principles of modern physics

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NEIL ASHBY

STANLEY C. MILLER

University of Colorado

HOLDEN-DAY, INC.

San Francisco

Cambridge

London

Amsterdam

Holden-Day, Inc.,
500 Sansome Street
San Francisco, California

library of Congress Catalog
Card Number: 71-1 13182
Manufactured in
the United States of America

HOLDEN-DAY SERIES IN PHYSICS

McAllister Hull and David S. Saxon, Editors

preface

This book is intended as a general introduction to modern physics for science and engineering students. It is written at a level which presumes a prior full year's course in classical physics, and a knowledge of elementary differential and integral calculus.

The material discussed here includes probability, relativity, quantum mechanics, atomic physics, statistical mechanics, nuclear physics and elementary particles. Some of these topics, such as statistical mechanics and probability, are ordinarily not included in textbooks at this level. However, we have felt that for proper understanding of many topics in modern physics--such as quantum mechanics and its applications--this material is essential. It is our opinion that present-day science and engineering students should be able to work quantitatively with the concepts of modern physics. Therefore, we have attempted to present these ideas in a manner which is logical and fairly rigorous. A number of topics, especially in quantum mechanics, are presented in greater depth than is customary. In many cases, unique ways of presentation are given which greatly simplify the discussion of there topics. However, few of the developments require more mathematics than elementary calculus and the algebra of complex numbers; in a few places, familiarity with partial differentiation will be necessary.

Unifying concepts which halve important applications throughout modern physics, such as relativity, probability and the laws of conservation, have been stressed. Almost all theoretical developments are linked to examples and data taken from experiment. Summaries are included at the end of each chapter, as well as problems with wide variations in difficulty.

This book was written for use in a one-semester course at the sophomore or junior level. The course could be shortened by omitting some topics; for example, Chapter 7, Chapter 12, Chapters 13 through 15, and Chapter 16 contain blocks of material which are somewhat independent of each other.

The system of units primarily used throughout is the meter-kilogram-second system. A table of factors for conversion to other useful units is given in Appendix 4. Atomic mass units are defined with the C^{12} atom as the standard.

We are grateful for the helpful comments of a large number of students, who used the book in preliminary form for a number of years. We also thank our colleagues and reviewers for their constructive criticism. Finally, we wish to express our thanks to Mrs. Ruth Wilson for her careful typing of the manuscript.

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APPENDICES

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1 introduction

.1 HISTORICAL SURVEY

The term modern physics generally refers to the study of those facts and theories developed in this century, that concern the ultimate structure and interactions of matter, space and time. The three main branches of classical physics-mechanics, heat and electromagnetism---were developed over a period of approximately two centuries prior to 1900. Newton's mechanics dealt successfully with the motions of bodies of macroscopic size moving with low speeds, and provided a foundation for many of the engineering accomplishments of the eighteenth and nineteenth centuries. With Maxwell's discovery of the displacement current and the completed set of electromagnetic field equations, classical technology received new impetus: the telephone, the wireless, electric light and power, and a host of other applications followed.

Yet the theories of mechanics and electromagnetism were not quite consistent with each other. According to the Galilean principle of relativity, recognized by Newton, the laws of mechanics should be expressed in the same mathematical form by observers in different inertial frames of reference, which are moving with constant velocity relative to each other. The transformation equations, relating measurements in two relatively moving inertial frames, were not consistent with the transformations obtained by Lorentz from similar considerations of form-invariance applied to Maxwell's equations. Furthermore, by around 1900 a number of phenomena had been discovered which were inexplicable on the basis of classical theories.

The first major step toward a deeper understanding of the nature of space and time measurements was due to Albert Einstein, whose special theory of relativity (1905) resolved the inconsistency between mechanics and electromagnetism by showing, among other things, that Newtonian mechanics is only a first approximation to a more general set of mechanical laws; the approximation is, however, extremely good when the bodies move with speeds which are small compared to the speed of light. Among the important results obtained by Einstein was the equivalence of mass and energy, expressed in the famous equation $E = mc^2$.

From a logical standpoint, special relativity lies at the heart of modern physics. The hypothesis that electromagnetic radiation energy is quantized in bunches of amount $h\nu$, where ν is the frequency and h is a constant, enabled

Planck to explain the intensity distribution of black-body radiation. This occurred several years before Einstein published his special theory of relativity in 1905. At about this time, Einstein also applied the quantum hypothesis to photons in an explanation of the photoelectric effect. This hypothesis was found to be consistent with special relativity. Similarly, Bohr's postulate-that the electron's angular momentum in the hydrogen atom is quantized in discrete amounts— enabled him to explain the positions of the spectral lines in hydrogen. These first guesses at a quantum theory were followed in the first quarter of the century by a number of refinements and ad hoc quantization rules; these, however, achieved only limited success. It was not until after 1924, when Louis de Broglie proposed, on the basis of relativity theory, that waves were associated with material particles, that the foundations of a correct quantum theory were laid. Following de Broglie's suggestion, Schrödinger in 1926 proposed a wave equation describing the propagation of these particle-waves, and developed a quantitative explanation of atomic spectral line intensities. In a few years thereafter, the success of the new wave mechanics revolutionized physics.

Following the discovery of electron spin, Pauli's exclusion principle was rigorously established, providing the explanation for the structure of the periodic table of the elements and for many of the details of the chemical properties of the elements. Statistical properties of the systems of many particles were studied from the point of view of quantum theory, enabling Sommerfeld to explain the behavior of electrons in a metal. Bloch's treatment of electron waves in crystals simplified the application of quantum theory to problems of electrons in solids. Dirac, while investigating the possible first order wave equations allowed by relativity theory, discovered that a positively charged electron should exist; this particle, called a positron, was later discovered. These are only a few of the many discoveries which were made in the decade from 1925-l 935.

From one point of view, modern physics has steadily progressed toward the study of smaller and smaller features of the microscopic structure of matter, using the conceptual tools of relativity and quantum theory. Basic understanding of atomic properties was in principle achieved by means of Schrodinger's equation in 1926. (In practice,. working out the implications of the Schrödinger wave mechanics for atoms and molecules is difficult, due to the large number of variables which appear in the equation for systems of more than two or three particles.) Starting in 1932 with the discovery of the neutron by Chadwick, properties of atomic nuclei have become known and understood in greater and greater detail. Nuclear fission and nuclear fusion are byproducts of these studies, which are still extrernely active. At the present time some details of the inner structure of protons, neutrons and other particles involved in nuclear interactions are just beginning to be unveiled.

Over fifty of the so-called elementary particles have been discovered. These particles are ordinarily created by collisions between high-energy particles of some other type, usually nuclei or electrons. Most of the elementary particles are unstable and decay into other more stable objects in a very short time. The study of these particles and their interactions forms an important branch of present-day research in physics.

It should be emphasized that one of the most important unifying concepts in modern physics is that of energy. Energy as a conserved quantity was well-known in classical physics. From the time of Newton until Einstein, there were no fundamentally new mechanical laws introduced; however, the famous variational principles of Hamilton and Lagrange expressed Newtonian lows in a different form, by working with mathematical expressions for the kinetic and potential energy of a system. Einstein showed that energy and momentum are closely related in relativistic transformation equations, and established the equivalence of energy and mass. De Broglie's quantum relations connected the frequency and wavelength of the wave motions associated with particles, with the particle's energy and momentum. Schrödinger's wave equation is obtained by certain mathematical operations performed on the expression for the energy of a system. The most sophisticated expressions of modern-day relativistic quantum theory are variational principles, which involve the energy of a system expressed in quantum-mechanical form. And, perhaps most important, the stable stationary states of quantum systems are states of definite energy.

Another very important concept used throughout modern physics is that of probability. Newtonian mechanics is a strictly deterministic theory; with the development of quantum theory, however, it eventually became clear that microscopic events could not be precisely predicted or controlled. Instead, they had to be described in terms of probabilities. It is somewhat ironic that probability was first introduced into quantum theory by Einstein in connection with his discovery of stimulated emission. Heisenberg's uncertainty principle, and the probability interpretation of the Schrödinger wavefunction, were sources of distress to Einstein who, not feeling comfortable with a probabilistic theory, later declared that he would never believe that "God plays dice with the world."

As a matter of convenience, we shall begin in Chapter 2 with a brief introduction to the concept of probability and to the rules for combining probabilities. This material will be used extensively in later chapters on the quantum theory ond on statistical mechanics.

The remainder of the present chapter consists of review and reference material on units and notation, placed here to avoid the necessity of later digressions.

1.2 NOTATION AND UNITS

The well-known meter-kiloglram-second (MKS) system of units will be used in this book. Vectors will be denoted by boldface type, such as **F** for force. In these units, the force on a point charge of Q coulombs, moving with velocity v in meters per second, at a point where the electric field is **E** volts per meter and the magnetic field is **B** webers per square meter, is the Lorentz force:

$$\mathbf{F} = Q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \tag{1.1}$$

where v x B denotes the vector cross-product of v and B. The potential in volts produced by a point charge Q at a distance r from the position of the charge is given by Coulomb's law:

$$V(r) = \frac{Q}{4\pi\epsilon_0 r} \tag{1.2}$$

where the constant ϵ_0 is given by

$$\frac{1}{(4\pi\epsilon_0)} = 9 \times 10^9 \text{ newtons-}m^2/\text{coulomb}^2 \tag{1.3}$$

These particular expressions from electromagnetic theory are mentioned here because they will be used in subsequent chapters.

In conformity with modern notation, a temperature such as "300 degrees Kelvin" will be denoted by 300K. Boltzmann's constant will be denoted by k_B, with

$$k_B = 1.38 \times 10^{-23} \text{ joules/molecule-K} \tag{1.4}$$

A table of the fundamental constants is given in Appendix 4.

1.3 UNITS OF ENERGY AND MOMENTUM

While in the MKS system of units the basic energy unit is the joule, in atomic and nuclear physics several other units of energy have found widespread use. Most of the energies occurring in atomic physics are given conveniently in terms of the *electron* volt, abbreviated eV. The electron volt is defined as the amount of work done upon an electron as it moves through a potential difference of one volt. Thus

$$\begin{aligned} 1 \text{ eV} &= e \times V = e(\text{coulombs}) \times 1 \text{ volt} \\ &= 1.602 \times 10^{-19} \text{ joules} \end{aligned} \tag{1.5}$$

The electron volt is an amount of energy in joules equal to the numerical value of the electron's charge in coulombs. To convert energies from joules to eV, or from eV to joules, one divides or multiplies by e, respectively. For example, for a particle with the mass of the electron, moving with a speed of 1% of the speed of light, the kinetic energy would be

$$\begin{aligned} \frac{1}{2} mv^2 &= \frac{1}{2}(9.11 \times 10^{-31} \text{ kg})(3 \times 10^6 \text{ m/sec})^2 \\ &= 4.1 \times 10^{-18} \text{ joules} \\ &= \frac{4.1 \times 10^{-18} \text{ j}}{(1.6 \times 10^{-19} \text{ j/eV})} \\ &= 2.6 \text{ eV} \end{aligned} \tag{1.6}$$

In nuclear physics most energies are of the order of several million electron volts, leading to the definition of a unit called the MeV:

$$
\begin{aligned}
1\ \text{MeV} &= 1\ \text{million eV} = 10^6\,\text{eV} \\
&= 1.6 \times 10^{-13}\ \text{joules} = (10^6 e)\ \text{joules} \qquad (1.7)
\end{aligned}
$$

For example, a proton of mass 1.667×10^{-27} kg, traveling with 10% of the speed of light, would have a kinetic energy of approximately

$$
\begin{aligned}
\frac{1}{2} Mv^2 &= \frac{1}{2}\,\frac{(1.67 \times 10^{-27}\,\text{kg})(3 \times 10^{7}\,\text{m/sec})^2}{(1.6 \times 10^{-13}\,\text{j/MeV})} \\
&= 4.7\ \text{MeV} \qquad (1.8)
\end{aligned}
$$

Since energy has units of mass x $(\text{speed})^2$, while momentum has units of mass x speed, for many applications in nuclear and elementary particle physics a unit of momentum called MeV/c is defined in such a way that

$$
\begin{aligned}
\frac{1\ \text{MeV}}{c} &= \frac{10^6\,e}{c}\ \text{kg-m/sec} \\
&= 5.351 \times 10^{-18}\ \text{kg-m/sec} \qquad (1.9)
\end{aligned}
$$

where c and e are the numerical values of the speed of light and electronic charge, respectively, in MKS units. This unit of momentum is particularly convenient when working with relativistic relations between energy and momentum, such as $E = pc$, for photons. Then if the momentum p in MeV/c is known, the energy in MeV is numerically equal to p. Thus, in general, for photons

$$
E(\text{in MeV}) = p(\text{in MeV}/c) \qquad (1.10)
$$

Suppose, for instance, that a photon has a momentum of 10^{-21} kg-m/sec. The energy would be $pc = 3 \times 10^{-13}$ joules = 1.9 MeV, after using Equation (1.7). On the other hand, if p is expressed in MeV/c, using Equation (1.9) we find that

$$
p = 10^{-21}\ \text{kg-m/sec} = 1.9\ \text{MeV}/c
$$

The photon energy is then $E = pc = (1.9\ \text{MeV}/c)(c) = 1.9$ MeV.

1.4 ATOMIC MASS UNIT

The atomic mass unit, abbreviated amu, is chosen in such a way that the mass of the most common atom of carbon, containing six protons and six neutrons in a nucleus surrounded by six electrons, is exactly 12.000000000 . . amu. This unit is convenient when discussing atomic masses, which are then always very close to an integer. An older atomic mass unit, based on an atomic mass of exactly 16 units for the oxygen atom with 8 protons, 8 neutrons, and 8 electrons, is no longer in use in physics research. In addition, a slightly different choice of atomic mass unit is commonly used in chemistry. All atomic masses appearing in this book are based on the physical scale, using carbon as the standard.

The conversion from amu on the physical scale to kilograms may be obtained by using the fact that one gram-molecular weight of a substance contains

Avogadro's number, N_0 = 6.022 x 10^{23}, of molecules. Thus, exactly 12.000 . . . grams of C^{12} atoms contains N_0 atoms, and

$$1 \text{ amu} = \frac{1}{12} \times \left(\frac{12 \text{ g}}{N_0}\right) \times 10^{-3} \text{ kg/g}$$
$$= 1.660 \times 10^{-27} \text{ kg} \tag{1.11}$$

1.5 PROPAGATION OF WAVES; PHASE AND GROUP SPEEDS

In later chapters, many different types of wave propagation will be considered: the de Broglie probability waves of quantum theory, lattice vibrations in solids, light waves, and so on. These wave motions can be described by a displacement, or amplitude of vibration of some physical quantity, of the form

$$\psi(x, t) = A \cos(kx \pm \omega t + \phi) \tag{1.12}$$

where A and ϕ are constants, and where the wavelength and frequency of the wave are given by

$$\lambda = \frac{2\pi}{k}, \quad \nu = \frac{\omega(k)}{2\pi} \tag{1.13}$$

Here the angular frequency is denoted by ω = o(k), to indicate that the frequency is determined by the wavelength, or wavenumber k. This frequency-wavelength relation, ω = w(k), is called a dispersion relation and arises because of the basic physical laws satisfied by the particular wave phenomenon under investigation. For example, for sound waves in air, Newton's second law of motion and the adiabatic gas law imply that the dispersion relation is

$$w = vk \tag{1.14}$$

where v is a constant.

If the negative sign is chosen in Equation (1.12), the resulting displacement (omitting the phase constant ϕ) is

$$\psi(x, t) = A \cos(kx - wt) = A \cos\left[k\left(x - \left(\frac{\omega}{k}\right)t\right)\right] \tag{1.15}$$

This represents a wave propagating in the positive x direction. Individual crests and troughs in the waves propagate with a speed called the phase speed, given by

$$w = \frac{\omega}{k} \tag{1.16}$$

In nearly all cases, the wave phenomena which we shall discuss obey the principle of superposition-namely, that if waves from two or more sources arrive at the same physical point, then the net displacement is simply the sum of the displacements from the individual waves. Consider two or more wave trains propagating in the same direction. If the angular frequency w is a function of the wavelength or wavenumber, then the phase speed can be a function of the wavelength, and waves of differing wavelengths travel at different speeds. Reinforcement or destructive interference can then occur as one wave gains on another of different wavelength. The speed with which the regions of constructive or destructive interference advance is known as the group speed.

To calculate this speed, consider two trains of waves of the form of Equation (1.15), of the same amplitude but of slightly different wavelength and frequency, such as

$$\begin{aligned} \psi_1 &= A \cos [(k + \tfrac{1}{2} Ak)x \quad (\omega + \tfrac{1}{2} \Delta\omega)t] \\ \psi_2 &= A \cos [(k - \tfrac{1}{2} Ak)x - (\omega - \tfrac{1}{2} \Delta\omega)t] \end{aligned} \qquad (1.17)$$

Here, k and ω are the central wavenumber and angular frequency, and Ak, $\Delta\omega$ are the differences between the wavenumbers and angular frequencies of the two waves. The resultant displacement, using the identity 2 cos A cos B = cos (A + 13) + cos (A − B), is

$$\psi = \psi_1 + \psi_2 = (2 A \cos \tfrac{1}{2} (Akx - \Delta\omega t)\} \cos (kx - wt) \qquad (1.18)$$

This expression represents a wave traveling with phase speed w/k, and with an amplitude given by

$$2 A \cos \tfrac{1}{2} (\Delta k x - Awt) = 2 A \cos \tfrac{1}{2} \Delta k \left(x - \frac{\Delta\omega}{\Delta k} t\right) \qquad (1.19)$$

The amplitude is a cosine curve; the spatial distance between two successive zeros of this curve at a given instant is $\pi/\Delta k$, and is the distance between two successive regions of destructive interference. These regions propagate with the group speed v_g, given by

$$v_g = \frac{\Delta\omega}{A\ k} \underset{\Delta k \to 0}{=} \frac{d\omega(k)}{dk} \qquad (1.20)$$

in the limit of sufficiently small Ak.

Thus, for sound waves in air, since ω = vk, we derive

$$v_g = \frac{d(vk)}{dk} = v = w \qquad (1.21)$$

and the phase and group speeds are equal. On the other hand, for surface gravity waves in a deep seo, the dispersion relation is

$$w = \{gk + k^3 T/\rho\}^{1/2} \qquad (1.22)$$

where g is the gravitational acceleration, J is the surface tension and ρ is the density. Then the phase speed is

$$w = \frac{\omega}{k} = \left\{ \frac{g}{k} + \frac{Tk}{\rho} \right\}^{1/2} \qquad (1.23)$$

whereas the group speed is

$$v_g = \frac{d\omega}{dk} = \frac{1}{2}\left(\frac{g + 3k^2T/\rho}{\{gk + k^3T/\rho\}^{1/2}}\right) \tag{1.24}$$

If the phase speed is a decreasing function of k, or an increasing function of wavelength, then the phase speed is greater than the group speed, and individual crests within a region of constructive interference-i.e. within a group of waves-travel from rear to front, crests disappearing at the front and reappearing at the rear of the group. This can easily be observed for waves on a pool of water.

1.6 COMPLEX NUMBERS

Because the use of complex numbers is essential in the discussion of the wavelike character of particles, a brief review of the elementary properties of complex numbers is given here. A complex number is of the form $\psi = a + ib$, where a and b are real numbers and i is the imaginary unit, $i^2 = -1$. The real part of ψ is a, and the imaginary part is b:

$$\mathrm{Re}(a + ib) = a$$
$$\mathrm{Im}(a + ib) = b \tag{1.25}$$

A complex number $\psi = a + ib$ can be represented as a vector in two dimensions, with the x component of the vector identified with $\mathrm{Re}(\psi)$, and the y component

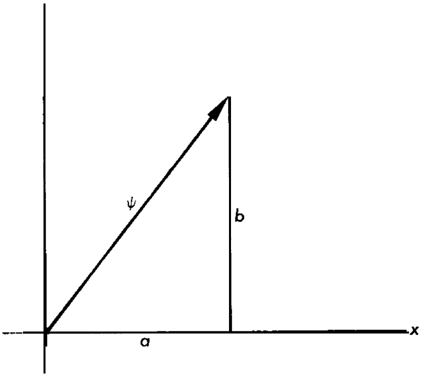


Figure 1.1. Two-dimensional vector representation of a complex number $\psi = a + ib$.

of the vector identified with $\mathrm{Im}(\psi)$, as in Figure 1.1. The square of the magnitude of the vector is

$$|\psi|^2 = a^2 + b^2 \tag{1.26}$$

The complex conjugate of $\psi = a + ib$ is denoted by the symbol ψ^* and is obtained by replacing the imaginary unit i by $-i$:

$$\psi^* = a - ib \tag{1.27}$$

We can calculate the magnitude of the square of the vector by multiplying ψ by its complex conjugate:

$$|\psi|^2 = \psi^*\psi = a^2 \quad (ib)^2 = a^2 + b^2 \tag{1.28}$$

The complex exponential function, $e^{i\theta}$, or exp $(i\theta)$, where θ is a real function or number, is of particular importance; this function may be defined by the power series

$$\begin{aligned} e^{i\theta} &= 1 + (i\theta) + \frac{(i\theta)^2}{2!} + \frac{(i\theta)^3}{3!} + \cdots \\ &= \sum_{n=0}^{\infty} \frac{(i\theta)^n}{n!} \end{aligned} \tag{1.29}$$

Then, replacing i^2 everywhere that it appears by -- 1 and collecting real and imaginary terms, we find that

$$\begin{aligned} e^{i\theta} &= 1 - \frac{\theta^2}{2!} + \frac{\theta^4}{4!} + \cdots + i\left(\theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} + \cdots\right) \\ &= \cos\theta + i\sin\theta \end{aligned} \tag{1.30}$$

Since $\{e^{i\theta}\}^n = e^{in\theta}$, we have de Moivre's theorem:

$$e^{in\theta} = \cos n\theta + i\sin n\theta = (\cos\theta + i\sin\theta\}^n \tag{1.31}$$

Since $(e^{i\theta})^* = e^{-i\theta}$, we also have the following identities:

$$\mathrm{Re}\, e^{i\theta} = \cos\theta = \frac{1}{2}(e^{i\theta} + e^{-i\theta}) \tag{1.32}$$

$$\mathrm{Im}\, e^{i\theta} = \sin\theta = \frac{1}{2i}(e^{i\theta} - e^{-i\theta}) \tag{1.33}$$

$$e^{i\theta}|^2 = e^{-i\theta}e^{i\theta} = e^0 = 1 \tag{1.34}$$

$$\frac{1}{(a+ib)} = \frac{1}{a+ib} \times \frac{a-ib}{a-ib} = \frac{a-ib}{a^2+b^2} \tag{1.35}$$

The integral of an exponential function of the form e^{cx} is

$$\int e^{cx} = \frac{e^{cx}}{c} + \text{constant} \tag{1.36}$$

and this is also valid when c is complex. For example,

$$\begin{aligned} \int_0^\pi e^{i\theta}d\theta &= \frac{e^{i\theta}}{i}\Big|_0^\pi = \frac{e^{i\pi} - e^0}{i} \\ &= \frac{(\cos\pi + i\sin\pi - 1)}{i} \\ &= \frac{(-1 + 0 - 1)}{i} = \frac{-2}{i} = +2i \end{aligned} \tag{1.37}$$

The complex exponential function is a periodic function with period 2π. Thus

$$\begin{aligned} e^{i(\theta+2\pi)} &= \cos(\theta + 2\pi) + i\sin(\theta + 2\pi) \\ &= \cos\theta + i\sin\theta \\ &\quad {}^{i\theta} \end{aligned} \tag{1.38}$$

More generally, if n is any positive integer or negative integer,

$$e^{i(\theta+2\pi n)} = e^{i\theta} \tag{1.39}$$

or $\exp(2n\pi i) = 1$. Conversely, if $\exp(i\theta) = 1$, the only possible solutions for θ are

$$\theta = 2\pi n, \quad n = 0, \pm 1, \pm 2, \pm 3, \ldots \tag{1.40}$$

2 probability

> We have ninety *chances in a* hundred.
>
> Napoleon at Waterloo, 1815

The commonplace meaning of the word "chance" is probably already familiar to the reader. In everyday life, most situations in which we act are characterized by uncertain knowledge of the facts and of the outcomes of our actions. We are thus forced to make guesses, and to take chances. In the *theory of* probability, the concepts of probability and chance are given precise meanings. The theory not only provides a systematic way of improving our guesses, it is also an indispensable tool in studying the abstract concepts of modern physics. To avoid the necessity of digressions on probability during the later development of statistical mechanics and quantum mechanics, we present here a brief introduction to the basic elements of probability theory.

When Napoleon uttered the statement above, he did not mean that if the Battle of Waterloo were fought a hundred times, he would win it ninety times. He was expressing an intuitive feeling about the outcome, which was based on years of experience and on the facts as he knew them. Had he known enemy reinforcements would arrive, and French would not, he would have revised the estimate of his chances downward. Probability is thus seen to be a relative thing, depending on the state of knowledge of the observer. As another example, a student might decide to study only certain sections of the text for an exam, whereas if he knew what the professor knew-namely, which questions were to be on the exam-he could probably improve his chances of passing by studying some other sections.

In physics, quantitative application of the concept of chance is of great importance. There are several reasons for this. For example, it is frequently necessary to describe quantitatively systems with a great many degrees of freedom, such as a jar containing 10^{23} molecules; however, it is, as a practical matter, impossible to know exactly the positions or velocities of all molecules in the jar, and so it is impossible to predict exactly what will happen to each molecule. This is simply because the number of molecules is so great. It is then necessary to develop some approximate, statistical way to describe the behavior of the molecules, using only a few variables. Such studies form the subject matter of a branch of physics called *statistical* mechanics.

Secondly, since 1926 the development of quantum mechanics has indicated that the description of mechanical properties of elementary particles can only be given in terms of probabilities. These results from quantum mechanics have profoundly affected the physicist's picture of nature, which is now conceived and interpreted using probabilities.

Thirdly, experimental measurements are always subject to errors of one sort or another, so the quantitative measurements we make always have some uncertainties associated with them. Thus, a person's weight might be measured as 176.7 lb, but most scales are not accurate enough to tell whether the weight is 176.72 lb, or 176.68 lb, or something in between. All measuring instruments have similar limitations. Further, repeated measurements of a quantity will frequently give different values for the quantity. Such uncertainties can usually be best described in terms of probabilities.

2.1 DEFINITION OF PROBABILITY

To make precise quantitative statements about nature, we must define the concept of probability in a quantitative way. Consider an experiment having a number of different possible outcomes or results. Here, the probability of a particular result is simply the expected fraction of occurrences of that result out of a very large number of repetitions or trials of the experiment. Thus, one could experimentally determine the probability by making a large number of trials and finding the fraction of occurrences of the desired result. It may, however, be impractical to actually repeat the experiment many times (consider for example the impossibility of fighting the Battle of Waterloo more than once). We then use the theory of probability; that is a mathematical approach based on a simple set of assumptions, or postulates, by means of which, given a limited amount of information about the situation, the probabilities of various outcomes may be computed. It is hoped that the assumptions hold to a good approximation in the actual physical situation.

The theory of probability was originally developed to aid gamblers interested in improving their income, and the assumptions of probability theory may be naturally illustrated with simple games. Consider flipping a silver dollar ten times. If the silver dollar is not loaded, on the average it will come down heads five times out of ten. The fraction of occurrences of heads on the average is $^5/_{10}$ or $\frac{1}{2}$ Then we say that probability $P(\text{heads})$ of flipping a head in one try is $P(\text{heads}) = \frac{1}{2}$. Similarly, the probability of flipping a tail in one try is $P(\text{tails}) = \frac{1}{2}$.

In this example, it is assumed that the coin is not loaded. This is equivalent to saying that the two sides of the coin are essentially identical, with a plane of symmetry; it is then reasonable to assume that since neither side of the coin is favored over the other, on the average one side will turn up as often as the other. This illustrates an important assumption of probability theory: When there are several possible alternatives and there is no apparent reason why they should occur with different frequencies, they are assigned ***equal*** probabilities. This is sometimes called the ***postulate of equal a priori probabilities.***

2.2 SUMS OF PROBABILITIES

Some general rules for combining probabilities are also illustrated by the coin-flipping experiment. In every trial, it is certain that either heads or tails will turn up. The fraction of occurrences of the result "either heads or tails" must be unity, and so

$$P(\text{either heads or tails}) = 1 \tag{2.1}$$

In other words, the probability of an event which is certain is taken to be 1.

Further, the fraction of heads added to the fraction of tails must equal the fraction of "either heads or tails," and so

$$P(\text{either heads or tails}) = P(\text{heads}) + P(\text{tails}) \tag{2.2}$$

In the special case of the fair coin, both P(heads) and P(tails) are ½, and the above equation reduces to $1 = \frac{1}{2} + \frac{1}{2}$.

More generally, if A, B, C, . . . are events that occur with probabilities P(A), P(B), P(C), . . . , then the probability of either A or B occurring will be given by the sum of the probabilities:

$$P(\text{either A or B}) = P(A) + P(B) \tag{2.3}$$

Similarly, the probability of either A or B or C occurring will be

$$P(\text{either A or B or C}) = P(A) + P(B) + P(C) \tag{2.4}$$

Here it is assumed that the labels A, B, C, . . . refer to mutually exclusive alternatives, so that if the event A occurs, the events B, C, . cannot occur, and so on. The above relation for combining probabilities simply amounts to addition of the fractions of occurrences of the various events A, B and C, to find the total fraction of occurrences of some one of the events in the set A, B, C.

These relations may easily be generalized for any number of alternatives. For example, consider an experiment with six possible outcomes, such as the six possible faces of a die which could be turned up when the die is thrown. Imagine the faces numbered by an index i that varies from 1 to 6, and let P_i be the probability that face i turns up when the die is thrown. Some one face will definitely turn up, and so the total probability that some one face will turn up will be equal to unity, Also, the probability that some one face will turn up is the same as the probability that either face one, or face two, or face three, or,. . . , or face six will turn up. This will be equal to the sum of the individual probabilities P_i. Mathematially,

$$1 = \sum_{i=1}^{6} P_i \tag{2.5}$$

In words, this equation expresses the convention that the probability of an event which is certain is equal to 1. It also utilizes a generalization of the rule given in Equation (2.3), which says the probability of either A or B is the sum of the probabilities of A and of B.

2.3 CALCULATION OF PROBABILITIES BY COUNTING

Given a fair die, there is no reason why the side with the single dot should come up more often than the side with five dots, or any other side. Hence, according to the postulate of equal a priori probabilities, we may say that *P,* = P,, and, indeed, that $P_1 = P_2 = P_3 = P_4 = P_5 = P_6$. Then $\sum_{i=1}^{6}$ P, $= 6P_1 = 1$, **or** $P_1 = {}^1\!/_6$ and hence $P_i = {}^1\!/_6$ for all i. This simple calculation has yielded the numerical values of the probabilities P,. A general rule which is very useful in such calculations may be stated as follows:

The probability of a particular event is the ratio of the number of ways this event can occur, to the *total* number of ways *all* possible events can occur.

Thus, when a die is thrown,, six faces can turn up. There is only one face that has two dots on it. Therefore, the number of ways a two dot face can turn up, divided by the total number of **ways** all faces can turn up, is ${}^1\!/_6$.

If one card is drawn at random from a pack of cards, what is the probability that it will be the ace of spades? Since the ace of spades can be drawn in only one way, out of a total of 52 ways for all possible cards, the answer is

$$P = \frac{(1\ \text{ace of spades})}{(52\ \text{possible cards})} \tag{2.6}$$

or $P = {}^1\!/_{52}$. Likewise, if one card is drawn from a pack, the probability that it will be an ace is (4 aces)/(52 possible cards) or $P = {}^4\!/_{52} = {}^1\!/_{13}$. We can also consider this to be the sum of the probabilities of drawing each of the four aces.

2.4 PROBABILITY OF SEVERAL EVENTS OCCURRING TOGETHER

Next we shall consider a slightly more complicated situation: flipping a coin twice. What is the probability of flipping two heads in succession? The possible outcomes of this experiment are listed in Table 2.1.

TABLE 2.1 Different possible outcomes for flipping a coin twice.

First Flip	Second Flip
heads	heads
heads	tails
tails	heads
tails	tails

Since there are two possible outcomes for each flip, there are two times two or four possible outcomes for the succession of two coin flips. Since there is no reason to assume that one of these four outcomes is more probable than another, we may assign each of the four outcomes equal probabilities of ¼ . The total number of outcomes is the product of the number of outcomes on the first flip and the number of outcomes on the second flip, while the number of ways of getting two heads is the product of the number of ways of getting a head on the first flip and the number of ways of getting a head on the second flip. Thus,

P(two heads in succession)

$$= \left\{\frac{\text{\# of ways for heads on flip 1}}{\text{\# of outcomes on flip 1}}\right\} \times \left\{\frac{\text{\# of ways for heads on flip 2}}{\text{\# of outcomes on flip 2}}\right\}$$

$$= \text{P(heads on flip 1)} \times \text{P(heads on flip 2)}$$

$$= \frac{1}{2} \times \frac{1}{2} = \frac{1}{4} \qquad (2.7)$$

nple If a die is rolled twice in succession, what is the probability of rolling the snake eye both times?

tion P(snake eye twice) = $(1/6) \times (1/6) = 1/36$.

These results illustrate another general property of probabilities: If two events A and *B* are independent-that is, if they do not influence each other in any way-then the probability of both A and *B* occurring is

$$P(A \text{ and } 6) = P(A)P(B) \qquad (2.8)$$

In words, the probability of two independent events both occurring is equal to the product of the probabilities of the individual events.

nple If you throw a six-sided die and draw one card from a pack, the probability that you throw a six and pick an ace (any ace) is equal to

$$\left(\frac{1}{6} \times \frac{4}{52}\right) = \frac{1}{78}$$

Another way to obtain the answer is to divide the number of ways of getting the six and any ace (1 x 4), by the total number of ways of getting all possible results (6 x 52), or

$$\frac{(1 \times 4)}{(6 \times 52)} = \frac{1}{78}$$

in this case.

2.5 SUMMARY OF RULES FOR CALCULATING PROBABILITIES

We may summarize the important features of the probability theory discussed so far in the following rules:

(1) The probability of an event that is certain is equal to 1.

(2) In a set of events that can occur in several ways, the probability of a particular event is the number of ways the particular event may occur, divided by the total number of ways all possible events may occur.

(3) (Postulate of equal a priori probabilities): In the absence of any contrary information, equivalent possibilities may be assumed to have equal probabilities.

(4) If A and B are mutually exclusive events that occur with probabilities P(A) and P(6), then the probability of either A *or* B occurring is the sum of the individual probabilities:

$$P(A \text{ or } B) = P(A) + P(B) \tag{2.9}$$

(5) If A and B are independent events that occur with probabilities P(A) and P(B), then the probability of both A and B occurring is the product of the individual probabilities:

$$P(A \text{ and } B) = P(A)P(B) \tag{2.10}$$

2.6 DISTRIBUTION FUNCTIONS FOR COIN FLIPPING

In order to introduce the idea of a distribution function, we continue with some examples of coin-tossing. Distribution functions are functions of one or more independent variables which label the outcomes of some experiment; the distribution functions themselves are proportional to the probabilities of the various outcomes (in some case's they are equal to the probabilities). The variables might be discrete or continuous. Imagine, for example, a single experiment consisting of flipping a coin N times, when N might be some large integer. Let n_H be the number of times heads turns up in a particular experiment. If we repeat this experiment many times, then n_H can vary from experiment to experiment. We shall calculate the probability that n_H heads will turn up out of N flips; this probability will be denoted by $P_N(n_H)$. Here the independent variable is n_H; and the quantity $P_N(n_H)$, which for fixed N is a function of n_H, is an example of a distribution function. In this case, the function only has meaning if n_H is a nonegative integer not greater than N.

To get at the problem of finding $P_N(n_H)$, we define P_{H1} to be the probability of getting a head in the first toss and P_{T1} to be the probability of getting a tail (both are ½ for a fair coin but differ from ½ for a weighted coin). Then $P_{H1} + P_{T1} = 1$. Likewise for the second toss, $P_{H2} + P_{T2} = 1$. If these two expressions are multiplied together, we get $P_{H1}P_{H2} + P_{H1}P_{T2} + P_{T1}P_{H2} + P_{T1}P_{T2} = 1$. Note that these four terms correspond to the four possibilities in Table 1, and that each term gives the probability of getting the heads and tails in a particular order.

In N tosses,

$$(P_{H1} + P_{T1})(P_{H2} + P_{T2}) \cdots (P_{HN} + P_{TN}) = 1 \tag{2.11}$$

and when the products on the left are carried out, the various terms give the probabilities of getting heads and tails in a particular order. For example, in three tosses, the product of Equation (2.1 1) contains eight terms, one of which is $P_{T1}P_{H2}P_{T3}$. This is equal to the probability of getting a tail, a head and a tail, in that order, in three tosses. If we were interested only in the probability of getting a given total number of heads n_H in N tosses regardless of order, we would take all the terms which contain n_H factors of the form P_{Hi}, regardless of the subscript numbers, and simply find their sum. This is equivalent to dropping all numerical subscripts and combining terms with similar powers of P,.

If the expression on the left of the equation, (P, + $P_T)^N$ = 1, is expanded, the term proportional to $(P_H)^{n_H}(P_T)^{N-n_H}$ is the probability of getting n_H heads ond N − n_H tails in N tosses, regardless of order. According to the binomial theorem.

$$(P_H + P_T)^N = \sum_{n_H=0}^{N} \left\{\frac{N!}{n_H!(N - n_H)!}\right\} P_H^{n_H} P_T^{N-n_H} \tag{2.12}$$

where zero factorial (0!) is defined to be one and n! = $n(n-1)(n-2)\cdots 3\cdot2\cdot1$. The reader may recognize the binomial coefficient $N!/n_H!(N -$ n,)! as the number of ways of selecting n_H objects from a total of N objects, regardless of order, or in our case, the number of ways of getting n_H heads in N tosses. Thus, a given term is the total number of different ways of getting n_H heads times the probability, $(P_H)^{n_H}(P_T)^{N-n_H}$, of getting n_H heads in one of these ways. Therefore, in the special case of a fair coin when $P_H = P_T = \frac{1}{2}$, the probability of getting n_H heads in N tosses, regardless of order, is

$$P_N(n_H) = \frac{N!}{n_H!(N - n_H)!}\frac{1}{2^N} \tag{2.13}$$

In Figures 2.1 through 2.4, the probability $P_N(n_H)$ of Equation 2.13 is plotted as o function of n_H for N = 5, 10, 30 and 100. It may he seen that as N becomes larger, the graph approaches a continuous curve with a symmetrical bell-like shape. The function $P_N(n_H)$ is called a probability *distribution function,* because it gives a probability as a function of some parameter, in this case n_H.

ple 1(a) Consider a coin which is loaded in such a way that the probability P_H of flipping a head is P_H = 0.3. The probability of flipping a tail is then P_T = 0.7. ‘What is the probability of flipping two heads in four tries?

ion Use Equation (2.13) with N = 4, n_H = 2; the required probability is

$$\frac{4!}{2!2!}(P_H)^2(P_T)^2 = 0.2646$$

ple 1 (b) What is the probability of getting at least one head in four tries, i.e. either one or two or three or four heads?

ion The probability of getting at least one head is the same as the probability of not getting four tails, which is one minus the probability of getting four tails. In this case,

$$P\ (\text{getting all four tails}) = \frac{4!}{0!4!}(P_H)^0(P_T)^4 = 0.2401;$$

Therefore,

$$P\ (\text{at least one head}) = 1 - 0.2401 = 0.7599$$

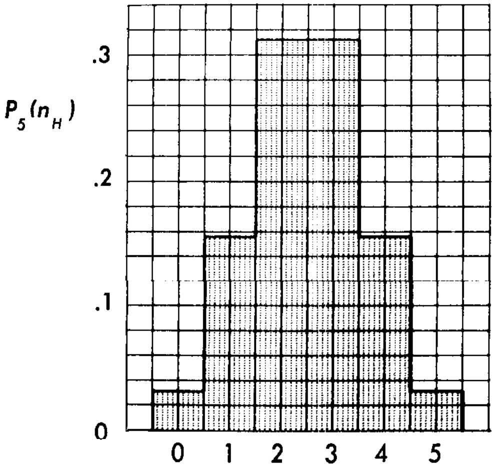


Figure **2.1.** Probability of getting n_H heads in 5 tosses.

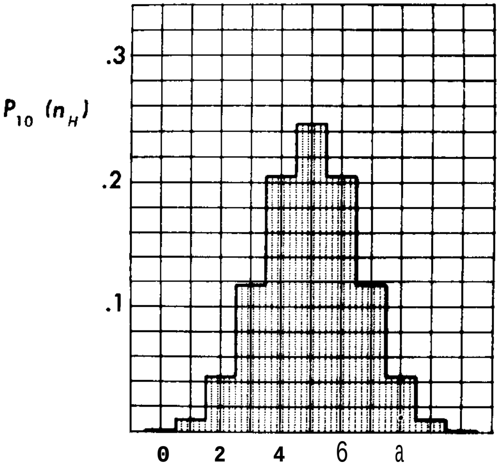


Figure 2.2. Probability of getting n_H heads in 10 tosses.

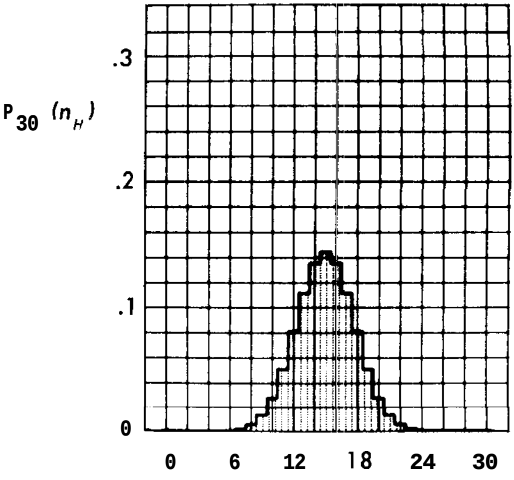


Figure 2.3. Probability of getting n_H heads in 30 tosses.

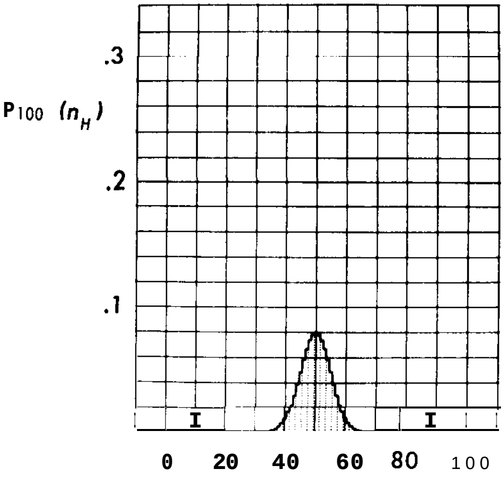


Figure 2.4. Probobility of getting n_H heads in 100 tosses.

ple 2(a) If the probability of getting all the forms filled out correctly at registration is 0.1, what is the probability of getting all forms filled out properly only once during registrations in three successive terms?

ion The probability of not getting the forms correct is 0.9 each time. Then the desired probability is

$$\frac{3!}{1!2!}(0.1)^1(0.9)^2 = 0.243$$

ple 2(b) What is the probability of filling out the forms correctly in one or more of the three registrations?

ion This is one minus the probability of doing it incorrectly every time or

$$1 - (0.9)^3 = 0.271$$

.7 DISTRIBUTION FUNCTIONS FOR MORE THAN TWO POSSIBLE OUTCOMES

Suppose we consider another experiment in which there are four possible results, A, B, C, and D, in a single trial. The probabilities for each result in this trial are, respectively, P_A, P_B, P_C and $P_D = 1 - P_A - P_B - P_C$. If the quantity on the left side of the equation

$$(P_A + P_B + P_C + P_D)^N = 1 \tag{2.14}$$

is expanded, the term proportional to

$$(P_A)^{n_A}(P_B)^{n_B}(P_C)^{n_C}(P_D)^{N-n_A-n_B-n_C}$$

is the probability that in N trials result A occurs n_A times, B occurs n_B times, C occurs n_C times and, of course, D occurs n_D times, with $n_D = N - n_A - n_B - n_C$. A generalized multinomial expansion may be written as follows:

$$(x + y + z + w)^N = \sum_{\substack{p,q,r \\ p+q+r\le N}} \left[\frac{N!}{p!q!r!(N-p-q-r)!}\right] x^p y^q z^r w^{N-p-q-r} \tag{2.15}$$

The probability that A occurs n_A times, B occurs n_B times, and C occurs n_C times in N trials is therefore

$$P_N(n_A, n_B, n_C) = \left[\frac{N!}{n_A!n_B!n_C!(N-n_A-n_B-n_C)!}\right](P_A)^{n_A}(P_B)^{n_B}(P_C)^{N-n_A-n_B-n_C} \tag{2.16}$$

The generalization to the case of any number of alternatives in the results of a single trial is obvious.

example In throwing a die three times, with six possible outcomes on each throw, the probability of throwing two fours and a three is

$$\frac{3!}{0!0!1!2!0!0!}\left(\frac{1}{6}\right)^0\left(\frac{1}{6}\right)^0\left(\frac{1}{6}\right)^1\left(\frac{1}{6}\right)^2\left(\frac{1}{6}\right)^0\left(\frac{1}{6}\right)^0=\frac{3\cdot 2}{2}\cdot\frac{1}{6^3}=\frac{1}{72}$$

2.8 EXPECTATION VALUES

One of the important uses of a probability distribution function arises in the computation of averages. We shall obtain a general formula for the computation of an average using a distribution function. Suppose that over several months a student took ten examinations and made the following grades: 91 once, 92 twice, 93 once, 94 four times, 95 twice. Figure 2.5 is a plot of the number,

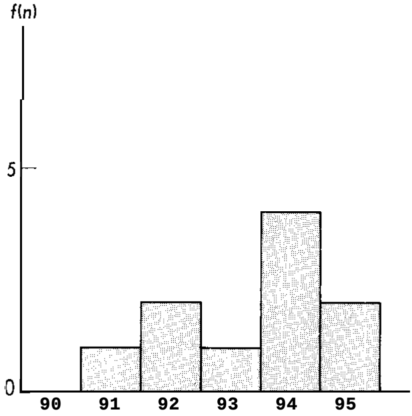


Figure 2.5. **Grade distribution function.**

f(n), of times the grade n was made, as a function of n. This function f(n) is also called a distribution function, but it is not a probability distribution function, since **f(n)** is the number of occurrences of the grade n, rather than the probability of occurrences of the grade *n*. To compute the average grade, one must add up all the numerical grades and divide by the total number of grades. Using the symbol **(n)** to denote the average of n, we have

$$(n) = \frac{91+92+92+93+94+94+94+94+95+95}{1+1+1+1+1+1+1+1+1+1} \qquad \textbf{(2.17)}$$

In the numerator, the grade 91 occurs once, the grade 92 occurs twice, 94 occurs four times, and, in general, the grade n occurs f(n) times. Thus, the numerator may be written as **(1 x 91) + (2 x 92) + (1 x 93) + (4 x 94) + (2 x 95)** or, in terms of n and *f(n),* the numerator is $\sum n\, f(n)$, where the summation is over all possible n. In the denominator, there is a 1 for each occurrence of an exam. The denominator is then the total number of exams or the sum of all the f(n). Thus, a formula for the denominator is $\sum f(n)$, summed over all n. Now we can write a general expression in terms of n and f(n) for the average value of n. It is

$$\langle n\rangle = \frac{\sum_n n f(n)}{\sum f(n)} \tag{2.18}$$

In this case, the average grade turns out to be 93.4. If the student were to take several more examinations, then, on the basis of past (experience, it could be expected that the average grade on these new examinations would be 93.4. For this reason, the average, $\langle n\rangle$, is also called the *expectation* value. Expectation values are of considerable importance in quonturn mechanics.

As a further example, suppose you made grades of 90, 80, and 90 on three examinations. The expectation value of your grade would be $(80 + 2 \times 90)/(1 + 2) = 86.67$.

2.9 NORMALIZATION

For any distribution function f(n), the value of the reciprocal of the sum $\sum f(n)$ is called the *normalization* of the distribution function. It $\sum f(n) = N$, we say that f(n) is normalized to the value N, and the normalization is I/N. Since the sum of the probabilities of all events is unity, when f(n) is a probability distribution function, it is normalized to unity:

$$\sum f(n) = 1 \tag{2.19}$$

Equation (2.18) refers to the expectation of the ndependent variable, $\langle n\rangle$. However, in some applications it might be necessary to know the expectation values of n^2, or n^3, or of some other function of n. In general, to find the average or expectation value of a function of n, such as A(n), one rnay use the equation:

$$(A(n)) = \frac{\sum A(n) f(n)}{\sum f(n)} \tag{2.20}$$

.10 EXPECTATION VALUE OF THE NUMBER OF HEADS

For a more detailed example of an expectation value calculation, we return to the flipping of a coin. As was seen before, if a number of experiments are performed in each of which the coin is flipped N times, we would expect that, on the average, the number of heads would be N/2, or $\langle n_H\rangle = N/2$. To obtain this result mathematically using Equation (2.18), we shall evaluate the sum

$$\langle n_H\rangle = \sum_{n_H=0}^{N} n_H P_N(n_H) \tag{2.21}$$

Here $\sum f(n) = \sum P_N(n_H) = 1$, since $P_N(n_H)$ is a probability distribution function with a normalization of unity. Therefore, the denominator has been omitted. From Equation (2.13), $P_N(n_H) = N!/\{2^N n_H!(N - n_H)!\}$ for a fair coin. Hence,

$$\langle n_H \rangle = \sum \frac{n_H N!}{[2^N n_H!(N - n_H)!]} \tag{2.22}$$

The result is indeed $N/2$. The reader who is not interested in the rest of the details of the calculation can skip to Equation (2.26).

We have to evaluate the summation in $\langle n_H \rangle = \sum_{n_H=0}^{N} n_H N!/[2^N n_H!(N - n_H)!]$. We can calculate this by a little bit of relabeling. First, note that the term corresponding to $n_H = 0$ does not contribute to the sum because the factor n_H is inside the sum, and in the denominator there is 0!, which is defined to be 1. Therefore, instead of going from 0 to N, the sum goes effectively from 1 to N. It is easily verified that after using the following identities:

$$N! = N(N-1)!; \quad \frac{n_H}{n_H!} = \frac{1}{(n_H - 1)!}; \quad (N - n_H)! = (N - 1 - [n_H - 1])! \tag{2.23}$$

and

$$2^N = 2 \cdot 2^{N-1} \tag{2.24}$$

Then factoring out an N/2, we get

$$\langle n_H \rangle = \frac{1}{2} N \sum_{n_H=1}^{N} \frac{(N-1)!}{[2^{N-1}(n_H - 1)!(N - 1 - [n_H - 1])!]} \tag{2.25}$$

Then, for $m = n_H - 1$, the summation over n_H from 1 to N can be rewritten as follows:

$$\langle n_H \rangle = \frac{1}{2} N \sum_{m=0}^{N-1} \frac{(N-1)!}{[2^{N-1} m!(N - 1 - m)!]} = \frac{1}{2} N \left(\frac{1}{2} + \frac{1}{2}\right)^{N-1} = \frac{1}{2} N \tag{2.26}$$

This result agrees with our intuitive idea of an expectation value. The result does not mean that, in an actual experiment, heads will come up exactly ½ N times, but heads will only come up ½ N times *on* the *average* after repeating the N tosses many times.

2.11 EXPERIMENTAL DETERMINATION OF PROBABILITY

Our previous discussion has suggested that we could experimentally measure the probability of some particular result by repeating the experiment many times. That is, the probability of an event should be equal to the fractional number of times it occurs in a series of trials. For example, if you know a coin is loaded, you cannot assume that $P(\text{heads}) = P(\text{tails})$, and it might be difficult to calculate these probabilities theoretically. One way to find out what P(heads) is, would be to flip the coin many times, compute n_H/N, and set the result equal to $P(\text{heads})$. Thus, if N is very large, we should find that

$$\frac{n_H}{N} \simeq \frac{\langle n_H \rangle}{N} = P(\text{heads}) \tag{2.27}$$

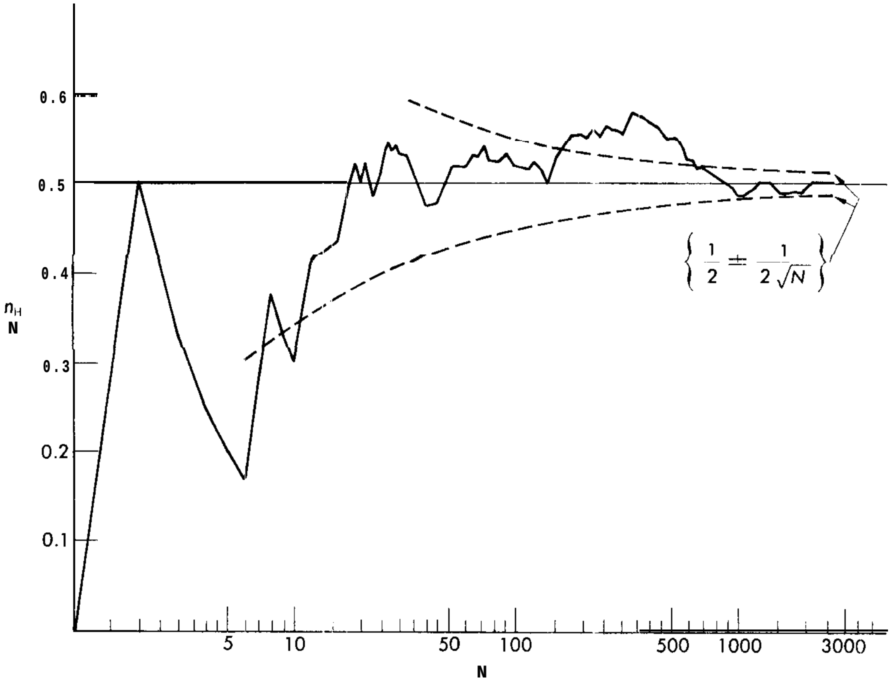


Figure 2.6. Graph of fractional number of heads in N tosses.

Figure 2.6 is a graph of n_H/N as a function of N in an actual experiment. Note the logarithmic horizontal scale. From the graph we see that for

$$N = 1, \quad \frac{n_H}{N} = 0;$$

$$N = 10, \quad \frac{n_H}{N} = 0.3;$$

$$N = 100, \quad \frac{n_H}{N} = 0.52$$

As N becomes very large, it is seen that n_H/N tends to ½. In this case, therefore,

$$P(\text{heads}) = \frac{\langle n_H \rangle}{N} = \lim_{N \to \infty} \frac{n_H}{N} = \frac{1}{2} \tag{2.28}$$

Although, as $N \to \infty$, one would obtain a unique value for $P(\text{heads})$, one may see from the graph that in actual practice the value of n_H/N for any finite N may be greater or less than ½, and generally could oscillate about ½ in some random fashion; the amplitude of these oscillations should decrease, however, as N increases.

2.12 EXPERIMENTAL ERROR

Since, in practice, we have to stop an experiment after some finite number of repetitions of the measurements, we would like to know how much error we are making on the average when we do this. In Figures 2.7 and 2.8 are given the

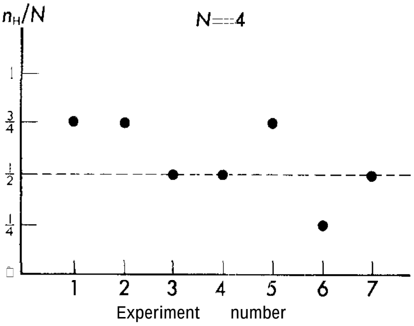


Figure 2.7.

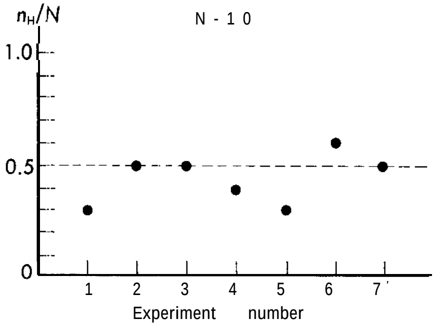


Figure 2.8.

actual fractions n_H/N, obtained in several repetitions of an experiment in which a coin was flipped N times. In the first experiment, N = 4; in the second, N = 10. One can see qualitatively that the points in the N = 10 case lie generally closer to the mean value of ½ than they do in the N = 4 case. Judging roughly from the scatter of the values of n_H/N in Figure 2.7, one might expect the error made in stopping at N = 4 to be about 0.2, whereas in Figure 2.8 it would be slightly smaller. Thus, generally speaking, we expect the error to decrease as the number of repetitions of the measurement increases.

2.13 RMS DEVIATION FROM THE MEAN

How can we define a precise numerical measure of the error? One way would be to average the distances of the points n_H/N from the mean value $\langle n_H\rangle/N$. In using such a measure we would have to be careful to take the magnitude of the distances; if we took some distances as positive and others as negative, we might calculate that the error was zero, which is not reasonable. A similar measure of error which is better for many purposes is the square root of the average of the squared differences of the points from the mean value. This is called the ***root* mean squared *deviation from the* mean.**

To illustrate what is meant, let us imagine that a coin is flipped N times. The mean $\langle n_H\rangle$ for a large number of experiments N should be ½ N. Consider the difference $n_H - \langle n_H\rangle$ for a single experiment with N flips. This difference is called the deviation from the mean. The squared deviation from the mean would be just $(n_H - \langle n_H\rangle)^2$. Here $\langle n_H\rangle$, as usual, is the average of n_H over many experiments, and n_H is the result for any one experiment. If we repeated the experiment many times and averaged this squared deviation from the mean, $(n_H - \langle n_H\rangle)^2$, over the experiments to obtain $\langle (n_H - \langle n_H\rangle)^2\rangle$, then this averaged squared deviation from the mean would be a measure of the square of the expected error. Thus, a measure of the expected error would be $\sqrt{\langle (n_H - \langle n_H\rangle)^2\rangle}$, the root mean squared deviation from the mean, or ***rms error*** for short.

The mean squared error may be reduced to another form which is also sometimes useful. First, write out the square as follows:

$$(n_H - \langle n_H\rangle)^2 = n_H^2 - 2n_H\langle n_H\rangle + \langle n_H\rangle^2 \tag{2.29}$$

If we take the average of both sides of this equation, then, since the average of a sum of terms may be computed term by term, we have

$$\langle (n_H - \langle n_H\rangle)^2\rangle = \langle n_H^2\rangle - \langle 2n_H\langle n_H\rangle\rangle + \langle\langle n_H\rangle^2\rangle \tag{2.30}$$

But from Equation 2.20, the average of a constant is just the same constant, so $\langle\langle n_H\rangle^2\rangle = \langle n_H\rangle^2$. Also from Equation 2.20, for any constant C we have $\langle C n_H\rangle = C\langle n_H\rangle$ and hence $\langle 2n_H\langle n_H\rangle\rangle = 2\langle n_H\rangle\langle n_H\rangle$. Combining these results, we obtain

$$\langle (n_H - \langle n_H\rangle)^2\rangle = \langle n_H^2\rangle - \langle n_H\rangle^2 \tag{2.31}$$

This result is quite general, for the mean squared error of any quantity; it was derived here using the variable n_H, but the derivation would be the same for any other variable. The equation states that the mean squared deviation from the mean is equal to the average of the square of the variable, minus the square of the average of the variable.

.14 RMS DEVIATION FOR COIN FLIPPING

To illustrate the use of rms error as a measure of error, we shall consider the case of coin flipping with a fair coin, and use the probability

$$P_N(n_H) = \frac{N!}{n_H!(N - n_H)!}\frac{1}{2^N} \tag{2.32}$$

to calculate the rms error as a function of N. We know that $\langle n_H\rangle = N/2$; hence, in this case, $\langle n_H\rangle^2 = N^2/4$. To calculate $\langle n_H^2\rangle$, we need to find

$$\sum_{n_H=0}^{N} \frac{n_H^2 N!}{n_H!(N - n_H)!}\frac{1}{2^N}$$

The result of the calculation is $n_H^2 = \frac{1}{4}N^2 + \frac{1}{4}N$. Anyone not interested in the details of this calculation should skip to the result in Equation 2.38.

As in the evaluation of n_H previously, we shall use a relabelling trick to evaluate the sum. We write $n_H^2 = n_H(n_H - 1) + n_H$, and use the fact that the average of a sum is the sum of averages. Then $\langle n_H^2\rangle = \langle n_H(n_H - 1)\rangle + \langle n_H\rangle$.

Since we already know that $\langle n_H \rangle = \frac{1}{2} N$, we need to calculate only $\langle n_H(n_H - 1)\rangle$. This is

$$\langle n_H(n_H - 1)\rangle = \sum_{n_H=0}^{N} n_H(n_H - 1)P_N(n_H)$$
$$= \sum_{n_H=0}^{N} \frac{n_H(n_H - 1)N!}{[2^N n_H!(N - n_H)!]} \tag{2.33}$$

The terms corresponding to $n_H = 0$ and $n_H = 1$ do not contribute because of the presence of the factor $n_H(n_H - 1)$ in the numerator. The sum then goes only over values of n_H from 2 through N. Now we will use the following identities to reduce the sum to something we can evaluate:

$$\frac{n_H(n_H - 1)}{n_H!} = \frac{1}{(n_H - 2)!}; \quad N! = N(N - 1)(N - 2)!;$$
$$(N - n_H)! = (N - 2 - [n_H - 2])!; \quad 2^N = 4 \cdot 2^{N-2} \tag{2.34}$$

Factoring out $\frac{1}{4} N(N - 1)$, we get

$$\langle n_H(n_H - 1)\rangle = \frac{1}{4} N(N - 1) \sum_{n_H=2}^{N} \frac{(N - 2)!}{[2^{N-2}(n_H - 2)!(N - 2 - [n_H - 2])!]} \tag{2.35}$$

The sum may be evaluated by letting $m = n_H - 2$. Then

$$\langle n_H(n_H - 1)\rangle = \frac{1}{4} N(N - 1) \sum_{m=0}^{N-2} \frac{(N - 2)!}{[2^{N-2} m!(N - 2 - m)!]}$$
$$= \frac{1}{4} N(N - 1)\left(\frac{1}{2} + \frac{1}{2}\right)^{N-2} = \frac{1}{4} N(N - 1) \tag{2.36}$$

Collecting the results, we have

$$\langle n_H^2 \rangle = \langle n_H(n_H - 1)\rangle + \langle n_H \rangle = \frac{1}{4} N(N - 1) + \frac{1}{2} N = \frac{1}{4} N(N + 1) \tag{2.37}$$

Finally, the root mean squared deviation from the mean is

$$\sqrt{\langle (n_N - \langle n_H \rangle)^2 \rangle} = \sqrt{\langle n_H^2 \rangle - \langle n_H \rangle^2} = \sqrt{\frac{1}{4} N(N + 1) - \frac{1}{4} N^2} = \frac{1}{2}\sqrt{N} \tag{2.38}$$

This rms deviation from the mean is the approximate number of heads by which we could usually expect the observation of n_H to differ from the expectation value, $\langle n_H \rangle = N/2$, in one series of N flips. We could call this the approximate error in finding the expectation value experimentally if we do one experiment with N flips. The fractional error in N tosses, i.e. the error in finding $\langle n_H \rangle / N$, is then the error divided by the number of tosses, or l/N times the rms deviation. The fractional error is therefore $\frac{1}{2}\sqrt{N}/N = 1/(2\sqrt{N})$. Thus, in attempting to measure a probability such as P(heads), we would have to say that after N flips in which n_H heads turned up, the probability would be equal to the fraction n_H/N but with a fractional error $1/(2\sqrt{N})$. Hence, we would write P(Heads) = $(n_H/N) \pm 1/(2\sqrt{N})$.

mple 1. After one flip of a fair coin, what would be the rms error in the measured probability?

ution $\frac{1}{2}/\sqrt{N} = \frac{1}{2}(1) = 0.5$.

mple 2. How many times would you have to flip the coin to reduce the uncertainty in the measured probability from 0.5 to 0.05?

ution $0.05 = \frac{1}{2}/\sqrt{N}$ or $N = \frac{1}{4}/(0.05)^2 = 100$ flips.

In Figure 2.6 the dashed lines are drawn at $\frac{1}{2} \pm \frac{1}{2}/\sqrt{N}$ to give an idea of the limits within which one could expect the graph to vary. This square root type behavior of an error occurs in many other places in physics. For example, in experiments in which the rate of decay of radioactive substances is measured, one simply counts the number N of decays in some time t. The measured counting rate is then N/f, and it can be shown by arguments very similar to those for coin flipping that the fractional error in the measured rate is of order of magnitude $1/\sqrt{N}$. Thus, to obtain good statistics, i.e. low error, in counting experiments, it is necessary to take large numbers of counts. To get the counting rate correct to three significant figures or a fractional error of 0.001, one would need around one million counts.

.15 ERRORS IN A COIN-FLIPPING EXPERIMENT

We may now compare this theory of the rms error with the experiments depicted in Figures 2.7 and 2.8. In Figure 2.7, each experiment (corresponds to N = 4. For this value of IV, the theory gives the fractional rms deviation to be $\frac{1}{2}/\sqrt{4} = 0.25$. Next, we will use the data of Figure 2.7 to find the experimental rms fractional deviation for this particular set of trails. To do this, we simply calculate the square root of the average of $[(n_H/N) - \langle n_H/N \rangle]^2$ over the seven experiments. The expectation value $\langle n_H/N \rangle$ is just the average of the results of these experiments and is 0.571. We may then obtain Table 2.2:

TABLE 2.2

Experiment Number	Deviation	(Deviation) ^{2}
1	0.179	0.0320
2	0.179	0.0320
3	-0.071	0.0050
4	-0.071	0.0050
5	0.179	0.0320
6	-0.321	0.1030
7	0.071	0.0050
		Sum = 0.2140

The average deviation squared is then $0.214/7 = 0.0306$, and the rms deviation is $\sqrt{0.0306} = 0.175$. Based on these seven experiments, the result of the first experiment could then be expressed as

$$\left\langle \frac{n_H}{N} \right\rangle = 0.750 \pm 0.175 \tag{2.39}$$

Likewise for the third experiment, $\langle n_H/N \rangle = 0.500 \pm 0.175$. This is in reasonable agreement with the theory, which supposes a very large number of experiments instead of seven and gives for the case $N = 4$,

$$\left\langle \frac{n_H}{N} \right\rangle = 0.500 \pm 0.25 \tag{2.40}$$

The reader can perform similar calculations for the data given in Figure 2.8 in the case $N = 10$. Here the experimental result for the rms deviation from the mean is 0.105. The theoretical result is

$$\left\langle \frac{n_H}{N} \right\rangle = 0.500 \pm 0.158 \tag{2.41}$$

2.16 ERRORS IN AVERAGES OF REPEATED EXPERIMENTS

Errors of the type we have described, depending on $1/\sqrt{N}$, also arise when repeating experiments which measure the average value of some physical quantity, such as the diameter of a cylinder or the length of an object. Suppose that an experiment is performed in which the quantity x is measured N times. It must be kept in mind here that a single experiment means N measurements of the value of the quantity, and the result of an experiment is the average value of the quantity for these N measurements. Then we ask: What is the error in the average value? If the experiment is repeated, it should give a new average value that does not differ from the previous one by much more than the error.

What is being measured here is an average itself. This average is not the same as the expectation value. The expectation value would be equal to the average if the number of measurements, N, approached infinity.

Suppose that the N individual measurements in one experiment are $x_1, x_2, \ldots, x_N$. The result of the experiment is then $(x_1 + x_2 + \cdots + x_N)/N$. Suppose the true, or expectation, value of the quantity is X. This would be the average of an extremely large number of measurements. The deviation from the true value X in a particular experiment is

$$\frac{x_1 + x_2 + \cdots + x_N}{N} - X$$

We can then get a measure of the experimental error by computing the rms error, averaged over many experiments of N measurements each. Call the error E_N.

Then

$$E_N = \sqrt{\left\langle\left(\frac{x_1 + x_2 + \cdots + x_N}{N} - X\right)^2\right\rangle} \tag{2.42}$$

To illustrate how this may be worked out, we shall take the case $N = 2$, only two measurements in an experiment. Then

$$\begin{aligned}
E_N &= \sqrt{\frac{\langle(x_1 + x_2 - NX)^2\rangle}{N^2}} \\
&= \sqrt{\frac{\langle([x_1 - X] + [x_2 - X])^2\rangle}{N^2}} \\
&= \sqrt{\frac{\langle(x_1 - X)^2 + 2(x_1 - X)(x_2 - X) + (x_2 - X)^2\rangle}{N^2}} \\
&= \sqrt{\frac{\{\langle(x_1 - X)^2\rangle + 2\langle(x_1 - X)(x_2 - X)\rangle + \langle(x_2 - X)^2\rangle\}}{N^2}}
\end{aligned} \tag{2.43}$$

for $N = 2$. Consider the term $\langle(x_1 - X)(x_2 - X)\rangle$. Whereas a term like $\langle(x_1 - X)^2\rangle$ is always positive, $(x_1 - X)$ is negative about as often as it is positive, and so is $(x_2 - X)$. Since the values of $(x_1 - X)$ and $(x_2 - X)$ are independent of each other,, their product will also be negative as often as it is positive, and the expectation value $\langle(x_1 - X)(x_2 - X)\rangle$ will be zero. Hence the only remaining terms produce:

$$E_N = \sqrt{\frac{\{\langle(x_1 - X)^2\rangle + \langle(x_2 - X)^2\rangle\}}{N^2}} \tag{2.44}$$

This was for the case $N = 2$. However it is easy to see that a similar argument applies for any N; all the expectation values of the cross-terms which arise in the square $[(x_1 - X) + (x_2 - X) + \cdots + (x_N - X)]^2$ will be nearly zero. Therefore,, for any N, we can say

$$E_N = \sqrt{\frac{\{\langle(x_1 - X)^2\rangle + \langle(x_2 - X)^2\rangle + \cdots + \langle(x_N - X)^2\rangle\}}{N^2}} \tag{2.45}$$

However, since the subscripts on the x's denote nothing more than the order in which the measurements are made, we expect that, on the average, the quantity $\langle(x_i - X)^2\rangle$ will be the same for all x_i, or

$$\langle(x_1 - X)^2\rangle = \langle(x_2 - X)^2\rangle = \langle(x_N - X)^2\rangle \equiv E_1^2 \tag{2.46}$$

We call this average E_1^2, since it is the mean squared error of a single measurement, averaged over many experiments. That is, E_1 is the rms deviation if we consider that the experiment consists of one measurement rather than N measurements. Then, since there are N terms like $\langle(x_i - X)^2\rangle$,

$$E_N = \sqrt{\frac{NE_1^2}{N^2}} = \frac{E_1}{\sqrt{N}} \tag{2.47}$$

Thus, the error in the result of an N-measurement experiment is less than the error in the result of a one-measurement experiment by a factor of $1/\sqrt{N}$. To see how this works in practice, Table 2.3 gives the actual results of 24 measurements of the diameter, in centimeters, of a cylinder, using vernier calipers. If we regard these as 24 separate experiments in which N = 1, then we can compute the mean value and the error for these 24 experiments. The mean of the 24 measurements, which we shall take as the true value, is X = 4.0754 cm and the rms error E_1 for one measurement is

TABLE 2.3 Results of Six Experiments, Each Consisting of Four Measurements of the Length of a Cylinder. Distances in Centimeters.

(1)	(2)	(3)	(4)	(5)	(6)
4.11	4.07	4.08	4.05	4.09	4.06
4.06	4.05	4.10	4.06	4.08	4.10
4.06	4.06	4.09	4.09	4.06	4.07
4.08	4.08	4.09	4.10	4.04	4.08
Av. = 4.0775	Av. = 4.065	Av. = 4.090	Av. = 4.075	Av. = 4.0675	Av. = 4.0775

Overall average of the results = 4.0754 cm

$$E_1 = \sqrt{\frac{\sum (\text{deviations})^2}{24}} = 0.018 \text{ cm} \tag{2.48}$$

Let us next regard the data as six experiments of four measurements each, in which the quantity being measured is the average of four measurements. In this case, N = 4, so the error in the average of the four measurements should be about $E_4 = E_1/\sqrt{5} = 0.009$ cm. By subtracting the overall average, 4.0754 cm, from each of the averages of the six experiments, we can find the experimental deviations of the averages from the mean. Then the experimental E_4 is

$$E_4 = \sqrt{\frac{\sum (\text{deviations of averages})^2}{6}} = 0.0081 \text{ cm} \tag{2.49}$$

This compares favorably with the result, 0.009 cm, obtained using Equation (2.47). Actually, while we used the mean of 24 experiments as the true value, this itself has an rms error associated with it. An estimate of this error, again using Equation (2.47), is $E_1/\sqrt{24} = 0.018/4.90 = .0037$ cm. The reader may well reflect that these differing measures of error for the same data look somewhat suspicious; however, this simply means that quoted errors often depend on the method of data handling.

2.17 PROBABILITY DENSITIES

So far, we have considered distribution functions which are functions of a discrete variable. In many cases, the independent variables are continuous. Consider, for example, a thin circular disc on a horizontal axle. If the disc is given a spin and then allowed to come to rest, what is the probability that some one point on the rim of the disc will be exactly on top? Obviously, since one point is only one of an uncountable infinity of points along the rim, the probability will be zero. However, let us introduce a coordinate system fixed in the wheel, and describe points on the rim in terms of an angle 0, with θ varying continuously from 0 to 2π to describe all different points on the rim. If there is no reason why one portion of the disc should come to the top more often than any other portion, then the probability that some portion in the infinitesimal range $d\theta$ will come up,, denoted by $P_{d\theta}$, is $P_{d\theta} = d\theta/2\pi$. The factor 27r in the denominator is chosen so that the total probability that some point (any point) on the rim comes to the top is unity. We can check this because

$$\sum_{\text{all } d\theta\text{'s}} P_{d\theta} = \int_0^{2\pi} \frac{d\theta}{2\pi} = \frac{2\pi}{2\pi} = 1 \tag{2.50}$$

Once an infinitesimal probability of this nature is known, it can be used to find the probability that an event takes place in a given range.. Thus, the probability that some point in the portion of the rim between $\pi/6$ and π will come to the top will be the integral of $d\theta/2\pi$ between the limits of $\pi/6$ and π. The result is $5/12$. The coefficient of $d\theta$ in the expression for $P_{d\theta}$ is called a probability density. In this special case, the probability density is $1/2\pi$. In general, for the continuous variable θ, if the probability of finding θ in the range $d\theta$ is given by an expression of the form $P_{d\theta} = p(\theta)\,d\theta$, then $p(\theta)$ is called the probability density. In our example, the probability density, p(B),. was a constant; but if, for instance, there were more friction on one side of the axle than the other, the wheel would be more likely to stop in certain positions, and $p(\theta)$ would not be independent of θ.

Similarly, with a different physical situation described by a variable x, and given the probability density p(x), the probability that x is to be found in the range dx will be $P_{dx} = p(x)\,dx$. A probability density is thus the probability per unit x, for the continuous variable x. Moreover, the probability that x will be

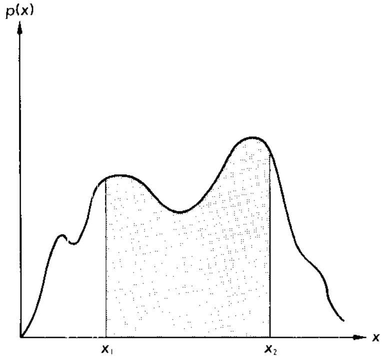


Figure 2.9. Crosshatched area under the probability density curve is the probability that a measurement of x will yield a value between x_1 and x_2

found in the range between x_1 and x_2 will be given by $\int_{x_1}^{x_2} p(x)\,dx$. This is just the area under the 'curve of p(x), versus x between the limits x_1 and x_2 (see Figure 2.9). Probability densities have the property that, when integrated over all possible values of x, the result must be the total probability that some value of x occurs, or $\int_{\text{all } x} p(x)\,dx = 1$.

2.18 EXPECTATION VALUES FROM PROBABILITY DENSITIES

We shall next show how to compute an average using a probability density. You recall that for a discrete probability distribution function, $P(x_i)$, of the discrete variable x_i, the rneon value of x is given by

$$\langle x\rangle = \sum_{\text{all } x_i} x_i\, P(x_i)$$

where $P(x_i)$ is the probability that x_i occurs. It is unnecessary to divide by $\sum_{\text{all } x_i} P(x_i)$ here, since the sum of the probabilities is unity. Now consider the entire range of the continuous variable x to be broken up into small increments Ax,. If x, is a point in Δx_i, then the probability $P(x_i)$ that it lies in the range Ax, will be given approximately by $P(x_i) = p(x_i)$ Ax,, where p(x) is the probability density. Thus, (x) = $\sum_{x_i} x_i\, p(x_i)\, \Delta x_i$. Taking the limit as $\Delta x_i \rightarrow 0$, we get

$$\langle x\rangle = \int_{\text{all } x} x p(x)\,dx. \tag{2.51}$$

example 1. Consider the probability density defined for $0 \le x \le 1$ by

$$p(x) = \begin{cases} 2, & 0 \le x \le ½ \\ 0, & ½ \le x \le 1 \end{cases}$$

A plot for p(x) is given in Figure 2.10. If we wish to compute the average value of some quantity using the given p(x), we should first check to see that p(x) is correctly normalized. It will be correctly normalized if the integral

$$\int_{\text{all } x} p(x)\,dx$$

is equal to one. In this case, $\int p(x)dx = \int_0^{1/2} 2dx = 1$, so the normalization is correct. The limits on the integral are 0 and ½, because in this special case, when $x > ½$, p(x) is equal to zero. To find the expectation value (x), we should compute the integral $\int x p(x) dx$. In this case also, the limits on the integral will be from 0 to ½ The integration may then be performed as follows:

$$\langle x\rangle = \int_0^{1/2} 2x\ dx = \frac{1}{4}$$

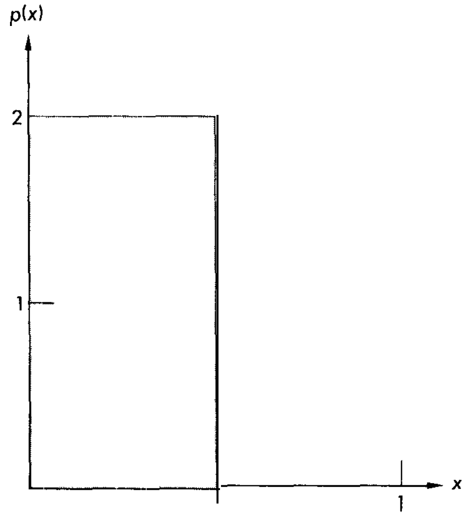


Figure 2.10.

ple 2. Consider a particle in a one dimensional box with ends at $x = 0$ and $x = 2$. The probability density for finding the particle outside the box is zero. In quantum mechanics the probability density is $\psi(x)|^2$, where the wave function $\psi(x)$ satisfies a wave equation called the *Schrödinger* ***equation.*** Suppose the probability density, $|\psi(x)^2$, is given by

$$|\psi(x)|^2 = p(x) = \frac{15}{16}\left(x^2 - \frac{1}{4}x^4\right)$$

for $0 \leq x \leq 2$. Outside this range, **p(x)** is zero. A plot of this function is shown in Figure 2.11. This probability density p(x) is correctly normalized so that

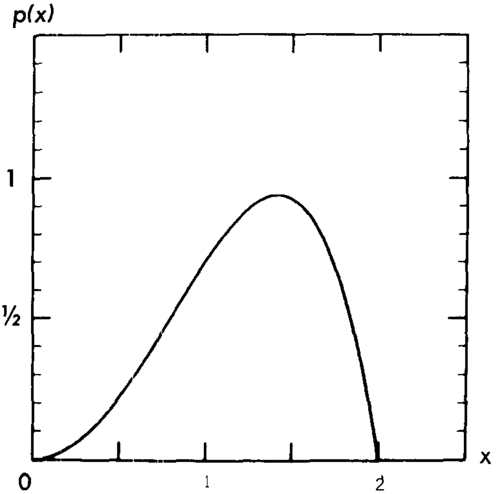


Figure 2.11.

$\int_0^2 p(x)dx = 1$. We can calculate the averuge value or expectation value of x as follows:

$$\langle x\rangle = \int_0^2 xp(x)\,dx = \frac{15}{16}\int_0^2 x\left(x^2 - \frac{1}{4}x^4\right)dx$$

$$= \frac{15}{16}\left(\frac{1}{4}x^4 - \frac{1}{24}x^6\right)\Bigg|_0^2 = \frac{5}{4}$$

Let us also calculate the rms deviation of x from the mean. This is a measure of the spread of the wave function $\psi(x)$. The rms deviation is

$$\langle(x - \langle x\rangle)^2\rangle^{1/2}$$

We know that the expectation value of x, $\langle x\rangle$, is $^5/_4$. Hence we wish to calculate the expectation value

$$\left\langle\left(x - \frac{5}{4}\right)^2\right\rangle = \langle x^2\rangle - \langle x\rangle^2 = \langle x^2\rangle - \frac{25}{16}$$

from Equation (2.31) It is

$$\left\langle\left(x - \frac{5}{4}\right)^2\right\rangle = \int_0^2 (x^2)p(x)\,dx - \frac{25}{16} = \frac{15}{16}\int_0^2\left(x^4 - \frac{1}{4}x^6\right)dx - \frac{25}{16}$$

$$= \frac{15}{16}\left(\frac{32}{5} - \frac{128}{28}\right) - \frac{25}{16} = \frac{17}{112} = 0.1518$$

Then the rms deviation from the mean is

$$\sqrt{\left\langle\left(x - \frac{5}{4}\right)^2\right\rangle} = \sqrt{0.1518} = 0.390$$

The same result can be obtained by straightforward calculation of

$$\left\langle\left(x - \frac{5}{4}\right)^2\right\rangle = \int_0^2\left(x^2 - \frac{5x}{2} + \frac{25}{4}\right)p(x)\,dx$$

but the algebra is more tedious.

2.19 GAUSSIAN DISTRIBUTION

An interesting probability density, called the *gaussian distribution,* arises when a fair coin is flipped an extremely large number of times. This same distribution arises in the majority of physical measurements involving random errors. In flipping a coin N times, the discrete probability distribution function was, from Equation (2.13),

$$P_N(n_H) = \frac{N!}{[2^N n_H!(N - n_H)]} \tag{2.52}$$

In the limit of very large N, this distribution function is sharply peaked about the average value of n_H, $\frac{1}{2}N$. This tendency may be seen by referring to Figures 2.1 through 2.4.

We can obtain an approximate analytical expression for $P_N(n_H)$, for large N, by using Stirling's approximation for the factorials: For large n, $\ln(n!) \cong \frac{1}{2}\ln(2\pi) + (n + \frac{1}{2})\ln(n) - n$. This, together with the approximation $\ln(1 + b) \cong b - \frac{1}{2}b^2$ for small b, leads to the following approximate result for $P_N(n_H)$:

$$P_N(n_H) \cong \sqrt{\frac{2}{\pi N}} \exp\left[\frac{-(n_H - N/2)^2}{N/2}\right] \tag{2.53}$$

when N is large and n_H is near its average, $\frac{1}{2}N$. A graph of Equation (2.53) is shown for N = 100 in Figure 2.12. The corresponding discrete curve of Figure 4 is shown on the same graph. It may be seen that for N = 100, the approximation of Equation (2.53) is already extremely good.

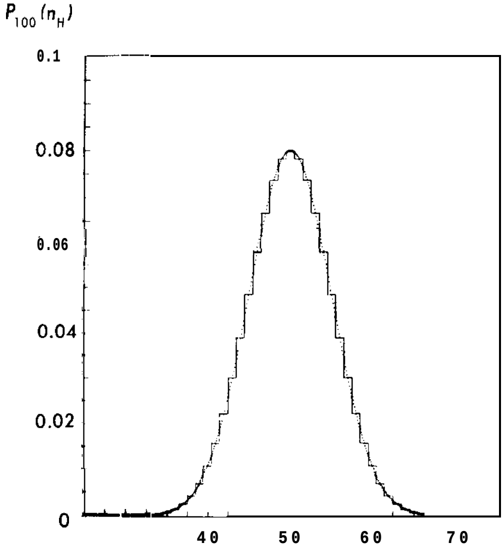


Figure 2.12. Comparison of the discrete probability distribution $P_{100}(n_H)$ with approximate function, a Gaussian. The Gaussian curve is drawn with a dashed line.

The exponential curve of Equation (2.53), peaked symmetrically about $\frac{1}{2}$ N, is called a gaussian or normal distribution. It occurs often in probability theory and in classical statistical mechanics. Although n_H is still a discrete variable taking on integral values, when N is sufficiently large we can lump many of these integral values together and regard $P_N(n_H)$ as a probability density.

20 EXPECTATION VALUES USING A GAUSSIAN DISTRIBUTION

In other chapters we will need a number of expectation values using the gaussian distribution. To illustrate the types of integrals which arise, let us find the root mean squared deviation of x for the gaussian probability density p(x), given by

$$p(x)\,dx = \frac{1}{\sqrt{2\pi}\,\sigma}\exp\left[\frac{-(x-x_1)^2}{2\sigma^2}\right]dx$$

Here x ranges from $-\infty$ to ∞, and the quantities x_1 and σ are constants. First, we check that this probability density is normalized to unity. Referring to the table of definite integrals, Table 2.4,

TABLE 2.4 Table of Integrals

$$\int_{-\infty}^{\infty}\exp\left(\frac{-y^2}{2\sigma^2}\right)dy = \sqrt{2\pi}\,\sigma$$

$$\int_{-\infty}^{\infty}y^2\exp\left(\frac{-y^2}{2\sigma^2}\right)dy = \sqrt{2\pi}\,\sigma^3$$

and letting $y = x - x_1$ with $dx = dy$, we find that

$$\int_{-\infty}^{\infty}p(x)\,dx = \frac{1}{\sqrt{2\pi}\,\sigma}\int_{-\infty}^{\infty}\exp\left(\frac{-y^2}{2\sigma^2}\right)dy = 1$$

In calculating the rms deviation from the mean of x, we need first to find the mean. Since the distribution is symmetric about $x = x_1$, it is clear that $\langle x\rangle = x_1$. If this were not obvious, the average value of x could be calculated by the equation

$$\langle x\rangle = \int_{-\infty}^{\infty}xp(x)\,dx \tag{2.54}$$

In the case of the gaussian, this is

$$\begin{aligned}\langle x\rangle &= \frac{1}{\sqrt{2\pi}\,\sigma}\int_{-\infty}^{\infty}x\exp\left[\frac{-(x-x_1)^2}{2\sigma^2}\right]dx\\ &= \frac{1}{\sqrt{2\pi}\,\sigma}\int_{-\infty}^{\infty}(x-x_1)\exp\left[\frac{-(x-x_1)^2}{2\sigma^2}\right]dx\\ &\quad+\frac{x_1}{\sqrt{2\pi}\,\sigma}\int_{-\infty}^{\infty}\exp\left[\frac{-(x-x_1)^2}{2\sigma^2}\right]dx\end{aligned} \tag{2.55}$$

The first integral on the right is zero because the integrand is odd in $(x - x_1)$. The second term is x_1. Thus, for a gaussian peaked about x_1, the average value of x is just the position of the center of the peak: $\langle x\rangle = x_1$.

Let us next calculate the rms deviation from the mean. This is $\sqrt{\langle (x-x_1)^2\rangle}$, so we first need to calculate the expectation value,

$$\langle (x-x_1)^2\rangle = \frac{1}{\sqrt{2\pi}\,\sigma}\int_{-\infty}^{\infty}(x-x_1)^2\exp\left[\frac{-(x-x_1)^2}{2\sigma^2}\right]dx \tag{2.56}$$

Again, with the substitution $y = x - x_1$, this reduces to the second integral in Table 2.4. Therefore, $\langle (x - x_1)^2 \rangle = \sigma^2$. Hence, the rms deviation from the mean is equal to σ. As a characteristic width of the gaussian curve, we might take the distance from x_1 to the point where the curve is half its maximum. This is at $x - x_1 = \sqrt{2 \ln 2}\,\sigma$ = 1.180. Thus we see that the width at half-maximum and the rms deviation are about the same.

summary

CALCULATION OF PROBABILITY

The probability of an event is equal to the number of possible ways of getting the particular result, divided by the total number of ways of getting all possible results. If A and B are two independent events, the total probability of getting either the result A or the result B is equal to the sum of the probabilities of getting A and of getting B separately:

$$P(\text{either } A \text{ or } B) = P(A) + P(B)$$

The probability of getting both A and B is equal to the product of the probabilities of getting A and of getting B separately:

$$P(\text{both } A \text{ and } B) = P(A)\,P(6)$$

The total probability of getting all possible results in a given situation is unity.

PROBABILITY DISTRIBUTION FUNCTIONS AND DENSITIES'

A probability P(n), which is a function of some discrete variable n, and which gives the probability of the event characterized by n, is called a probability distribution function. The normalization of a probability distribution function is unity:

$$\sum_{\text{all } n} P(n) = 1$$

A quantity p(x), which is a function of the continuous variable x, such that p(x) dx is the probability of finding x in the infinitesimal interval dx, is called a probability density.

$$\int_{\text{all } x} p(x)\,dx = 1$$

If f (n) is a distribution function, then the probability distribution function P(n) is given by $P(n) = f(n)/\sum_{\text{all } n} f(n)$. If f (x) is a function of the continuous variable x, then likewise, $p(x) = f(x)/\int f(x)\,dx$.

EXPECTATION VALUES

The average value of any quantity g(n) or g(x) is defined as:

$$\langle g\rangle = \frac{\sum g(n)\, f(n)}{\sum f(n)} = \sum g(n)\, P(n)$$

or

$$\langle g\rangle = \frac{\left(\int g(x)\, f(x)\, dx\right)}{\int f(x) dx} = \int g(x)\, p(x)\, dx$$

The average value is also called an expectation value, because in repetitions of the experiment, when average values are computed, it is to be expected that their values are equal to the expectation value.

EXPERIMENTAL DEFINITION OF PROBABILITY

If an experiment is performed which is repeated N times, and the event H occurs a total of n_H times, then the experimental definition of the probability of the event H is

$$\lim_{N\to\infty} \frac{n_H}{N} = P(H)$$

The root mean square (rms) deviation of n_H from the mean is defined as

$$\sqrt{\langle (n_H - \overline{n_H})^2\rangle} = \sqrt{\langle n_H^2\rangle - \langle n_H\rangle^2}$$

The rms deviation from the mean of a measured quantity is a good measure of the error, or uncertainty, in the measured value of the quantity.

If a measurement is repeated N times, the probable error in the average is proportional to $1/\sqrt{N}$ times the probable error for one measurement.

problems

1. If you draw 4 cards from a standard deck of playing cards, what is the probability that they are all aces?
   Answer: $(4\cdot 3\cdot 2\cdot 1)/(52\cdot 51\cdot 50\cdot 49) = 1/270{,}725$.
2. If you draw 4 cards from a standard deck of playing cards, what is the probability that none is an ace?
   Answer: $(48\cdot 47\cdot 46\cdot 45)/(52\cdot 51\cdot 50\cdot 49) = 38{,}916/54{,}145$.
3. If you draw 4 cards from a standard deck of playing cards, what is the probability that exactly one is an ace?
   Answer: $4\cdot(48\cdot 47\cdot 46\cdot 4)/(52\cdot 51\cdot 50\cdot 49) = 69{,}184/270{,}725$.
4. A jar contains 3 black balls and 4 white balls. If you draw 1 ball out of the jar, what is the probability that it will be white?
   Answer: 4/7.

5. A jar contains 4 black balls and 10 white balls. If you draw 2 balls out of the jar, what is the probability that both will be white?

   Answer: $(10 \times 9)(14 \times 13) = 45/91$.

6. A blind man in a cafeteria comes to pick up his silverware, which is stored in deep cans. Two of the cans contain forks. One can contains 1 salad fork, the other contains 99 regular forks and 1 salad fork. He sticks his hand at random into a can and picks a fork at random from the forks in the can. What is the probability that he will pick a salad fork?

   Answer: 0.505.

7. If the probability of missing the bull's-eye target shooting is 0.96, how many bull's-eyes would you expect to hit in 350 shots?

   Answer: 14.

8. What is the probability that in 10 throws of a die, a 2 comes up 5 times?

   Answer: $10!5^5/(5!)^2 6^{10} = 21{,}875/1{,}679{,}616$.

9. What is the probability that in 10 throws of a die, a 2 comes up 5 times and a 3 comes up 2 times?

   Answer: $10!4^3/5!2!3!6^{10} = 35/13122$.

10. If a rabbit runs past you and the probability of catching it is 0.05, then what is the probability of catching at least 2 rabbits if a herd of 160 rabbits runs by one at a time? What is the probability of catching exactly 2 rabbits?

    Answer: $1 - (0.95)^{160} - 160(0.95)^{159} \cdot (0.05) = 0.99743$;
    $160!(0.95)^{158}(0.05)^2/158!2! = 0.00961$

11. According to quantum mechanics, a free atom may have an intrinsic angular momentum $\sqrt{n(n+2)}\,\hbar/2$ associated with it, where n is an integer and $\hbar$ a constant. If a particular component is measured, it can have with equal probability $n + 1$ equally spaced values from $-\frac{1}{2} n\hbar$ to $\frac{1}{2} n\hbar$. If there are N such noninteracting atoms, what is the probability that there are m_1 with z components of $\frac{1}{2} n\hbar$, m_2 with $(\frac{1}{2} n - 1)\hbar, \ldots, N - (m_1 + m_2 + \cdots + m_n)$ with $-\frac{1}{2} n\hbar$?

    Answer: $N!/(n+1)^N m_1!m_2! \ldots [N - (m_1 + m_2 + \ldots + m_n)]!$

12. A crystal is grown by evaporating A and B type atoms, and then letting them condense to form the crystal. If, because of the forces involved, an A atom is twice as likely to stick to the crystal as a B atom, what is the probability that the final crystal will consist of $\frac{2}{3} A$ atoms if there are 3N total atoms? What is the probability in terms of N that it will consist of $\frac{2}{3}$ B atoms? Find the ratio of these probabilities if $N = 10^{22}$.

    Answer: $(3N)!2^{2N}/3^{3N}N!(2N)!$; $(3N)!2^N/3^{3N}N!(2N)!$;
    $2^{10^{22}} = 10^{(3 \times 10^{21})}$

13. Suppose a prism whose cross section is an equilateral triangle has the three faces forming the triangle marked A, B and C. If the triangle is dropped on a table, it is equally likely that any of these faces is on the bottom. If it is dropped N times, find an expression for the probability that the A face is on the bottom n times, B m times, and C $(N - n - m)$ times.

    Answer: $N!/3^N n!m!(N - n - m)!$

14. If, in the previous problem, the triangular cross section is not equilateral but is such that in one drop of the prism the probability that side A is down is p and that side B is down is q, what is the probability of n A's and m B's in N trials?

    Answer: $N!p^n q^m(1 \quad p - q)^{N-n-m}/n!m!(N \quad n - m)!$

15. A particle can move along the x axis, and is moved successively by the fixed amount Δx with equal probability either in the positive or the negative x direction. If

it is moved N times, what is the probability that it is $n\,\Delta x$ in the positive x direction away from where it started? Assume N and n are both even integers.

Answer: $N!/2^N \left(\frac{N+n}{2}\right)! \left(\frac{N-n}{2}\right)!$

16. If in a trial the probability of getting result 1 is p and that of getting result 2 is $q = 1 - p$, show that in N trials the expectation value of the number of times one gets result 1 is

$$\left[x \frac{d}{dx} \sum_{n=0}^{N} \frac{N!x^n q^{N-n}}{n!(N-n)!}\right]_{x=p} = \left[x \frac{d}{dx}(x+q)^N\right]_{x=p}$$

Find this expectation value. Also find the expectation value of the square of the number of times one gets result 1.

Answer: Np; N^2p^2 + Npq.

17. In quantum mechanics, it is found that a harmonic oscillator consisting of a mass m and a spring of constant k can have energies of $E_n = (n + \tfrac{1}{2})\hbar\omega$, where $\hbar$ is a constant, $\omega = \sqrt{k/m}$, and n is an integer or zero. As you will see in the statistical mechanics chapter, the probability that it has an energy E_n, when the Kelvin temperature is J, is

$$\frac{\exp(-E_n/k_B T)}{\sum_{n=0}^{\infty} \exp(-E_n/k_B T)}$$

where k_B is a constant called *Boltzmann's* constant. The denominator is a geometric series whose sum is given by

$$\sum_{n=0}^{\infty} \exp\left(\frac{-E_n}{k_B T}\right) = \frac{\exp(-\tfrac{1}{2}\,h\omega/k_B T)}{1 - \exp(\hbar\omega/k_B T)}$$

Show that the expectation value of the energy is given by

$$\left[-\frac{d}{dx}\ln\left(\sum_{n=0}^{\infty} e^{-E_n x}\right)\right]_{x=1/k_B T}$$

and evaluate it.

Answer: $h\omega\{1 + 1/[\exp(h\omega/k_B T) - 1]\}$.

18. Suppose N noninteracting particles are confined in a volume V. What is the probability that any one particle will be found inside a volume V', which is inside V? What is the probability of finding all N particles in V'?

Answer: V'/V; $(V'/V)^N$.

19. An unfair coin is tossed 10 times, with $p(H) =: 0.6$. Calculate the rms deviation from the mean of n_H. See Problem 16.

Answer: 1.549.

20. Suppose N noninteracting particles are confined in a volume V, and all momenta are equally probable so long as their components lie between p_x and $p_x + P_x$, p_y and $p_y + P_y$, and p_z and $p_z + P_z$. What is the probability that the ith particle lies in the volume $dx_i dy_i dz_i$ inside V and lies in the momentum range dp,,, dp_{yi}, dp,, inside the momentum bounds? What is the total probability that these N particles are in

$dx_1, dy_1, dz_1, , dx_N, dy_N$ and dz_N, and $dp_{x_1}, , dp_{zN}$? This 6N dimensional space of coordinates and momenta is called phase space.

Answer: $\dfrac{dx_i\, dy_i\, dz_i\, dp_{x_i}\, dp_{y_i}\, dp_{z_i}}{VP_xP_yP_z}$; $\dfrac{dx_1\, dy_1 \ldots dz_N\, dp,\, dp_{x_1} \ldots dp_{zN}}{(VP_xP_yP_z)^N}$.

21. The displacement of a mass executing harmonic motion is given by $x = x_0 \cos \omega t$. The time it spends in dx is dx/v in a given half cycle, where $v = \omega x_0 \sin \omega t$. A half period is π/ω. In terms of dx, t, ω, x_0, what is the probability of finding the mass in dx? This probability can be written as f(x) dx, where f(x) is the distribution function. Find f(x). Find the expectation value for x and x^2.

Answer: $dx/\pi x_0 \sin \omega t|$; $f(x) = 1/\pi\sqrt{x_0^2 - x^2}$, $\langle x\rangle = 0$, $(x') = \frac{1}{2}x_0^2$.

22. The distribution of weights x in lb, of a large set of objects is given by the distribution function $f(x) = e^{-10x}$, where $0 \leq x \leq \infty$. What is the normalization constant C such that $Cf(x)$ is the probability density? What is the average value of the weight x? What is the rms deviation from the mean?

Answer: 10; $\frac{1}{10}$; $\frac{1}{10}$.

23. If an arrow is dropped on a uniform table, all directions are equally probable. Find the distribution function $f(\theta)$ where the probability that it points in the increment $d\theta$ is f(%)d%. Find the expectation value of θ, and of θ^2 if θ varies between $-\pi$ and π.

Answer: $1/(2\pi)$; 0 ; $\pi^2/3$.

24. A piece of sand falls in an hourglass a distance h. At the instant it hits, another piece starts falling, etc. What in terms of the distance y down from the top, is the probability of finding a piece of sand in the increment dy at the distance $y < h$? What is the expectation value of y for a moving piece of sand?

Answer: $dy/2\sqrt{hy}$; $h/3$.

25. A fair coin is tossed 360,000 times. Estimate the ratio of the probability that heads turn up 179,000 times, to the probability that heads turns up 180,000 times (assume the gaussian distribution).

Answer: *0.00387.*

3 special theory of relativity

In this chapter it will be seen that the laws of Newtonian mechanics, when used to describe objects of very high energies, or traveling at very high speeds, give predictions which disagree with experiment. The understanding of the fundamental reasons for these disagreements and the discovery of the theory of relativity, which agrees with experiment, are due to Albert Einstein (1879-1955). His theory is based on some simple experimental facts and on a careful analysis of the processes of measurement of length and time.

We shall discuss how length and time measurements are related in frames of reference which are moving with respect to each other. These relationships are called the *Lorentz* transformation *equations* and are basic to the later development of the laws of physics, when speeds are comparable to that of liight. Historically, the primary experiment which helped convince other physicists that Einstein's theory was correct was the Michelson-Morley experiment, to be discussed in Section 3.12. However, we shall first look at some other discrepancies between the predictions of classical physics and experiment; such discrepancies also necessitate the introduction of the theory of relativity.

3.1 CONFLICT BETWEEN ULTIMATE SPEED AND NEWTON'S LAWS

In Newtonian or classical mechanics, the basic law which describes the motion of any particle of mass m under the action of a net applied force F and with acceleration a is Newton's second law of motion, $F = ma$. This law agrees with experiment for most ordinary situations, but it breaks down in extreme situations, such as for particles going at very high speeds.

Imagine, for example, an electron of mass 9.11×10^{-31} kg acted on by an electric field of 10^6 volts/m over a distance of ten meters. The force is the charge times the field or 1.6×10^{-13} nt. By Newton's second law, the acceleration is $F/m = 1.76 \times 10^{17}$ m/sec^2. If the electron starts from rest, the kinematic expression for the speed v is $v = \sqrt{2as}$, where s is the distance the particle has moved. In this example for s = 10 m, the final speed is $v = 1.9 \times 10^9$ m/sec.

However, it is now a well-known fact, substantiated by multitudes of experiments with cyclotrons and other accelerating machines, that no particle can be made to go faster than the speed of light, c = 2.9974 x 10^8 m/sec (hereafter we will use 3 x 10^8 m/sec for c). Thus, Newtonian mechanics disagrees with experiment. The error is either in the second law of motion, or in the kinematics, or both. However, since the kinematical relation follows directly from the definitions of velocity and acceleration, we would expect that it is the law of motion which must somehow be modified in order to resolve the discrepancy.

3.2 CLASSICAL MOMENTUM AND ENERGY CONSERVATION—CONFLICT WITH EXPERIMENT

The laws of conservation of mechanical energy and momentum follow from Newton's laws of motion, which were seen to be of suspect validity by the preceding example. Now we shall apply these classical conservation principles to the problem of an elastic collision between two bodies of equal mass. Comparison of our prediction for high speed experiments will show a discrepancy, giving further evidence that the laws of motion must be modified, and that the definitions of energy and momentum will also have to be modified if we are to retain our concept of the existence of conserved physical quantities.

For a particle of mass *m* and velocity v colliding elastically with another of the same mass initially at rest, conservation of energy gives

$$\frac{1}{2}mv^2 = \frac{1}{2}mv_1^2 + \frac{1}{2}mv_2^2 \qquad v^2 = v_1^2 + v_2^2 \tag{3.1}$$

where $\mathbf{v}_1$ and $\mathbf{v}_2$ are the velocities of the two particles after the collision. (See Figure 3.1.) Likewise, conservation of momentum gives us

$$m\mathbf{v} = m\mathbf{v}_1 + m\mathbf{v}_2 \quad \text{or} \quad \mathbf{v} = \mathbf{v}_1 + \mathbf{v}_2 \tag{3.2}$$

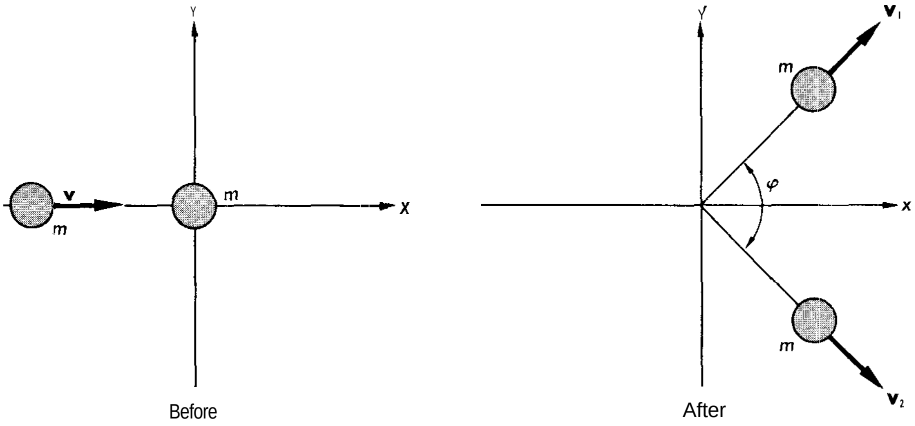


Figure 3.1. Collision of particles with equal rest mass.

The scalar product of the latter equation with itself leads to

$$v^2 = v_1^2 + 2\mathbf{v}_1 \cdot \mathbf{v}_2 + v_2^2 \tag{3.3}$$

Comparison with Equation (3.1) shows that $\mathbf{v}_1 \cdot \mathbf{v}_2$ is zero. Then, if neither final velocity is zero, the angle between the final velocities must be ninety degrees.

The photographs in Figures 3.2 and 3.3 show some experimental results. Figure 3.2 is a multiple flash photograph of two colliding billiard balls of equal mass. The angle between the paths of the outgoing balls can be measured directly from the photographs; it is found to be essentially ninety degrees, as predicted. In Figure 3 a track is shown in a nuclear emulsion of a collision between an electron traveling with a speed of nearly 3×10^8 m/sec, and an electron initially at rest in the emulsion. We would expect energy to be conserved in this collision, because conservative forces are involved and little radiation is emitted during the collision. As in Figure 3.2, the plane of motion is the same as the plane of the paper. From the photograph, the angle between the outgoing particles is found to be around 19 degrees, much different from the predicted ninety degrees. Into the classical prediction went the classical laws of energy and momentum conservation. Also, since the same mass was used on both sides of the equations, conservation of mass was assumed. Therefore, one or more of these classical laws must be incorrect.

3.3 CONSERVATION OF MASS-CONFLICT WITH EXPERIMENT

Let us finally look at experiments relating directly to the conservation of mass. In chemical reactions, such as $2H_2 + O_2 \rightarrow 2H_2O$, it is well substantiated from experiment that the total mass after the reaction occurs is equal to the total mass before the reaction. This mass conservation law is sometimes called Dalton's Law. In such chemical reactions, the forces involved are electrical in nature and act between particles separated by distances of the order of 10^{-10} meters. Atomic nuclei are bound together very tightly by a different, extremely strong force, called the strong interaction, which acts between particles separated by distances of the order of 10^{-15} meters. This leads to nuclear interaction energies that are around a million times greater than in chemical reactions. For example, suppose a proton and a neutron combine to form a deuteron.

The mass of a proton is: 1.6724×10^{-27} kg;
The mass of a neutron is: 1.6747×10^{-27} kg;
The sum of the masses is: 3.3471×10^{-27} kg.

When these particles combine, the mass of the resulting deuteron is 3.3431×10^{-27} kg. This is less than the total original mass, so that mass is not conserved. Therefore, if the energies of interaction are high enough, significant departures from the conservation of mass law can be observed.

Of the two other conservation laws known in classical physics-conservation of angular momenturn and of charge-experiment shows that whereas the first must be modified for high energy particles,, the charge conservation law remains generally valid under all circumstances.

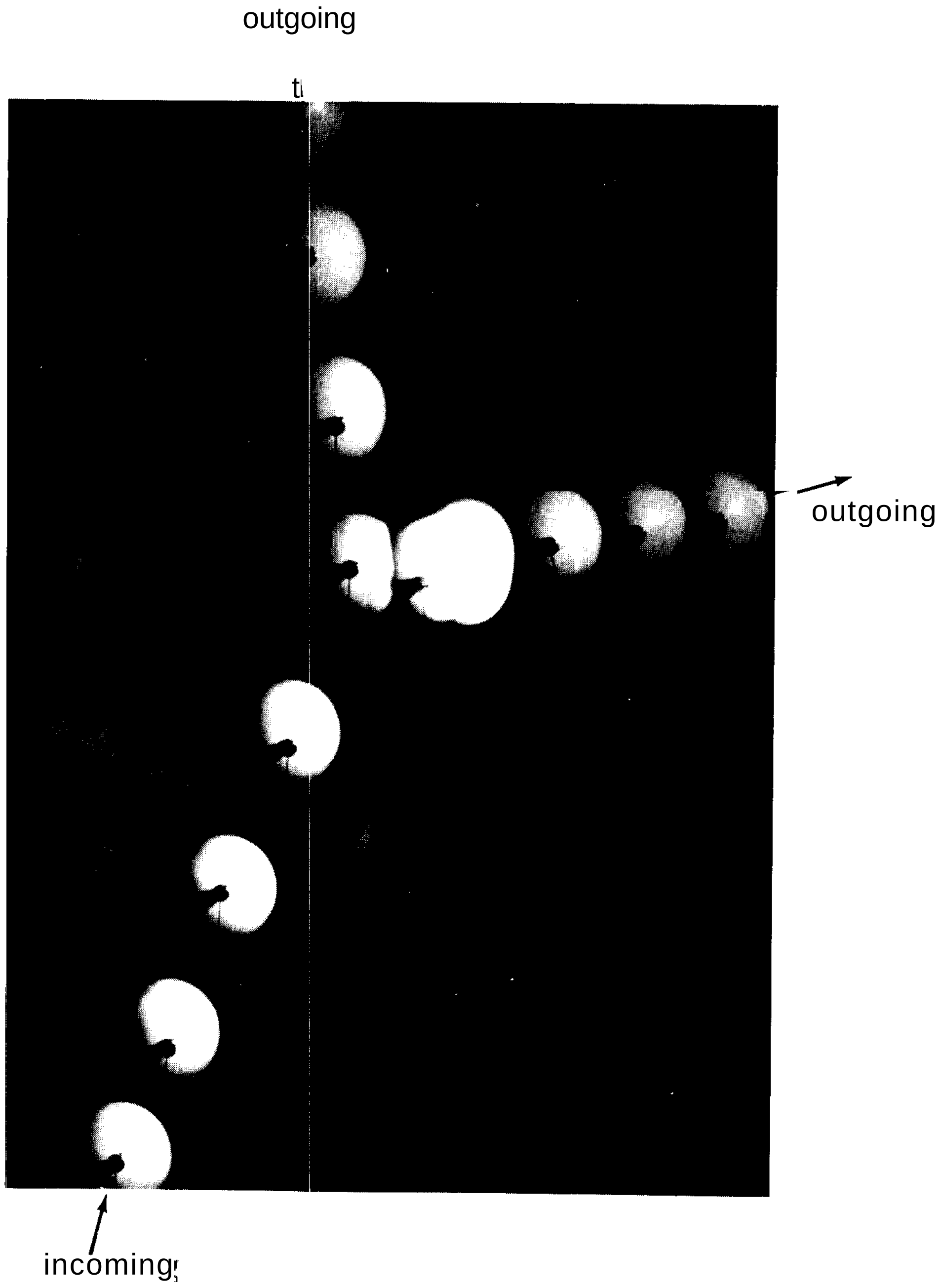


Figure 3.2. Elastic collision of two billiard balls.

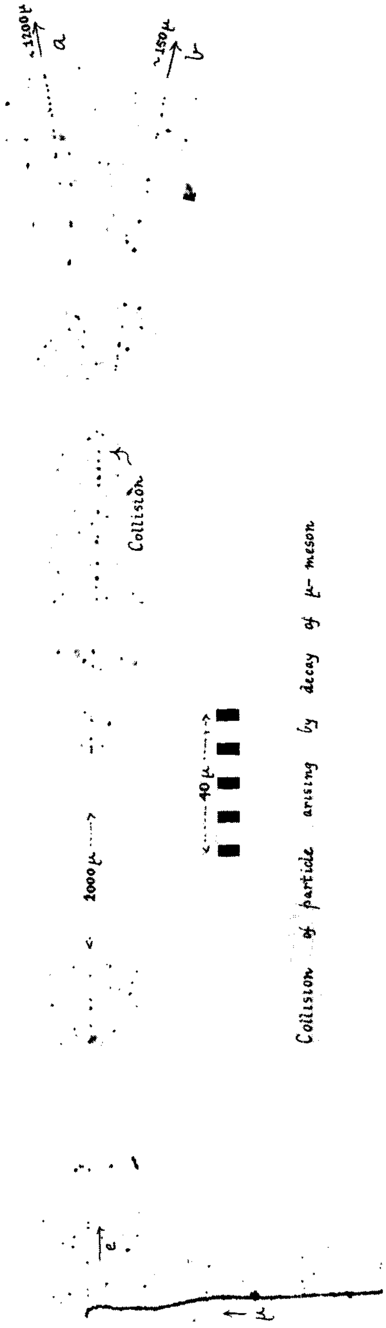
Figure 3.3

Collision with an electron of the charged particle formed by the β-decay of a p-meson

The charged particle emitted in the P-decay of a p-meson makes a collision with an electron in the emulsion. The tracks before and after the collision are long enough to allow the momenta of the particles to be determined. An analysis of the dynamics of the collision can therefore be made, assuming it to be elastic so that no appreciable energy is emitted in the form of photons. It may thus be shown that if track (a) is clue to the recoiling electron, the mass of the particle producing the track (b) is 3 ± 2m_e; and if track (b) is due to an electron, the mass of the other particle is I ·5 ± 1 . Om,. This observation therefore proves that the particle produced in the decay of the p-meson is of small rest-mass and gives very strong support for the view, commonly held, that it is an electron.

Although the collision is almost certainly due to two particles of equal mass, of which one was originally "at rest," the subsequent directions of motion of the two particles are not at right angles, since the velocities are in the relativistic region.

From The Study of Elementary Particles by the Photographic Method, Powell, Fowler and Perkins.



3.4 CORRESPONDENCE PRINCIPLE

In the next chapter we will develop the generalizations of mechanics, due to Albert Einstein, that will resolve the difficulties encountered above. The correspondence principle, to be discussed in this section, serves as a useful guide in finding the generalization of a law that is valid for one range of a variable, but which hos to be modified for another range of that variable.

Suppose there existed a t'heory of mechanics that gave results in agreement with experiment for all speeds $v \lesseqqgtr c$. The difficulties with Newtonian mechanics show up mainly when we are dealing with high speeds. Then in the case of very low speed, $v \ll c$, the predicted results of this new theory must be identical to the predicted result of Newton's laws of motion.

Newton's laws are so well verified in terrestrial and astronomical experiments that they must be an accurate representation of nature in those cases. About the highest speed available in such experiments with large objects is the speed of the planet Mercury, 10^5 mi/hr or 5×10^4 m/sec. Since this speed is small compared to c, we would expect any deviations from the predictions of Newton's laws of motion to be very small. However, in modern accelerating machines particles are accelerated to speeds (approaching the speed of light, c, and Newton's second law does not apply. The newer theory, the special theory of relativity, applies to all particles going with any speed up to c.

The correspondence principle states that any new theory which applies to a broader range of experiments than an old theory, must give the same predicted results as the old theory in those experiments with which the old theory is in agreement. The new theory---in our case, the special theory of relativity-must give the same results as Newton's laws of motion when applied, for instance, to problems involving motion of artificial satellites.

Another way of stating the correspondence principle is: Any new theory which contains an older theory as a special case must give the same predictions as the old theory in the special cases to which the old theory applies.

As we will see, special relativity explains why the mass of a deuteron might not equal the sum of the neutron and proton masses. Also in accord with the correspondence principle, relativity gives Dalton's law when applied to chemical reactions. The correspondence principle is also satisfied in the other examples discussed above.

3.5 INERTIAL SYSTEMS

Hoving seen in preceding sections that the Newtonian laws of motion do not always agree with experiment, we shall now proceed to analyze in more detail the conditions under which the laws are known to hold. One of the most important restrictions, and one which also applies in special relativity, is that the laws can be valid only in certain frames of reference called *inertial* frames. Consider, for example, Newton's first law of motion: If the net force acting on a body is zero, the body will either remain at rest or will continue to move with constant velocity in a straight line. An inertial frame, by definition, is one in which the first law-the law of inertia—holds.

To measure the position and velocity of a particle, we need a coordinate system, set up with clocks and measuring rods (rulers) at rest in it, to observe the motions of bodies. There are many different coordinate systems we could choose. For example, we could pick a rectangular xyz system, as in Figure 3.4,

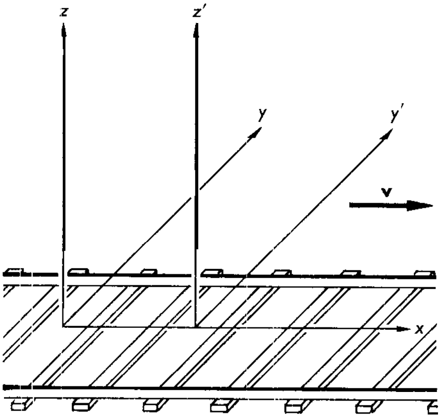


Figure 3.4. Two inertial reference frames.

with its z axis pointing up, and its origin in the middle of some railroad tracks with the x axis pointing parallel to the rails. Also, let us pick a second coordinate system with origin fixed in a train going along the tracks with constant velocity **v** relative to the tracks. We call this system the x'y'z' system, with z' axis up, and x' axis parallel to the tracks. A passenger in the train might observe a book lying on the seat and say that relative to the x'y'z' system, the book is at rest, and therefore by Newton's first law, there must be no force on the book.

On the other hand, a person standing in the middle of the railroad tracks might say that the book is traveling with constant velocity v relative to the xyz system. Therefore, for him also the force is zero by Newton's first law.

To simplify the discussion, we shall designate the observers by letters, calling the observer on the train G. and the one on the tracks R. G. goes and R. remains. We shall call their coordinate systems G and R, respectively. G.'s coordinate system, G, is the x'y'z' set; R.'s set, R, is the xyz set.

Now according to R., the book is traveling with constant velocity, **v.** The net force acting on it is therefore zero, in accordance with Newton's first law in R. Likewise, the motion of the book in G.'s system, G, satisfies the first law since the book is at rest. A system of coordinates in which Newton's first law of motion is satisfied is called an ***inertial system*** because, when no force acts on it, the inertia of a body causes it to continue in a state of rest or of motion with constant velocity. Thus, since the book in G.'s coordinate system is at rest and has no net force acting on it, the x'y'z' coordinate system (the G system), would be an inertial system of coordinates. (At this point, we are neglecting the earth's rotation and planetary motion.) Likewise, R.'s system is an inertial system

3.6 NON-INERTIAL SYSTEMS

Not all coordinate systems are inertial systems. Imagine a rotating coordinate system $(x''y''z'')$ fixed in a merry-go-round, as in Figure 3.5, which is rotating

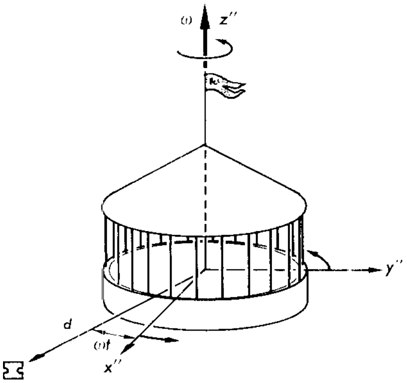


Figure 3.5. Coordinate system fixed in a merry-go-round which is rotating with angular velocity ω.

with the angular velocity ω, relative to the ground. The origin of the coordinate system is on the axis of rotation. A ticket stub lying on the ground a distance d from the axis of rotation will have x" and y" coordinates, $x'' = d \cos \omega t$, $y'' = d \sin \omega t$. The equation of the path of the stub in $x''y''$ coordinates, that is, as seen by an observer fixed to the merry-go-round, is thus $(x'')^2 + (y'')^2 = d^2$, the equation of a circle. The net force acting on the ticket stub from all physical causes such as gravity and contact with the ground is zero. The path of the stub in the $x''y''$ coordinates is a circle. Therefore, the first law of motion is invalid in this rotating coordinate system, and it is not an inertial system.

The earth we live on rotates approximately once per day relative to the sun. A coordinate system fixed relative to the earth also rotates once a day. Then the sun undergoes circular motion relative to such a coordinate system fixed in the earth. (See Figure 3.6.) We conclude that this coordinate system fixed in the earth is, therefore, not an inertial system. We have defined an inertial system as a system of coordinates in which the first law of motion holds. Clearly, if an observer is accelerating, the first law will not hold because an object not acted on by forces will appear to accelerate. Thus, a coordinate system fixed on the surface of the earth is not exactly an inertial system, both because of the centripetal acceleration that bodies have on the earth's surface and because it is a rotating coordinate system.

The magnitude of the centripetol acceleration of a man on the equator is

$$\omega^2 r = (2\pi/86400 \text{ sec per revolution})^2(\text{about } 4000 \text{ miles})$$
$$= 2.1 \times 10^{-5} \text{ mi/sec}^2 = 0.11 \text{ ft/sec}^2$$

The acceleration of a car which speeds up from rest to 15 mi/hr in 60 seconds

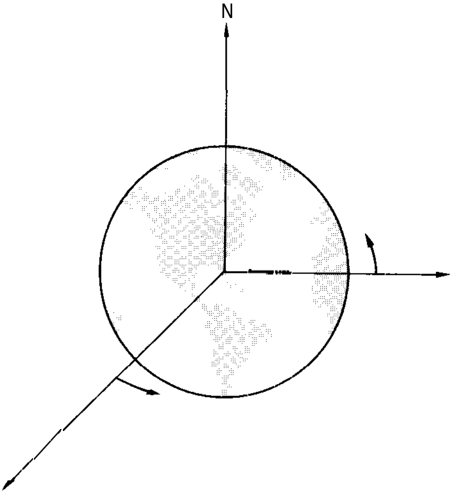


Figure 3.6. A coordinate system fixed on the surface of the earth is a non-inertial system.

is 6.9 x 10^{-5} mi/sec^2, which is of the same order of magnitude as the centripetal acceleration at the equator. Suppose a coordinate system were fixed in a car which is accelerating, and that a passenger in the car is observing a ticket stub lying on the road. Then the net force on the stub from all physical causes is zero. As seen from the car's coordinate system, however, the stub is accelerating. Therefore, the accelerating system is not an inertial system, since Newton's, first law does not hold; similarly, the man on the equator is not in an inertial reference frame.

3.7 AXES RELATIVE TO FIXED STARS

Suppose that instead of axes fixed in the earth, we choose a set of axes with center at the center of the earth, but with the x axis pointing along the direction of orbital motion and the y axis pointing toward the sun. This is still not an inertial system, because the coordinate system will rotate once a year; also, the earth has a small centripetal acceleration toward the sun. We can go a step further and take a coordinate system with origin at the sun's center, one axis normal to the plane of our galaxy and another along the line from the center of the sun to the center of the galaxy. This is again not an inertial system, because the sun orbits around the galactic center. However, this is close enough for most purposes, as seen in Table 3.1, because the acceleration of the sun toward the galactic center is very small compared to ordinary accelerations we measure on earth. From here on, we shall assume that, to a good approximation, a coordinate system with origin fixed at the center of the sun and axes pointing toward "fixed" stars is an inertial system of coordinates, because it has negligible acceleration and negligible rate of rotation. Then the path of a free particle (no forces acting on it) relative to this system will, to a high degree of approximation, appear to be a straight line.

TABLE 3.1 Accelerations of Origins of Possible Reference Frames

acceleration of	towards	$a = v^2/r$
point on equator	center of earth	2.1×10^{-5} mi/sec^2
center of earth	sun	1.5×10^{-6} mi/sec^2
sun	center of galaxy	1.5×10^{-13} mi/sec^2

3.8 GALILEAN TRANSFORMATIONS

Suppose R. is at rest relative ta the inertial system with origin in the sun, and consider G., in the x'y'z' system, moving with same constant velocity v relative ta R. Let's choose x and x' axes parallel ta v, as shown in Figure 3.7. The motion of a free particle looks like straight line, constant velocity motion, ta G. as well as ta R., so the systems of bath G. and R. are inertial systems. We shall exumine this in mare detail, in order ta find *transformation* relations between the two coordinate systems. Suppose that at a certain instant t, as measured by R., the free particle is at the point (x,y,z). As measured by clocks in G.'s system, the time is t' when this observation is made. If in G and R there are clacks which beat seconds and which are set ta $t = t' = 0$ at the instant the origins in G and R pass each other, the Newtonian assumption of absolute time gives

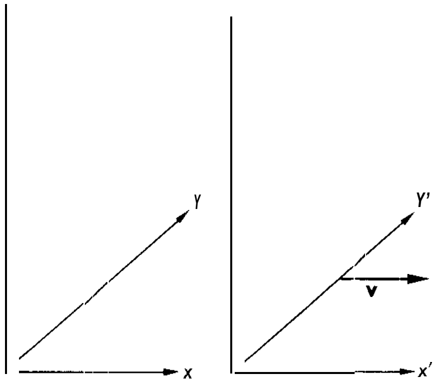


Figure 3.7. R and G inertial frames. G moves with velocity v relative to *R.*

$$t' = t \tag{3.4}$$

We will later see that this equation, which seemed so obvious ta Newton and to generations of physicists thereafter, is not valid in special relativity.

After time t, referring ta Figure 3.8, the origins are separated by a distance equal ta vt, since G. travels with speed v relative ta R. Thus, the position x' of the particle at the instant $t' = t$, as measured by G., can be expressed as

$$x' = x - vt \tag{3.5}$$

Also, if the y' axis is chosen parallel to y, and z' is parallel ta z, we have, at the same instant $t' = t$, the fallowing relations between G.'s and R.'s measure-

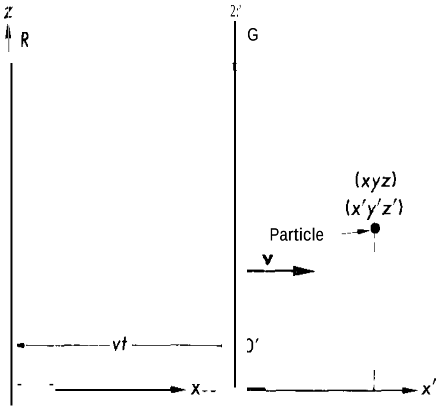


Figure 3.8. Separation between origins at time t is vt.

ments of the particle's position:

$$y' = y, \quad z' = z \tag{3.6}$$

Of course, R. and G. must each use measuring rods at rest in their respective coordinate systems. The four equations, Equations (3.4), (3.5), and (3.6), are called the *Galilean* transformation equations. The equation $t' = t$ was, in Newtonian mechanics, simply taken to be self-evident; other intuitive assumptions went into the other equations, such as the assumption that all lengths appear the same in the two coordinate systems. It will be seen that, when the relative speed of G and R becomes large, these assumptions are erroneous, indicating that intuition can't always be trusted.

3.9 GALILEAN VELOCITY TRANSFORMATIONS

Next, let us find the relation between the particle velocities, as measured in the two coordinate systems, using the Galilean transformations. The x components of velocity in the two systems, R and G, are dx/dt and dx'/dt', respectively. However, since if time is (absolute dt and dt' are equal, we don't have to distinguish between them. Differentiation of Equation (3.5) with respect to t, remembering that v is constant, results in

$$\dot{x}' = \dot{x} - v \tag{3.7}$$

where the dots mean time derivatives. Similarly, Equations (3.5) lead to

$$\dot{y}' = \dot{y}, \quad \dot{z}' = \dot{z} \tag{3.8}$$

The result states that if R. observes a particle going with constant velocity, and G. is moving with constant velocity relative to R., then G. will observe the particle moving with constant velocity. Hence, if R. is in an inertial system, so is G.

Hence, all inertial frames are completely equivalent as far as the statement of the first law of motion is concerned; if the first law is valid in one inertial frame, it is valid in every other inertial frame.

This result is a first indication of the significance of this discussion of inertial frames. The similarity of the statements of the first law of motion in various inertial frames means that there is no way to pick and choose among the infinity of inertial frames (using the first law), in the hope that by judicious choice the expression of the law might be made simpler. One inertial frame is as good as another. One may draw the analogy of attempting to pick a better origin for coordinates for the expression of the rules of plane analytic geometry-actually, one origin is as good as another.

It will be seen below that this equivalence property of the law of inertia is also satisfied by the other laws of motion. Hence no mechanical law can be used to draw essential distinctions between inertial frames. Nevertheless, Newton and many other physicists of the eighteenth and nineteenth centuries maintained a belief in the existence of an absolute space and an absolute time. "Absolute space" referred to space coordinates measured with respect to one preferred inertial frame, which was supposed to be absolutely at rest. Absolute time flowed uniformly, independent of the motion of the observer with respect to absolute space, and the belief in the existence of absolute time was the origin of the assumption in Equation (3.4).

10 SECOND LAW OF MOTION UNDER GALILEAN TRANSFORMATIONS

Let us look at the expression of the second law of motion in the two relatively moving coordinate systems, R and G. We shall put primes on all quantities such as $\mathbf{F}'$, m', $\mathbf{a}'$, to denote quantities measured by G. We shall ask how the quantities $\mathbf{F}'$, m', $\mathbf{a}'$, for general motion of a particle, are related1 to the corresponding physical quantities $\mathbf{F}$, m, $\mathbf{a}$, measured by R. In Newtonian mechanics, it is always assumed that all observers will measure a particle to have the same mass, i.e. mass is an absolute quantity. So for a given particle, if m' is the particle's mass as measured in G, and m is its mass as measured in R, then $m' = m$. Similarly, forces are absolutes, and are assumed to be the same in two inertial systems. For example, a book weighs the same on a scale on the ground as on a scale in a car moving at constant velocity. Then $\mathbf{F}' = \mathbf{F}$. By using Equations (3.7) and (3.8), we can find a relationship between the two accelerations $\mathbf{a}'$ and $\mathbf{a}$. Differentiating these equations with respect to time (t or t'), we find that

$$a_x' = a_x, \quad a_y' = a_y, \quad a_z' = a_z \tag{3.9}$$

Thus, the accelerations are the same in the two inertial systems.

We see that the three quantities in $\mathbf{F} = m\mathbf{a}$, the second law, are equal to the corresponding quantities $\mathbf{F}'$, m', $\mathbf{a}'$ in the other inertial frame. It follows that $\mathbf{F}' = m'\mathbf{a}'$. In Newtonian mechanics, the second law of motion has the same form in all inertial frames; this law,. therefore, cannot be used to pick out some preferred inertial frame in which the law would be different.

11 THIRD LAW UNDER GALILEAN TRANSFORMATIONS

Finally, the third law, the law of action and reaction, is the same in various inertial systems; in other words, the law is form-invariant under Galilean transformations. We can see this because if particles A and B interact in the R system, the third law gives $\mathbf{F}_{(A \text{ on } B)} = -\mathbf{F}_{(B \text{ on } A)}$. But for any force, F = F'. So this equation is the same as $\mathbf{F}'_{(A \text{ on } B)} = -\mathbf{F}'_{(B \text{ on } A)}$, which is the third law for the same interaction in system G. Hence, all the Newtonian laws of motion are form-invariant under Galilean transformations. Therefore, there is no hope of finding one preferred inertial system, in which the laws of mechanics take a simpler mathematical form, and which we could say is absolutely at rest.

3.12 MICHELSON-MORLIE'Y EXPERIMENT

In spite of the fact that *all* classical mechanical laws are form-invariant under Galilean transformations, Newton's philosophical beliefs led him to assert that there existed a preferred inertial frame, at rest in absolute space.

Later on in the nineteenth century, people came to believe that light waves were supported by a medium called the "ether," which was at rest in absolute space. Relative to the ether, light was supposed to propagate at the speed c; hence, by the Galilean velocity transformation, Equation (3.7), observers in motion with respect to the ether should be able to observe light rays propagating at various speeds, depending on the direction of propagation and on the motion of the observer with respect to the ether. The apparent variation in the speed of propagation of light would mean, in other words, that the laws describing light waves are not form-invariant under Galilean transformations. Hence, detection of the motion of an observer with respect to the absolute rest frame, or with respect to the ether, by means of experiments with light, appeared at first to be feasible.

A very accurate experiment designed to detect the absolute motion of the earth was performed by Michelson and Morley in 1881. This was an experiment

TABLE 3.2 Trials of the Michelson-Morley Experiment

Observer	Year	Place	Ratio of expected to observed time differences
Michelson	1881	Potsdam	2
Michelson & Morley	1887	Cleveland	40
Morley & Miller	1902-04	Cleveland	80
Miller	1921	Mt. Wilson	15
Miller	1923-24	Cleveland	40
Miller (sunlight)	1924	Cleveland	80
Tomaschek (starlight)	1924	Heidelberg	15
Miller	1925-26	Mt. Wilson	13
Kennedy	1926	Pasadena & Mt. Wilson	35
Illingworth	1927	Pasadena	175
Piccard & Stahel	1927	Mt. Rigi	20
Michelson et al.	1929	Mt. Wilson	90
Joos	1930	Jena	375
Townes, Javan, Murray, Jaseja	1962	long Island	1000

in which light was sent along two arms of an interferometer, of equal length's, placed parallel and perpendicular to the direction of the earth's orbital velocity. The difference in light speed, or travel time differences, along these two arms could be measured with precision great enough to detect the earth's orbital velocity, 30 km/sec. When the experiment was first performed, physicists were surprised to learn that the time difference was zero—i.e. the experiment gave a *null* result. This means that, to within the accuracy of the experiment, the light speed is independent of direction and hence-which is not reasonable--that the earth seemed to be at rest in absolute space. This experiment has been performed many times since 1881 with greatly increased accuracy, always with a null result. Some of these results are given in Table 3.2. Many other extremely accurate experiments involving moving charges, moving telescopes, interferometers with unequal arms, etc., performed to detect the earth's motion have given null results.

13 POSTULATES OF RELATIVITY

All of the efforts to detect the absolute motion of the earth by optical experiments have failed in spite of the large magnitude of the expected effect. This tends to indicate that absolute motion is simply not detectable by means of optical experiments. We have also seen that no preferred inertial system can be detected by means of Newtonian mechanics. Einstein concluded from this that it must be a fundamental fact of nature that there is no experiment of any kind, performed in an inertial system, by means of which it is possible to detect absolute motion or to select a preferred inertial system.

A deeper analysis of the relations between the inertial systems G and R is necessary. If there is no way of detecting a preferred frame of reference, we can never say that, of two observers, G. and R., who are moving relatively to each other in inertial frames, one is at rest absolutely. Only relative motion is observable. (See Figure 3.9.) Thus, R. can say, "G. is moving with velocity **v** relative to me," but not, "I am at rest in absolute space and G. is moving." If G. is in an

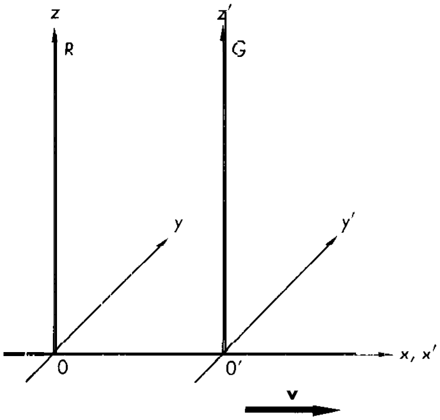


Figure 3.9. Reference frame G moves with velocity **v** along the positive x,x' direction with respect to R.

inertial system, the experiments he performs using apparatus at rest in that system would be described by some set of equations which express physical laws. If R. performed identical experiments using apparatus at rest in his inertial frame, these experiments would be described by physical laws in *R* which would be the same in form as the physical laws in G. So, in principle, there is no difference in the form of the equations which express physical laws discovered by G. and those discovered by R. This is one of the basic assumptions of the theory of relativity, called the ***principle of*** relativity, and may be stated as follows: ***All the laws of physics are the same in all inertial frames.*** This principle is a general statement which restricts the possible physical laws to those having the property of form-invariance with respect to transformations. between inertial systems. Although it is consistent with the results of mechanical and optical experiments, it is not true that all conceivable experiments have already been performed, or that all physical laws have been discovered. Hence the principle has very broad implications.

Measurements at the (earth's surface show that light propagates in a vacuum with speed $c \cong 3 \times 10^8$ m/sec, independent of direction. If R. measures the speed of a light wave in vacuum, it will be c. If the laws describing light waves are valid laws of physics, and if G. measures the speed of some light wave, it should be c. Both would measure the speed to be c even if it were the same light wave whose speed they were measuring. This very important principle was taken by Einstein as the second fundamental assumption of his theory: ***In vacuum the speed of light, c, is a constant,*** irrespective ***of the state of motion of the source.***

Thus, if G., traveling at velocity $\mathbf{v}$ relative to R., shines his flashlight in the $+x'$ direction, it follows that he will observe a light wave that travels with speed c. R. will observe the same wave traveling with the same speed c. (See Figure 13.10.)

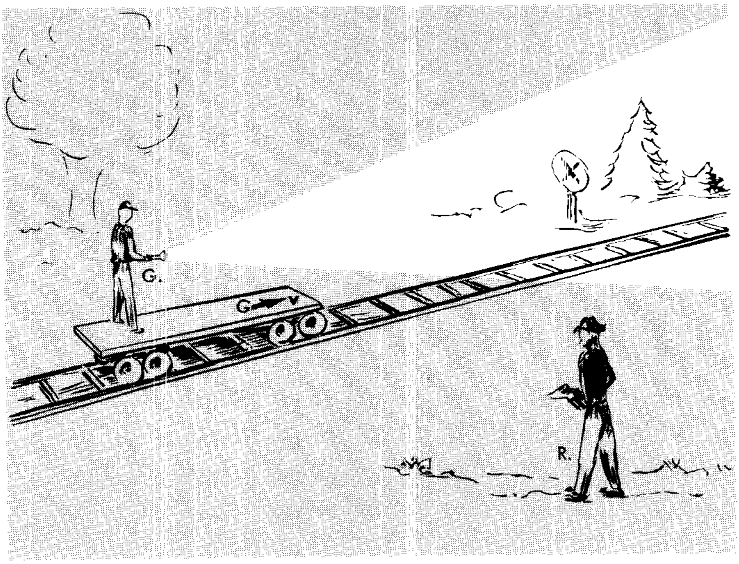


Figure 3.10. Both G. and R. see light from the flashlight moving with the same speed *c* relative to themselves.

This contradicts the Galilean velocity transformations, Equations (3.4), (3.5) and (3.6), which tell us that the speed of light wave sent out by G. as observed by R., is c + v. Therefore, if the postulate of the constancy of the speed of light is correct, as indicated by experiment, the Galilean transformations must be incorrect. Since the Galilean transformations depend solely on distance and time measurements, and since a speed is a distance divided by a time, somehow the distance and time measurements must be modified in relativity so that the speed of light remains a universal constant.

Summarizing, Einstein was led to base a new theory on two postulates. These are:

I. The principle of relativity:

No inertial system is preferred. The equations expressing the laws of physics have the same form in all inertial systems.

II. The principle of the constancy of the speed of light:

The speed of light, c, is a universal constant independent of the state of motion of the source.

14 EXPERIMENTAL EVIDENCE FOR THE SECOND POSTULATE

Most of the experiments performed to test the predictions of relativity theory largely confirmed the first postulate but did not test the second postulate directly. We shall now describe an experiment which was performed to test the validity of the second postulate, that the speed of light is a constant independent of the motion of the light source.

Suppose R. has a light source at rest in his lab and he measures the speed of

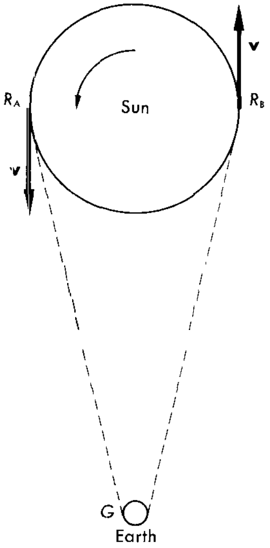


Figure 3.11. Light emitted from positions A and B on the sun's equator comes from sources moving with different velocities relative to the earth.

light using apparatus at rest in his lab. He finds the speed to be c. Then, if G. is moving toward R.'s light source with speed v, the light's speed in G would be c if the second postulate is correct, but c + v if the Galilean transformations are correct. If G. is moving away from R.'s light source, with speed v, the Galilean transformations imply that the light's speed in G would be c v. The difference between these two observed speeds would be 2v.

Imagine that R. is sitting in a lab at rest on the sun's equator, as in Figure 3.1 1. The sun rotates about an axis which is nearly normal to the line of sight of G., who is supposed to be on the earth. The sun has a radius of 695,000 km and rotates with angular velocity 2.9 x 10^{-6} rad/sec. The speed with which a point A or *B* (see Figure 3.1 1) at the edge of the visible equator moves either toward or away from the earth is *v* = ***or* = 2** km/sec = 2000 m/sec. Hence, if G. measures the speed of light, (emitted by a source at rest relative to R, for both points A and *B*, he should see a difference of 4000 m/sec if the Galilean transformations are correct and no difference if the second postulate is correct.

When the experiment was actually performed by the Russian physicist Bonch-Bruevich, the speed difference was observed to be 63 ± 230 m/sec, where the figure ±230 m/sec indicates the size of the probable error in the measurements. This experiment is in far better agreement with the principle of the constancy of the speed of light than with the Galilean transformations. Bench-Bruevich calculated that, given the result 63 ± 230 m/sec and the predicted result of the Galilean transformation of 4000 m/sec, the chance that the Galilean transformation could be right is 1 in 10^{45}. A reproduction of that paper is given on the following page.

3.15 GALILEAN TRANSFORMATIONS AND THE PRINCIPLE OF RELATIVITY

The Galilean Transformations connecting the measurements of G. with those of R. may be written as:

$$x' = x - vf \qquad y' = Y$$
$$f' = t \qquad z' = z \tag{3.10}$$

These transformations are completely consistent with the principle of relativity (Postulate I) taken by itself. This may be seen by solving for x, y, z, *t* in terms of x', y', z't:

$$x = x' + vt' \qquad Y = Y'$$
$$t = t' \qquad z = z' \tag{3.11}$$

Examining the last four equations, it is seen that they are of the same *form* as the first four except for the sign of the relative velocity and the interchange of primed and unprimed variables. This formal difference in the two sets of transformations, which occurs in the sign of the relative velocity, is one manifestation of the

LETTERS TO THE EDITOR

A DIRECT **EXPERIMENTAL** CONFIRMATION OF THE SECOND **POSTULATE** OF THE SPECIAL THEORY OF RELATIVITY

(in connection with Dingle's note)

A. M. Bonch-Bruevich

Received 18 February 1960

It is well known that the Special Theory of Relativity is based on the postulate of the relativity of motion and the postulate that the velocity of light is constant.[1] The first postulate is a direct consequence of the negative results of repeated attempts to detect a privileged coordinate system in observing optical and electrical pheonomena. Experiments for this purpose, repeated over several decades after the formulation of the Special Theory of Relativity, have confirmed the first postulate with increasing accuracy.[2-5] The second postulate of the Theory was not based on direct experimental results, and in the decades that followed it was not confirmed directly because of the great difficulties encountered in setting up the appropriate experiments.

The Special Theory of Relativity no longer needs any additional support. None the less, as Academician S. I. Vavilov pointed out more than ten years ago, a direct experiment showing that the velocity of light is independent of the velocity of the source of radiation relative to the observer is important, due to the basic significance of this postulate. Dingle published a note on this recently.[6] It appears from this note that the author is not acquainted with the result:; of the experiment to confirm the second postulate directly, carried out in 1955.[7-9]

In this experiment, a comparison was made of the times tl and t_2 required for light emitted by two moving sources to traverse a distance L = 2000 meters. The sun's equatorial edges were used as sources. Switching from the radiation of the sun's eastern edge to that of its western edge corresponds to changing the velocity of the source of radiation by 3.9 km/sec in the plane of the ecliptic. We used a phase method to show to the required accuracy that under these conditions the transit time over the hase L remains constant. The intensity of the light radiated along the base by the left or right equatorial edges of the sun was modulated at a frequency of about 12 Mc/s. The phasemeter of a high resolving-power fluorometer was then used to measure the phase shift $\Delta\varphi$ of the modulation of the light trawling along the base when the transition was made from one edge of the sun to the other.[10]

A statistical analysis of the results of more than 1700 measurements of At = t2 ▪ tl showed that in our experiment the change in the transit time over the base L of the light emitted by the left and right equatorial edges of the sun was At = (1.4 ± 5.1) X 10^{-12} sec.

We note that if the classical law of compounding velocities were valid, the quantity At for our apparatus would have had the value 75 X 10^{-12} sec, which lies far outside the limits of experimental error. In addition, the value At = 0 lies inside these limits.

As was shown,[9] these experimental results can be statistically analyzed along different lines, and used to compare the probabilities that the classical or relativistic laws of compounding velocities are valid. This shows that the probability that the velocity of light is independent of the velocity of motion of tie source exceeds by 1045 times the probability that the classical law of compounding velocities is valid.

The experimental results appear convincing to us, and it seems of little importance to repeat them in another variation at present (for instance, using excited atoms or ions as a moving source of radiation)

From Optics 6 Spectroscopy, 9, 73 (1960).

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principle that neither of the inertial systems is preferred. Hence the correct transformation laws in relativity must have a similar property; it is mainly the constancy of the speed of light which brings about major changes in the form of the transformations.

3.16 TRANSFORMATION OF LENGTHS PERPENDICULAR TO THE RELATIVE VELOCITY

We shall now begin the derivation of the correct transformation laws which will replace the Galilean transformations. These new transformations will have to be valid for all physical values of the relative velocity v. Experimentally, the largest possible magnitude of the relative velocity of two physical objects is c. When the relative velocity v is such that $v << c$, however, the correspondence principle requires that the more general transformations reduce to the Galilean transformations. To find the modified transformations, we will consider several thought experiments.

We first consider the measurement of distances oriented perpendicular to the direction of relative velocity between the two frames, that is, along the y or z directions. To find G.'s coordinate y' in terms of the unprimed coordinates measured by R., suppose that G. and R. each have meter sticks which, when at rest relative to each other, are identical. Then lay one meter stick with midpoint on each of the z and z' axes, and arrange the two sticks parallel to the y, y' axes as in Figure 3.12. Imagine that G. and R. drive nails into the sticks at the ends to provide definite markers for the end points, and that then G. moves past R. with some large constant velocity v along the x axis. If the nails in G.'s stick pass between the nails in R.'s stick, we would have to say that G.'s meter stick was contracted due to its motion. Because R. is moving with speed v relative to G., then

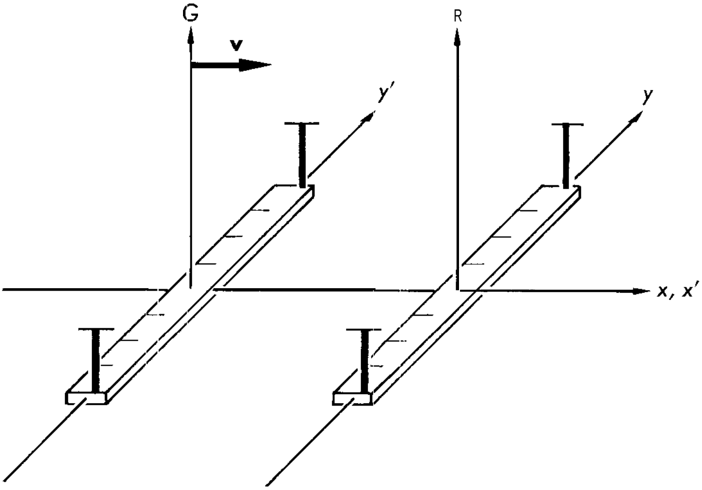


Figure 3.12. Thought experiment showing lengths oriented perpendicular to the direction of relative motion are unchanged by motion.

by the principle of relativity, R.'s nails must also pass between G.'s nails. However, it is not consistent to say that G.'s nails pass between R.'s, and R.'s pass between G.'s; the only way this can be consistent is if the nails hit each other. This would tell us, in general, that the transformation between y and y' is:

$$Y' = Y \tag{3.12}$$

A similar argument results in:

$$z' = z \tag{3.13}$$

So no matter what the relative velocity is, as long as it is normal to the y' and z' axes, we must still have y' = y and z' = z, just as in the Galilean transformations. However, we still have to obtain x' and t' in terms of x and t, which is a less straightforward process.

17 TIME DILATION

Let us consider another thought experiment to see how time intervals and lengths oriented along the x axis vary from one inertial frame to another. Suppose G. puts a mirror a distance L' out along his z' axis at M' in Figure 3.13, and arranges it so that a light ray which passes from his origin 0' to *M'* will be reflected right back to 0'. The principle of the constancy of the speed of light means that G. will find that the light ray travels with speed c. The time it takes to go from 0' to *M'* and back to 0' is then

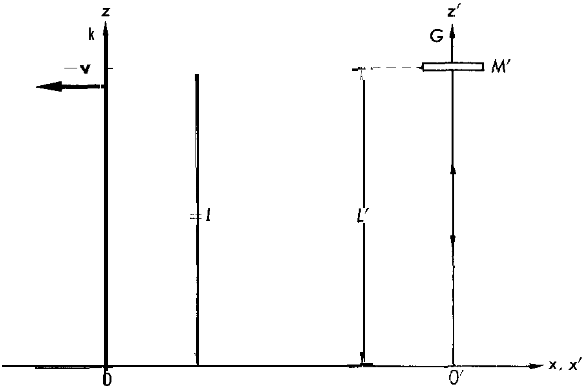


Figure 3.13. **Thought experiment as seen by G.; light travels from 0' to the stationary mirror M' and** back.

$$\Delta t' = \frac{2L'}{c} \tag{3.14}$$

Next we consider the same light ray from R.'s point of view, and calculate the time interval At for the light ray to go from 0 to M' and come back to the origin 0'. We assume here that 0 and 0' coincide when the light ray is first emitted. In Figure 3.14, the dashed rectangle represents the position of the mirror at the time the ray strikes it. Since z' = z and z' = l' for the mirror, R. will observe that the mirror is out in the z direction a distance L = l'. Let's call the time

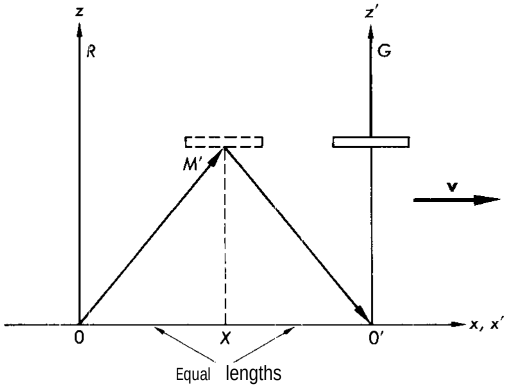


Figure 3.14. Thought experiment as seen by R.; light travels obliquely from 0 to the moving mirror M' and back to 0'.

at which R. observes that the ray strikes the mirror At,,. The x coordinate of this event, "ray strikes mirror," if G. moves with velocity v, will be $(v)(\Delta t_{go})$. In the triangle OMX in the figure, the hypotenuse OM is therefore of length $(L'^2 + [v\Delta t_{go}]^2)^{1/2}$. Since the speed of light relative to R. is c, the time it takes for light to go from 0 to M' will be given by

$$\Delta t_P = \frac{(L'^2 + [v\Delta t_{go}]^2)^{1/2}}{c} \tag{3.15}$$

When this equation is solved for At,, , the result is

$$\Delta t_{go} = \frac{(L'/c)}{(1 - v^2/c^2)^{1/2}} \tag{3.16}$$

It takes as much time for the ray to come from M' back to 0', as to go from 0 to M'. Therefore, the total time, At, for the ray to go from 0 to M to 0' is $2\Delta t_{go}$, or

$$At = \frac{(2L'/c)}{(1 - v^2/c^2)^{1/2}} \tag{3.17}$$

We have thus analyzed an event-the collision of the light ray with O'—from two different points of view. G. says that for this event,

$$x' = 0 \quad \text{and} \quad \Delta t' = \frac{2L'}{c} \tag{3.18}$$

R. says that for this event,

$$x = v\Delta t = \frac{(2vL'/c)}{(1 - v^2/c^2)^{1/2}} \tag{3.19}$$

and

$$\Delta t = \frac{(2L'/c)}{(1 - v^2/c^2)^{1/2}} \tag{3.20}$$

There are several things we can do with this information. For example, the ratio of At to At' can be obtained. Division of the equation for Δt by that for At' gives $\Delta t/\Delta t' = (1 - v^2/c^2)^{-1/2}$, or

$$\Delta t = \frac{\Delta t'}{(1 - v^2/c^2)^{1/2}} \tag{3.21}$$

That is, the observers obtain different times for the occurrence of the event.

To give a numerical example, if $v = 4c/5$, $1 - v^2/c^2 = \frac{9}{25}$ and At $= \Delta t'/(\frac{9}{25})^{1/2} = (\frac{5}{3})\Delta t'$. So if G.'s clock, at 0', reads 3 sec elapsed time, then a clock at rest in R.'s system, which is at the position of 0' when the ray strikes it, will have beat 5 seconds.

Hence the "moving" clock, G.'s clock, beats more slowly than R.'s clocks. In this experiment G.'s clock at O' was the only clock he used in making the measurements. However, R. used one clock at his origin to mark the time the ray went out, and one clock at the final position to mark the time of arrival of the ray back at 0'. These two clocks in R.'s system cannot be the same clock because we assumed in the thought experiment that all R.'s clocks remain at rest in R. R., therefore, used at least two clocks. We may conclude that for the speed of light to have the same value for all observers, it must be true that clocks moving relative to a system beat slower than clocks at rest in the system. However, the observer at rest must use at least two clocks to see the effect, while the moving observer carries one clock along with him. This effect is called time *dilation.*

In this experiment,, the clock carried by the "moving" observer, G., appears to beat more slowly than the two clocks in the "rest" system, that of R. If we analyze a similar experiment from the point of view of G., in which we regard G.'s system as the rest system, then by the principle of relativity we must find that a single clock carried along by R. will beat slower than G.'s clocks. In this latter experiment, by the principle of relativity,

$$At' = \Delta t\sqrt{1 - \frac{v^2}{c^2}} \tag{3.22}$$

just the opposite of Equation (3.21). This shows that the student should not attempt to learn the equations of relativity in terms of primed and unprimed variables, but in terms of the physical interpretation of the equations; confusion regarding the sense of the various contraction and dilation effects is then less likely to result.

mple Suppose someone your own age gets in a rocket ship and moves past you with a speed v such that $(1 \quad v^2/c^2)^{1/2} = \frac{1}{2}$ Suppose that in 10 seconds, by his own reckoning, he counts that his heart beats 10 times. You would observe that in ten seconds, by your own reckoning, his clocks have recorded less than ten seconds, or $(\frac{1}{2})(10) = 5$ sec, so you would observe that his heart beats only 5 times. If he goes to Mars and returns, he will then be younger than you when he gets back.

This time dilotion effect has been observed in experiments in which the average lifetimes of high speed particles called p-mesons are measured. μ-mesons at rest decay into electrons after an average lifetime of 2.2×10^{-6} sec. This decay can be thought of as an internal clock in the meson. When the mesons are moving rapidly, it appears to us that the internal clock beats slower, so the meson's average lifetime appears to be longer. Table 3.3 gives some experimentally observed lifetimes, together with corresponding values calculated from Equation (3.21) for differing values of v/c. The measurements were obtained by B. Rossi and D. B. Hall, who counted the number of cosmic ray μ mesons at different heights above the earth's surface. Since the μ's are produced by high energy cosmic ray particles striking the earth's outer atmosphere, the number of μ's counted at a given height was a measure of the number of μ's surviving after being created in the primary collisions. From these measurements, along with independent measurements of speeds of the μ's, the lifetimes as a function of speed could be found.

TABLE 3.3 μ-Meson Lifetimes As a Function of Speed

v/c	$T_{average}$ (obs.)	$T_{average}$ (calc.)
0.9739	10.6 ± 3.5 μsec	9.3 μsec
0.9853	13.3 ± 5.8 μsec	13.0 μsec
0.990	15.6 ± 5.8 μsec	15.7 μsec

3.18 LENGTH CONTRACTION

The results of the thought experiment, from which we obtained the time dilation effect, can also be used to derive a length contraction effect for rods oriented parallel to the relative velocity. Suppose R. has a measuring rod along his x axis, on which he makes a scratch at his origin 0 and another scratch at the point where the light ray hits 0' after reflection from the moving mirror. Let us call the distance between scratches in R.'s system Ax. Since Ax is the distance between 0 and 0' after the time At, during which G. is moving away with speed v,

$$Ax = v\Delta t \tag{3.23}$$

Now the distance, Ax', measured by G. between the scratches is a distance between scratches on a rod which is moving with speed v relative to him. It is also the distance between O and 0', measured after the time, At', when the light after going from 0' to M' arrives back at 0'. Then the distance between scratches is, for G.,

$$\Delta x' = v\Delta t' \tag{3.24}$$

Division of the expression for Ax' by that for Ax leads to

$$\frac{\Delta x'}{Ax} = \frac{At'}{\Delta t}. \tag{3.25}$$

But from the time dilation 'equation, Equation (3.21),

$$\frac{\Delta t'}{\Delta t} = \left(1 - \frac{v^2}{c^2}\right)^{1/2} \tag{3.26}$$

Therefore,

$$\Delta x' = \left(1 - \frac{v^2}{c^2}\right)^{1/2} \Delta x \tag{3.27}$$

Here Ax is the length of an object measured in a system in which the object is at rest. The object is moving with speed v relative to the G system in which the corresponding length Ax' is measured. Thus, if an object is moving relative to the observer with velocity v, it appears contracted in the dimension parallel to v by the factor, $(1 - v^2/c^2)^{1/2}$. Since y = y' and z = z', the object is not changed in size in directions perpendicular to v. For example, if $v/c = 4/5$, Ax' = $(3/5)$ Ax. This result says that a stick of any length Ax at rest relative to R., when measured by G., appears to be shorter. This effect, in which moving rods appear contracted in the direction of motion, is a necessary consequence of the assumption that the speed of light has the same value for all observers.

Suppose G. and R. both have meter sticks parallel to the x and x' axes. To R., the length of G.'s stick appears to be less than a meter. Also to G., R.'s stick is less than a meter long. How can each measure the other's stick to be shorter? The reason is that to measure a moving length one must find the positions of the two ends *simultaneously,* and then measure the distance between these positions. The two observers simply disagree about what measurements are simultaneous, as we shall see. It should be noted that if the physical situation is reversed so that the length is at rest relative to G., Equation (3.27) would become $\Delta x = (1 - v^2/c^2)^{1/2}\,\Delta x'$. So, as in the case of time dilation, one should not learn the equation in terms of where the prime goes but in terms of the physical situation corresponding to the given equation.

.19 LORENTZ TRANSFORMATIONS

With the information gained from these thought experiments, we can now find the Lorentz transformations which give the relativistic relations between coordinates of events, observed from different inertial frames. Two of the equations are unchanged: y' = y and z' = z. We will assume in our transformations that $t = t' = 0$ when the origins 0 and 0' coincide. This can be done by simply setting the clocks to zero at that instant.

Suppose an object at P' in figure 3.15 is at rest relative to G. The distance x in the figure is the x coordinate of P' relative to R; it is the distance measured parallel to the x axis, from x = 0 to P'. As measured by R.. the distance from 0' to P' is Δx = x − vt. To G., the distance O'P' is simply x' = Ax'. Also, we note that Ax' is a distance between points at rest in the moving system G. Thus Ax is less than Ax' by the factor $(1 - v^2/c^2)^{1/2}$. We then have Ax' = $\Delta x/(1 \quad v^2/c^2)^{1/2}$. But as we found above, Ax' = x' and Ax = x − vt. Therefore, we obtain the following transformation equation relating x'to x and t:

$$x = \frac{1}{(1 - v^2/c^2)^{1/2}}(x \quad vt) \qquad (3.28)$$

This applies if P' is any point whatever. Hence, if some event occurs relative to R at position x and at time t, then substitution of x and t into this transformation equation gives the value of x' at which G. observes the event. Equation (3.28) is the same as the 'corresponding Galilean equation, except for the factor

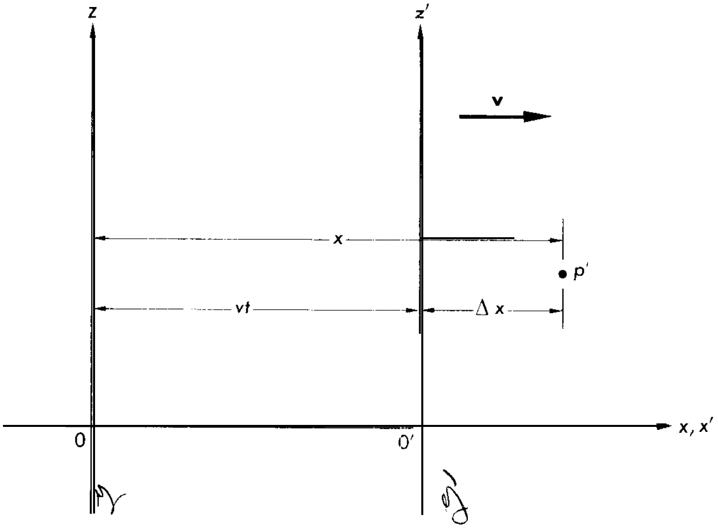


Figure 3.15. x coordinate of on object at rest in G and observed by R.

$1/(1 - v^2/c^2)^{1/2}$. As v/c approaches zero, this factor approaches one. Therefore, the correspondence principle is satisfied.

The principle of relativity implies that the equation giving x in terms of x' and t' is of the same form as the transformation equation, Equation (3.28), but with the sign of v reversed. Hence, in terms of x' and t', we must have

$$x = \frac{1}{(1 - v^2/c^2)^{1/2}}(x' + vt') \tag{3.29}$$

Finally, we want to find the transformation equation which gives the time t' in terms of measurements made by the observer R. To do this, we use the expression for x' of Equation (3.28) to eliminate x' in Equation (3.29). The resulting equation is

$$x = \frac{1}{(1 - v^2/c^2)^{1/2}}\left[\frac{1}{(1 - v^2/c^2)^{1/2}}(x - vt) + vt'\right] \tag{3.30}$$

On solving this last equation for t', we find that

$$t' = \frac{1}{(1 - v^2/c^2)^{1/2}}\left(t - \frac{vx}{c^2}\right) \tag{3.31}$$

This is the desired relationship giving t' in terms of t and x. Likewise from the principle of relativity, expressing t in terms of t' and x', we must have

$$t = \frac{1}{(1 - v^2/c^2)^{1/2}}\left(t' + \frac{vx'}{c^2}\right) \tag{3.32}$$

For v << c, the two equations, (3.31) and (3.32), both reduce to $t' = t$. Therefore, the correspondence principle is satisfied.

These equations were found using the length contraction equation. They also agree with the time dilation formula. We con see this by supposing that a single clock is at rest in the moving system G at x' = 0. The equation

$$t = \frac{1}{(1 - v^2/c^2)^{1/2}}\left(t' + \frac{vx'}{c^2}\right) \qquad (3.33)$$

becomes, for this clock, $t = t'/(1 - v^2/c^2)^{1/2}$. The time t', read on this single clock at rest in the moving system G, is therefore less than the time t measured by a coincident clock in the rest system *R*. This agrees with Equation (3.13), found previously from a thought experiment.

The set of transformations we have found between x'y'z't' and xyzt are:

$$x' = \frac{1}{(1 - v^2/c^2)^{1/2}}(x - vt),$$

$$y' = y,$$

$$z' = z,$$

$$t' = \frac{1}{(1 - v^2/c^2)^{1/2}}\left(t - \frac{vx}{c^2}\right) \qquad (3.34)$$

These are called the ***Lorentz transformations.*** We have seen that they satisfy the correspondence principle. They were derived by repeated use of the two postulates of the theory of relativity.

mple Suppose that G. is moving away from R. in the positive x direction at a speed such that $v/c = 5/13$. If R. sets off a firecracker at $y = z = 0$, $x = 10{,}000$ *m*, $t = 10^{-4}$ sec, where and when does G. observe it?

lution For $v/c = 5/13$, $(1 - v^2/c^2)^{1/2} = 12/13$. Then substitution into Equations (3.34) gives $y' = z' = 0$, $x' = 1667$ m, $t' = 0.944 \times 10^{-4}$ sec.

.20 SIMULTANEITY

Aside from the time dilation factor $(1 - v^2/c^2)^{-1/2}$, the equation for t' in the Lorentz transformations differs from the Galilean transformations by a term

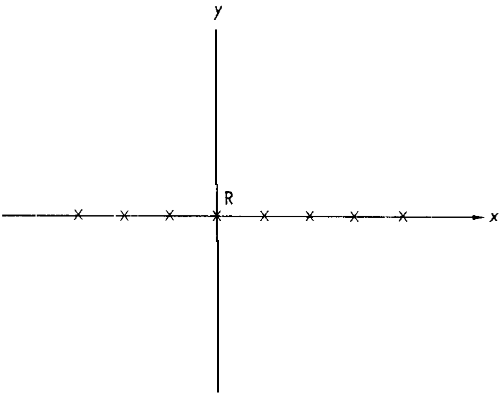


Figure 3.16. A number of explosions ot different positions along the *x* axis are simultoneous in *R*.

proportional to x. To see the physical significance of this term, suppose that R. sets off a number of explosions along the x axis, which by his own clocks occur simultaneously, at the instant $t = 0$. (See Figure 3.16.) The equation $t' = (t - vx/c^2)/(1 - v^2/c^2)^{1/2}$, tells us that for $t = 0$ but for different positions x, $t' = -vx/c^2(1 - v^2/c^2)^{1/2}$. These are then the readings on the various clocks of G. for the different explosions, all of which are observed simultaneously in R. at $t = 0$. Thus, for positive x, these clocks in G appear to be set behind what R. would call the correct time by the amounts $vx/c^2(1 - v^2/c^2)^{1/2}$, which depend on position. Hence events that appear simultaneous to R. do not appear simultaneous to G.; the times of their occurrence depend on the x positions of the events. Simultaneity is thus a concept which has no absolute meaning.

Perhaps we may understand this by considering the observer R. standing, as in Figure 3.17, halfway between two light detectors D_1 and D_2, that record the time at which light hits them. If R. turns on the light bulb he is holding, then, since it takes the same time for the wavefront to travel from R. to D_1 as to D_2, the detectors record equal times when light hits them. R. would say that the light hit the detectors simultaneously.

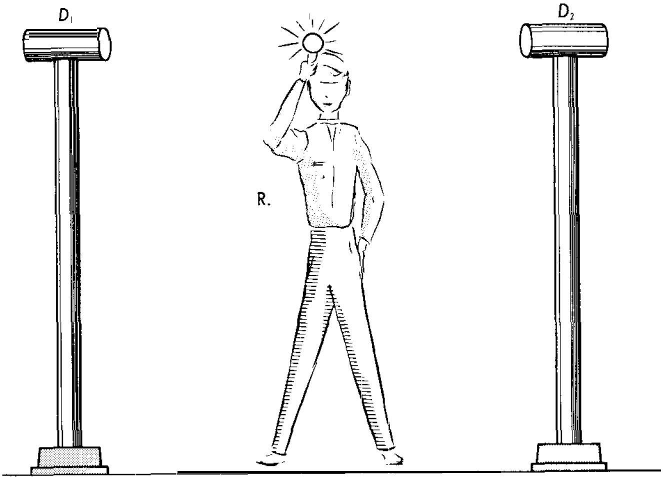


Figure 3.17. Light emitted from a point halfway between two detectors at rest in ***R*** arrives simultaneously at the two detectors in R.

However, if, as shown in Figure 3.18, G. is moving past R.'s position at the instant R. turns on the light, then as far as G. is concerned, he sees D_1 and D_2 moving backward with speed v. Then, in G.'s system, the light wave going forward and the detector D_2 are approaching each other, while D_1 is moving parallel to the light wave going backward, The light wave going forward thus appears to have traveled less distance before it strikes the detector. Therefore, in G.'s system, the light hits D_2 before it hits D_1, and the events which were simultaneous in R are not simultaneous in G. Since G. believes that the light hits D_2 first, but D_1 and D_2 record the same time, G. says that the timer at D_2 is set fast compared to that at D_1. That is, the timers are not synchronized in G.

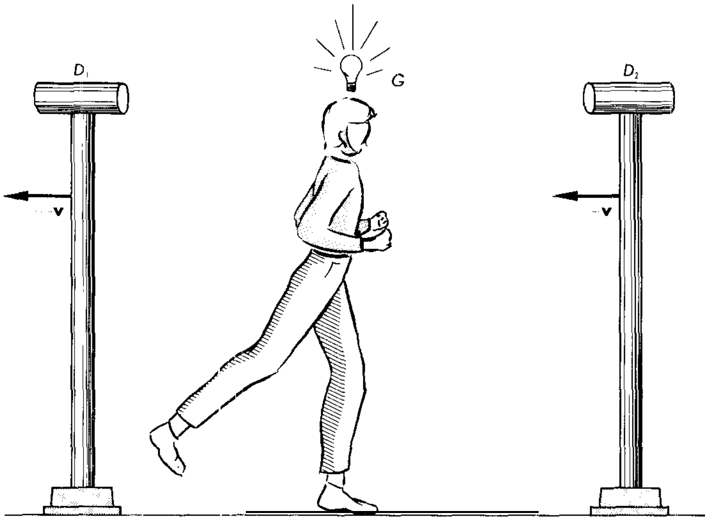


Figure 3.18. Light emitted as G. passes the midpoint between two moving detectors does not arrive at the detectors simultaneously in G.

mple 1. Two events at $x = \pm 100$ km are observed by R. at the instant $t = 0$. When are these events observed by G. if G.'s velocity in the positive x direction relative to R has magnitude $c/10$? (Assume $t' = t = 0$ when $x' = x = 0$.)

ution $t' = -vx/c^2(1 - v^2/c^2)^{1/2} - 0.1(\pm 100)/(3 \times 10^5)(0.99)^{1/2}$
$= \pm 3.35 \times 10^{-6}$ sec.

mple 2. If the relative velocity has magnitude $9c/10$, when are they seen?

ution $t' = 0.9(\pm 100)/(3 \times 10^5)(0.19)^{1/2} = \pm 6.88 \times 10^{-4}$ sec.

When a length measurement of a moving object is made, the positions of both ends of the rod must be marked at the same time. (See Figure 3.19.) Thus, for

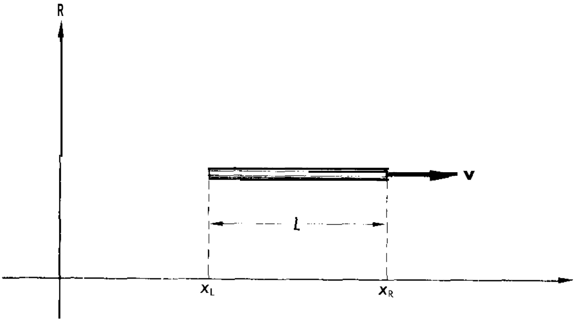


Figure 3.19. To measure **the length of a moving rod, R. makes marks simultaneously at the positions of the left and right ends, x_L and x_R. $L = L_{marks}$.**

a rod of length L at rest in G, R. could measure its apparent length L by noting the position of its left end, x_L, and the position of its right end, x_R, at the **same *time,*** and then measuring the difference $x_R - x_L$. Suppose, for example, that when G.'s speed is 10,000 ft/sec, R. waits 10^{-3} seconds to mark the right end of the rod after he marks the left end. The error he would make in his length measurement would be (1 OOOO)(1 0^{-3}) = 10 ft.

Let R. mark the positions of two ends of the rod at time t. Then, from the Lorentz transformations, G. would say the right mark was made at the time $t'_R = (t - vx_R/c^2)/(1 - v^2/c^2)^{1/2}$. Also, G. would say the left mark was made at the time $t'_L = (t - vx_L/c^2)/(1 - v^2/c^2)^{1/2}$. Since these times are not the same, the marks do not appear to be made simultaneously in G; rather, it appears the right end is marked first. The difference between these times is $\Delta t' = t'_L - t'_R$, given by

$$\text{At'} = \frac{v(x_R \quad x_L)}{c^2(1 - v^2/c^2)^{1/2}} = \frac{vL}{c^2(1 - v^2/c^2)^{1/2}} \tag{3.35}$$

In this time, relative to G. the R system moves a distance $v\Delta t'$ to the left. Hence, the righthand mark approaches the left end of the rod by a distance

$$v\Delta t' = \frac{v^2 L}{c^2(1 - - v^2/c^2)^{1/2}} \tag{3.36}$$

Thus, if to G. the length of the rod is l', the distance between the marks is

$$L'_{\text{marks}} = L' - \frac{v^2 L}{c^2(1 - - v^2/c^2)^{1/2}} \tag{3.37}$$

To R., of course, the distance between the marks is $L_{\text{marks}} = L$, the apparent length of the rod.

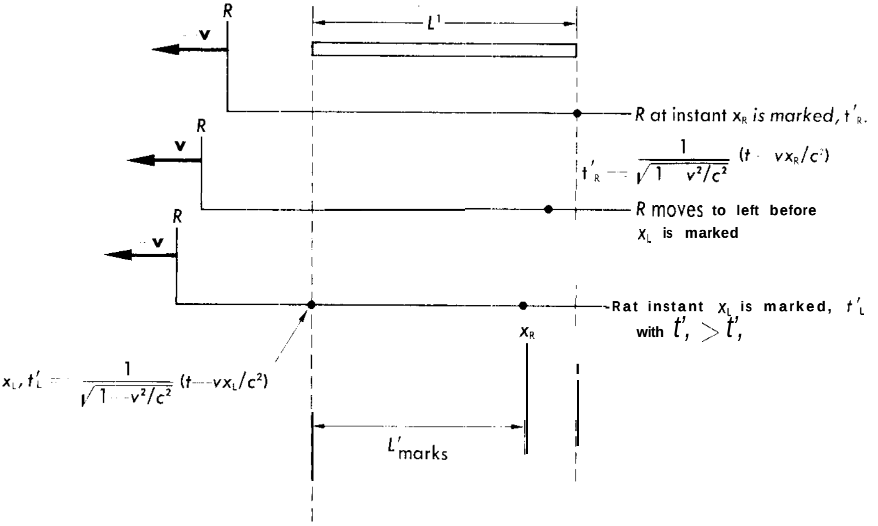


Figure 3.20. R.'s measurements of the length of the rod in G, as seen by G.

The above result can be used to check the length contraction effect, for suppose the ratio of the apparent length of a moving rod to that of an identical rod at rest is denoted by $1/\gamma$, where γ is some constant depending on relative speed. Then since to R. the rod at rest in G is moving, $L_{\text{marks}} = L = L'/\gamma$. However, to G. the marks at rest in *R* are moving with the same speed, so $L'_{\text{marks}} = L/\gamma$. Thus, eliminating L' and L'_{marks} from Equation (3.37),

$$\frac{L}{\gamma} = \gamma L - \frac{v^2 L}{c^2(1 - v^2/c^2)^{1/2}} \tag{3.313}$$

This quadratic equation for γ has solutions $\gamma = 1/(1 - v^2/c^2)^{1/2}$ and $\gamma = -(1 - v^2/c^2)^{1/2}$. Since the second solution becomes -1 as v/c goes to zero, it does not satisfy the correspondence principle and may be discarded. The first solution agrees with the length contraction found previously from another thought experiment. Since the present argument is based on the disagreement regarding simultaneity between the two frames, we see that this is the basic reason why lengths in one system may appear shortened in another system, and vice-versa.

2 1 TRANSFORMATION OF VELOCITIES

It is extremely useful to know how velocity measurements made by different observers are related. Suppose, as is illustrated in Figure 3.21, that R. observes

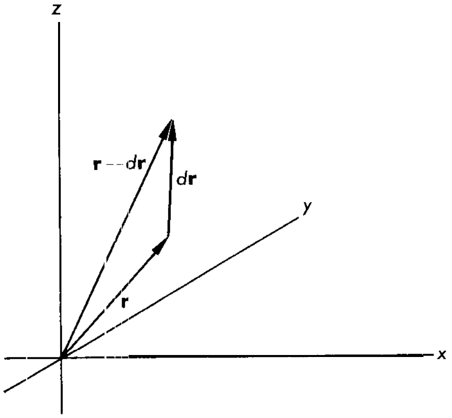


Figure 3.21. The position vector of o particle changes by dr in time *dt*.

a particle moving in time dt from the point with coordinates *x,y,z* to x + *dx*, y + *dy*, z + dz. In R the velocity then has components of *dx/dt*, *dy/dt*, and *dz/dt*. Suppose G. observes the very same particle going from x', y', z' to x' + dx', y' + dy', z' + *dz'* in the time interval *dt'*. The velocity components in G are then *dx'/dt'*, *dy'/dt'*, and *dz'/dt'*. We shall use the Lorentz transformation equations to find dx', *dy'*, dz', and dt' in terms of the unprimed differential quantities. The use of the velocity definitions just stated will then lead to the velocity transformations.

One of the equations of the Lorentz transformation, Equations (3.34), is

$$x' = \frac{1}{(1 - v^2/c^2)^{1/2}}(x - vt) \tag{3.39}$$

the differential form of this equation is

$$dx' = \frac{1}{(1 - v^2/c^2)^{1/2}}(dx - vdt) \tag{3.40}$$

This was obtained simply by differentiation, understanding that the relative velocity of the two observers is kept constant, i.e. that v is constant. The increment dt' is obtained in the same way from the equation,

$$t' = \frac{1}{(1 - v^2/c^2)^{1/2}}\left(t - \frac{vx}{c^2}\right) \tag{3.41}$$

It is

$$dt' = \frac{1}{(1 - v^2/c^2)^{1/2}}\left(dt - \frac{vdx}{c^2}\right) \tag{3.42}$$

Hence, the x' component of velocity is

$$\frac{dx'}{dt'} = \frac{dx - vdt}{dt - vdx/c^2} \tag{3.43}$$

If we divide the numerator and denominator through by dt, on the righthand side we get $(dx/dt) - v$ in the numerator and $1 - v(dx/dt)/c^2$ in the denominator. (We shall use the dot notation for time derivatives, $\dot{x} = dx/dt$, the x component of velocity in R; likewise in G, $\dot{x}' = dx'/dt'$.) Equation (3.43) is, in this notation,

$$\dot{x}' = \frac{dx'}{dt'} = \frac{(\dot{x} - v)}{(1 - v\dot{x}/c^2)} \tag{3.44}$$

Thus, for example, if a particle goes with an x component of velocity, x = $-\frac{1}{2}$ c relative to R, and v = $\frac{1}{2}$ c, then G. will measure the $\dot{x}'$ component of velocity to be

$$\dot{x}' = \frac{(-\frac{1}{2}c - \frac{1}{2}c)}{(1 + \frac{1}{4})} = -\left(\frac{4}{5}\right)c$$

On the other hand, the Galilean transformation would give $\dot{x}' = \dot{x} - v = -\frac{1}{2}c - \frac{1}{2}c = -c$.

To obtain the transformation equation for $\dot{y}$, we have $\dot{y} = dy/dt$ and $\dot{y}' = dy'/dt'$. Since y' = y, we have dy' = dy. Also, for the differential dt', we may use the expression in Equation (3.42). Therefore,

$$\dot{y}' = \frac{dy'}{dt'} = \frac{dy\sqrt{1 - v^2/c^2}}{(dt - vdx/c^2)} \tag{3.45}$$

Hence, dividing numerator and denominator by dt, we obtain

$$\dot{y}' = \frac{(1 - v^2/c^2)^{1/2}\,\dot{y}}{(1 - v\dot{x}/c^2)} \tag{3.46}$$

By a similar derivation, we get for i':

$$\dot{z}' = \frac{(1 - v^2/c^2)^{1/2}\,\dot{z}}{(1 - v\dot{x}/c^2)} \tag{3.47}$$

ple If a particle is observed by R. to move with velocity components (10,000,; 42,000; 128,000) km/sec, then when G. passes R. with a speed ½ c in the positive x direction, what will be the velocity components he observes?

tion $1 - v\dot{x}/c^2 = 1 - [10^4][1.5\times 10^5]/[3\times 10^5]^2 = {}^{59}/_{60}$;

$\sqrt{1 - v^2/c^2} = \sqrt{1 - 1/4} = \sqrt{3/2}$;

$\dot{x}' = (10^4 - 1.5\times 10^5)/({}^{59}/_{60}) = 1.42\times 10^5$ km/sec;

$\dot{y}' = \tfrac{1}{2}\sqrt{3}(4.2\times 10^4)/({}^{59}/_{50}) = 3.70\times 10^4$ km/sec;

$\dot{z}' = \tfrac{1}{2}\sqrt{3}(12.8\times 10^4)/({}^{59}/_{60}) = 11.3\times 10^4$ km/sec.

Equations (3.47), (3.46) and (3.44) are the desired velocity transformations. These transformations satisfy the principle of relativity, for the inverse transformations from G to *R* are of the same mathematical form, except for the sign of v. We may show this, for example, by solving Equation (3.44) for $\dot{x}$ in terms of $\dot{x}'$:

$$\dot{x}'\left(1 - \frac{v\dot{x}}{c^2}\right) = \dot{x}' - \frac{v\dot{x}'\dot{x}}{c^2} = \dot{x} - v, \tag{3.48}$$

or

$$\dot{x}\left(1 + \frac{v\dot{x}'}{c^2}\right) = \dot{x}' + v, \tag{3.49}$$

giving

$$\dot{x} = \frac{\dot{x}' + v}{1 + v\dot{x}'/c^2} \tag{3.50}$$

Comparison with Equation (3.44) shows clearly that the principle of relativity is satisfied. The other transformation equations, Equations (3.46) and (3.47), also have this property. If all terms involving factors of v/c in Equations (3.44), (3.46), (3.47) are neglected, we obtain the Galilean transformation, thus showing that the correspondence principle is satisfied.

ple If a light ray in R has velocity components $\dot{y} = c\sin\theta$, $\dot{x} = c\cos\theta$, so that the magnitude of the velocity is c, show that in another inertial system the speed is also c, so that the principle of the constancy of the speed of light is satisfied.

ion $\dot{x}' = (c\cos\theta - v)/(1 - v\cos\theta/c)$;

$\dot{y}' = \sqrt{1 - v^2/c^2}\, c\sin\theta/(1 - v\cos\theta/c)$.

$$(\dot{x}')^2 + (\dot{y}')^2 = \frac{[(c^2\cos^2\theta - 2cv\cos\theta + v^2) + (c^2\sin^2\theta - v^2\sin^2\theta)]}{[1 - (2v/c)\cos\theta + (v^2/c^2)\cos^2\theta]}.$$

Since $\cos^2\theta + \sin^2\theta = 1$, this becomes

$$(\dot{x}')^2 + (\dot{y}')^2 = \frac{[c^2 - 2cv\cos\theta + v^2\cos^2\theta]}{[1 - (2v/c)\cos\theta + (v^2/c^2)\cos^2\theta]} = c^2.$$

summary

LAWS OF CLASSICAL MECHANICS

In classical (Newtonian) mechanics, there were five quantities conserved: mass, energy, momentum, angular momentum and charge. In relativistic mechanics, all of the corresponding conservation laws are modified except conservation of charge.

CORRESPONDENCE PRINCIPLE

The correspondence principle is a useful guide in the derivation of new theories. It states that any new theory containing an old, well-established theory as a special case, but applicable over a greater range of phenomena, must give the same prediction as the old where the old applies.

INERTIAL SYSTEM

An inertial system of coordinates is one in which the first law of motion is satisfied. A good <Approximation to an inertial system may be obtained by choosing an origin of axes at the center of the sun and allowing the axes to point toward fixed stars. Then the acceleration and rate of rotation of the axes are negligible.

GALILEAN TRANSFORMATIONS

A system moving with constant velocity relative to an inertial system is also an inertial system. The coordinates of events in a system S' moving with velocity v relative to the inertial system S are given by the Galilean transformations:

$$\mathbf{r}' = \mathbf{r} - \mathbf{v}t$$
$$t' = t$$

MICHELSON-MORLEY EXPERIMENT

If the ether exists, and light propagates with speed c relative to the ether, and if the Galilean transformation laws are correct, then it should be possible to detect the motion of the earth through the ether. The Michelson-Morley experiment, performed with an interferometer, gave a null result for this velocity, as did many other experiments designed to detect the motion of the earth through the ether.

POSTULATES OF RELATIVITY

The postulates of relativity are:

I. Principle of Relativity: All the laws of physics are the same in form, in all inertial frames.
II. Principle of the Constancy of the Speed of Light: The speed of light, c, is a constant irrespective of the state of motion of the source.

It follows that an observer in any inertial frame will observe light to travel with speed c.

BONCH-BRUEVICH'S EXPERIMENT

The experiment of Banch-Bruevich in which the difference of the speed of light coming from opposite limbs of the sun was found to be zero, shows that liight does not obey the Golilean law for the addition of velocities.

TIME DILATION

A moving clock, which reads the time interval At', when compared with a series of clocks at rest relative to the observer that read the time interval At, will be observed to beat more slowly. If the velocity of the moving clock is v, relative to the other clocks, then

$$\Delta t' = \sqrt{1 - \frac{v^2}{c^2}}\,\Delta t$$

This time dilation is observed experimentally in the decay in flight of p-mesons.

LENGTH CONTRACTION

An observer comparing the length of a moving rod, oriented parallel to the direction of relative velocity v, with rods placed at rest, will observe the length AL of the moving rod to be shorter than its length AL' as measured by an observer at rest relative to it.

$$AL' = \frac{1}{\overline{1 - v^2/c^2}}\,AL$$

SIMULTANEITY

Simultaneity is a concept which depends on the observer. Two events which are simultaneous when viewed in one inertial frame are not necessarily simultaneous when viewed in an inertial frame moving relative to the first. An observer S' observing events which to S appear simultaneous at x_1 and x_2, will see a time difference of magnitude

$$\Delta t' = \frac{-1}{\sqrt{1 - v^2/c^2}} \frac{v(x_2 - x_1)}{c^2}$$

LORENTZ TRANSFORMATIONS

The Lorentz transformations are a set of four equations giving relations between coordinates of events as measured in the inertial system S', which is moving with relative speed v with respect to S in the x, x' directions. If the origins are chosen so that $t = t' = 0$, when the origins pass, then the Lorentz transformations are:

$$x' = \frac{1}{\sqrt{1 - v^2/c^2}}(x - vt); \quad y' = y; \quad z' = z; \quad t' = \frac{1}{\sqrt{1 - v^2/c^2}}\left(t - \frac{vx}{c^2}\right)$$

VELOCITY TRANSFORMATIONS

If a particle in the S' system has velocity components ($\dot{x}'$, $\dot{y}'$, $\dot{z}'$) and the S' system moves with speed v in the x direction relative to S, then the unprimed and primed velocity components are related by:

$$\dot{x}' = \frac{\dot{x} - v}{1 - \dot{x}v/c^2} \quad \dot{y}' = \sqrt{1 - \frac{v^2}{c^2}}\frac{\dot{y}}{1 - \dot{x}v/c^2}; \quad \dot{z}' = \sqrt{1 - \frac{v^2}{c^2}}\frac{\dot{z}}{1 - \dot{x}v/c^2}$$

problems

1. Prove that the classical law of conservation of momentum in a two-particle collision is form-invariant under Galilean transformations, if mass is conserved.
2. If two objects, of masses m_1 and m_2 and velocities V_1 and V_2, whose relative velocity toward each other is $V = V_2 - V_1$ collide inelastically and stick together, show using Newtonian mechanics that the kinetic energy lost is an invariant under Galilean transformations. What conservation laws do you have to assume in order to prove this?

   Answer: Conservation of momentum, conservation of mass.
3. Prove that Newton's second law of motion is not form-invariant under a transformation between an inertial system and a second coordinate frame which has a constant acceleration relative to the first.
4. There are a number of double stars called *eclipsing binaries*, where the two bodies revolve about their common center of mass. As seen from earth, in each revolution one star passes in front of the other so that the second star's light cannot be seen,

When photographs of these stars are made in different colors or wavelengths, the periods for this eclipse are found to be identical. Since these stars may be thousands, of light-years away (one light-year is the distance light travels in a year), what conclusion can you draw about variation of the speed of light with wavelength?

5. It was at one time suggested that the speed of light is not constant relative to an ether but is constant relative to the object emitting it, and that Galilean transformations could then be used. Argue from the observations on eclipsing binaries discussed in the previous problem that this cannot be the case.

6. The electron beam in the picture tube of a TV set can move across the screen at a speed faster than c. How can this be consistent with special relativity?

7. If in one second a moving stopwatch in good working condition is seen to register ½ sec, how fast is it moving relative to you?

   Answer: $0.866c$.

8. If a person's heart beats 70 times per minute, what would be the apparent pulse rate if he were moving at a speed of $0.9c$?

   Answer: 30.5 per min.

9. In one second of your time, how much change of time would a stop watch register if it were moving at a speed relative to you of (a) 19/181 c; (b) 4/5 c; (c) 60/61 c.

   Answer: 180/181 sec; 3/5 sec; 1 1/61 sec.

10. Consider two observers, S and S'. S' is moving relative to S with speed v. S shines a light ray out with a component of velocity V parallel to the direction of relative motion and a component perpendicular to that direction. S' observes the light moving parallel to his y axis (y being normal to V). Assuming $y' = y$, and the constancy of the speed of light, derive the time dilation formula by analyzing measurements that S and S' could make.

11. A beam of protons coming out of an accelerator is contaminated by π^+-mesons which have a lifetime when at rest of 2.54×10^{-8} sec and travel with speed 0.990 c. How far from the beam port *must* a target be placed in order that nearly all the mesons will have decayed before striking the target? Assume the mesons have 3 lifetimes in their rest system before striking target.

    Answer: 160 m.

12. A hydrogen atom emits some light of wavelength 6563 Angstroms in the frame of reference at rest with respect to the atom. If the atom were moving at $^5/_{13}$ the speed of light relative to you in a direction perpendicular to the displacement of the atom relative to you, what would be the wavelength of the light you would observe? (Use the time dilation formula to find the ratio of frequencies and the fact that the wavelength is the speed of light divided by the frequency.) 1 Angstrom = 10^{-10} m.

    Answer: 7110 Angstroms.

13. What is the apparent length of a meter stick if it is moving relative to you parallel to its length at a speed of (a) 0.1 c; (b) 0.8 c; (c) 0.99 c?

    Answer: 0.995 m; 0.600 m: 0.141 m.

14. Repeat the previous problem if in its rest frame the meter stick is at 60° relative to the velocity.

    Answer: 0.999 m; 0.916 m 0.869 m.

15. It was pointed out that if one twin went to another planet and back, he would be younger than the stay-at-home twin, because his clocks would run slow compared to earth clocks. If the traveler's speed is v and the planet's distance away is L, the time it takes on earth for the round trip is $2L/v$. Using the distance of the trip as seen by the spaceman, find the time as far as he is concerned.

Answer: $\dfrac{2L\sqrt{1 - v^2/c^2}}{v}$.

16. Two twin astronauts, A_1 and A_2, are to make trips to distant planets, distances d, and d_2 away, respectively, with $d_1 \neq d_2$. They wish to choose their speeds so their age difference upon returning to earth is zero. Show that they should choose their speeds v_1 and v_2 such that

$$\frac{d_1}{v_1}\left(1 \quad \sqrt{1 \quad v_1^2/c^2}\right) = \frac{d_2}{v_2}\left(1 - \sqrt{1 - v_2^2/c^2}\right)$$

or equivalently,

$$\frac{v_1}{d_1} = \frac{2v_2d_2[1-(1-v_2^2/c^2)^{1/2}]}{[v_2^2(d_1^2-d_2^2)/c^2] + 2d_2^2[1-(1-v_2^2/c^2)^{1/2}]}$$

17. Solve the velocity transformation equations algebraically for $\dot{x}$, $\dot{y}$, $\dot{z}$ in terms of $\dot{x}', \dot{y}', \dot{z}'$, and show that the inverse transformations result from changing v to $-v$ and interchanging primed and unprimed symbols.

18. Consider the Lorentz transformations, $x' = (\sqrt{1 - v^2/c^2})^{-1}(x - vt)$, $t' = (\sqrt{1 - v^2/c^2})^{-1}(t\,vx/c^2)$. Imagine that R. has a stick of length L along the x axis at rest in his system, with the left end at $x = 0$. Suppose G. marks the ends of the stick simultaneously in the primed system at $t' = 0$, and measures the length L'. Show that $L' = \sqrt{1 - v^2/c^2}\,L$. Find the times at which R. sees G. measure the two ends; show that this lack of simultaneous measurement and G.'s contracted measuring rods as seen by R. are sufficient to account for G.'s measurement of L', $L' = \sqrt{1 - v^2/c^2}\,L$, so far as R. is concerned.

19. A student is given an examination to be completed in 1 hr by the professor's clock. The professor moves at a speed of 0.97c relative to the student, and sends back a light signal when his clock reads 1 hr. The student stops writing when the light signal reaches him. How much time did the student have for the exam?

Answer: $\sqrt{\dfrac{1 + v/c}{1 \quad v/c}}$ 1 hrs.

20. In an inertial system, a number of clocks are synchronized. If you move at 30 km/sec relative to the system, how far apart in the direction of your velocity do clocks appear to be which to you are 1 sec out of synchronism?

Answer: 3×10^9 km.

21. Two clocks on the x axis in a system moving at $^3/_5c$ relative to you appear to be synchronized. They appear to be 10 m apart. How much do the clocks appear to be out of synchronism in the rest frame of the clocks?

Answer: 2.5×10^{-8} sec.

22. Two colliding beams of electrons each have velocities of .50 c as observed in the lab. What is the relative speed of the electrons in the inertial system in which one of the beams of electrons is at rest?

Answer: 0.8 c.

relativistic mechanics and dynamics

Because of the modifications of the velocity transformations introduced by relativistic effects, the concepts, of energy, momentum and angular momentum in special relativity must be redefined so that the laws of physics are form-invariant with respect to Lorentz transformations. The reader should already be familiar with the Newtonian laws of conservation of energy, momentum and angular momentum. It is still possible in relativity to define momentum, angular momentum and energy in such a way that the general conservation laws are valid. However, then new effects arise, such as the variation of mass with velocity, and the equivalence of mass and energy, which is expressed by the famous equation, $E = mc^2$. These effects will be derived and discussed in this chapter.

.1 LORENTZ TRANSFORMATIONS

Recall that when two observers are moving relative to each other, as in Figure 4.1, where G. moves past R. with velocity v, their observations of the space-time coordinates of an event are related not by means of the Galilean transformations, but by the Lorentz transformations. If primed quantities $(x', \ldots, t')$

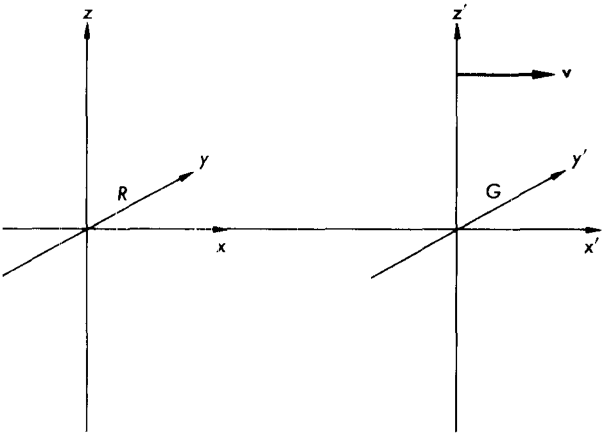


Figure **4.1.** **Inertial systems of R. and G.**

are used to denote measurements made by G. and unprimed quantities $(x, \ldots, t)$ are used to denote R.'s measurements, the Lorentz transformations are

$$x' = \frac{1}{\sqrt{1 - v^2/c^2}}(x - vt); \quad y' = y; \quad z' = z;$$

$$t' = \frac{1}{\sqrt{1 - v^2/c^2}}\left(t - \frac{vx}{c^2}\right) \tag{4.1}$$

Also, if a particle moves so that its velocity components relative to R. are $\dot{x}, \dot{y}, \dot{z}$, then its velocity components relative to G. are

$$\dot{x}' = \frac{(\dot{x} - v)}{(1 - v\dot{x}/c^2)}; \quad \dot{y}' = \sqrt{1 - \frac{v^2}{c^2}}\,\frac{\dot{y}}{(1 - v\dot{x}/c^2)};$$

$$\dot{z}' = \sqrt{1 - \frac{v^2}{c^2}}\,\frac{\dot{z}}{(1 - v\dot{x}/c^2)} \tag{4.2}$$

We shall frequently refer to these transformations in discussing momentum and energy.

4.2 DISCREPANCY BETWEEN EXPERIMENT AND NEWTONIAN MOMENTUM

Momentum in Newtonian mechanics is defined as mass times velocity, and the total momentum is conserved when particles collide. The question is, can we also find a quantity in relativistic mechanics which is conserved when particles collide? We ultimately have to do this by looking to experiment. However, by using the general principles we have previously discussed to analyze a thought experiment, we can predict what we might expect the experimental results to be. First of all, the relativistic quantity which we shall call momentum must reduce to the Newtonian expression, mass times velocity, when the speed is much less than c, according to the correspondence principle.

Let us next ask, can a relativistic expression for momentum still be given simply as $m_0\mathbf{v}$ when m_0 is the Newtonian mass? The mass of a proton is 1.67×10^{-27} kg. The maximum speed a proton can have is $c = 3 \times 10^8$ m/sec. Hence, if this expression is correct, the maximum momentum a proton can have is 5.0×10^{-19} kg-m/sec. However, in *some* cosmic rays, which are high energy particles striking the earth from outer space, fast protons having momenta on the order of 10^{-8} kg-m/sec are observed. Such large particle momenta can be measured in principle by allowing the proton to collide with another particle, thus giving up some momentum; then allowing the proton and the other particle to collide with other particles, sharing their momenta; and so on, until the proton has caused a large number of particles to be traveling with generally low speeds. Then the momenta of each of these particles can be measured by measuring their mass and velocity. By assuming that momentum is conserved, one can work backward to find the initial momentum of the incident proton. We conclude that the

Newtonian expression $m_0\mathbf{v}$ cannot be a valid expression for momentum in the 'case of high velocities.

1.3 MOMENTUM FROM A THOUGHT EXPERIMENT

Nevertheless, we shall attempt to find theoretically an expression of the form mv for the relativistic momentum of a particle, such that the total momentum is conserved in collisions. Experimenters have discovered that there indeed exists such a vector quantity; however, in relativistic mechanics the factor **m**, multiplying v is not a constant independent of speed. We shall define m as the mass. The mass m_0 that a particle has at rest we shall call the rest ***mass.*** **If** $v \ll c$, **the** 'correspondence principle requires that $m = m_0$. From our above arguments about cosmic rays, we would expect m to increase as the speed increases.

Suppose that G. and R. have identical guns that shoot identical bullets. When we say "identical" bullets, we mean that the bullets have equal rest masses, m_0. The guns are assumed to shoot the bullets out with equal muzzle velocities, denoted by U. G. shoots his bullet along the negative y' axis. Thus, the y' component of velocity that G. sees is

$$\dot{y}'_G = -U \tag{4.3}$$

He sees no x component of velocity for the bullet, i.e. $\dot{x}'_G = 0$. (See Figure 4.2.) R., watching G.'s bullet, sees a y component of velocity,

$$\dot{y}_G = -\sqrt{1-\frac{v^2}{c^2}}\,U \tag{4.4}$$

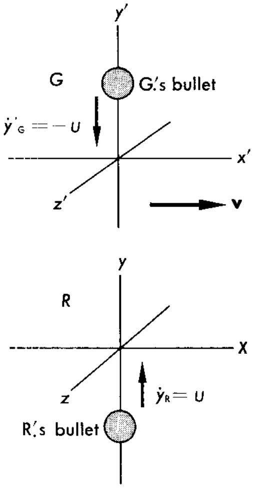


Figure 4.2. **Bullets fired with muzzle speeds U in their respective rest systems, arranged so that a collision occurs.**

by Equations (4.2). Let R. shoot his bullet along the positive y axis. It will then have a y component of velocity, as observed by R., of

$$\dot{y}_R = +U \tag{4.5}$$

Again using Equations 4.2, since $\dot{x}_R = 0$, the bullet shot by R. has a y' component of velocity when observed by G. of

$$\dot{y}_R' = \sqrt{1 - \frac{v^2}{c^2}}\,U \tag{4.6}$$

A prime or lack of a prime on the velocity component means it is observed by G. or R., respectively. The subscript G or R means the bullet is shot by G. or R., respectively.

Now we suppose that the bullets collide and stick together, and that momentum in the y direction is conserved during the collision. This experiment has been set up so that there is complete symmetry between the coordinate systems. Both R. and G. are shooting bullets that have the same rest masses, with the same muzzle velocities, in their own systems of coordinates. They both shoot normal to the direction of relative motion between the coordinate systems. By the principle of relativity, then, neither coordinate system is preferred,, and both R. and G. must observe the same experimental results in their respective coordinate systems. From the symmetry between the two coordinate systems, if G. observes a final y' velocity that is negative, i.e. a velocity component which is parallel to the original velocity of his bullet, then R. must observe a final y velocity which is parallel to the original y velocity of his bullet and which has a positive sign. However, from the results of the Lorentz velocity transformations, Equations 4.2, $\dot{y}$ cannot be positive while $\dot{y}'$ is negative. Thus, the final y component of velocity of the bullets after collision must be zero. Since we assumed that the momentum is mv, this means that the final y component of momentum of the two bullets is zero. So if momentum is to be conserved, the total y component of momentum of the two bullets before collision must also be zero in both systems of coordinates.

Let us look at the initial momentum from the point of view of R. Suppose he observes that his bullet has a mass m_R. Then he sees a momentum for this bullet of $m_R U$. If G.'s bullet, as observed by R., has a mass m_G and a y component of velocity $\dot{y}_G$, then the y component of momentum of this bullet, as seen by R., is $m_G \dot{y}_G$. Thus, the total momentum seen by R. is

$$m_R U + m_G \dot{y}_G = 0 \tag{4.7}$$

By Equation (4.4), the velocity component, $\dot{y}_G$, of G.'s bullet observed by R. is $--(1\quad v^2/c^2)^{1/2}U$. On substituting this into Equation (4.7) and solving for m_G, we find that

$$m_G = \frac{m_R}{(1 - v^2/c^2)^{1/2}} \tag{4.8}$$

This equation is valid for all values of U, which has canceled out. In the limit in which U, the muzzle velocity, approaches zero, R.'s bullet is at rest relative to R., and $m_R = m_0$, the rest mass. The speed of G.'s bullet relative to R. is then the same as that of G., and is equal to v. Hence, the moss of the moving (G.'s) bullet, as observed by R., is given in terms of its rest mass m_0 and its speed v by

$$m\ (=m_G) = \frac{m_0}{(1 - v^2/c^2)^{1/2}} \text{(relativistic mass)} \tag{4.9}$$

Thus, if the relativistic momentum of a rapidly moving particle is proportional to v, the momentum must be of the form

$$p = \frac{m_0 v}{(1 - v^2/c^2)^{1/2}} \tag{4.10}$$

for momentum to be conserved.

If we had written down the law of conservation of momentum, Equation (4.7), from the point of view of G. rather than of R., the results would have been the same: The mass of a moving object is increased by the factor $(1 - v^2/c^2)^{-1/2}$ over the mass the same object possesses when at rest.

Consider the expression for the mass of a particle, $m_0/(1 - v^2/c^2)^{1/2}$. In the limit as v approaches c, this mass increases without limit. Thus, arbitrarily large momenta are possible without having arbitrarily large velocities.

nple If a particle moves with 0.8 the speed of light, what will its mass be in terms of the rest mass?

tion $(1 - 0.8^2)^{1/2} = 0.6$. Then $m = m_0/0.6 = 1.667 m_0$.

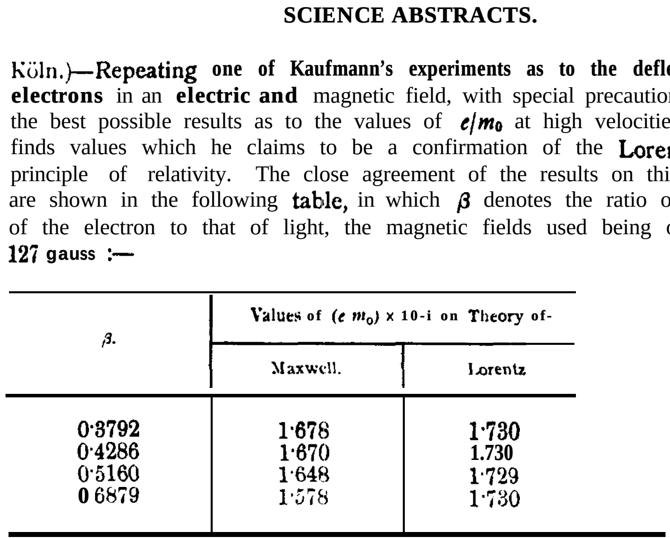
In the limit as v becomes very small compared to c, the mass m of a particle of rest mass m_0 is given by $m = m_0$, because in this limit $(1 - v^2/c^2)^{1/2}$ is unity. This result is in agreement with the correspondence principle.

1.4 EXPERIMENTAL VERIFICATION OF MASS FORMULA

The increase of mass with velocity was observed in an experiment performed by Biicherer **in 1908. By projecting electrons into crossed electric and magnetic** fields, he was able to select electrons of known velocity. The subsequent deflection of the electrons in a magnetic field gave the mass. Given in Table 4.1 are the values of **m/m,,** as a function of v/c for the electrons observed by Biicherer. The

TABLE 4.1 Increase of Moss With Speed

v/c	m/m_0 (observed)	m/m,, (theory)
0.3173	1.059	1.055
0.4286	1.106	1.107
0.6879	1.370	1.376

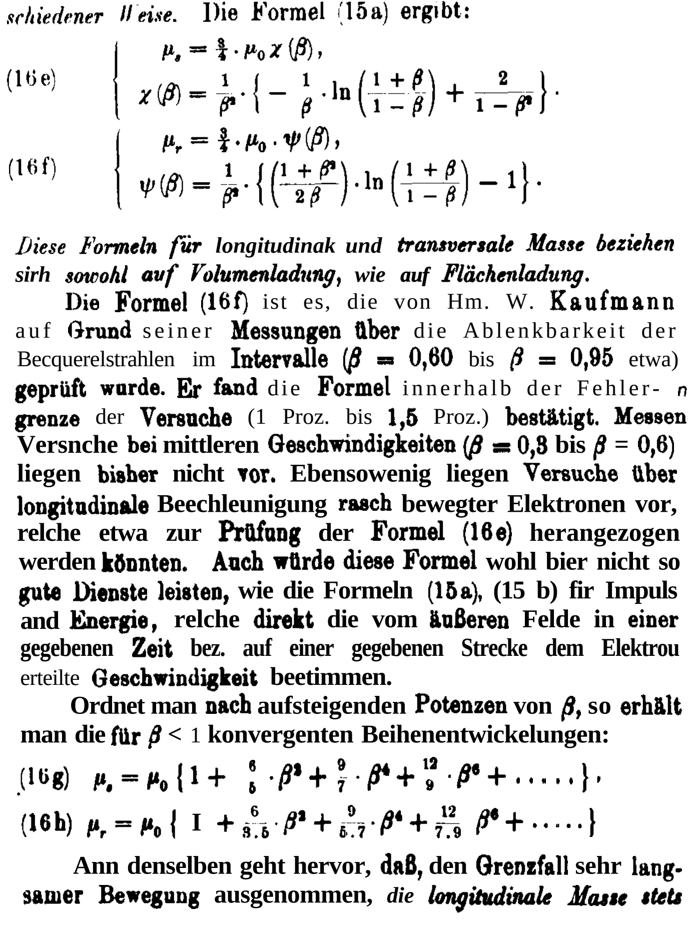


SCIENCE ABSTRACTS.

Köln.)—**Repeating one of Kaufmann's experiments as to the deflection of** the **electrons** in an **electric and** magnetic field, with special precautions to obtain the best possible results as to the values of e/m_0 at high velocities, the author finds values which he claims to be a confirmation of the Lorentz-Einstein principle of relativity. The close agreement of the results on this principle are shown in the following table, in which β denotes the ratio of the speed of the electron to that of light, the magnetic fields used being of the order 127 gauss :—

β.	Values of (e m_0) x 10-i on Theory of-	
	Maxwell.	Lorentz
0·3792	1·678	1·730
0·4286	1·670	1.730
0·5160	1·648	1·729
0 6879	1·578	1·730

Science Abstracts, 11, 687 (1908).



schiedener Weise. Die Formel (15a) ergibt:

$$(16e)\quad \left\{\begin{aligned} \mu_s &= \tfrac{3}{4}\cdot\mu_0\,\chi(\beta),\\ \chi(\beta) &= \frac{1}{\beta^2}\cdot\left\{-\frac{1}{\beta}\cdot\ln\left(\frac{1+\beta}{1-\beta}\right)+\frac{2}{1-\beta^2}\right\}.\end{aligned}\right.$$

$$(16f)\quad \left\{\begin{aligned} \mu_r &= \tfrac{3}{4}\cdot\mu_0\cdot\psi(\beta),\\ \psi(\beta) &= \frac{1}{\beta^2}\cdot\left\{\left(\frac{1+\beta^2}{2\beta}\right)\cdot\ln\left(\frac{1+\beta}{1-\beta}\right)-1\right\}.\end{aligned}\right.$$

Diese Formeln für longitudinale und transversale Masse beziehen sich sowohl auf Volumenladung, wie auf Flächenladung.

Die Formel (16f) ist es, die von Hrn. W. Kaufmann auf Grund seiner Messungen über die Ablenkbarkeit der Becquerelstrahlen im Intervalle ($\beta = 0,60$ bis $\beta = 0,95$ etwa) geprüft wurde. Er fand die Formel innerhalb der Fehlergrenze der Versuche (1 Proz. bis 1,5 Proz.) bestätigt. Messende Versuche bei mittleren Geschwindigkeiten ($\beta = 0,3$ bis $\beta = 0,6$) liegen bisher nicht vor. Ebensowenig liegen Versuche über longitudinale Beschleunigung rasch bewegter Elektronen vor, welche etwa zur Prüfung der Formel (16e) herangezogen werden könnten. Auch würde diese Formel wohl hier nicht so gute Dienste leisten, wie die Formeln (15a), (15 b) für Impuls und Energie, welche direkt die vom äußeren Felde in einer gegebenen Zeit bez. auf einer gegebenen Strecke dem Elektron erteilte Geschwindigkeit bestimmen.

Ordnet man nach aufsteigenden Potenzen von β, so erhält man die für $\beta < 1$ konvergenten Reihenentwickelungen:

$$(16g)\quad \mu_s = \mu_0\left\{1+\frac{6}{5}\cdot\beta^2+\frac{9}{7}\cdot\beta^4+\frac{12}{9}\cdot\beta^6+\ldots\ldots\right\},$$

$$(16h)\quad \mu_r = \mu_0\left\{1+\frac{6}{3.5}\cdot\beta^2+\frac{9}{5.7}\cdot\beta^4+\frac{12}{7.9}\,\beta^6+\ldots\ldots\right\}$$

Aus denselben geht hervor, daß, den Grenzfall sehr langsamer Bewegung ausgenommen, *die longitudinale Masse stets*

Figure 4.3. A page from Annalen der Physik 10, 152 (1902) showing the "Maxwell" mas formulas referred to by Bücherer

third column gives the corresponding values calculated from Equation (4.9). Innumerable experiments since 1908 have continued to be in excellent agreement with theory. (See Figure 4.3) Also experiments verify that with the expression for momentum found above, nomentum is always conserved in collisions between particles.

.5 RELATIVISTIC SECOND LAW OF MOTION

In Newtonian mechanics, the second law for a particle can be written $\mathbf{F} = m\, d\mathbf{v}/dt$; where m is a constant. Hence, in the nonrelativistic case, we do not have to consider the effect of changes in m. However, the question arises in relativistic mechanics as to whether the correct relativistic expression is: (a) $\mathbf{F} = m\, d\mathbf{v}/dt$; or (b) $\mathbf{F} = d(m\mathbf{v})/dt$; or (c) some other intermediate expression. We may (answer this in part by considering a constant force F_0 acting on an electron in the x direction. This force could be obtained by letting the electron move in a [uniform electric field. Let us take case (a), $F_x = F_0 = m dv_x/dt$, and show that it leads to an unreasonable result. Imagine an electron starting from rest, under the action only of the constant force, F_0, in the x direction, so that $v_x = v$. Inserting the expression for m from Equation (4.6), we have

$$\frac{m_0}{\sqrt{1 - v^2/c^2}}\frac{dv}{dt} = F_0 \qquad (4.11)$$

This can be written: $dv/\sqrt{1 - v^2/c^2} = F_0/m_0\, dt$. The initial condition we assumed on v is that at $t = 0$, $v = 0$. The solution is $v = c \sin(F_0 t/m_0 c)$. This is easily verified by substitution into the differential equation. The expression for v says that for the time when, for instance, $F_0 t/m_0 c = 3\pi/2$, the velocity is negative. Also, the velocity has a magnitude of c periodically. These conclusions do not seem reasonable. More important, they disagree with experiment. So the possibility $\mathbf{F} = m d\mathbf{v}/dt$ is eliminated.

In the following section, it will be shown that case (b), $\mathbf{F} = d/dt\,(m\mathbf{v})$ leads directly to the law of conservation of momentum for collisions between particles. Thus case (b) seems highly reasonable, and, in fact, its correctness is borne out by experiment. In other words, force is time rate of change of momentum:

$$\mathbf{F} = \frac{d}{dt}(m\mathbf{v}) \qquad (4.12)$$

Of course, this form is also valid for Newtonian mechanics.

.6 THIRD LAW OF MOTION AND CONSERVATION OF MOMENTUM

If the force is given by $\mathbf{F} = d(m\mathbf{v})/dt$, then if the third law is also valid, we can show that relativistic momentum is conserved in a collision. Newton's third law of motion states that if particle number one acts on particle number two with a force

$\mathbf{F}_{1\text{ on }2}$, and if particle number two acts on one with $\mathbf{F}_{2\text{ on }1}$, during a collision, then

$$\mathbf{F}_{1\text{ on }2} + \mathbf{F}_{2\text{ on }1} = 0 \tag{4.13}$$

If $\mathbf{p}_1 = m_1\mathbf{v}_1$ is the momentum of particle number one, then (assuming no other forces act)

$$\mathbf{F}_{2\text{ on }1} = \frac{d\mathbf{p}_1}{dt} \tag{4.14}$$

Similarly,

$$\mathbf{F}_{1\text{ on }2} = \frac{d\mathbf{p}_2}{dt} \tag{4.15}$$

Adding these two equations and using the law of action and reaction, we find

$$\frac{d(\mathbf{p}_1 + \mathbf{p}_2)}{dt} = 0 \tag{4.16}$$

Integration once over the time gives

$$\mathbf{p}_1 + \mathbf{p}_2 = \mathbf{C} \tag{4.17}$$

where c is a constant. Hence, the momentum is constant, or total momentum after the collision is equal to the total momentum before the collision. In other words, the third law of motion leads to conservation of momentum in collisions. The result can be extended for a system of an arbitrary number of particles.

4.7 RELATIVISTIC ENERGY

In Newtonian mechanics, the work done on a body when a force is exerted which moves the body through some distance, goes into increasing the energy of the body. This is also true in relativity, and work is still defined the same way. If E is the energy of a body, and a force F exerted is moved through a distance dr in doing work on the body, then the increase in energy E is:

$$dE = \mathbf{F}\cdot d\mathbf{r} \tag{4.18}$$

Since $\mathbf{F} = d(m\mathbf{v})/dt$, the expression for dE becomes

$$dE = \frac{d(m\mathbf{v})}{dt}\cdot d\mathbf{r} \tag{4.19}$$

We can reinterpret the right side of this equation by writing the dt underneath the dr and noting that $d\mathbf{r}/dt = \mathbf{v}$. Then

$$dE = d(m\mathbf{v})\cdot\mathbf{v} = dm(\mathbf{v}\cdot\mathbf{v}) + m(d\mathbf{v}\cdot\mathbf{v}) \tag{4.20}$$

All the quantities on the right side of this equation are functions of the velocity, v. We shall express the right side as an exact differential in order to find an expression for energy in terms of velocity. We first write the scalar products in terms of the scalar speed v: $\mathbf{v}\cdot\mathbf{v} = v^2$ and $\mathbf{v}\cdot d\mathbf{v} = \frac{1}{2} d(\mathbf{v}\cdot\mathbf{v}) = \frac{1}{2} dv^2$. So

$$dE = dm(v^2) + \frac{1}{2} md(v^2) \tag{4.21}$$

The m here is the relativistic mass, $m_0/(1 - v^2/c^2)^{1/2}$. Therefore,

$$dm = \frac{\frac{1}{2} m_0 d(v^2)}{[c^2(1 - v^2/c^2)^{3/2}]} \tag{4.22}$$

Substituting this expression for dm into Equation (4.21), and combining terms, we get

$$dE = m_0c^2 \frac{\frac{1}{2} d(v^2/c^2)}{(1 - v^2/c^2)^{3/2}} \tag{4.23}$$

The right side can now easily be integrated, yielding

$$E = \frac{m_0c^2}{(1 - v^2/c^2)^{1/2}} + \text{constant} \tag{4.24}$$

It is very convenient to set the constant of integration equal to zero. If this is done, the result can be expressed in terms of m:

$$\boxed{E = mc^2 \text{ (relativistic energy)}} \tag{4.25}$$

One thing which this implies is that associated with an increase in mass is an increase in energy and vice versa. Another thing which is implied is that if $v = 0$, the energy is $E = m_0c^2$; this may be interpreted as the rest energy a body has by virtue of the fact that it possesses mass.

KINETIC ENERGY

That part of the energy which is due to the particle's motion is called kinetic energy. It is simply the total energy mc^2 minus the energy with no motion, m_0c^2. If we denote kinetic energy by the symbol T, then

$$T = mc^2 - m_0c^2 = m_0c^2\left(\frac{1}{\sqrt{1 - v^2/c^2}} - 1\right) \tag{4.26}$$

Let us first find the rest energy of a proton. Its mass is 1.67 x 10^{-27} kg. Then the rest energy is

$$E = m_0c^2 = (1.67 \times 10^{-27})(3 \times 10^8)^2 = 1.50 \times 10^{-10}\ \mathrm{J}$$

Next suppose the proton is traveling at speed $(\frac{4}{5})c$ relative to an observer. Its kinetic energy is

$$T = m_0c^2\left(\frac{1}{\sqrt{1 - v^2/c^2}} - 1\right) = (1.50 \times 10^{-10})\left(\frac{5}{3} - 1\right) = 1.00 \times 10^{-10}\ \mathrm{J}$$

The classical expression for the kinetic energy would give $\frac{1}{2} m_0 v^2 = \frac{1}{2}(1.157 \times 10^{-27})(2.4 \times 10^8)^2 = 0.48 \times 10^{-10}$ j. On the other hand, if the speed of the proton is as small as $(\frac{1}{20})c$, the relativistic kinetic energy is 1.88×10^{-13} j, and to this number of significant figures the classical expression gives the same result.

We see from this example that when the speed is much less than c, the relativistic and classical kinetic energy agree. This is in accord with the correspondence principle. We may prove that the expressions agree in general for small v/c. We shall need to expand $(1 - v^2/c^2)^{-\frac{1}{2}}$ for small v/c. For this, we use the binomial theorem, $(a - b)^n = a^n \quad na^{n-1}b + \ldots$. Then, with $a = 1$, $b = v^2/c^2$, and $n = -\frac{1}{2}$, it follows that $(1 - v^2/c^2)^{-1/2}$ is approximately $1 + \frac{1}{2} v^2/c^2$. Here we are (dropping terms of order v^4/c^4 or higher because they are assumed to be very small. Then, approximately,

$$T = m_0c^2 \left[\left(1 + \frac{1}{2}\frac{v^2}{c^2}\right) - 1\right] = \frac{1}{2} m_0 v^2 \tag{4.27}$$

Note that just as the classical expression, $\frac{1}{2} m_0 v^2$, is not correct for the kinetic energy at high energies, neither is $\frac{1}{2} mv^2$.

4.9 POTENTIAL ENERGY AND CONSERVATION OF ENERGY

The energy changes considered so far are changes in kinetic energy due to forces which may be either conservative or nonconservative. If a conservative force, $\mathbf{F}_c$, is present, then

$$\int_{r_1}^{r_2} \mathbf{F}_c \cdot d\mathbf{r} = -(V_2 \quad V_1) \tag{4.28}$$

where V is the potential energy depending only on the position and not on the integration path. If there are no forces other than the conservative ones, from the definition of energy,

$$\int_{r_1}^{r_2} dE = \int_{r_1}^{r_2} \mathbf{F}_c \cdot d\mathbf{r} = m_2c^2 - m_1c^2 \tag{4.29}$$

On equating the right sides of Equations (4.28) and (4.29) and rearranging, we find that

$$m_1c^2 + V_1 = m_2c^2 + V_2 \tag{4.30}$$

This is the conservation of energy equation.

.10 EXPERIMENTAL VERIFICATION OF EQUIVALENCE OF MASS AND ENERGY

Equation (4.25) indicates as we have seen, that there is energy-rest (energy--associated with the rest mass, i.e. $E_0 = m_0c^2$. There is plenty of evidence in nuclear physics that indicates that rest mass is indeed equivalent to energy, and that mass can be converted to energy and vice versa.

An example of this occurs when lithium is bombarded by fast protons: the lithium nucleus, ${}_3Li^7$, and a proton, ${}_1p^1$, combine to form an unstable nucleus which splits into two fast helium nuclei, ${}_2He^4$: ${}_1p^1 + {}_3Li^7 \rightarrow {}_2He^4 + {}_2He^4$. The rest masses of these particles are given in Table 4.2, in atomic mass units (amu). (1 amu is the mass of an atom of C^{12}; 1 amu = 1.660×10^{-27} kg. These mass units were discussed in Chapter 1.)

TABLE 4.2 Masses of particles participating in reaction P + Li → 2He, in amu

P	**1.0073**
Li	**7.0143**
He	**4.0015**

The sum of the p and Li masses is the total mass of the incoming particles; it is 8.0216 amu. The total rest mass of the outgoing particles is 8.0030 amu. Thus, rest mass is not conserved. However, energy is conserved in the overall nuclear reaction, for very precise measurements of the difference between the kinetic energy of the incoming proton and the total kinetic energy of the He nuclei gives AE = $(2.770 \pm 0.005) \times 10^{-12}$ j. The increase in rest mass is 0.0186 amu, or 0.309×10^{-28} kg. Then the increase in rest energy is $\Delta m_0c^2 = \mathbf{2.78} \times 10^{-12}$ j. It thus appears that the increase in mass is accounted for quantitatively by a corresponding decrease in kinetic energy.

nple A mass of 1 gm has a rest energy of

$$m_0c^2 = (10^{-3}\ \text{kg})(3 \times 10^8\ \text{m/sec})^2 = 9 \times 10^{13}\ \text{j}.$$

If this energy could be converted into electricity and sold at a rate of 6¢ per kilowatt-hour, how much would it be worth?

tion $(9 \times 10^{13})(1/[3.6 \times 10^6]\ \text{kw-hr/j})(0.06)$ = 1.5 million dollars.

11 RELATIONSHIP BETWEEN ENERGY AND MOMENTUM

In Newtonian mechanics, the relationship between kinetic energy and momentum is

$$T = \frac{1}{2}mv^2 = \frac{\tfrac{1}{2}(mv)^2}{m} = \frac{p^2}{2m} \qquad (4.31)$$

A general relation between energy and momentum is of considerable utility in special relativity. We may use the expressions for energy and momentum, Equations (4.10) and (4.25), to obtain such a relation mathematically. We have, upon squaring Equation (4.25),

$$E^2 = m^2c^4 = \frac{m_0^2c^4}{(1 - v^2/c^2)} \tag{4.32}$$

In the same way,

$$c^2p^2 = \frac{m_0^2c^2v^2}{(1 - v^2/c^2)} \tag{4.33}$$

Then, subtracting,

$$E^2 - c^2p^2 = m_0^2c^2\left(\frac{c^2 - v^2}{1 - v^2/c^2}\right) = m_0^2c^4 \tag{4.34}$$

Since the rest energy plus kinetic energy should be positive, Equation (4.34) can be solved for E by taking the positive square root: $E = \sqrt{p^2c^2 + m_0^2c^4}$. In the limit asp becomes very small, the binomial theorem may be used to expand the right side of the equation $E = \sqrt{c^2p^2 + m_0^2c^4}$, to obtain, approximately, $T = E - m_0c^2 = p^2/2m_0$ in agreement with the Newtonian result.

example 1. In Chapter 1 a unit of energy called the electron volt (eV) was defined as 1 eV = 1.602 x 10^{-19} joules = e joules. Also, 1 MeV = 10^6 eV. The rest moss of an electron is approximately 9 x 10^{-31} kg. Find its rest energy in MeV.

solution $E_0 = m_0c^2 = (9 \times 10^{-31})(3 \times 10^8)^2/1.6 \times 10^{-13}$ j/MeV = 0.5 MeV. To three significant figures, the correct value is 0.511 MeV.

example 2. If an electron is emitted from a nucleus in a beta decay with a kinetic energy of 0.5 MeV, what is its momentum in MeV/c?

solution $E^2 = c^2p^2 + m_0^2c^4$ or $p = (E^2 - m_0^2c^4)^{1/2}/c$.
E is $J + m_0c^2$, so that $E^2 - m_0^2c^4 = J(J + 2m_0c^2) = 0.5(0.5 + 2[0.511]) =$ 0.761 MeV^2. The momentum in MeV/c is numerically the square root of this number: $p = \sqrt{0.761}$ = 0.872 MeV/c. In kg-m/set, this would be

$$\frac{(0.872)(1.6 \times 10^{-13}\ \text{j/MeV})}{(3 \times 10^8)} = 4.65 \times 10^{-22}\ \text{kg-m/sec.}$$

4.12 REST MASS OF Λ^0 FROM EXPERIMENT

We shall now consider in detail a more elaborate example, which shows how one may use the relativistic equations to find experimentally an unknown particle mass, in terms of known masses and measured energies and momenta. The rest mass of the particle will be measured using bubble chamber photographs in which a Λ^0 particle decays into a proton and a π meson. If you wish to follow along on the measurements, you will need to use a protractor, a flexible plastic ruler and a slide rule.

A charged particle moving rapidly through a bubble chamber leaves a trail of very tiny bubbles that render its track visible and that can be photographed. In the experiment discussed here, a beam of very high energy negatively charged particles called K^- mesons was allowed to penetrate into a bubble chamber filled with a mixture of organic liquids, so that there were large numbers of the more ordinary constituents of matter, e.g. protons,. neutrons and electrons, present in the chamber. These K^- mesons (the superscript means a particle having a negative charge) may combine with the protons (p’) and neutrons (n) to produce particles called pions (π) and uncharged $(^0$ superscript) Λ^0 hyperon:;, in the following reactions:

$$K^- + p^+ \rightarrow \Lambda^0 + \pi^0$$
$$K^- + n \rightarrow \Lambda^0 + \pi^- \qquad (4.35)$$

The charged particles interact electrically with the fluid molecules to produce ionization which leads to observable bubbles. Since the Λ^0 and π^0 are uncharged, their tracks in the chamber will not be visible. However, in a very short time the Λ^0 decays into a proton and a π^- meson, according to the reaction:

$$\Lambda^0 \rightarrow p^+ + \pi^- \qquad \textbf{(4.36)}$$

Since both p^+ and π^- are charged, their tracks will be visible in the chamber. The π^0 would decay into uncharged photons, which again, are not easily visible.

A diagram representing a typical series of such events is shown in Figure 4.4. A magnetic field applied to the chamber causes charged particles to move in curved paths, for which the radius of curvature is proportional to the momentum.

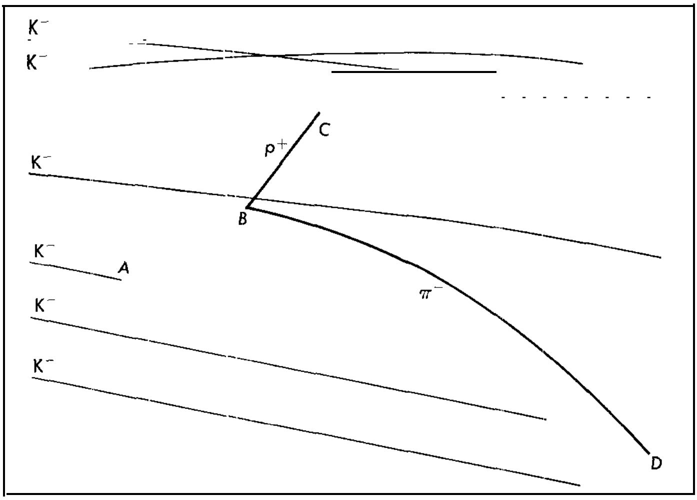


Figure 4.4. Diagram of a typical bubble chamber photograph of Λ^0 decay, showing p^+ and π^- tracks.

Here, the K^- tracks are easily identified, since all the K^- mesons have the same curvature. At point A, a K^- disappears, according to one of the reactions given in Equation (4.35). A Λ^0 is produced, which travels to *B,* where it decays. Since the decay products are oppositely charged, the forces due to the magnetic field are in opposite directions for the two particles, and their tracks will curve in opposite directions.

The p^+ and π^- gradually lose their kinetic energies in collisions with the molecules of the liquid in the chamber, and will finally slow down and come to rest. In Figure 4.5, this occurs at C and *D*. The track length, or range, for any given particle moving in any particular medium is a well-defined function of the particle's initial momentum or energy. By measuring the range, the energy and momentum may be measured whenever previously determined range versus momentum curves are available.

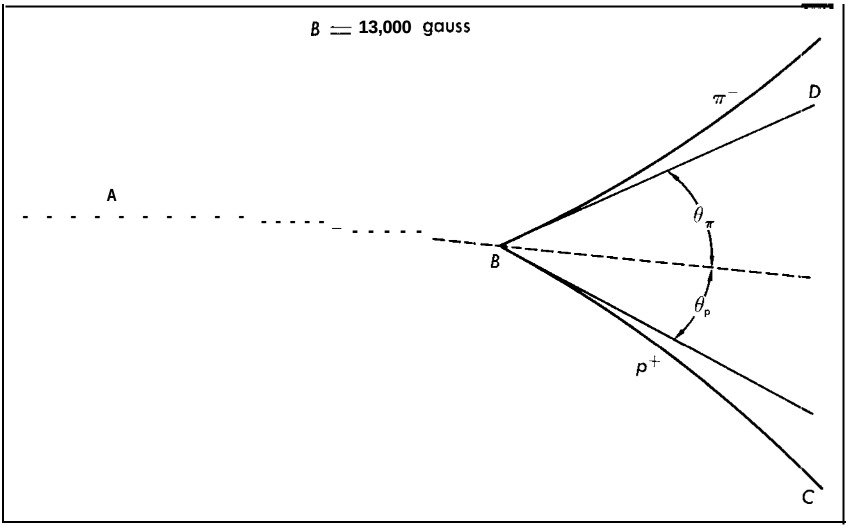


Figure 4.5. Angles used in the calculation of the Λ^0 rest mass.

In this example, we shall apply the relativistic laws of conservation of energy and momentum to the decay which occurs at *B,* coupled with range and direction measurements of the p^+ and π^- tracks, for the purpose of measuring the rest mass $m_{0\Lambda}$ of the invisible Λ^0 particle. Referring to Figure 4.5, the dashed line represents the path of the Λ^0, which we will assume has velocity $\mathbf{v}_\Lambda$ and energy,

$$E_\Lambda = \frac{m_{0\Lambda}c^2}{\sqrt{1 - v_\Lambda^2/c^2}} \tag{4.37}$$

If the pion and proton are created initially with total energies E_π and E_p, respectively, then, by conservation of energy, we have

$$E_\Lambda = E_\pi + E_p \tag{4.38}$$

Further, if θ_π and θ_p are the initial angles at which the pion and proton are projected, measured as indicated in the diagram, then, by conservation of momentum,

$$p_\Lambda = p_\pi \cos\theta_\pi + p_p \cos\theta_p \tag{4.39}$$

and

$$0 = p_\pi \sin\theta_\pi - p_p \sin\theta_p \tag{4.40}$$

Dividing Equation (4.39) by Equation (4.38) and using $p = mv = Ev/c^2$, we have

$$\frac{v_\Lambda}{c} = \frac{p_\Lambda c}{E_\Lambda} = \frac{(p_\pi c\cos\theta_\pi + p_p c\cos\theta_p)}{(E_\pi + E_p)} \tag{4.41}$$

The combination of Equations (4.37) and (4.38) leads to

$$m_{0\Lambda} c^2 = (E_\pi + E_p)\sqrt{1 - \frac{v_\Lambda^2}{c^2}}. \tag{4.42}$$

All the quantities on the right side of Equations (4.41) and (4.42) may be obtained directly or indirectly from the photographs; hence, from Equation (4.42), the rest mass of the Λ^0 may be determined.

Figure 4.6 is a reproduction of a carefully selected bubble chamber photograph, in which the Λ^0 decay products travel in the plane of the picture. The angles θ_π and θ_p may be (measured with ruler and protractor. To aid in the measurements, dashed lines have been drawn on the photograph along the path of the Λ^0 and also along the paths of the π^- and p^+. The measurement gives θ_p = 17" and θ_π = 31". Then $\cos\theta_p = 0.96$ and $\cos\theta_\pi = 0.86$. Next, the ranges may be measured by laying a flexible plastic rule along the curved paths of the π^- and p^+. The ranges measured in this way must be corrected because of the fact that the reproduction is not lifesize. A centimeter calibration scale is reproduced on the photograph for this correction. After applying the correction, we find the ranges

$$R_p = 2.45 \text{ cm} \quad \text{and} \quad R_\pi = 17.4 \text{ cm}$$

These ranges may be converted into kinetic energies by using the tvvo range-energy curves in Figure 4.7. Then the momenta may be obtained from the momentum-energy equation:

$$p = \frac{\sqrt{E^2 - m_0^2c^4}}{c} = \frac{\sqrt{T^2 + 2m_0c^2T}}{c} \tag{4.43}$$

From the curves, the kinetic energies are $T_p = 44$ MeV and $T_\pi = 60$ MeV for the proton and pi meson, respectively. The rest energy of the proton is 938 MeV. The proton momentum is, therefore, from Equation (4.22)

$$p_p = [44(44 + 1876)]^{1/2} = \frac{291\text{ MeV}}{c}$$

The π^- rest energy is 139.6 MeV; so its momentum is

$$p_\pi = [60(60 + 279.2)]^{1/2} = \frac{143\text{ MeV}}{c}$$

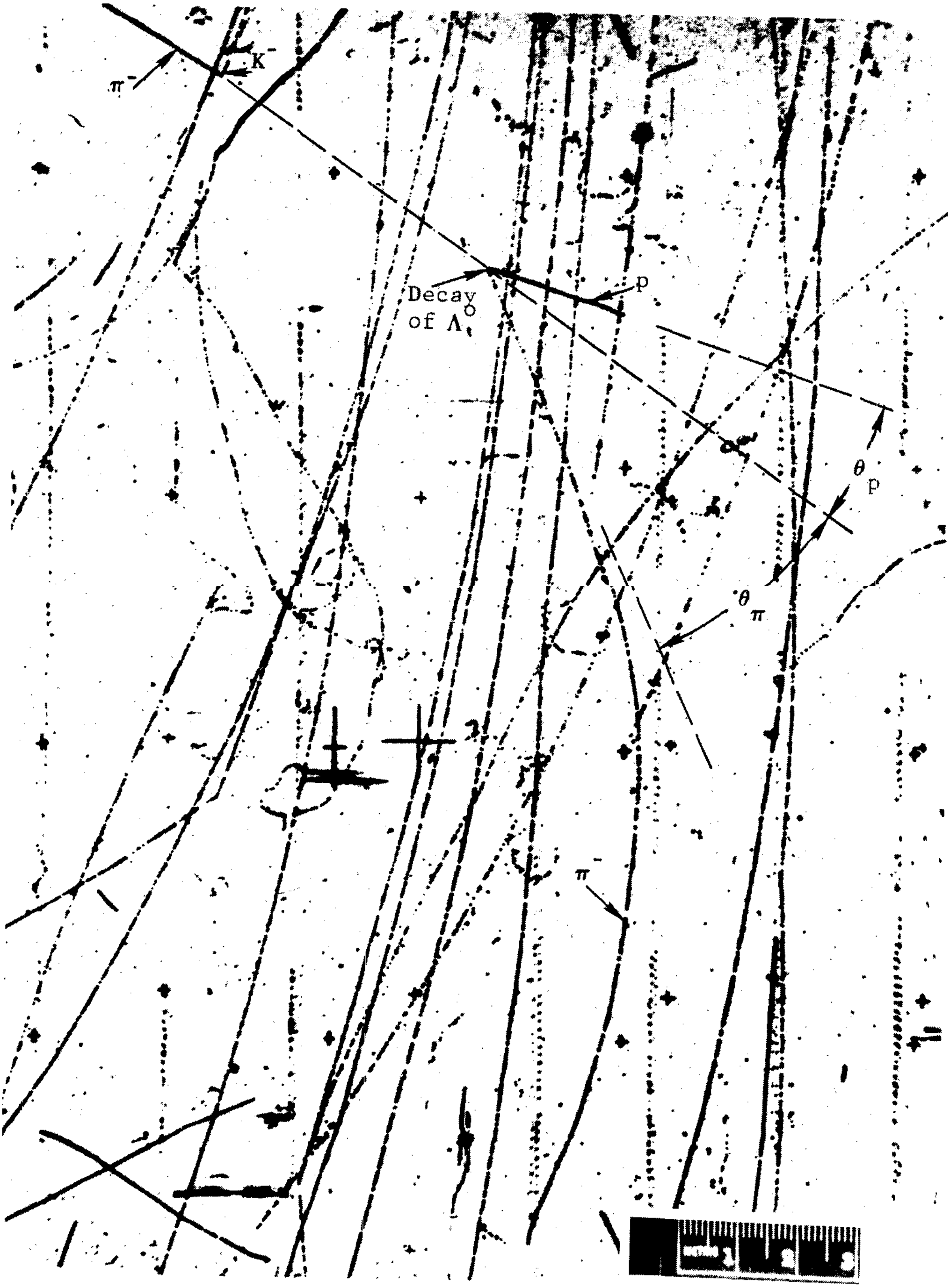


Figure 4.6. Bubble chamber photograph of Λ^0 decay.

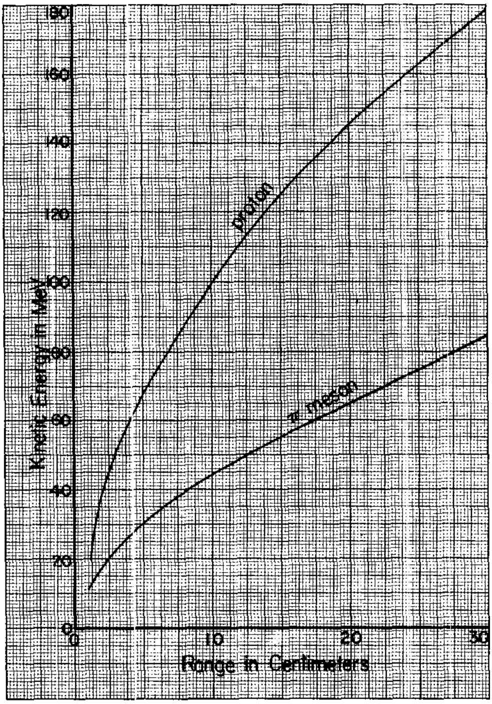


Figure 4.7. Range curves for photographs in Figures 4.6 and 4.8.

From Equation (4.41),

$$\frac{v_\Lambda}{c} = \frac{[(143)(0.86) + (291)(0.96)]}{[(139.6 + 60) + (938 + 44)]} = 0.340$$

Finally, from Equation (4.42), the Λ^0 rest energy is

$$m_{0\Lambda}c^2 = [(139.6 + 60) + (938 + 44)][1 - (0.34)^2]^{1/2} = 1111 \text{ MeV}$$

The accepted value for this rest energy is 1115 MeV. Similar analysis of other photographs gives results which agree closely with the value, 1115 MeV. This not only provides a value for the lambda's mass, but is o direct experimental verification of the validity of relativistic mechanics.

As one further check, one may test whether relativistic momentum, in the direction transverse to the Λ^0's motion, is conserved according to Equation 4.20. Using the measured values from the photograph,

$$0 = 143 \sin 31^\circ - 291 \sin 17''$$
$$0 = 74 - 85$$

which agrees as well as can be expected, to the accuracy with which the angles were measured.

4.13 TRANSFORMATION PROPERTIES OF ENERGY AND MOMENTUM

As a preliminary to the discussion of the form-invariance of the laws of quantum physics, we shall, in this section, derive the transformation laws connecting the energies and momenta of a particle, measured by two relatively moving observers. In deriving these transformations, we shall need to use the time dilation formula, which says that a clock moving with speed v relative to an observer appears to that observer to beat slow by the factor $\sqrt{1-v^2/c^2}$. Consider, as in Figure 4.8, three inertial systems S_0, R, and G. S_0 is the system in which a clock and a particle are at rest. Let $-\mathbf{u}$ be the velocity of R relative to S_0, and let $-\mathbf{u}'$ be the velocity of G relative to S_0. Then, corresponding to the proper time interval dt_0 in S_0, there is a time interval dt in ?, with

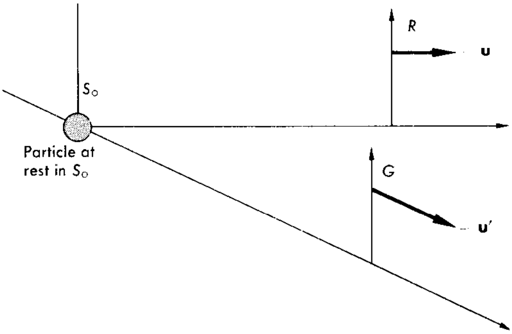


Figure 4.8. Instantaneous rest system of o particle.

$$dt_0 = dt\sqrt{1-\frac{u^2}{c^2}} \tag{4.44}$$

Similarly, the corresponding time interval in G is dt'; where

$$dt_0 = dt'\sqrt{1-\frac{u'^2}{c^2}} \tag{4.45}$$

Combining the last two results, we have the equation,

$$dt'\sqrt{1-\frac{u'^2}{c^2}} = dt\sqrt{1-\frac{u^2}{c^2}} \tag{4.46}$$

In other words, the quantity $dt\sqrt{1-u^2/c^2}$ is form-invariant with respect to Lorentz transformations. This result applies to any infinitesimal time interval between specific events along the path of a particle, measured by the two observers; u and u', the velocities relative to the particle, can be in any arbitrary directions relative to each other.

We may use the invariance of the interval, Equation (4.46), to obtain the transformations for momentum and energy. Imagine a particle of rest mass m_0, placed at the origin of S_0. Then with our choice of velocity $-\mathbf{u}$ of R relative to

So, the particle will have a velocity +u relative to R. Similarly, relative to G the particle will have a velocity i-u'. We shall assume that G is moving relative to R, with velocity v along the x', x axes, i.e. that G and R are related by the Lorentz transformations given previously. Consider the y component of momentum of the particle measured by R. It is just

$$p_y = \frac{m_0 u_y}{\sqrt{1-u^2/c^2}} = \frac{m_0}{\sqrt{1-u^2/c^2}} \frac{dy}{dt} \tag{4.47}$$

Relative to G, the y component of momentum is

$$p_y' = \frac{m_0}{\sqrt{1-u^2/c^2}} \frac{dy'}{dt'} \tag{4.48}$$

However, from the Lorentz transformation between R and G for the y coordinate, dy' = dy. Using this and the result in Equation (4.46), we find that the relation between p_y and p_y' is simply

$$p_y' = p_y \tag{4.49}$$

In a similar fashion, it is easily proved that the connection between z components of momentum is

$$p_z' = p_z \tag{4.50}$$

We next find the transformation for the x components of momentum. From the definition of momentum,

$$p_x' = \frac{m_0}{\sqrt{1-u'^2/c^2}} \frac{dx'}{dt'} \tag{4.51}$$

But using the invariance property in Equation (4.46) and the expression for dx' which arises from the Lorentz transformation,

$$dx' = \frac{1}{\sqrt{1-v^2/c^2}}(dx - v\,dt) \tag{4.52}$$

we obtain

$$p_x' = \frac{1}{\sqrt{1-v^2/c^2}}\left(\frac{m_0\,dx}{\sqrt{1-u^2/c^2}\,dt} - v\frac{m_0}{\sqrt{1-u^2/c^2}}\right) \tag{4.53}$$

In terms of p_x and the energy $E = m_0c^2/\sqrt{1-u^2c^2}$, this reduces to

$$p_x' = \frac{1}{\sqrt{1-v^2/c^2}}\left(p_x - \frac{vE}{c^2}\right) \tag{4.54}$$

Thus, p_x' depends on both the energy and momentum of the particle measured in the rest system R.

Lastly, to obtain the transformation for energy, we need the Lorentz transformation for the time interval dt':

$$dt' = \frac{1}{\sqrt{1-v^2/c^2}}\left(dt - \frac{v}{c^2}\,dx\right) \tag{4.55}$$

This combined with Equation (4.46) and the expression for energy in terms of rest mass, $E' = m_0c^2/\sqrt{1 - u'^2/c^2}$, gives us

$$\frac{E'}{c^2} = \frac{m_0}{\sqrt{1 - u'^2/c^2}}\frac{dt'}{dt'}$$

$$= \frac{1}{\sqrt{1 - v^2/c^2}}\left(\frac{m_0}{\sqrt{1 - u^2/c^2}} - \frac{v}{c^2}\frac{1}{\sqrt{1 - u^2/c^2}}\frac{dx}{dt}\right) \qquad (4.56)$$

In terms of E/c^2 and p_x, this reduces to

$$\frac{E'}{c^2} = \frac{1}{\sqrt{1 - v^2/c^2}}\left(\frac{E}{c^2} - \frac{v}{c^2}p_x\right) \qquad (4.57)$$

To summarize, we have used the definitions of energy and momentum of a particle, and the invariance relation $dt\sqrt{1 - u^2/c^2} = dt'\sqrt{1 - u'^2/c^2}$, together with the Lorentz transformations, to derive the transformation formulas for energy and momentum of a particle as measured by observers moving with relative speed v. There is a complete analogy between the Lorentz transformations of (x, y, z, t) and the transformations of $(p_x, p_y, p_z, E/c^2)$. The transformations are:

(1) $x' = \dfrac{1}{\sqrt{1 - v^2/c^2}}(x - vt);$ $\qquad p_x' = \dfrac{1}{\sqrt{1 - v^2/c^2}}\left(p_x - v\dfrac{E}{c^2}\right)$

(2) $y' = y;$ $\qquad PC = p_y$

(3) $z' = z;$ $\qquad p_z' = p_z$

(4) $t' = \dfrac{1}{\sqrt{1 - v^2/c^2}}\left(t - \dfrac{v}{c^2}x\right);$ $\qquad \dfrac{E'}{c^2} = \dfrac{1}{\sqrt{1 - v^2/c^2}}\left(\dfrac{E}{c^2} - \dfrac{v}{c^2}p_x\right)$

(4.58)

Just as the quantity $c^2t^2 - x^2 - y^2 - z^2$ is an invariant (it is the equation of a spherical light wave if set equal to zero), so is the quantity

$$c^2\left(\frac{E}{c^2}\right)^2 - p_x^2 - p_y^2 - p_z^2$$

a relativistic invariant as may be seen by finding $c^2(E'/c^2)^2 - p_x'^2 - p_y'^2$ $p_z'^2$ using Equations (4.58—1,2,3,4). The invariant may be evaluated in the rest frame of the particle where p = 0 and $E = m_0c^2$. This gives again the energy-momentum relation for particles of rest mass m_0:

$$E^2 = p^2c^2 + m_0^2c^4 \qquad (4.59)$$

or, for zero rest mass, $E = pc$.

As an example of the application of these energy-momentum formulae.. suppose a particle of rest mass m_0 has a speed of magnitude v in the negative x direction, relative to R. Its energy in terms of m_0 and v, relative to G, is then given by Equation (4.28):

$$E' = \frac{c^2}{\sqrt{1 - v^2/c^2}}\left[\frac{m_0}{\sqrt{1 - v^2/c^2}} - \frac{v}{c^2}\left(- \frac{m_0 v}{\sqrt{1 - v^2/c^2}}\right)\right]$$

$$= m_0 c^2 \left(\frac{1 + v^2/c^2}{1 - v^2/c^2}\right) \qquad \textbf{(4.60)}$$

4.14 TRANSFORMATIONS FOR FREQUENCY AND WAVELENGTH

The reader is probably familiar with the decrease in apparent frequency of a sound wave as a moving source approaches and then recedes. This phenomenon, known as the Döppler effect, also occurs when one observes the frequency of a moving light source. We shall obtain the relativistic transformations relating the frequencies and wavelengths of a light wave as measured by two observers, G. and R., as G moves relative to R with a speed v along their mutually parallel x', x axes. These transformations will provide a means of (comparing with energy momentum transformations to see if the quantum relation, $E = h\nu$, is form-invariant under Lorentz transformations.

We imagine that observers G. and R., situated at their respective origins, measure the frequency of a light wave with plane wave fronts by counting the number of fronts which pass their origins in some specified time interval. Let the observed directions of propagation be denoted by angles θ' (in G) and θ (in R), with respect to the positive x' (in G), x (in R) axes. The situation is diagrammed in Figure 4.9. In relating the frequencies ν' (in G) and ν (in R) of the wave, we

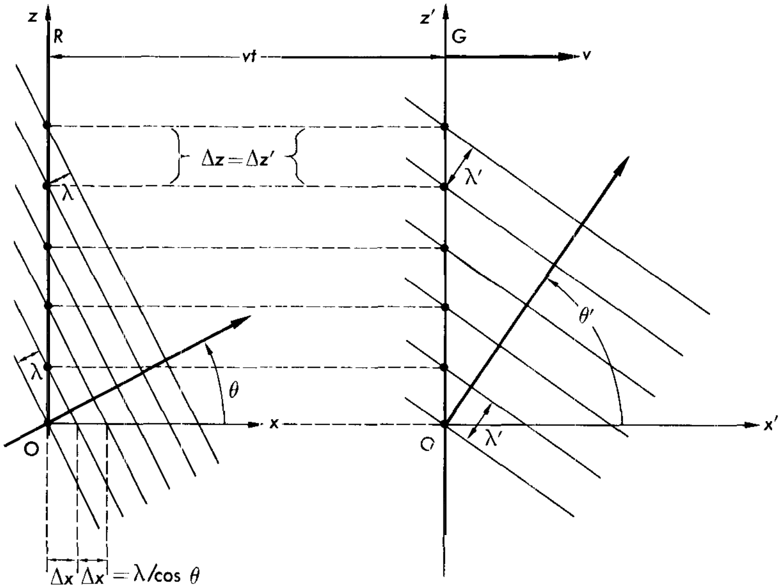


Figure 4.9. Measurement of frequency of a light wave by observers in relative motion.

must take into account two effects: First, the clock at the origin of G beats slower than the clocks in R, and second, the origin of G is moving with respect to that of R so that at any given instant there may be wave fronts which have passed R, but have not yet reached G.

Suppose that starting at the instant $t = t' = 0$ when the origins coincide, G. counts wave fronts for a time t', and that their observed frequency is ν'; the number of fronts which he counts is then $t'\nu'$. Similarly, beginning at the same instant, let R. count wavefronts passing 0: he will obtain $t\nu$. But $t\nu$ is not equal to $t'\nu'$, since there are fronts between the two origins which, in Figure 4.9, have been counted by R. but not by G. The number of these fronts lying between 0 and 0' may be found by dividing the distance between origins, vt, by the horizontal distance Δx between fronts. From Figure 4.9, $\Delta x = \lambda/\cos\theta = c/\nu\cos\theta$, so the additional number of fronts measured by R. is $vt/\Delta x = \nu vt\cos\theta/c$. Therefore,

$$t\nu = t'\nu' + \nu vt\frac{\cos\theta}{c} \qquad (41.61)$$

Solving for $t'\nu'$, we obtain

$$t'\nu' = \left(1 - \frac{v}{c}\cos\theta\right)t\nu \qquad (4.62)$$

If t were equal to t', this would be identical to the Doppler effect in sound for an observer moving relative to a source. In this expression, t refers to a time measured in the rest frame R, both on a clock at 0 and on one at 0'; at the same instant, t' (on a single clock at 0') is measured in the moving frame G. Hence, t and t' are related by the simple time dilation formula, $t' = t\sqrt{1 - v^2/c^2}$. So, substituting for t in the above equation and canceling t', we obtain

$$\nu' = \frac{\nu(1 - v/c\cos\theta)}{\sqrt{1 - v^2/c^2}} \qquad (4.63)$$

From this we may also obtain the transformation formula for wavelengths, since $\nu'\lambda' = \nu\lambda = c$:

$$\lambda' = \frac{\lambda\sqrt{1 - v^2/c^2}}{(1 - v/c\cos\theta)} \qquad (4.64)$$

The relation between the angles of propagation θ' and θ may be obtained by noting that, since measurements of distance along the z, z' axes are related by $z' = z$, the two observers agree that the distances between two successive points where the wavefronts intersect the z or z' axes are equal: $\Delta z' = \Delta z$. But from Figure 4.9,

$$\lambda' = \Delta z'\sin\theta', \quad \lambda = \Delta z\sin\theta \qquad (4.65)$$

Hence,

$$\frac{\lambda'}{\sin\theta'} = \frac{\lambda}{\sin\theta} \qquad (4.66)$$

and from Equation (4.64),

$$\sin \theta' = \frac{\sin \theta \sqrt{1 - v^2/c^2}}{(1 - v/c \cos \theta)} \tag{4.67}$$

The cosine of the angle θ' may be obtained by simplifying the trigonometric formula:

$$\cos 6' = \sqrt{1 - \sin' \theta'} = \sqrt{\frac{(1 - v/c \cos \theta)^2 - \sin^2 \theta (1 - v^2/c^2)}{(1 - v/c \cos \theta)^2}}$$

$$= \sqrt{\frac{\cos^2 \theta - 2v/c \cos \theta + v^2/c^2}{(1 - v/c \cos \theta)^2}} = \frac{\cos \theta - v/c}{1 - v/c \cos \theta} \tag{4.68}$$

where the positive sign of the square root was chosen in order that $\cos \theta' = \cos \theta$ in the special case $v = 0$, when the observers are not in relative motion

The relativistic transformation Equations (4.63), (4.64), (4.67) and (4.68) are the principal results of this section; we shall now discuss a few applications.

.15 TRANSVERSE DÖPPLER EFFECT

Suppose that to an observer in the rest system *R*, the direction of propagation is perpendicular, or transverse. to the direction of motion of G. Then 6' = 90°, and Equation (4.63) becomes

$$\nu' = \frac{\nu}{\sqrt{1 - v^2/c^2}} \tag{4.69}$$

This change in frequency is simple to understand solely as the result of the time dilation effect. Since R. sees the waves propagating parallel to his z axis, each wave that passes 0 will simultaneously (to R.) pass 0' (see Figure 4.10). Thus, both observers agree on the number of wavefronts they have counted, but G.'s clocks beat more slowly, so the frequency of the waves will appear higher to G., in order that equal numbers of wavefronts be counted by both observers.

Suppose G. carries along a source of light which emits plane waves of natural frequency $\nu' = \nu_0$. If R. then observes the light transversely, at 90" from the direction of motion, the frequency will be given by

$$\nu = \nu_0 \sqrt{1 - \frac{v^2}{c^2}} \tag{41.70}$$

and since Xv = c, the wavelength will be

$$\lambda = \frac{\lambda_0}{\sqrt{1 - v^2/c^2}} \tag{4.71}$$

Thus the wavelength will appear to be increased, or red-shifted. The transverse Döppler effect could be used to obtain a direct experimental verification of the time dilation predicted by special relativity; however, such experiments are

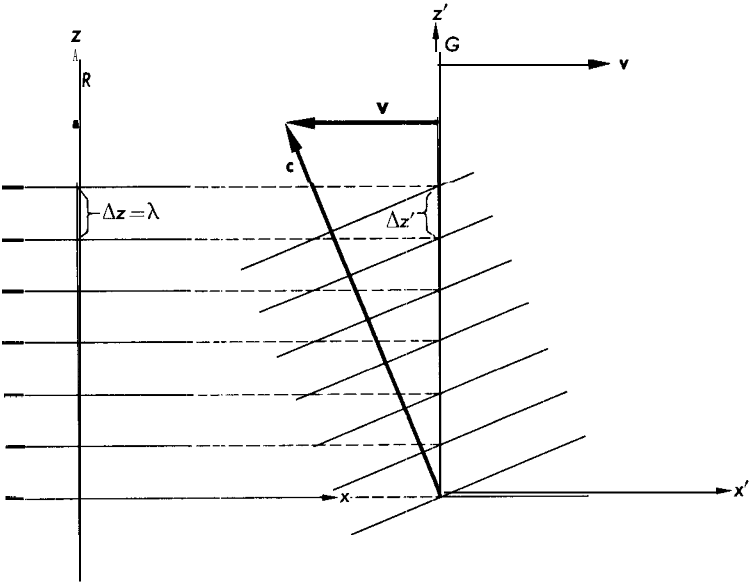


Figure 4.10. Transverse Doppler effect

difficult, because it is hard to arrange matters so that an appreciable amount of light of known proper frequency ν_0 comes in at exactly 90". Errors in angle will yield corrections of order v/c, whereas the transverse effect is of order $(v/c)^2$.

4.16 LONGITUDINAL DÖPPLER EFFECT

In the longitudinal Doppler effect, the observed light is traveling parallel to the direction of relative motion of the source. In this case, $\theta = 0$ or π. Suppose again that G. carries along a light source of frequency ν_0 and that $\theta' = 0$. The diagram, Figure 4.9, is drawn so that the light is propagating to the right ($\theta = 0$) in R, and hence we must imagine the source to be positioned far out on the negative x' axis and approaching the observer R. Therefore, substituting 6' = 0 in Equation (4.63), we obtain the expression for the frequency ν observed by R.:

$$\nu_0 = \frac{\nu(1 - v/c)}{\sqrt{1 - v^2/c^2}} \tag{4.72}$$

Or, since the factor $(1 - v/c)/\sqrt{1 - v^2/c^2}$ can be simplified by writing it as

$$\frac{1 - v/c}{\sqrt{1 - v^2/c^2}} = \sqrt{\frac{(1 - v/c)(1 - v/c)}{(1 - v/c)(1 + v/c)}} = \sqrt{\frac{1 - v/c}{1 + v/c}} \tag{4.73}$$

we have

$$\nu = \nu_0\sqrt{\frac{1 + v/c}{1 - v/c}} \tag{4.74}$$

for an approaching source of proper frequency ν_0. Since Xv = c, the corresponding expression for wavelength is

$$\lambda = \lambda_0\sqrt{\frac{1 - v/c}{1 + v/c}} \tag{4.75}$$

If the source is receding, we have instead, by reversing the sign of v (or changing θ from 0 to a),

$$\nu = \nu_0\sqrt{\frac{1 - v/c}{1 + v/c}}, \quad \lambda = \lambda_0\sqrt{\frac{1 + v/c}{1 - v/c}} \tag{4.715}$$

This indicates that for a receding source, the apparent wavelength is redshifted.

If a source of natural wavelength 5000 Angstroms is moving with velocity v = $4c/5$ directly toward the observer, the observed wavelength would be blueshifted and Equation (4.75) would apply. The observed wavelength would be

$$\lambda = (5000\ \text{Å})\,\text{If----}\,\frac{1 - 0.8}{1 + 0.8} = \frac{5000\ \text{Å}}{3} = 1667\ \text{A}$$

The longitudinal Doppler effect can be used to interpret the spectra of light received from distant galaxies. Bright spectral lines from these galaxies are identified by comparison with spectra of the elements, produced on earth. The identification shows the lines are systematically redshifted. For nearby galaxies whose distances can be measured by observing cepheid variable stars, the fractional redshift $\Delta\lambda/\lambda$ is directly proportional to the distance. This is expressed in Hubble's relation,

$$c\frac{\Delta\lambda}{\lambda} = Hr \tag{4.77}$$

where H, Hubble's (constant, is approximately 75 km/sec per 10^6 parsecs. (1 parsec = 3.26 light-years.)

TABLE 4.3 Redshifts of Some Quasi-Stellar Objects (Quasars, by Kohn and Palmer, Harvard Univ. Press, 19'67).

Catalogue Number	Redshift $z = \Delta\lambda/\lambda$	Recession velocity, $\beta = v/c$
3c 2738	0.158	0.146
3c 249.1	0.311	0.264
3c 345	0.595	0.436
3c 48	0.367	0.303
3c 279	0.536	0.405
1116+12	2.1 la	0.813
PHL 256	0.131	0.122
PHL 938	1.93	0.791
BSO 1	1.24	0.668

Recent observations of quasars, for which no independent distance measurements are available, have revealed enormous redshifts, indicating that the objects from which this light was emitted may be receding from our galaxy at speeds of over 80% of the speed of light. Some of these recent observations are given in Table 4.3. The redshifts, if interpreted as Döppler shifts, imply that the entire visible universe is expanding and hence that at some distant time in the past all the matter in the universe must have been concentrated in one region. The galactic redshifts are the primary experimental evidence on which the big bang theory of the origin of the universe is based.

summary

TRANSFORMATIONS OF ENERGY AND MOMENTUM

The transformation formulae for energy and momentum of a particle E', p' as observed from a system of reference moving with speed v along the x, x' axes relative to an observer who measures the values E, p for the same particle, are given by

$$p'_x = \frac{1}{\sqrt{1 - v^2/c^2}}\left(p_x - v\frac{E}{c^2}\right) \qquad p'_y = p_y$$

$$\frac{E'}{c^2} = \frac{1}{\sqrt{1 - v^2/c^2}}\left(\frac{E}{c^2} - \frac{v}{c^2}p_x\right) \qquad p'_z = p_z$$

The four quantities p_x, p_y, p_z, E/c^2, are thus analogous to x, y, z and t.

TRANSFORMATIONS FOR FREQUENCY AND WAVELENGTH

The transformation formulae for frequency ν', wavelength λ' and angle of propagation 19' of a light wave, observed from a system of reference moving with speed v along the x,x' axes, relative to an observer who measures the values ν, λ, and θ for the same wave, are

$$\nu' = \frac{\nu(1 - v/c \cos\theta)}{\sqrt{1 - v^2/c^2}}$$

$$\lambda' = \frac{\lambda\sqrt{1 - v^2/c^2}}{(1 - v/c \cos\theta)}$$

$$\cos\theta' = \frac{(\cos\theta - v/c)}{(1 - v/c \cos\theta)}$$

$$\sin\theta' = \frac{\sin\theta\sqrt{1 - v^2/c^2}}{(1 - v/c \cos\theta)}$$

Since $E = h\nu$ and $p = h/\lambda$ for light, these are identical to the transformation equations for energy and momentum of a particle of zero rest mass.

DÖPPLER EFFECT

A light source of natural frequency ν_0 (wavelength λ_0) will have its frequency shifted when measured by an observer moving with respect to the source. If the light is observed at 90° from the direction of motion of the source, then the frequency is redshifted due to time dilation:

$$\nu = \nu_0 \sqrt{1 - \frac{v^2}{c^2}} \qquad \lambda = \frac{\lambda_0}{\sqrt{1 - v^2/c^2}}$$

If the source is receding from the observer with speed v and the light is observed parallel to v, then

$$\nu = \nu_0 \sqrt{\frac{1 - v/c}{1 + v/c}} \qquad \lambda = \lambda_0 \sqrt{\frac{1 + v/c}{1 - v/c}}$$

For an approaching source, the sign of v is reversed.

problems

1. Suppose a particle with rest mass m_0 is initially at rest at $x = 0$. If it is acted on by a constant force F in the x direction, find x as a function of time. Check to see if this gives the same as the nonrelativistic equations given for small velocity, i.e. small time. Also show that the speed approaches c as t approaches infinity
   Answer: $x = (c^2 m_0/F)[\sqrt{1 + (Ft/m_0 c)^2} - 1]$.
2. Suppose a force F acts on a particle in the same direction as the velocity. Show that the power expended by the force is $m_0 v(dv/dt)/(1 - v^2/c^2)^{3/2}$, and hence show that the energy of the particle is mc^2.
3. Show that $dE/dp = v$, the speed of the particle.
4. An electron of mass $m_0 = 9.1 \times 10^{-31}$ kg and a proton of mass $M_0 = 1.67 \times 10^{-27}$ kg are each accelerated from rest through a total potential energy difference of 1.6×10^{-11} J. What is the increase in mass of each particle? What is the fractional increase in mass of each particle? What is the final speed of each?
   Answer: 1.78×10^{-28} kg; 1.78×10^{-28} kg; $196\, m_0$; $0.107\, M_0$; $0.999987c$; 0.43 c.
5. Suppose 1.00 cubic kilometer of water at 0°C were changed to ice by extracting heat. How much would the mass change? (Heat of fusion = 80 kcal/kg = 3.35×10^5 J/kg.)
   Answer: 3.73 kg.
6. The energy radiated from the sun in the form of neutrinos has the intensity 0.12 J/cm²/min at the earth's surface. The earth-sun distance is 1.5×10^8 km and the sun's mass is 2.0×10^{30} kg. Calculate the fractional loss in mass from the sun in 10^{10} years (age of the universe), from the radiation of neutrinos.
   Answer: 9.9×10^{-6}.
7. An oil-powered ship obtains energy at the rate of 4 x 10” cal/lb from its fuel. A

nuclear-powered ship obtains energy by converting about 0.0003% of its fuel from moss to energy. For o given moss of fuel, calculate the ratio of the distances the two ships should be able to travel.

Answer: Nuclear-powered ship travels 7,320 times as far.

8. In a certain kind of instrument used for focusing o beam of high energy particles onto o point, the maximum kinetic energy for which the instrument works is $T = 1.22$ times the rest energy. 'What speed do particles of this kinetic energy have?

Answer: 2.68×10^8 m/sec.

9. Show that in terms of the kinetic energy, T, the magnitude of the momentum is $pc = \sqrt{T^2 + 2Tm_0c^2}$, where m_0 is the rest mass.

10. Find the correction terms of order v^4/c^4 to the kinetic energy expression ½ m_0v^2 in the correspondence limit.

Answer: ⅜ $m_0c^2\,(v^4/c^4)$.

11. If o particle has a momentum of 5.60×10^{-19} kg-m/sec and a kinetic energy of 7.52×10^{-11} j, find its speed. Find its rest mass in kg.

Answer: 2.24×10^8 m/sec; 1.67×10^{-27} kg.

12. An electron has a kinetic energy of 1.6×10^{-13} j, and is incident on a proton at rest in the laboratory. The center of momentum frame, an inertial frame in which the total momentum of both particles is zero, is moving with what speed relative to the laboratory? The rest moss of the electron is 9.11×10^{-31} kg, and that of the (proton is 1.67×10^{-27} kg.

Answer: 4.54×10^5 m/sec.

13. Using the equations for transformation of velocity components, show that when $E^2 = p^2c^2 + m_0^2c^4$, for on inertial system in which p has the components p_x, p_y, p_z and the energy is E, then in another system moving at velocity **v** in the positive x direction relative to the first, the momentum and energy are $p_x' = (p_x - vE/c^2)/\sqrt{1 - v^2/c^2}$, $p_y' = p_y$, $p_z' = p_z$, and $E' = (E \quad vp_x)/\sqrt{1 \quad v^2/c^2}$. Note the similarity to the x, y, z, t transformations.

14. Using the Lorentz transformations for coordinates, show that

$$d\tau = \sqrt{dt^2 - (dx^2 + dy^2 + dz^2)/c^2} = dt\sqrt{1 - v^2/c^2}$$

is *invariant* under *Lorentz* transformations. Here dx, dy, dz ore infinitesimal displacements of a particle and v is the speed of an inertial system relative to the rest frame of the particle. Show that the momentum and $E/c = \sqrt{p^2 + m_0^2c^2}$ are given by $\mathbf{p} = m_0\,d\mathbf{r}/d\tau$, $E/c = m_0(c\,dt)/d\tau$. Thus, since $d\tau$ is an invariant, the momentum and E/c transform like **r** and ct. This is an olternate way of working Problem 13.

15. Suppose a particle of rest moss m_0, moving in the positive x direction, has o total energy (rest plus kinetic) of E_1 It hits o similar particle (rest moss m_0), which is at rest. Express the total momentum p_x ond the total energy of the two particles in terms of E_1 and m_0c^2. Using the results of Problem 13, find, in terms of E_1 and m_0c^2, the speed v of the system in which the momentum is zero, i.e. $p_x' =$ ʋ. 'Aiso 'tin'c E' in terms of E_1, m_0c^2, and v. Eliminate v to show that $E' = \sqrt{2(E_1 + m_0c^2)(m_0c^2)}$. This total energy in the center of momentum system is important in studying nuclear reactions.

Answer: $\sqrt{(E_1/c)^2 - m_0^2c^2}$; $E_1 + m_0c^2$; $v = c\sqrt{E_T^2 \quad m_0^2c^4}/(E_1 + m_0c^2)$.

In the following collision problems, use the facts that total energy and total momentum are conserved. By squaring the energy equation twice, quantities like $\sqrt{p^2 + m_0c^2}$ con be eliminated. An alternative procedure would be to tronsform to the center of momentum system as indicated in Problem 15. The solution is much simpler in that system.

16. A particle with speed v hits another at rest. If both have rest mass m_0, and the final velocities are along the same straight line, what are the final velocities?

Answer: 0; v.

17. A particle with momentum p and rest mass m_1 hits another at rest with mass m_2. If the final velocities are along the same straight line, what are the final momenta'?

Answer: $$2pm_2\left(\frac{m_2+\sqrt{(p/c)^2+m_1^2}}{m_1^2+m_2^2+2m_2\sqrt{(p/c)^2+m_1^2}}\right);$$

$$p\,\frac{m_1^2-m_2^2}{m_1^2+m_2^2+2m_2\sqrt{(p/c)^2+m_1^2}}$$

18. Two particles have momenta p and $-\mathbf{p}$. They collide elastically. What are the magnitudes of the final momenta, and what is the angle between them?

Answer: p, p, 180" (this is the center of momentum frame for these particles).

19. Two particles of rest masses m_1 and m_2 have momenta p_1 and p_2, respectively. If the final velocities after an elastic collision are along the same straight line, what is the final momentum of particle 1?

Answer:

$$p_1' = \frac{p_1(m_1^2-m_2^2)c^2 + 2p_2\left(-p_1p_2 + m_1^2c^2 + \sqrt{p_1^2+m_1^2c^2}\sqrt{p_2^2+m_2^2c^2}\right)}{m_1^2c^2 + m_2^2c^2 - 2p_1p_2 + 2\sqrt{p_1^2+m_1^2c^2}\sqrt{p_2^2+m_2^2c^2}}.$$

20. Two particles with rest masses m_1 and m_2 have momenta p_1 and p_2, respectively, along the same straight line. What is the final speed of the combination if they stick together on collision? What is the rest mass of the combination? (It is not $m_1 + m_2$.)

Answer: $c(p_1+p_2)/\left(\sqrt{p_1^2+m_1^2c^2}+\sqrt{p_2^2+m_2^2c^2}\right)$;

$$\sqrt{m_1^2+m_2^2-2\left(p_1p_2-\sqrt{p_1^2+m_1^2c^2}\sqrt{p_2^2+m_2^2c^2}\right)/c^2}.$$

21. Two particles of the same rest mass, m_0, collide elastically. One particle was initially at rest, and the other had momentum p. If the final velocities are the same in magnitude, what is the angle between these velocities? Nonrelativistically, this would be 90".

Answer: $$\theta = \cos^{-1}\left(\frac{\sqrt{p^2+m_0^2c^2}-m_0c}{\sqrt{p^2+m_0^2c^2}+3m_0c}\right).$$

22. In Figure 4.11 is given another bubble chamber photograph of the production and decay of a Λ^0 hyperon. Using the method illustrated in the text, find the rest mass of the Λ^0 from this photograph.

23. Verify that light moving parallel to the y axis in one inertial system goes at the angle

$$\tan^{-1}\left(\frac{v}{\sqrt{c^2-v^2}}\right)$$

relative to the y' axis in a system moving with velocity $\mathbf{v}$ along the x axis relative to the first system. In the first system, $E_y = E_z = B_y = B_x = 0$, $B_z = E_x/c \neq 0$. The transformation of the field components perpendicular to $\mathbf{v}$ is:

$$\mathbf{E}'_\perp = \frac{(\mathbf{E}_\perp + \mathbf{v}\times\mathbf{B})}{\sqrt{1-v^2/c^2}},\quad \mathbf{B}'_\perp = \frac{(\mathbf{B}_\perp - \mathbf{v}\times\mathbf{E}/c^2)}{\sqrt{1-v^2/c^2}}$$

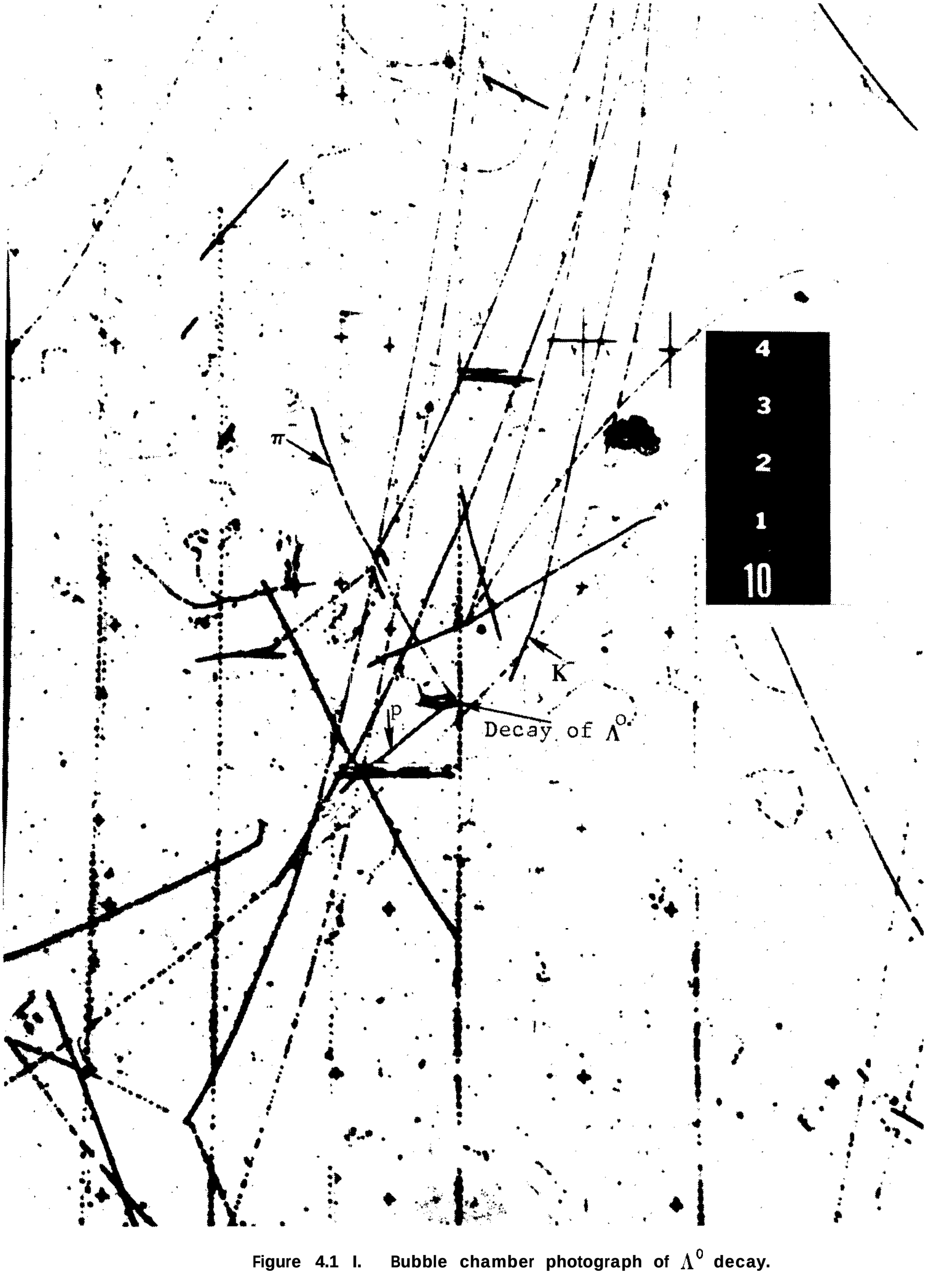


Figure 4.1 I. Bubble chamber photograph of Λ^0 decay.

Find what the transformation of the E components parallel to **v** must be for the light wave to be transverse in the second system. If $E_y = E_x = B_y = B_z = 0$, $B_x = E_z/c \neq 0$, find how the **B** component parallel to **v** transforms.

Answer: $E'_\parallel = E_\parallel$, $B'_\parallel = B_\parallel$.

24. A light source emits light in its rest system of 4000 Angstroms wavelength at the violet end of the visible spectrum. If in a second system the light goes perpendicular to the relative velocity and has a wavelength of 7000 Angstroms at the red end of the visible spectrum, what is the relative velocity?

Answer: 2.46×10^8 m/sec.

25. Due to the sun's rotation, a point at the surface of the sun on its equator has a speed relative to the center of 1.85 km/sec. If an atom at rest emits light of wavelength 5400 Angstroms, what is the wavelength difference for this light emitted from opposite edges of the sun's equator as seen from the earth?

Answer: 0.0666 Angstrom.

26. light at the natural wavelength 6328 Angstroms is emitted from a source which is approaching at 0.45 the speed of light. Calculate the observed wavelength and frequency. If the light source were receding, what would be the observed energy of single photons received from the source?

Answer: $\lambda = 3897$ Angstroms; $\nu = 7.70 \times 10^{14}$ sec^{-1}; 1.93×10^{-19} j = 1.21 eV

27. Light of wavelength 5000 Angstroms from a flashlight you hold hits a mirror moving away from you at 0.8c. What is the frequency of the light reflected back to you?

Answer: 6.67×10^{13} sec^{-1}

28. The phase of a plane sinusoidal wave, $k_x x + k_y y + k_z z - \omega t$ with $c = \omega/k = \omega/\sqrt{k_x^2 + k_y^2 + k_z^2}$, is invariant under a Lorentz transformation. A wavecrest in one system must look like a wavecrest in another system. Show that this is so if $k_x, k_y, k_z, \omega/c$ transform under a Lorentz transformation just as x, y, z, ct do. Since $k = 2\pi/\lambda$, the magnitude of the momentum of a photon is $kh/2\pi$, and likewise the energy is $h\nu = \omega h/2\pi$. Verify that these are consistent with the transformation equations for momentum and energy.

29. Consider two twins R. and G., and let G. travel with speed v out towards a distant light *source*, for a total distance L as observed by R. G. then returns along the same path to his starting point with speed v. Suppose both G. and R. observe light of a definite frequency coming from the distance source. Use the equations of the longitudinal Döppler effect, and the fact that at the end of the trip both G. and R. will have counted the same total number of wavecrests, to show that the travelling twin is younger by the factor $\sqrt{1 - v^2/c^2}$.

5 quantum properties of light

The classical electrodynamics of Faraday, Ampere and Maxwell-as expressed in Maxwell's equations--was successful in predicting the existence of electromagnetic oscillations, and led to many useful applications, culminating in the invention of radio in 1896. By the early part of the twentieth century, however, other electromagnetic phenomena had been discovered, which could not be adequately explained by the classical theory. Among the most significant of these phenomena were the emission of electrons from a metal surface when irradiated by light (photoelectric effect), the change of wavelength of light scattered by free electrons (the Compton effect), the discreteness of optical spectra emitted by hot gases, and the energy distribution with frequency of radiation emitted by hot bodies.

An important prediction of the classical theory was that an accelerated charge should always emit radiation. If an atom is pictured as a heavy positively charged core with an electron revolving in some orbit about the core, then the electron should emit energy because it is continually being accelerated toward the core by the Coulomb attraction. This energy loss should cause the electron to spiral in toward the core and eventually collide with it in about 10^{-10} seconds. Thus this classical model contradicted the fact that an atom can be a stable physical system. Further, the theory predicted that all frequencies should be present in the emitted radiation, corresponding to the fact that all rotation frequencies are possible in the classical orbits. This is in contrast to the observed fact that often a hot gas emits light only at a discrete set of frequencies.

Another important consequence of the classical theory was that the intensity of energy transported by a light wave through free space is proportional to the square of the amplitude of the oscillating electric (or magnetic) field. Also, these electric and magnetic field amplitudes could have continuous arbitrary numerical values, not dependent on the frequency. This led to serious difficulties in explaining the observed properties of the electromagnetic radiation contained in a cavity inside a hot body. The classical theory of this "black-body" radiation assumed that the radiation inside a large cavity consisted of standing electromagnetic waves with a continuous distribution of energies. The resulting theoretical calculations gave a distribution of energy with frequency which disagreed with experiment, except at very low frequencies.

Max Planck was the first to give an acceptable quantitative explanation of black-body radiation. Instead of assuming that the distribution of energies of the standing waves is continuous, he assumed that the waves could have only discrete energies, differing in amount by integral multiples of $h\nu$, where ν is the frequency and h is a constant having the value 6.63 x 10^{-34} joules-seconds. The result of Planck's theoretical calculation agreed with experiment in all respects.

Thus, when electromagneti,: waves of frequency ν are emitted or absorbed1 by matter, the energy has to be emitted or absorbed in amounts $E = h\nu$. Since, when a particle is emitted or absorbed by matter, a definite discrete amount of energy is transferred, a light wave appears in this respect to act very much like a particle, when interacting with matter. When propagating from one point io another, however, it must still behave like a wave because it is capable of exhibiting interference and diffraction. The standing waves of frequency ν inside a cavity can be thought of as consisting of a number of quanta, or photons, each of energy $h\nu$. When energy $h\nu$ is emitted by one wall of the cavity, the number of photons of this frequency inside the cavity will increase by unity. Photons of many different frequencies can be present in the cavity. The subsequent absorption of energy $h\nu$ by another wall of the cavity can, in some respects,, be considered equivalent to the passage of a particle (a photon) from one wall to another. The reality of this particle-like picture of the states of the electromagnetic field has been verified in many experiments.

In this chapter we shall begin by examining, from the point of view of special relativity, the hypothesis that light waves are particles which carry energy in discrete amounts $E = h\nu$. If the relation $E = h\nu$ is to be a valid physical law, it follows from the first postulate of relativity that it must be valid in any inertial frame. The equations of relativity tell us how to relate space and time measurements, and hence also frequency, wavelength, energy, and momentum measurements, made by observers in relative motion. We may then apply the relativistic transformations to the Planck relation E = hu, to see if it is form-invariant with respect to Lorentz transformations.

5.1 ENERGY TRANSFORMATION FOR PARTICLES OF ZERO REST MASS

In the previous chapter, transformation equations for energy and momentum of particles were obtained. We now wish to investigate the possibility that, according to Planck's hypothesis, a light wave can be considered to act like a particle which, because the particle has speed c, must have zero rest mass. This may be seen from the comparison of the two alternate expressions for energy

$$E = \sqrt{(pc)^2 + (m_0c^2)^2} = \frac{m_0c^2}{\sqrt{1 - v^2/c^2}} \tag{5.1}$$

In order that the energy and rnomentum be non-vanishing for $m_0 = 0$, we must have $v = c$, in which case the latter expression becomes indeterminate:

$$E = \frac{m_0 c^2}{\sqrt{1 - v^2/c^2}} = \frac{\text{zero}}{\text{zero}} \tag{5.2}$$

But then the former expression reduces to simply $E = pc$.

The relation $E = pc$ is entirely consistent with the classical electromagnetic theory of a plane electromagnetic wave, where

$$(\text{Energy density}) = c \times (\text{Momentum density}) \tag{5.3}$$

or, in a given volume, $E = pc$ for electromagnetic waves.

Since for zero rest moss particles we have $E = pc$, then $p_x = p \cos\theta = E\cos\theta/c$, where θ is the direction of travel of the particle with respect to the x axis in R. Also, in the G coordinate system, $p_x' = E'\cos\theta'/c$. Substituting into the transformation equation (Equation 4.57), we get

$$\frac{E'}{c^2} = \frac{(E/c^2)(1 - v/c\cos\theta)}{\sqrt{1 - v^2/c^2}} \tag{5.4}$$

Note the similarity to the transformation equation for frequency,

$$\nu' = \frac{\nu(1 - v/c\cos\theta)}{\sqrt{1 - v^2/c^2}} \tag{5.5}$$

5.2 FORM-INVARIANCE OF $E = h\nu$

In fact, it is at once clear that if Planck's equation $E = h\nu$ for a single photon is valid in the system R, then upon using the transformations (5.4) and (5.5), the corresponding relation in the G system must be $E' = h\nu'$. The Planck equation is thus relativistically invariant, provided the constant h has the same numerical value in all inertial frames.

Furthermore, if the energy is a function only of frequency, the relation $E = h\nu$ is the only possible relation between energy and frequency which is relativistically invariant. Suppose, for example, that Planck had proposed $E = h\nu^n$, where n is some exponent not equal to unity. This relation would not be relativisticolly form-invariant, and therefore could not be a valid physical law, as it leads to the relation

$$E' = h\,(\nu')^n\left(\frac{1 - v/c\cos\theta}{\sqrt{1 - v^2/c^2}}\right)^{n-1} \tag{5.6}$$

in the other reference frame. Thus, it is a remarkable fact that the only possible relativistically invariant relation between energy and frequency is precisely the relation which enabled Planck to explain all the properties of black-body radiation. Further, if $E = h\nu$, there is a definite relation between momentum and wavelength, which can be derived by noting that $E = h\nu = pc$, and $\lambda\nu = c$. Solving for p in terms of the wavelength λ,

$$p = \frac{h\nu}{c} = \frac{h\nu}{\lambda\nu} = \frac{h}{\lambda} \tag{5.7}$$

Since this relation between momentum and wavelength is equivalent to $E = h\nu$, it is also form-invariant.

We may conclude that, if there exists a discrete energy related only to frequency for light,, which is considered to be a particle of zero rest mass, then to be relativistically invariant, the only possible relation is $E = h\nu$, where h is a universal constant. Also, the only possible relation between momentum and wavelength has to be $p = h\lambda$. Thus:

$$\boxed{E = h\nu = pc \qquad p = h/\lambda \quad \text{for photons}} \tag{5.8}$$

These relations for a single photon state the relationship of momentum and energy to wavelength and frequency under the assumption that light transports energy and momentum in discrete amounts. If there are n photons, the expressions for E and p should each be multiplied by n. Note that the expression for energy does not contain the amplitude of the electromagnetic field oscillations. On the other hand, in classical electromagnetic theory the **energy is proportional to the squared amplitude of the fields. Therefore, the physical meaning of the squared amplitwde will have to be reconsidered.**

The relations, Equation (5.8), are subject to verification by experiment. In the following sections, we shall consider experiments in which the quantization of energy carried by photons is important, and in which the value of h can be determined independently. The value of h obtained from black-body radiation experiments wash = 6.547 $\times 10^{-34}$ joules-seconds.

5.3 THE DUANE-HUNT LAW

One phenomennn which may be explained by using the quantum relation $E = h\nu$ **is the short-wavelength cutoff (high-frequency cutoff) of the continuous x-ray** spectrum. Figure 5.1 represents a typical x-ray tube, consisting mainly of a hot

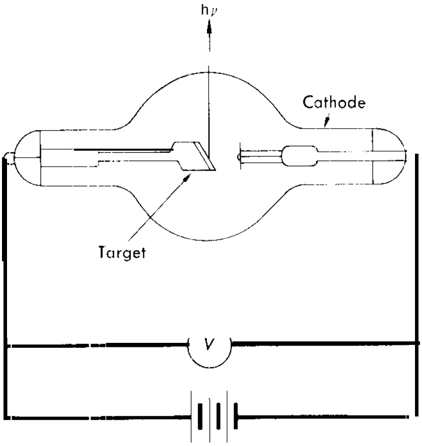


Figure 5.1. Production of x rays by stopping fast electrons in dense materials.

cathode which emits electrons, and a source of potential which can accelerate the electrons from the cathode up to many thousands of electron volts kinetic energy. The electrons then strike a dense target, usually made of tungsten or molybdenum, and are brought suddenly to rest, i.e. they are decelerated. According to classical theory, such a decelerated charge should emit radiation, and this is what is observed experimentally. If the accelerating potential V is upwards of 10,000 volts, then the frequencies of emitted radiation lie in the x-ray region.

Suppose $I(\lambda)d\lambda$ is the amount of energy emitted with wavelengths in the range from λ to $\lambda + d\lambda$. This intensity $I(\lambda)$ is a quantity which can be observed experimentally; a typical set of experimental results is given in Figure 5.2,

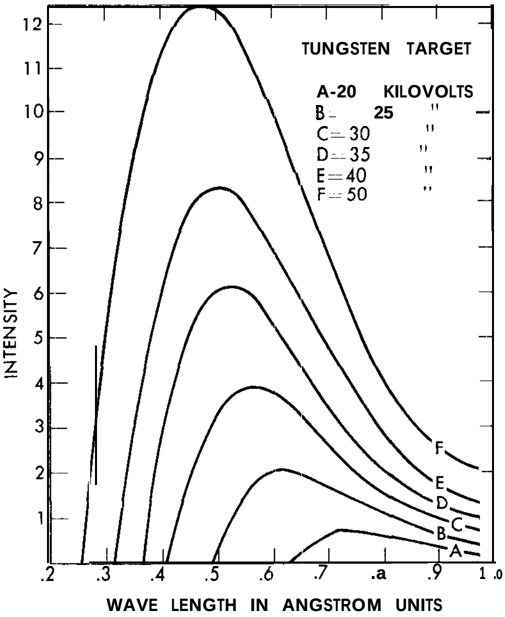


Figure 5.2. Intensity distribution of x rays produced at different accelerating voltages.

in which $I(\lambda)$ is plotted as a function of λ. Note that as the accelerating voltage V is increased, there is a general increase in the intensity of x rays produced, and also that there is for each V a minimum wavelength (or maximum frequency) emitted. This can be understood as follows: We assume that the x rays are radiated discontinuously in the form of quanta of energy $h\nu$ when the electron comes to a stop. Some electrons may emit many quanta, but it is possible that an electron is stopped so suddenly that all its kinetic energy goes into a single quantum of energy $h\nu_{max}$. This ν_{max} would be the maximum frequency of a quantum which could be (emitted. The electron is initially accelerated and is given kinetic energy by passage through a difference of potential V, so the kinetic energy it gains there will be $T = eV$. By conservation of energy, if in the collision all this is given to a single quantum of frequency ν_{max}, then

$$h\nu_{max} = eV \tag{5.9}$$

This equation is called the *Duane-Hunt law.* It can be checked against the experimental data given in Figure 5.2. From the graph, which is plotted in terms of wavelength, the minimum wavelengths can be read off for given accelerating Potential. In terms of ν_{max}, $\lambda_{min} = \frac{c}{\nu_{max}}$, so in terms of λ_{min} the constant h could be expressed as

$$h = \frac{eV\lambda_{min}}{c} \tag{5.10}$$

For example, at V = 40,000 volts, λ_{min} from the graph is 0.31 Angstroms. This gives, using $e = 1.6 \times 10^{-19}$ coul., a value for h: $h = 6.61 \times 10^{-34}$ i-sec. Similarly, other values for h can be obtained from the data of Figure 5.2. The results are given in Table 5.1; the values all agree reasonably well with each other and with the value of *h* determined from black-body radiation experiments.

TABLE 5.1 Duane-Hunt Law

V (volts)	λ_{min} (Angstroms)	$h = eV\lambda_{min}/c$
20,000	.62	6.61×10^{-34} j-sec.
25,000	.49	6.53×10^{-34} j-sec.
30,000	.405	6.48×10^{-34} j-sec.
35,000	.35	6.35×10^{-34} i-sec.
40,000	.31	6.61×10^{-34} i-sec.
50,000	.255	6.80×10^{-34} i-sec.
		6.56×10^{-34} j-sec. (average)

.4 PHOTOELECTRIC EFFECT

Historically the first application of Planck's equation $E = h\nu$ to another phenomenon was made by Einstein, when he showed how the photoelectric effect

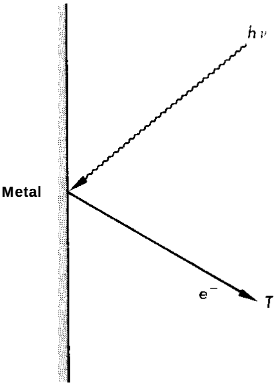


Figure 5.3. Photoelectric Effect: A single incident photon of energy $h\nu$ con cause on electron to be ejected from a metal surface if the frequency is sufficiently high.

may be explained. In the photoelectric effect, light is allowed to fall on a metal surface as illustrated in Figure 5.3, and electrons of various kinetic energies are then ejected from the surface due to absorption of light energy. One may measure the kinetic energies T of the ejected electrons, and the numbers of ejected electrons, as functions of both the frequency, and the intensity, of the incident light. Five important features of this effect could not be explained by the classical theory. We shall consider these features one by one, and show how they may be explained using $E = h\nu$ and the concept of the photon, or quantum of light.

5.4.1 Emission from a given surface does *not* occur unless the frequency of the *light is greater than* a certain *critical* frequency denoted *by* ν_c, *which* is independent *of the intensity of* the incident *light.*

That is, no matter how intense the light is, no electrons will come off unless the frequency exceeds ν_c. This is difficult to understand classically, because the more intense the light is, the more energy should be available to make the electrons come off.

Electrons are normally kept from flying off the surface of a metal by the Coulomb attractions between the electrons and the positive ions. It takes a certain amount of energy to overcome this attraction at room temperature, and from experiments on thermionic emission these energies can be measured. The minimum energy required to remove one electron is defined as the *work* function Φ of the metal. Typical values of the work function are given in Table 5.2. These work functions are typically of the order of a few electron volts. These are only the minimum energies required to remove an electron from a metallic surface. It might actually require more energy than $h\nu_c$ to remove an electron, because an electron far down inside the metal might have to collide with several obstacles, thus losing energy, before it could get out. Also, some electrons inside the metal have less kinetic energy than others to begin with.

TABLE 5.2 Work Functions for Some Typical Metals

Element	Work Function
Molybdenum	4.20 eV
Nickel	5.03 eV
Silver	4.73 eV
Tungsten	4.54 eV
Zinc	4.30 eV

Suppose an electron absorbs one photon, which gives it just enough energy to overcome the work function and escape. The energy of this photon is $E = h\nu$. In terms of Φ, $h\nu = \Phi$. If $h\nu$ *were* less than Φ, the electron could not escape. Therefore, there is a critical frequency, ν_c, determined by $\nu_c = \Phi/h$, such that for lesser frequencies, an electron cannot escape by absorbing a photon. For example, the critical frequency for Zinc is

$$\nu_c = \frac{\Phi}{h} = \frac{e \times 4.30\ \text{eV}}{h} = \frac{1.60 \times 10^{-19}\ \text{coul} \times 4.30\ \text{eV}}{6.63 \times 10^{-34}\ \text{j-sec}}$$

$$= 1.04 \times 10^{15}\ \text{sec}^{-1}$$

(Note that work functions in the table are given in units of electron volts.)

The incident light beam, at a frequency lower than the critical frequency, could be made more intense by increasing the number of quanta in the beam. So if n quanta per unit area per unit time fall on the metal, the intensity is given in terms of n and ν by $I = nh\nu$. Since the light is absorbed in quanta of amount $h\nu$, and not nhu, increasing the intensity of the beam will not cause electrons to come off in this case.

Suppose that we consider next the case of incident frequencies greater than the critical frequency. Then electrons can come off when quanta are absorbed. In general, the electrons will come off with a distribution of energies because of losses due to collisions inside the metal, and so forth. So we shall consider only those electrons coming off with maximum possible kinetic energies, T_{max}. The energy absorbed from the light, $h\nu$, goes into overcoming the work function and in giving kinetic energy to the electron. Thus, by conservation of energy,

$$h\nu = T_{max} + \Phi \tag{5.11}$$

This is known as the Einstein *photoelectric* equation.

ple If $\Phi = 2.04$ eV and visible light of wavelength $\lambda = 4000$ Angstroms is used, then the maximum kinetic energies are

$$T_{max} = h\nu - \Phi = \frac{hc}{\lambda} - \Phi$$

$$= \frac{(6.63 \times 10^{-34}\ \text{j-sec}) \times (3 \times 10^{8}\ m/\text{sec})}{(4 \times 10^{-7}\ \text{m}) \times (1.6 \times 10^{-19}\ \text{j/eV})} - 2.04\ \text{eV}$$

$$= 1.07\ \text{eV}$$

For such problems, since T_{max} is a few electron volts, while the rest energy of an electron is 510,000 eV, we can use the approximate nonrelativistic expression for kinetic energy, $T = \frac{1}{2} m_0 v^2$, to obtain the maximum electron velocity. Then the photoelectric equation can be written in the form:

$$T_{max} = \frac{1}{2} m_0 v_{max}^2 = h\nu - \Phi \tag{5.12}$$

.2 T_{max} does not depend on the *intensity* of the incident light.

Classically, it would seen that the more energy contained in the incident light, the more a particular electron could absorb. However, the photoelectric equation does not predict any dependence of T_{max} on the intensity, $I = nhu$.

5.4.3 T_{max} increases with increasing frequency of light.

This follows directly from the photoelectric equation. If T_{max} is measured1 and plotted as a function of frequency, the slope of the curve should be equal to h. The intercept on the frequency axis should be Φ/h. The energy T_{max} may be measured by placing an electrode near the metal surface and applying to it a negative potential, -V, with respect to the metal. This is illustrated in Figure 5.4.

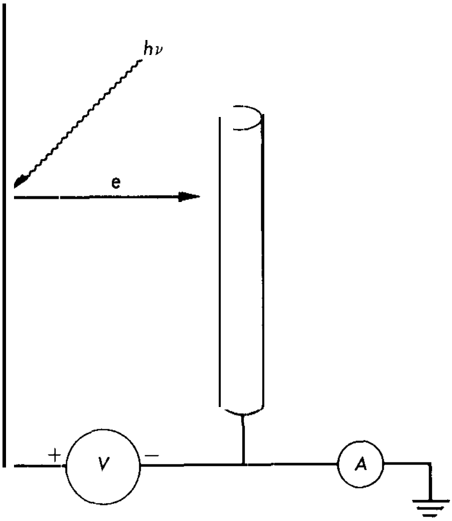


Figure 5.4. Rough diagram of apparatus for measurement of h/e.

This stopping potential V is increased until no current is collected by the electrode, that is, until V is just large enough to turn back electrons with the energy T_{max}. Then the change in potential energy as the electron travels from the metal surface to the electrode is just eV, and is equal to T_{max}. So $eV = h\nu - \Phi$, and if V is

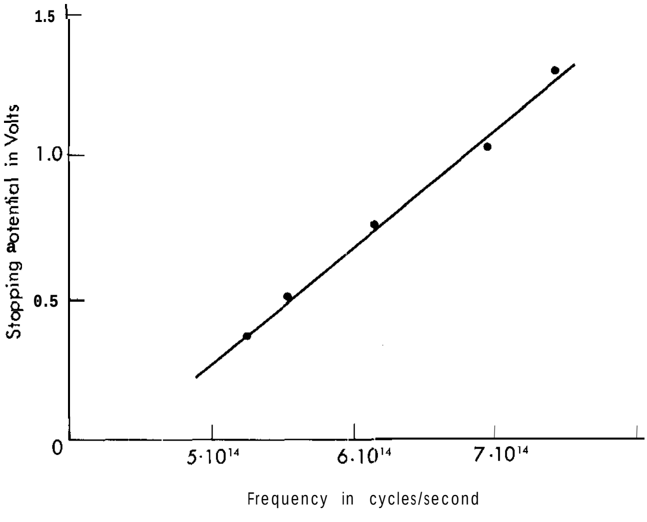


Figure 5.5. Graph of stopping potential vs. frequency.

measured and plotted as a function of frequency, the slope of the curve should be equal to *h/e.* In Figure 5.51 are given some experimental data for the measurement of V as a function of frequency for a particular metal surface. From the data, using the known value of the electronic charge e, Planck's constant can be independently determined. The value obtained from the graph is h = 6.65×10^{-34} j-sec.

1.4 The number of photoelectrons emitted per second is proportional to the intensity of the light.

Classically, this is consistent with conservation of energy, but it is not clear why the increase in available energy as the intensity is increased shouldn't increase T_{max}. if, however, the intensity is $nh\nu$, with $\nu > \nu_c$, then for every photon absorbed, only one electron can be given off. If the intensity is then doubled, keeping the frequency fixed, the number n of quanta is doubled, so that the number of electrons given off should also be doubled. Thus, the quantum theory explains this fact completely.

1.5 Emission of photoelectrons may occur immediately, *regardless* of the intensity of *the* light.

This means that if the intensity is made smaller and smaller, then no matter how small it is, immediately after the light is turned on, some electrons may come 'off. It is not too difficult to arrange for the intensity to be so low that it should take several hours for 5.0 eV of energy to be absorbed by an atom in the metal --that is, provided the intensity is proportional to the square of the amplitude. However, on the basis of the cluantum picture, if there is any light at all, there will have to be at least one quantum present, so an electron could absorb it and leave the surface.

Suppose, for example, that the intensity were so low that 5.0 eV of energy every ten minutes were incident on a surface of work function 2.5 eV, ond that the frequency of the incident light were such that $h\nu = 5.0$ eV. Then, on the average, six electrons would come off every hour; but it turns out to be impossible to predict exactly when these electrons would come off. They would do so at [random times, rather than regularly every ten minutes. Hence, only the probability of ejecting an electron at a given instant can be predicted. This probability can be correctly calculated using the classical formula, which says the square of the amplitude is proportional to the intensity. The intensity is related, on the average, to the number of quanta present. This will be discussed below in detail.

5.5 COMPTON EFFECT

If light waves strike a free electron, as in Figure 5.6, then, according to classical electrodynamics, the electric field vector should cause the electron to oscillate. Hence the electron will be accelerated, and should emit radiation at the same fre-

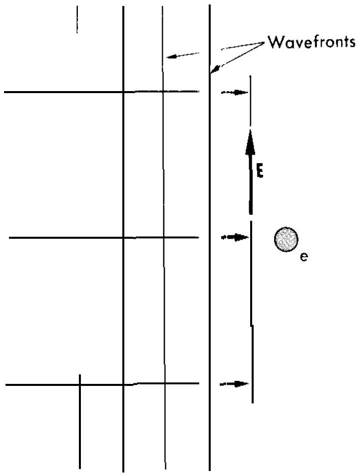


Figure 5.6. Electric field in an electromagnetic wave striking an electron causes the electron to accelerate. Classically, radiation of the same frequency should be emitted, but a shift of wavelength with angle is observed.

quency as that of the incident light. However, experimental observations show that the light reradiated by the electron is changed in frequency (and so in wavelength). For example, considering only the light scattered at 90" from the incident direction, experiments show that the change of wavelength of the light is $\Delta\lambda$ = 0.024 Angstrom. This, of course, is a very small shift in wavelength. In order to observe this shift, it is necessary to do the experiment with x rays.

The effect can be understood as the absorption of a photon of energy, $E = h\nu$, and momentum, $p = h/\lambda$, a subsequent re-emission of a photon of different energy, $E' = h\nu'$, and momentum, $p' = h/\lambda'$, with a recoil of the electron from

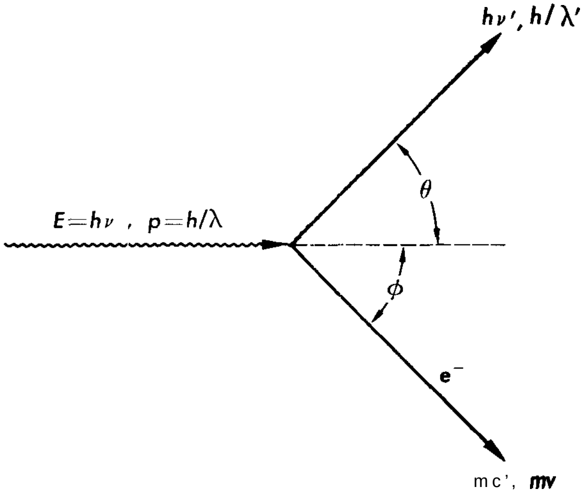


Figure 5.7. Diagram of collision between a photon of energy $E = h\nu$ and a free electron.

the state in which it was initially at rest-i.e. a relativistic collision between two particles. We shall treat the electron as a relativistic particle which, after the collision, has velocity **v** at on angle ϕ relative to the incident direction. The relativistic mass m is then

$$m = \frac{m_0}{\sqrt{1 - v^2/c^2}} \tag{5.13}$$

Let us write down the conservation of energy equation. Referring to Figure 5.7, before the collision the total energy is that of the photon, $h\nu$, and that of the electron at rest, m_0c^2. After the collision, the new photon has an energy $h\nu'$, and the energy of the electron is mc^2. So the law of conservation of energy is

$$h\nu + m_0c^2 = h\nu' + mc^2 \tag{5.14}$$

or since $\nu = c/\lambda$ and $\nu' = c/\lambda'$,

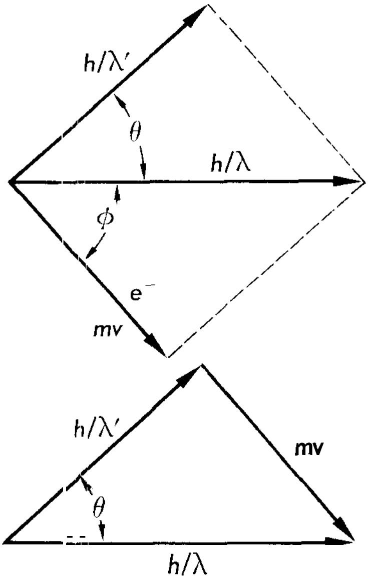


Figure 5.8. Momentum conservation diagrams for photon-free electron collision.

$$\frac{h}{\lambda} + m_0c = \frac{h}{\lambda'} + mc \tag{5.15}$$

Next, we write down the conservation of momentum equations. The relationships between the momentum vectors are diagrammed in Figure 5.8. The initial momentum is that of the incident photon only, since the electron is initially at rest. This initial momentum is equal to the vector sum of the final momenta, of magnitudes h/λ' for the photon and *mv* for the electron. The x component of momentum is conserved. This gives the conservation law,

$$\frac{h}{\lambda} = \frac{h}{\lambda'}\cos\theta + mv\cos\phi \tag{5.16}$$

For conservation of they component of momentum, we have

$$0 = \frac{h}{\lambda'}\sin\theta - mv\sin\phi \tag{5.17}$$

These equations can be manipulated in various ways to yield useful information about the collision process. Note that the equations combine relativistic mechanics for the electron, with the equations $E = pc = h\nu$ for the photons. For our purposes, we wish to calculate the wavelength λ' of the scattered photon in terms of λ and the angle θ, through which the photon is scattered. This means that in the above three equations, (5.15, 5.16, and 5.17), we must eliminate the variables ϕ and v. There are several ways to proceed with the algebra; the result is given in Equation (5.23). The quickest way to eliminate the angle ϕ is to use the vector triangle in Figure 5.8, and apply the law of cosines, which in this case gives us

$$p^2 = (mv)^2 = \left(\frac{h}{\lambda}\right)^2 + \left(\frac{h}{\lambda'}\right)^2 - \frac{2h^2}{\lambda'\lambda}\cos\theta \tag{5.18}$$

The final momentum, p, of the electron in Equation (5.18) can be eliminated by means of the relation $E^2 = p^2c^2 + m_0^2c^4$ or $p^2 = E^2/c^2 - m_0^2c^2$. Then, since $E = mc^2$,

$$p^2 = m^2v^2 = m^2c^2 - m_0^2c^2 \tag{5.19}$$

We may now obtain an expression for p^2 in terms of the initial and final wavelengths, X,X'. Write the conservation of energy equation (5.15) as

$$mc = m_0c + \frac{h}{\lambda} - \frac{h}{\lambda'} \tag{5.20}$$

Squaring this last equation and solving for $m^2c^2 - m_0^2c^2$, *we* get

$$m^2c^2 - m_0^2c^2 = 2m_0c\left(\frac{h}{\lambda} - \frac{h}{\lambda'}\right) + \left(\frac{h}{\lambda} - \frac{h}{\lambda'}\right) \tag{5.21}$$

Thus, combination of equations (5.19) and (5.21) gives us

$$p^2 = m^2v^2 = 2m_0c\left(\frac{h}{\lambda} - \frac{h}{\lambda'}\right) + \left(\frac{h}{\lambda} - \frac{h}{\lambda'}\right) \tag{5.22}$$

Then, eliminating p^2 between Equations (5.22) and (5.18), after some cancellation and reduction to common denominators, one may solve for $\lambda' - \lambda$. The result is

$$\lambda' - \lambda = \frac{h}{m_0c}(1 - \cos\theta) \tag{5.23}$$

This last equation gives the change in wavelength in terms of the universal constants, h/m_0c, and the scattering angle θ. In the derivation, apart from the relationship $p^2 = E^2/c^2 - m_0^2c^2$, we used conservation equations for energy and momentum, and simply eliminated the unwanted variables involving the momentum of the electron.

At a scattering angle of $\theta = 90^\circ$, Equation (5.23) predicts that $\lambda' \quad \lambda = h/m_0c$. For the electron, $m_0 = 9.11 \times 10^{-31}$ kg, and $h = 6.63 - 10^{-34}$ joule-set; calculating $\lambda' \quad \lambda$ in Angstroms gives us

$$\lambda' - \lambda = \frac{6.63 \times 10^{-34}\text{j-sec}}{9.11 \times 10^{-31}\text{kg} \times 3 \times 10^{8} m/\text{sec}} = .0243 \text{ Angstrom} \quad (5.24)$$

This is in extremely good agreement with the experimental value for the shift at **90".**

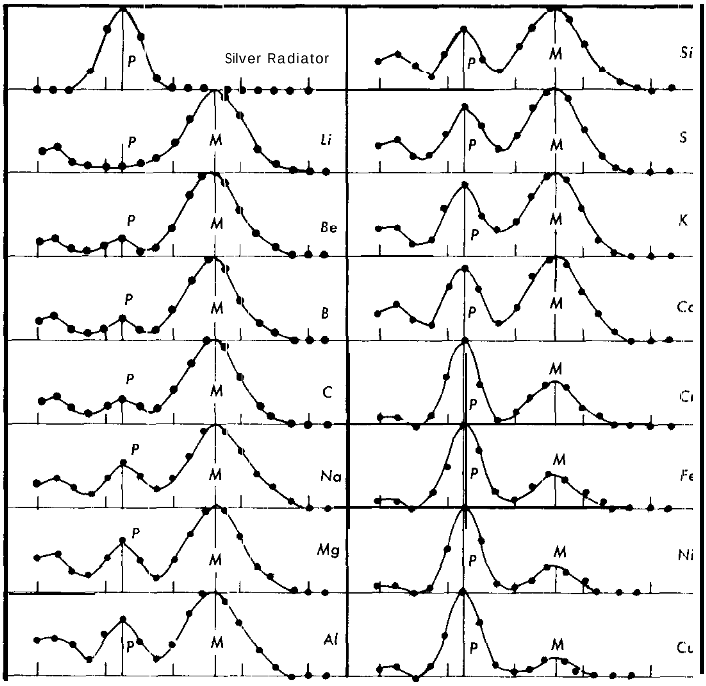


Figure 5.9. Modified and unmodified Compton lines.

The constant $h/m_0c = 2.43 \times 10^{12}$ is called the Compton ***wavelength*** and is a characteristic quantum length associated with the electron.

In Figure 5.9 are shown graphs of intensity versus wavelength of the lines observed at a scattering angle of $90°$, for scattering by the electrons in a number of substances. Notice there are two lines, one at a position corresponding to zero change in λ, the other slightly displaced from it. The displaced line is that due to Compton scattering from free electrons, and is called the ***modified*** line. The other is called the ***unmodified*** line, and is due to scattering from bound electrons. Here, in place of the moss m_0 for electrons in the Compton wavelength, a mass comparable to atomic masses should be used, so the shift of wavelength is negligible. In elements with higher valuer of Z, and hence with more tightly bound electrons, there are relatively fewer free electrons, and so the intensity of the modified line becomes smaller in comparison to that of the unmodified line.

.6 PAIR PRODUCTION AND ANNIHILATION

Another phenomenon in which the quantum properties of light enter is ***pair production***, where a photon of sufficiently high energy (called a gamma ray), reacts to form an electron and another particle, a positron, which has positive charge +e and rest mass equal to the rest mass of the electron, m_0. Symbolically, the process is represented by

$$\gamma \rightarrow e^- + e^+$$

where "e^-" represents the electron and "e^+" the other particle, a positron. Let us ask whether such a process can occur in free space. In this process, we assume the photon of energy $h\nu$ and momentum $h\nu/c$ disappears, and, for simplicity, that the positron and electron continue along in the same direction together, with equal speeds v as in Figure 5.10. Applying the conservation laws, we have, for conservation of energy,

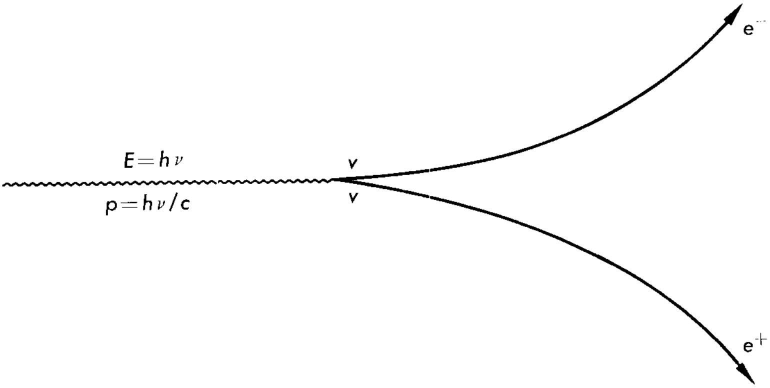


Figure 5.10. Pair production by a photon in free space is impossible as energy and momentum cannot be simultaneously conserved.

$$h\nu = \frac{2m_0c^2}{\sqrt{1-v^2/c^2}} \tag{5.25}$$

Conservation of momentum gives

$$\frac{h\nu}{c} \quad \frac{2m_0v}{\sqrt{1-v^2/c^2}} \tag{5.26}$$

Eliminating the frequency ν from the above equations, one can solve for the speed v. This can be done, for example, by dividing the second equation into the first, giving us

$$c = \frac{c^2}{v} \tag{15.27}$$

or v = c. This immediately implies that the rest mass must vanish, and hence we arrive at a contradiction: The process as we have assumed it to occur is impossible. This is because energy *and* momentum (cannot simultaneously be conserved in free space in this process. Assuming different speeds or directions for the two particles would not alter these conclusions.

However, if the high-energy gamma ray passes near a very heavy particle, then the heavy particle can soak up all the momentum without carrying away a significant amount of energy. To show this, the process is pictured as in Figure 5.11: The γ gives much of its momentum to the heavy particle, and almost all

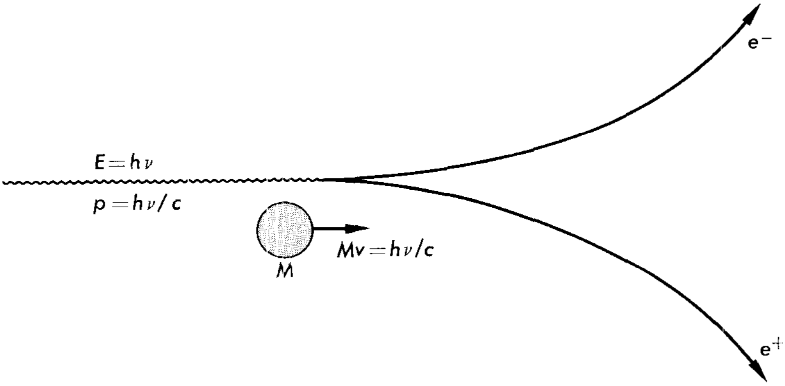


Figure 5.1 1. A high-energy gamma ray passing near matter can create an electron-positron pair-material nuclei soaking up momentum but not energy.

its energy to the electron-positron pair. let us see why this is so. The ratio R of energy carried off by the heavy particle to energy available is

$$R = \frac{\frac{1}{2} Mv^2}{h\nu} \tag{5.28}$$

where we may use the nonrelativistic expression for the heavy particle if the most energetic γ rays we consider have energies of no more than about '10 MeV, which is small compared to the rest energy of a heavy particle such as a proton. If all the momentum of the x ray is assumed to go into momentum of the heavy particle, then $h\nu/c = Mv$. Solving this last equation for v, we have $v = h\nu/Mc$. Substituting v into the ratio R, after some cancellation, we get

$$R = \frac{\frac{1}{2} M(h\nu/Mc)^2}{h\nu} = \frac{1}{2}\frac{h\nu}{Mc^2}$$

Thus, since $h\nu \ll Mc^2$, the ratio R is very small, and the fraction of energy carried away by the heavy particle is negligible, even when it takes up all the momentum. In general, not all the momentum is given to the heavy particle, but it takes up enough to allow the reaction to take place.

Having accounted for momentum conservation with the presence of the heavy particle, we have only to consider energy conservation in the pair creation process. Thus, if v_+ and v_- are the velocities of positron and electron, respectively, then

$$h\nu = \frac{m_0c^2}{\sqrt{1 - v_+^2/c^2}} + \frac{m_0c^2}{\sqrt{1 - v_-^2/c^2}}$$

The minimum gamma-ray energy required to create a pair will occur when the final energies of both particles. are minimum. This will occur when $v_+ = v_- = 0$. Such a minimum kinetic energy for a process to occur is called the threshold *energy,* and

$$h\nu\big|_{\text{threshold}} = 2m_0c^2 \tag{5.29}$$

Since the rest energy of an electron is 0.511 MeV, the threshold gamma energy is 1.022 MeV. It is indeed observed experimentally that when gamma rays of energies greater than 1.022 MeV pass through matter-so that many heavy particles are present-electron-positron pairs are created.

An electron and a positron can also combine in a collision in which they annihilate each other and give off a burst of radiation. Suppose the electron and positron were initially at rest. Their total energy is 1.022 MeV. If they annihilate each other, giving off one photon only, momentum could not be conserved because the initial momentum is zero, whereas the final single particle would have to possess some momentum. Thus, at least two photons must be emitted. If two photons are emitted, then in order to conserve momentum they must go off in opposite directions, with momenta of equal magnitudes. Thus, their energies will be equal (see Figure 5.12). Each photon will then have to carry away an energy of 0.511 MeV. This is observed experimentally.

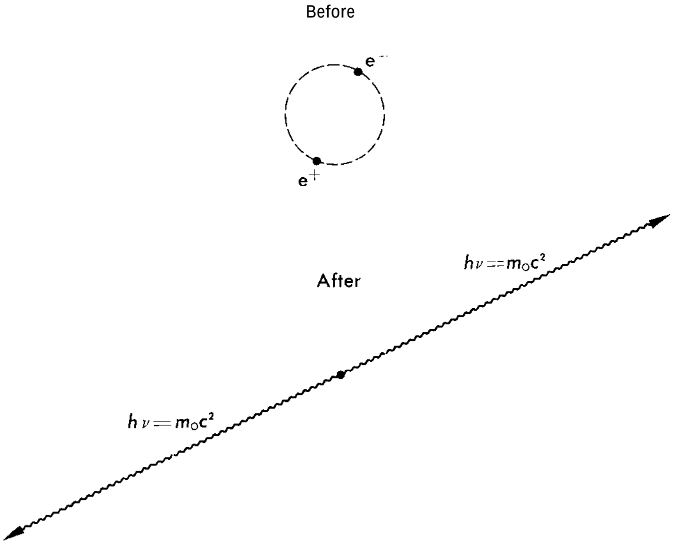


Figure 5.12. Pair annihilation at rest causes at least two photons to be given off, which travel in opposite directions with equal energies.

Whereas the phenomena of pair creation and annihilation do not give an independent way of measuring Planck's constant, because the frequency of the photon is much too high to be measured, they show clearly that the photon must carry energy and momentum, and that total energy and momentum of the particles in a reaction are both conserved.

5.7 UNCERTAINTY PRINCIPLE FOR LIGHT WAVES

It is a general physical fact that any measurement of a physical quantity generates uncontrollable disturbances which may alter the value of the physical quantity being measured. For example, to measure the temperature of a gas, a thermometer must be introduced into the gas, which may decrease the volume slightly and hence heat up the gas. In addition, there might be some heat exchange between gas and thermometer. When analyzed in detail, all physical measurements can be shown to have a similar disturbing character. We are interested here in the uncertainties introduced into the values of frequency (energy) and wavelength (momentum) of light waves by attempts to measure their values, ν and λ.

Consider a measurement of frequency. A frequency is a number of cycles per unit of time, so to measure a frequency, we have to count the number N of wave crests that pass a given point in a given time Δt; then the frequency will be given by

$$\nu = \frac{N}{At} \tag{5.30}$$

Here, At is the time interval over which the measurement extends. In counting N, the number of crests, various difficulties may arise. If the wave is not a pure sine wave, then it will consist, perhaps, of a superposition of several frequencies, and repeated measurements of N will not agree. Even if the wave is a pure sine wave, when we count crests over a fixed time interval At, then for a particular measurement we might not know whether we should include the last portion of a wave as a crest or not. To put it another way, suppose we chop the pure sine wave so that it only lasts a time At. Then the sharp variations in amplitude at the ends can be represented in terms of a superposition of waves of many different frequencies, so that repeated measurements of N would not always give the same value. It is not difficult to make an order-of-magnitude estimate of the range of uncertainty, AN of N. It will be about 1, since in counting crests we may miss one or more crests at the ends. Thus, if the uncertainty in N is AN $\simeq$ 1, there will be a corresponding uncertainty $\Delta\nu$ in our measurement of frequency, and this will be

$$\Delta\nu = \frac{\Delta N}{\Delta t} \simeq \frac{1}{\Delta t} \tag{5.31}$$

Thus, the product:

$$\Delta\nu\Delta t \simeq 1 \tag{5.32}$$

This result arises purely because of the wave nature of the light; it is not only valid for light but for all other classical wave disturbances, and also for other waves such as those arising in quantum theory.

From Equation (5.32), we can obtain a corresponding uncertainty relation for energy. The energy of a photon of frequency ν is $E = h\nu$, so the uncertainty in energy will be related to the uncertainty in frequency by AE = h Au. Therefore,

$$\Delta E\Delta t \simeq h \tag{5.33}$$

This result states that the product of the time Δt over which the measurement is conducted, times the uncertainty in the measurement of energy of a photon, is approximately h.

TABLE 5.3 **Typical Data From a Frequency Counter: Time Interval**

$\Delta t = 1.0$ sec. Numbers of counts in repeated measurements:

100404	100485	100485	100482	100485
100485	100485	100484	100483	100485
100486	100485	100486	100484	100484
100484	100485	100485	100482	100485
100485	100486	100484	100482	100484
100485	100485	100479	100484	100485
100485	100484	100482	100483	100484
100485	100484	100482	100484	100486
100485	100485	100483	100485	100485
100485	100485	100483	100485	100485
100485	100484	100484	100485	100486

Average number of counts = 100484.31

RMS deviation from the mean of the number of counts = 1.28 counts.

In Table 5.3 are given the numbers of counts in repeated measurements by an electronic wave crest counter, which has counted crests of a wave put out by an audio signal generator over a time interval $\Delta t = 1.00$ sec. The root mean square deviation from the mean of N can be taken as a measure of the uncertainty in N. From the table, one can find the uncertainty in frequency of the measurements; it is 1.28 sec^{-1}. Thus the uncertainty product is

$$\Delta \nu \Delta t \sim 1.28$$

in accord with the uncertainty principle, Equation (5.33).

5.8 MOMENTUM, POSITION UNCERTAINTY

An uncertainty relation may be obtained in a similar way, which relates momentum and distance. Imagine freezing a pure sine wave and measuring the number of wave crests, N, within the distance Δx on the meter stick. Then the wavelength λ is given by $\lambda = \Delta x/N$. The momentum will be

$$p = \frac{h}{\lambda} = \frac{hN}{\Delta x}$$

However, again because near the endpoints it will not be clear whether we have included the last wavecrest correctly or not, repeated measurements may give differing values for N. Again, the uncertainty in N will be roughly $\Delta N \simeq 1$, and the corresponding uncertainty in momentum will be

$$\Delta p \simeq \frac{h}{\Delta x}$$

or

$$\Delta p \Delta x \simeq h \tag{5.34}$$

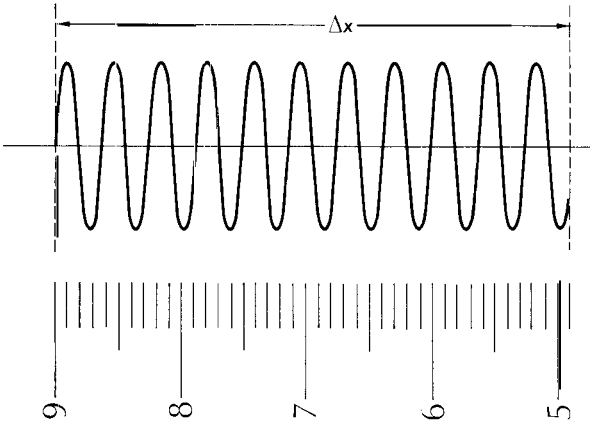


Figure 5.13. **Basic uncertainties arise in attempts to measure wavelength or momentum.**

If we take as a measure of Δp and Ax the rms deviations from the mean, this uncertainty relation can be made more precise. As one might guess, there is a wave shape that makes the uncertainty product $\Delta x\, \Delta p$ *a* minimum. It turns out that this minimum occurs when the wave shape is a sine wave modulated by a gaussian, of the form $ce^{-x^2/2\sigma^2}$, with c and σ constants. For this wave, Ax Ap = $h/4\pi$. So, in general,, we could say that $\Delta x\, \Delta p \geq h/4\pi$.

In terms of wavelength, the uncertainty in λ is

$$\Delta\lambda = \left|\Delta\left(\frac{\Delta x}{N}\right)\right| = \frac{\Delta x}{N^2}\,\Delta N = \left(\frac{\Delta x}{N}\right)^2 \cdot \frac{\Delta N}{\Delta x} \qquad \textbf{(5.35)}$$

and this gives, in terms of the measured value $\lambda = \Delta x/N$,

$$\Delta\lambda\,\Delta x \geq \frac{\lambda^2}{4\pi} \qquad \textbf{(5.36)}$$

The uncertainty relation $\Delta p\ \Delta x \geq h/4\pi$ for light waves, states that a measurement of momentum of a light wave which is carried out over a spatial interval Ax will have an uncertainty such that the product of Ax times the uncertainty in momentum is greater than $h/4\pi$.

These results show that there are basic limitations on our ability to simultaneously measure certain properties of light waves; later, we shall see that very similar uncertainty relations hold for material particles such as electrons,, protons and atoms. No conceivable measurement process can give rise to knowledge of physical quantities which violates these relations.

i.9 PROBABILITY INTERPRETATION OF AMPLITUDES

We have seen in detail how light waves carry energy $E = h\nu$ and momentum $p = h/\lambda$, and that when they interact with matter, photons are emitted and absorbed and have many particle-like properties. We now have to reconcile these results with the fact that in calculations of interference and diffraction, the experimental results are very well explained by using wave-like properties, namely superposition of wave amplitudes. In a diffraction calculation, illustrated in Figure 5.14, the square $|\psi(\theta)|^2$ of the amplitude $\psi(\theta)$ is proportional to the intensity of the light arriving at the screen at the angle θ, where $\psi(\theta)$ is obtained as a linear superposition of contributions $\psi_i(\theta)$ from each of the individual point sources of Huyghen's wavelets. Mathematically, the intensity is given by

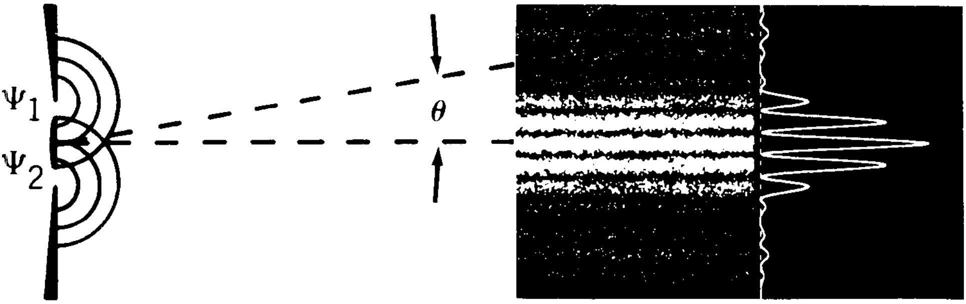


Figure 5.14. Double-slit diffraction pattern for light must be interpreted in terms of probabilities.

$$I(\theta) = k\,|\psi(\theta)|^2 = k\left|\sum_i \psi_i(\theta)\right|^2 \tag{5.37}$$

where k is some proportionality constant. In order to explain the form of the diffraction pattern, it is said that the energy going into the angle θ is proportional to the absolute square, or magnitude of the square, of the total amplitude ψ.

However, if, according to the quantum theory of light, we are actually dealing with photons of frequency ν, and if the flux of photons going into the angle θ is n, then $I = nh\nu$; thus the square of the amplitude would be proportional to the number of photons going into the angle θ. Imagine that the screen on which the photons are allowed to fall is fluorescent, so that whenever a photon strikes the screen at some point, this is made evident by a visible flash. Then, when the intensity of the incident photon beam is large, there are many photons, and there will be many flashes on the screen. The number of flashes at a given point is proportional to the square of the amplitude calculated classically.

Suppose now that the intensity of the beam is reduced to such a low value that only one photon at a time goes through the slit system. Then only one flash at a time will be seen on the screen, at some definite position. Sometimes, the flash will be at one point, sometimes at another. That is, the exact position at which a given photon strikes the screen will be unpredictable. However, suppose the screen is replaced by a film and a long exposure is made, so that over a long period many, many photons hit the film, one at a time. When this experiment is performed, the pattern on the film is precisely that predicted classically, i.e. the diffraction pattern. Thus, even though only one photon at a time goes through the slit system, so that one might think photons could not interfere with each other, one still obtains the diffraction pattern.

Therefore, the squared amplitude does not tell exactly where a photon will go--which is unpredictable--- but it does tell what happens on the average to many photons. It can only be interpreted as a probability. The square of the amplitude, $|\psi(\theta)|^2$, is thus proportional to the probability that a given photon will be found at the angle θ. $\psi(\theta)$ is then referred to as a probability ***amplitude.***

To obtain the probability that a photon will be found at the angle θ, one calculates the sum, or superposition, of all the probability amplitudes which contribute to $\psi(\theta)$. Then $|\psi(\theta)|^2 = |\sum_i \psi_i(\theta)|^2$ is proportional to the probability of finding a given photon at position θ. This probability interpretation of the amplitude squared is verified by many experiments.

summary

THE PLANCK RELATION BETWEEN ENERGY AND FREQUENCY FOR LIGHT

In order to explain the observed properties of black-body radiation, Planck postulated that light carried energy in discrete bundles called quanta, or photons. If the frequency of the light is ν, then the photon energy is $E = h\nu$. The total energy could be $nh\nu$, where n is some integer. This law is relativistically form-invariant. Since $E = pc$ for photons where p is the momentum, it follows that $p = h/\lambda$. The presently accepted value of h is:

$$h = 6.6262 \times 10^{-34} \text{ joules-sec.}$$

Another useful constant is:

$$\frac{hc}{e} = 1.2399 \times 10^{-6} \text{ j-m/coul.}$$

DUANE-HUNT LAW

If electrons are accelerated through a potential difference V, they acquire kinetic energy eV. Then, if they are suddenly stopped, the maximum energy that can be emitted by an electron will be $eV = h\nu_{max}$.

PHOTOELECTRIC EFFECT

The work function Φ of a metal surface is defined as the minimum energy necessary to remove one electron from the surface. If light of frequency ν is incident on the surface, electrons may be ejected. The maximum kinetic energy T_{max} of an electron is given by the Einstein photoelectric equation,

$$T_{max} = h\nu - \Phi$$

If $h\nu < \Phi$, no electrons can come off. The critical frequency ν_c, at which some electrons are barely able to escape, is given by $h\nu_c = \Phi$. The value of T_{max} is independent of the intensity of the incident light; the number of electrons emitted is proportional to the intensity $nh\nu$ of the light.

COMPTON EFFECT

When a photon of initial wavelength λ is scattered by a free electron, itself initially at rest, then the scattered photon has its wavelength changed an amount given by:

$$\lambda' - \lambda = \frac{h}{m_0 c}(1 - \cos\theta)$$

where θ is the angle through which the photon is scattered.

PAIR PRODUCTION AND ANNIHILATION

A photon of energy greater than $2m_0c^2$ can, when passing near a heavy particle, be changed into an electron-positron pair. An electron and positron at rest can annihilate each other to produce two or more photons. If two photons are produced, they each have energies of m_0c^2.

UNCERTAINTY PRINCIPLE

A single measurement of frequency of a photon, which lasts over a time interval, Δt, necessarily has on uncertainty given by $\Delta\nu\Delta t \geq 1$. Then the energy is uncertain by an amount ΔE, where $\Delta E \Delta t \geq h$. In a measurement of momentum of a photon, where the position of the photon is known to within an accuracy Δx, there will be an uncertainty Δp in momentum given by $\Delta p \Delta x \geq h/4\pi$.

PROBABILITY INTERPRETATION OF AMPLITUDES

Experiments performed with low intensity light waves indicate thot the squared amplitude of the wave may be interpreted as the probability that a photon will be found at a certain position.

problems

1. What energy would an electron require in order to have the same momentum as an 8 MeV photon?
Answer: 8.0163 MeV.
2. Find the wavelengths for photons of the following energies: (a) 10.2 eV corresponding to the shortest wavelength emitted by a hydrogen atom; (b) 100 keV x ray; (c) 500 MeV gamma my.
Answer: (a) 1216 Angstroms;(b) 0.1243 Angstroms; (c) 2.49 x 10^{-5} Angstroms.
3. Find the kinetic energy in MeV of an electron with momentum equal to c times its rest mass. Compare with $\frac{1}{2} m_0 v^2$.
Answer: $(\sqrt{2} - 1)m_0c^2 = 0.212$ MeV; $\frac{1}{2} m_0 v^2 = \frac{1}{4} m_0 c^2 = 0.128$ MeV.
4. Two particles travel in the lab system with equal but opposite speeds and collide. If the kinetic energy of each particle is 9 times the rest energy (m_0c^2) as observed from the lob, then what is the kinetic energy of one of the particles as observed from a system in which the other particle is at rest?
Answer: $198 m_0c^2$.
5. A proton with total energy $\gamma m_0 c^2$ and momentum $\gamma m_0 c^2$, where $\gamma = 1/\sqrt{1 - v^2/c^2}$ and v is the proton speed, hits a proton at rest in the laboratory system. Use the transformation equations for the total energy, $(\gamma + 1)m_0c^2$, and momentum, $\gamma m_0 v$, of the two-proton system to find the energy and momentum in a frame moving with speed v' relative to the laboratory system. Take the relative velocity parallel to the velocity of the first proton. Show that if $v' = \gamma v/(\gamma + 1)$, the momentum is zero. This center *of momentum* system is classically the center of mass system. Show that in thot system,

$$\frac{1}{\sqrt{1 - v'^2/c^2}} = \sqrt{\frac{(\gamma + 1)}{2}}$$

and thus that the total energy in the center of momentum system is

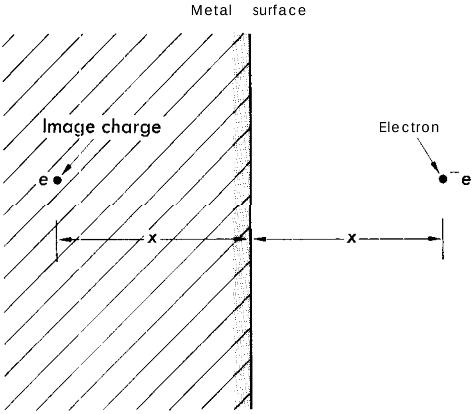
$$\sqrt{2(\gamma + 1)}m_0c^2$$

6. An electron has a kinetic energy of 1 MeV in one inertial system. Find the magnitude of the momentum of the electron in MeV/c in a system moving relative to the first at c/2, (a) in the same direction as the electron velocity in the first system; (b) perpendicular to the electron velocity in the first system. The electron rest mass corresponds to 0.51 1 MeV.
Answer: (a) 0.770 MeV/c; (b) 1.669 MeV/c.
7. What would be the wavelength of the most energetic x rays produced by electrons of 50 keV kinetic energy striking a lead target?
Answer: 0.249 Angstrom.
8. For what wavelength of incident light will photoelectrons ejected from zinc have a maximum velocity of $\frac{1}{10}$ of the speed of light?
Answer: 4.83 Angstroms.
9. A gamma ray of energy 5.7 MeV is Compton scattered at an angle of 60” from free electrons. Find the energy in MeV of the outcoming photon.
Answer: 0.867 MeV.

10. Find the least frequency of incident light that will knock electrons out of the surface of a metal with a work function of 3 eV.

Answer: 7.24 x 10^{14} sec^{-1}.

11. The potential barrier of electrons at the surface of a metal which leads to the work function is due to electrons which get slightly outside the surface, inducing a positive charge inside the surface. This leads to a force which is the same as if an image charge equal and opposite to that of the electron were attracting the electron, as shown in the diagram. Verify qualitatively that the lines of force between electron and image charge would satisfy the condition that they must be perpendicular to the conducting surface. Show that the electron has a potential energy of $-e^2/(16\pi\epsilon_0 x)$ where x is the distance to the metal surface. This image force should no longer be present once the electron is a distance from the surface comparable to the metal atom spacings, say 1 Angstrom. Compute the electron potential energy at that distance and compare in order of magnitude with work functions given in Table 5.2.



Answer: 3.6 eV.

12. Find the maximum kinetic energy in eV of electrons knocked out of a surface with a work function of 1.5 eV by light of wavelength 6000 Angstroms.

Answer: 0.57 eV.

13. The threshold wavelength for emission of electrons from a Cs surface is 6540 Angstroms. Calculate the work function of Cs in eV, and calculate the maximum energy in eV photoelectrons would have if photons of wavelength 4000 Angstroms were incident on the surface.

Answer: 1.90 eV; 1.20 eV.

14. An x-ray photon is scattered by a free electron at rest through an angle of 60°. The wavelength changes by 15%. What is the incident wavelength?

Answer: 0.0486 Angstrom.

15. Compute the wavelength shift for photons backscattered (θ = 180°) from free protons.

Answer: 2.65 x 10^{-5} Angstroms.

16. Show that when a photon is scattered by a free electron at rest, the product of the initial frequency and electron rest mass divided by the product of the final frequency and final electron mass is $1 - v/c \cos \Phi$, where v is the final electron speed and Φ is the angle between the scattered electron and photon.

17. A 150,000 eV photon collides with a free electron at rest and scatters at 90°. What is the final kinetic energy of the electron?

    Answer: 34 keV.

18. Derive an expression for the kinetic energy of the recoil electron which has just been Compton scattered, in terms of the initial photon energy $h\nu$ and the initial and final wavelengths, λ, λ' of the photon.

    Answer: $T = h\nu \dfrac{\Delta\lambda}{\lambda + \Delta\lambda}$ where $\Delta\lambda = \lambda' - \lambda$.

19. An electron traveling with speed $v = (\frac{4}{5})c$ is hit head-on by a photon of energy $h\nu$ and is brought to a dead stop. There is a scattered photon which goes back along the path of the incident photon. Calculate the energy $h\nu$ of the initial and $h\nu'$ of the final photons in MeV.

    Answer: $h\nu = 0.17$ MeV; $h\nu' = 0.511$ MeV.

20. A positron of kinetic energy 1 MeV annihilates with an electron at rest. If the resulting two photons have equal energies find the angle between their momenta.

    Answer: 90.6°.

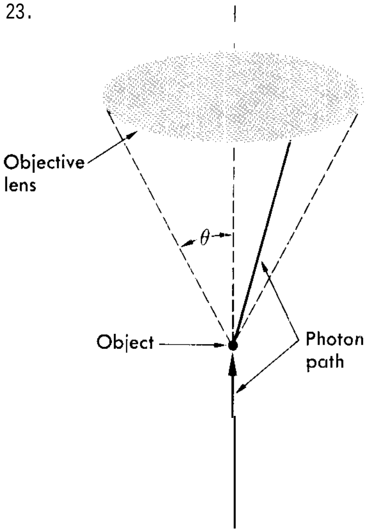
21. A 2 MeV photon creates an electron-positron pair. If the resulting electron has a kinetic energy of ¼ MeV, what is the kinetic energy of the positron?

    Answer: 0.728 MeV.

22. In the hydrogen atom the light given off when an electron goes from one energy state to another is not quite monochromatic. Estimate the wavelength spread in light given off at close to 6563 Angstroms using the uncertainty principle, if it takes around 10^{-8} seconds for such a transition between energy states to take place.

    Answer: 0.0014 Angstrom.

23.



Suppose that the position of an object is to be measured by means of scattering single photons from it and observing the photons through a microscope. The radius of the objective lens subtends θ at the object. Show that due to the scattering of a photon with momentum $h\nu/c$, the uncertainty in momentum of the object is of order $\Delta p = (h\nu \sin\theta)/c$. Show that in a plane perpendicular to the lens axis, the distance between field maxima for the scattered photon can be as high as $\Delta x = \lambda/\sin\theta$. This can be taken as the error in position measurement of the object. Find $\Delta x \Delta p$.

6 matter waves

It has already been seen how in some situations electromagnetic field quanta may have particle-like attributes: They carry energy in discrete amounts $E = h\nu$, and are emitted and absorbed by matter as though they were particles. When traveling through a slit system, however, they can still behave like waves, in the sense that the probability that a photon will be found at some angle θ from its original direction is proportional to the classically calculated diffraction intensity pattern.

Another remarkable fact of nature is that particles such as electrons, neutrons and others can also display wave-like character under appropriate experimental conditions. Since experimentally it is found that atoms emit light at only discrete frequencies, just as a stretched string only emits sound waves at a discrete set of frequencies, it might be expected that a wavelike character of particles would provide the key to an understanding of atomic spectra. Just as the discrete frequencies of a stretched string are due to standing 'waves on the string, so the discrete frequencies of atomic spectra could be due to standing waves within the atoms.

The wavelike properties of particles were postulated by Louis de Broglie in 1924. He was led to this discovery when he noted certain similarities in the properties of particles and waves, under Lorentz transformations. We shall take up the fundamental study of these *waves-de* Broglie waves-in this chapter. De Broglie assumed that, associated with a particle of speed V, was a wave having some phase speed not equal to c. This phase speed w is related to V by a simple equation, which we shall derive below. That a phase speed can be associated with a particle in a consistent way depends on some special features of the relativistic Lorentz transformations. Let us begin by examining the transformation properties of plane waves of any kind under Lorentz transformations between inertial frames.

6.1 PHASE OF A PLANE WAVE

A plane wave may be conveniently described in terms of its propagation vector **k** and angular frequency, $\omega = 2\pi\nu$. If the wavelength in the inertial rest system R is λ, then the propagation vector is defined as a vector of magnitude $2\pi/\lambda$, pointing in the direction of propagation of the wave. The propagation vector far a plane wave is thus normal to the wave fronts.

For a wave propagating along the positive x axis, one possible sinusoidal like wave form has the wave amplitude, or wave function,

$$\psi = Ae \exp\left[i\left(\frac{2\pi x}{\lambda} - 2\pi\nu t\right)\right] \tag{6.1}$$

where A is a constant and $\nu = \omega/2\pi$ is the frequency. This wovefunction is more simply expressed in terms of the angular frequency ω and the wavenumber k = k |:

$$\psi = Ae^{i(kx \quad \omega t)} \tag{6.2}$$

The term kx can be written in vector form, since in this case, k is parallel to the x axis. Thus, if r is the position vector of some point in space, then

$$kx = k_x x = k_x x + k_y y + k_z z = \mathbf{k} \cdot \mathbf{r} \tag{6.3}$$

because $k_y = k_z = 0$. The wavefunction in terms of k . r is

$$\psi = Ae^{i(\mathbf{k}\cdot \mathbf{r} - \omega t)} \tag{6.4}$$

Since the wavefunction is now written in terms of vectors, Equation (6.4) gives the wavefunction no matter what the direction of propagation is. For example, if the wave were propagating in the x-y plane at an angle of θ relative to the x axis, then the x and y components of k would be

$$k_x = k \cos\theta, \quad k_y = k \sin\theta \tag{6.5}$$

So, in terms of k and θ, k r $= kx \cos\theta + ky \sin\theta$, and the wavefunction would be A exp $[i(kx \cos\theta + ky \sin\theta -$ wt)].

The function $\mathbf{k}\cdot\mathrm{r} - \omega t$ is called the phase of the wave; that is, the phase is the coefficient of i in the exponent of the wavefunction. If the wave amplitude has a trigonometric form such as $\psi = A \cos(\mathbf{k}\cdot\mathrm{r} - \omega t)$, then the phase is the argument of the trigonometric function. Each time the phase of the wave changes by 2π, the wave amplitude goes through one complete cycle of oscillation. If we fix our attention on a locus of points of constant phase, such as

$$\mathbf{k}\cdot\mathrm{r} - \omega t = \text{constant} \tag{6.6}$$

then, as the time increases, the positions r which satisfy this equation move with a velocity w, called the phase velocity. These points of constant phase define a wavefront, and hence the phase velocity is just the velocity with which the wavefronts propagate. The phase speed can be written in terms of k and ω by using the definitions:

$$w = \nu\lambda = \frac{2\pi\nu \cdot \lambda}{2\pi} = \frac{\omega}{k} \tag{6.7}$$

This could also be obtained by differentiating Equation (6.6):

$$\mathbf{k}\cdot\frac{d\mathbf{r}}{dt} = \omega \tag{6.8}$$

Since the velocity $d\mathbf{r}/dt$ for the wavefront is parallel to the direction of propagation, $kw = \omega$.

example If, at a fixed point r, the amplitude is observed for 12 periods of oscillation, what is the net change in phase of the wave?

solution The period is T = $2\pi/\omega$; observing for a time Δt = 12T = $24\pi/\omega$ results in a change of phase $\Delta(\mathbf{k}\cdot\mathbf{r} - \omega t) = -\omega\Delta t = -24\pi$.

If N wavecrests propagate past a given point, this means that the phase has changed by 27rN. Thus we arrive at the main point of the discussion so far: The change in phase of the wave is proportional to, and hence is a measure of, the number of wavecrests which pass a given point.

6.2 INVARIANCE OF THE PHASE OF A PLANE WAVE

A pure sine or cosine wave in an inertial frame R will also appear to be a pure sine or cosine wave in another frame, if the wave amplitude is the solution of a wave equation which is relativistically invariant. We will assume this to be the case. Then, by considering Figure 6.1, it is easy to see that the phase of a plane wave is a relativistic invariant; that is, it has the same numerical value at corresponding physical points in all inertial frames. Zeros of the amplitude in R will appear to be zeros of the amplitude in G, and similarly for the maxima and minima. So for every wavefront in R, there will be a wavefront in G. For example, suppose the wavefront of zero phase passes the origins 0 and 0' in Figure 6.1 at the instant 0 and 0' coincide. If this wavefront is observed at some later time at position $P'(\mathbf{r}', t')$ in G, which coincides with P(r, t) in R, then it will still have zero phase. The same holds for every other plane of constant phase, at any point in space and time. Thus, the phases of the plane wave as observed in the two inertial frames are equal, and the phase is a relativistic invariant. This invariance will allow us to derive some interesting things about the transformation properties of k and ω.

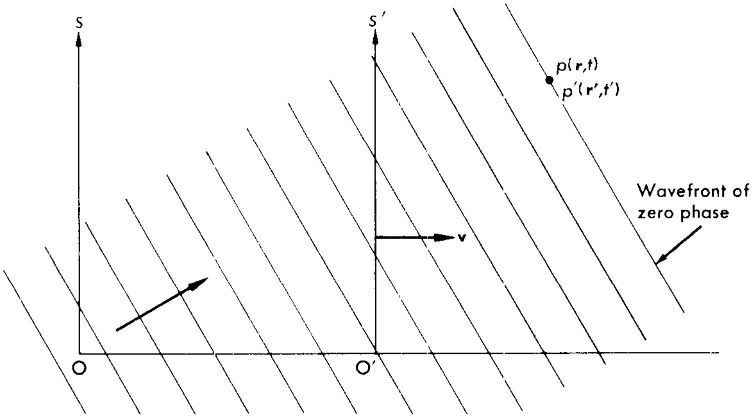


Figure 6.1. A plane wave observed in two inertial systems.

If $t = t' = 0$ when the origins coincide, and the phase in G is $\mathbf{k}'\cdot\mathbf{r}' - \omega' t'$, the phase in R is $\mathbf{k}\cdot\mathbf{r} - \omega t$. So in mathematical form the invariance of the phase can be written as:

$$\mathbf{k}'\cdot\mathbf{r}' - \omega' t' = \mathbf{k}\cdot\mathbf{r} - \omega t \tag{6.9}$$

This equation reflects the fact that a wavefront, such as a maximum of the wave amplitude, has physical reality, and all observers, can agree on the number of wavecrests which pass by a given physical point. Hence, they can agree on the value of the phase.

6.3 TRANSFORMATION EQUATIONS FOR WAVEVECTOR AND FREQUENCY

Use of the invariance property, Equation (6.9), allows us to obtain the transformation equations for $\mathbf{k}'$ and ω' in terms of $\mathbf{k}$ and ω. We first write out the invariance equation in more detail, using components of $\mathbf{k}$: k_x, k_y, k_z, and of $\mathbf{k}'$: k'_x, k'_y, k'_z We get

$$k'_x x' + k'_y y' + k'_z z' - \omega' t' = k_x x + k_y y + k_z z - \omega t \tag{6.10}$$

This equation is valid for all values of the two sets of space and time coordinates which refer to the same physical point and which are, therefore, connected by the Lorentz transformations. If we express x, y, z and t in terms of x', y', z' and t', then, since R moves with speed v relative to G, we have the Lorentz transformations, Equations (3.16) and (3.18):

$$\begin{aligned} x &= \frac{1}{\sqrt{1 - v^2/c^2}}(x' + vt'), \\ y &= y' \\ z &= z' \\ t &= \frac{1}{\sqrt{1 - v^2/c^2}}\left(t' + \frac{vx'}{c^2}\right) \end{aligned} \tag{6.11}$$

Substitution of these values of x, y, z, t into Equation (6.10) gives the result,

$$\begin{aligned} k'_x x' + k'_y y' + k'_z z' - \omega' t' &= k_x \frac{1}{\sqrt{1 - v^2/c^2}}(x' + vt') + k_y y' + k_z z' \\ &\quad - \frac{\omega}{\sqrt{1 - v^2/c^2}}\left(t' + \frac{vx'}{c^2}\right) \end{aligned} \tag{6.12}$$

This last equation must now be true for all values of x', y', z' and t'. For example, if we consider an observation on the z axis when the origins coincide so that $x' = y' = t' = 0$ with $z' \neq 0$, the equation reduces to

$$k'_z z' = k_z z' \tag{6.13}$$

After cancellation of z', we obtain

$$k'_z = k_z \tag{6.14}$$

Similarly, by taking $x' = z' = t' = 0$, $y' \neq 0$, we can show that

$$k'_y = k_y \tag{6.15}$$

To obtain k'_x in terms of k_x and ω, we set $y' = z' = t' = 0$ with x' unequal to zero. We get

$$k'_x x' = \frac{k_x x'}{\sqrt{1 - v^2/c^2}} - \frac{\omega v x'/c^2}{\sqrt{1 - v^2/c^2}} \tag{6.16}$$

or

$$k'_x = \frac{1}{\sqrt{1 - v^2/c^2}} \left(k_x - \frac{v\omega}{c^2}\right) \tag{6.17}$$

Lastly, using $x' = y' = z' = 0$ and $t' \neq 0$, we can find ω' in terms of ω and k_x. The result is

$$\omega' = \frac{1}{\sqrt{1 - v^2/c^2}} (\omega - vk_x) \tag{6.18}$$

Collecting the four results, we have the transformation equations:

$$k'_x = \frac{1}{\sqrt{1 - v^2/c^2}} \left(k_x - v\frac{\omega}{c^2}\right) \tag{6.19}$$

$$k'_y = k_y \tag{6.20}$$

$$k'_z = k_z \tag{6.21}$$

$$\omega' = \frac{1}{\sqrt{1 - v^2/c^2}} (\omega - vk_x) \tag{6.22}$$

These results were obtained simply by showing that the phase of any plane wave, going with any phase speed, has the same numerical value in all inertial frames. In other words, the phase $(\mathbf{k} \cdot \mathbf{r} - \omega t)$ is a relativistic invariant. Combining this with the Lorentz transformations, we were led directly to the transformation equations for $\mathbf{k}$ and ω, by equating coefficients of x', y', z' and t' on both sides of the equation.

If we considered these equations in the limiting case of phase speed $w = \omega/k = c$, the speed of light, they would lead back to the equations for the Doppler effect for light found in Chapter 4.

Equations (6.19) through (6.22) resemble very closely the relativistic transformation laws for momentum and energy of a particle, which are:

$$\begin{aligned} p'_x &= \frac{1}{\sqrt{1 - v^2/c^2}} \left(p_x - \frac{vE}{c^2}\right) \\ p'_y &= p_y \\ p'_z &= p_z \\ E' &= \frac{1}{\sqrt{1 - v^2/c^2}} (E - vp_x) \end{aligned} \tag{6.23}$$

This is a very suggestive comparison.

.4 PHASE SPEED OF DE BROGUE WAVES

With the transformations in Equations (6.19)—(6.22), we can examine in detail the hypothesis of de Broglie, namely that with each particle there can be associated a wave which travels along with the particle as the particle moves, with some phase speed w which may be different from the particle speed V. The transformation equations suggest that the wave vector k and angular frequency ω might be closely related to the momentum p and energy E of the particle. In fact, we will see that if particles have waves associated with them, the only possible relations must be of the form

$$\mathbf{p} = \hbar \mathbf{k} \qquad E = \hbar\omega$$

where $\hbar$ is a constant.

Let us first derive the relation between phase speed and particle speed. In the above transformation 'equations, ω'/c^2 is analogous to E'/c^2, and k' is analogous to p'. It was proved eorlier that $c^2(E/c^2)^2 - p$ was a relativistic invariant. In the same way, we could show that $c^2(\omega/c^2)^2 - k^2$ is a relativistic invariant or that it has the same value in all inertial frames. Mathematically, this can be expressed as:

$$\rule{2cm}{0.4pt}\; k'^2 = \frac{\omega^-}{\;} - k^2 = \text{invariant} = C \qquad \textbf{(6.24)}$$

where C is a constant independent of the inertial frame in which w and ***k* are** measured.

In the special case of light, which consists of zero rest mass particles, the value of the invariant, $\omega^2/c^2 - k^2$, is equal to zero. This suggests that when a wove of angular frequency w and wave number k is associated with a material particle, then the value of the invariant $\omega^2/c - k^2$ might be related to the particle's mass.

De Broglie's hypothesis was that, associated with a particle having speed V, was a wove having phase speed w. He assumed that the energy in the wave traveled along with o group speed $v_g = d\omega/dk$, which was identical with the particle speed V. The group speed $v_g = d\omega/dk$ can be calculated using the invariant expression in Equation (6.24), by differentiating with respect to k. The result is

$$2\omega/c^2 \frac{d\omega}{dk} - 2k = 0 \qquad \textbf{(6.25)}$$

Solving for the group speed, we get

$$v_g = \frac{dw}{dk} = c^2 \frac{k}{w} \qquad (6.26)$$

Since the phase speed is w = w/k, the group speed in terms of w is

$$v_g = \frac{c^2}{w} \qquad \textbf{(6.27)}$$

If we identify the particle speed V with the group speed, then

$$v_g = V = \frac{c^2}{w} \qquad (6.28)$$

or

$$wV = c^2 \qquad (6.29)$$

This relation, $wV = c^2$, is form invariant, since its derivation was based on a relativistic invariant. Thus, if in another inertial system G the particle speed is V', then upon identifying the group speed $d\omega'/dk'$ in G with the particle speed V', one would obtain, by an analogous argument, $w'V' = c^2$.

Since particle speeds must be less than c, in general the phase speed will be greater than c. Indeed, for particles whose velocities approach zero, the corresponding phase speed must approach infinity. Although the phase speed is greater than the speed of light, this does not contradict special relativity, because the energy travels along with the particle speed V, which is identical with the group speed. The individual wave crests travel with the phase speed, whereas the energy travels with the speed of the envelope of the waves, the group speed.

To illustrate the relation between phase and group speeds, imagine the analogy, as in Figure 6.2, of a plane light wave traveling with speed c incident upon a screen at an angle i from the normal. The point of intersection of a wavefront with the screen travels along *the screen* with a speed $w = c/\sin i$. This speed can approach infinity, ii i approaches 0. However, the energy travels along the screen only with the speed $V = c \sin i$. Hence, in this example, $wV = c^2$.

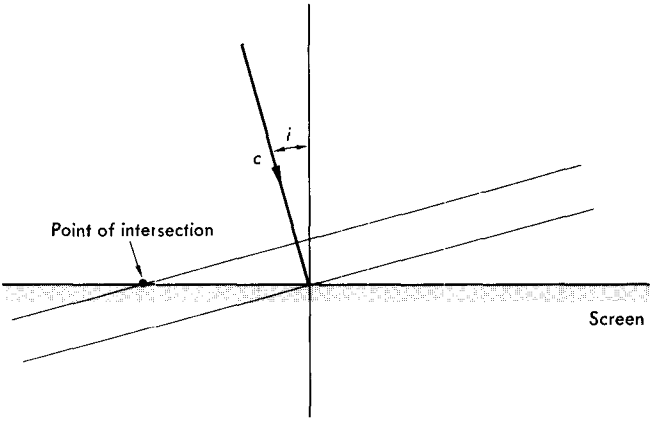


Figure 6.2. A plane wave hitting a screen obliquely.

From Equation (6.29) a useful relation between energy, momentum, wavelength and frequency of a particle can be derived. We know that $w = w/k$, $E = mc^2$, and $P = mV$. By means of these three relations, we can eliminate w, V and c^2 in $wV = c^2$. The result is $(\omega/k)(p/m) = E/m$, or

$$\frac{w}{k} = \frac{E}{P} \qquad (6.30)$$

.5 PARTICLE INCIDENT ON INTERFACE

The discussion above had to do with arbitrary particles (waves) traveling through free space, and we have established that for a wave of phase speed w to be associated with a particle of speed V, it is necessary that $wV = c^2$. Now we wish to show that relations of the form $p = hk$ and $E = \hbar\omega$, where A is a constant, are valid.

We can obtain more information about p and k by considering a situation in which the particle (wave) is incident on a piece of material which acts like a refractive medium for the wave. This refraction simply corresponds to a (change in phase speed. As far as the particle is concerned, the refraction takes place because the new region has a different constant potential energy U than the potential energy in free space. (We use U for potential energy here, since V is used for particle speed.) For electrons, for example, this situation could be realized approximately by letting an electron pass into a metal. Let's first treat the situation assuming we are dealing with particles. In Figure 6.3, $\mathbf{p}_1$ is the incident

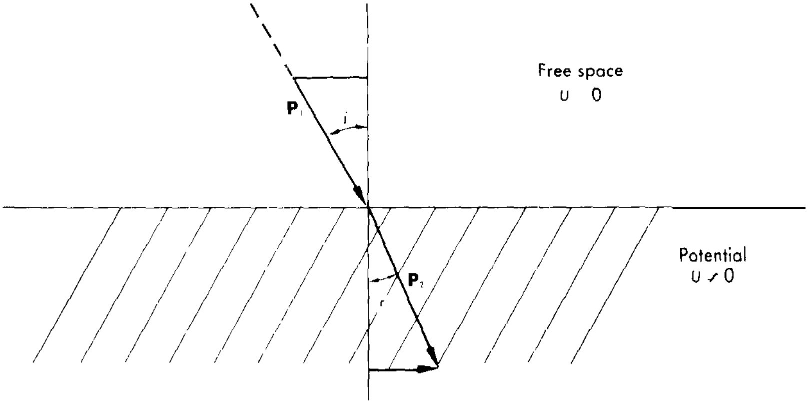


Figure 6.3. A particle passing from one region of constant potential energy into another of different potential energy.

momentum at an angle of i from the normal to the surface. The quantity $\mathbf{p}_2$ is the momentum after the particle passes into the region of constant potential energy, $U \neq 0$, at an angle r from the normal. The only force acting on the particle is one acting normal to the surface, as the particle passes the surface. There is no force acting parallel to the surface, so the components of $\mathbf{p}_1$ and $\mathbf{p}_2$ parallel to the surface are equal. In other words, the components of momentum, in the directions along which no force acts, are conserved. In terms of i and r, the angles of incidence and refraction, this can be written mathematically as

$$p_1 \sin i = p_2 \sin r \tag{6.31}$$

or

$$\frac{p_2}{p_1} = \frac{\sin i}{\sin r} \tag{6.32}$$

6.6 WAVE RELATION AT INTERFACE

Next, let us treat the situation assuming we are dealing with waves. In Figure 6.4, OA is a wavefront in free space, and A travels with speed w_1, from A

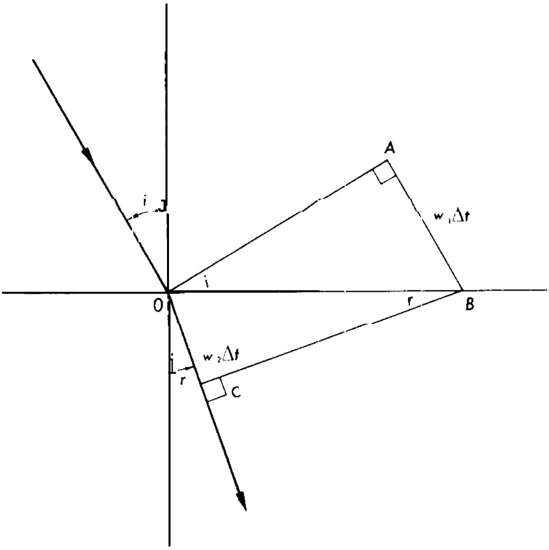


Figure 6.4. **A** wave passing from one medium into another, where the phase speed is different, changes direction by Huyghen's principle.

to B in time Δt. Angles OAB and OCB are right angles, and side OB is common to both triangles. Thus, since angle $AOB = i$ and angle OBC = r, *we* have $w_2\Delta t$ = OB sin r and $w_1\Delta t = OB$ sin i. This latter set of equations can be written, by dividing out Δt and OB, as

$$\frac{w_2}{w_1} = \frac{\sin r}{\sin i} \tag{6.33}$$

If this result is applied to light waves, it is just Snell's law. The derivation is the same as that used in deriving Snell's law.

Combining the results of Equations (6.32) and (6.33), we can write

$$\frac{p_2}{p_1} = \frac{\sin i}{\sin r} \tag{6.34}$$

$$\frac{w_2}{w_1} = \frac{\sin r}{\sin i} \tag{6.35}$$

and therefore,

$$p_1w_1 = p_2w_2 \tag{15.36}$$

Thus, as the particle (wave) travels into the region of nonzero potential, the product pw remains constant. In terms of k and ω, w = wk, so the product $p\omega/k$ remains constant. Now if a linear boundary condition is assumed, such as assuming that the wave amplitude or its derivative is continuous across the surface, the frequencies ω_1 and ω_2 must be equal; otherwise, the amplitudes would get out of phase and the boundary condition could not be satisfied for all time. Although we do not yet know all the physical laws obeyed by de Broglie waves, it will be seen later that linear boundary conditions do exist and, therefore, the frequency remains the same. Hence, since $p\omega/k$ does not change in crossing the surface, the quantity p/k remains the same, or, in terms of p_1, p_2, k_1 and k_2,

$$\frac{p_1}{k_1} = \frac{p_2}{k_2}$$

6.7 DE BROGLIE RELATION

As the electron moves across an interface between two media, the ratio p/k remains constant. If it then moved into a third medium, p/k would still remain unchanged. Thus, no matter what the speed of the particle is, p/k will remain unchanged. Since p/k remains unchanged, we can write:

$$\boxed{p = \hbar k \qquad \text{de Broglie Relation}} \tag{6.37}$$

where $\hbar$ (read h bar) is a constant independent of speed. This is precisely the relation assumed by de Broglie. Since a general inertial frame of reference was used, this result is independent of the frame of reference and should be relativistically invariant. The theoretical discussion does not tell whether A depends on the kind of particle or is a constant independent of particle type. The answer to this question must be obtained by performing experiments on various particles. Experiments show that the constant is independent of particle type, and thus this $\hbar$ is the same as that discussed in connection with photons, with

$$\hbar = \frac{h}{2\pi} \tag{6.38}$$

a universal constant. One such experiment is discussed in the next section.

If de Brogiie waves carry momentum $p = \hbar k$, we can derive a corresponding relation between energy and frequency. It was shown that in free space, $\omega/k = E/p$ [see Equation (6.30)]. Thus, since $p = hk$,

$$\boxed{E = \hbar\omega \qquad \text{de Broglie relation}} \tag{6.39}$$

In terms of the frequency, $\nu = \omega/2\pi$, the energy can be written as:

$$E = 2\pi\hbar\nu = h\nu \tag{6.40}$$

If $E = \hbar\omega$ and $p = \hbar k$ in the inertial system R, then from the comparison of the transformation equations for energy and momentum with the transformations for **k** and w in Equations (6.19) through (6.22), the relation between E' and ω' in G must be

$$E' = \hbar\omega' \tag{6.41}$$

and the relation between p' and k' must be

$$p' = \hbar k' \tag{6.42}$$

The de Broglie relations are thus relativistically form-invariant.

Finally, if E = $\hbar\omega$ and p = Ak, then the invariant,

$$\frac{E^2}{c^2} - p^2 = m_0^2 c^2 \tag{6.43}$$

can be used to calculate the unknown constant C in Equation (6.24). The result is

$$\frac{\omega^2}{c^2} - k^2 = \left(\frac{m_0 c}{\hbar}\right)^2$$

From Equation (6.38), we see that for electrons the constant $m_0 c/\hbar$ is 27r divided by the Compton wavelength, $h/m_0 c$.

To summarize briefly the logical arguments leading to de Broglie's relations, if a particle has wave-like properties so that a wave of phase speed w is associated with the particle in Free space, then $wV = c^2$, where V is the particle or group speed. If these waves carry energy and momentum, with E = $\hbar\omega$ and p = $\hbar k$, then the transformation laws for k and ω are equivalent to those for p and E. So, instead of two different sets of transformation equations, there is only one set. Further, all these relations are relativistically form-invariant, provided the constant $\hbar$ has the same value in every other inertial frame.

6.8 EXPERIMENTAL DETERMINATION OF $\hbar$

De Broglie predicted that electrons would behave like waves with a wavelength λ = h/p. When these waves enter a crystal with regular lattice spacing, they should scatter and show interference, much as light does on a grating. These matter waves were demonstrated in 1927 by Davisson and Germer, who observed diffraction peaks in a beam of electrons scattered from a Nickel crystal. The experimental arrangement is diagramed in Figure 6.5. The hot cathode F emits electrons which are accelerated through the electron gun, which strike a crystal of Ni and are diffracted back at an angle ϕ into a detector. Knowing the accelerating potential V, one may compute the electrons' momentum, and knowing ϕ and the lattice spacing of Ni, one may compute the wavelength λ, or k = $2\pi/\lambda$. Hence, one can measure the value of $\hbar$ for electrons. The positions of the diffraction maxima are determined by constructive interference between waves scattered from different sets of parallel planes within the crystal. This is called Bragg diffraction.

In the next few paragraphs, we shall derive the relation between the diffraction angle ϕ and the wavelength λ_1 of the incident electrons. Anyone not interested in the details of this derivation should skip to the result in Equation (6.48).

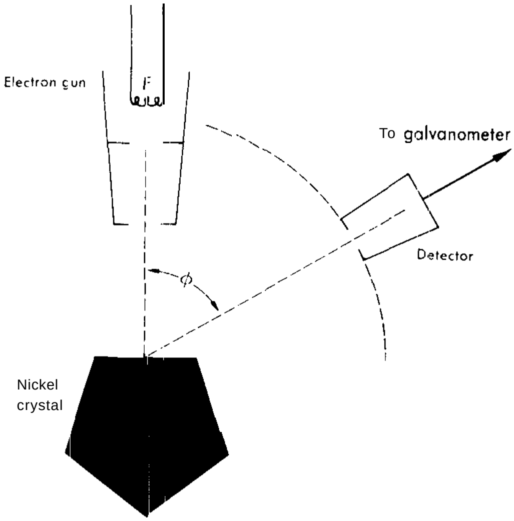


Figure 6.5. **The experimental arrangement in the electron diffraction experiments of Davisson and Germer.**

9 BRAGG EQUATION

Let the wavelength of the particles be λ_1 outside the crystal, and let the wavelength inside the crystal be λ_2. The wavelength is, in general, different inside the crystal, because the electron has different kinetic energy inside. The electrons are incident normally on the crystal surface and pass straight into the crystal. They then undergo Bragg diffraction from some set of parallel planes of atoms inside the crystal (See Figure 6.6). Let θ be the angle of incidence between the incoming beam and the normal to some set of parallel planes. We will first find the Bragg equation for diffraction maxima. Figure 6.7 is an enlarged picture of a portion of two atomic planes, P_1 and P_2. Lines A and B are two particle wave rays which reflect partially at O_2 on plane P_2 and at O_1 on plane P_1, respectively. For

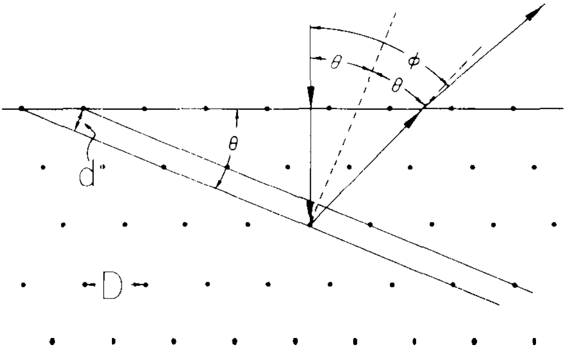


Figure 6.6. Incident and reflected electron beams near the surface of a nickel crystal in the Davisson-Germer experiment.

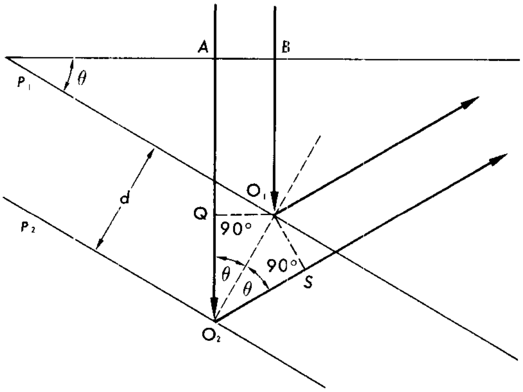


Figure 6.7. Beams incident on different partially reflecting parallel planes interfere due to different path lengths.

the two reflected rays to add constructively, the path difference, QO_2S, of the rays must be an integral number n times the wavelength λ_2. From triangle $O_2\,O_1$ Q, the distance QO_2 is d cos θ. The path difference is then twice this distance, or

$$QO_2S = 2d\cos\theta \tag{6.44}$$

Then the Bragg condition is $2d\cos\theta = n\lambda_2,\ n = 1, 2, \ldots$

The most intense diffraction peaks will occur due to reflections from planes rich in atoms. It is found that the dominant diffraction comes from the planes indicated in the diagram of Figure 6.6, where the dots indicate lines normal to the paper containing nickel atoms. The distance D between planes of densest packing in the diagram is D = 2.15 Angstroms for nickel. The spacing between diffracting planes can be expressed in terms of the distance D between atoms in the crystal, For the two parallel planes in the diagram, in terms of θ,

$$d = D\sin\theta \tag{6.45}$$

Therefore, for Bragg diffraction, in terms of D and the angle 2θ ($2\cos\theta\sin\theta = \sin 2\theta$),

$$n\lambda_2 = D\sin 28 \tag{6.46}$$

6.10 DIFFRACTION OF ELECTRONS

The diffracted electrons come back toward the crystal surface; their angle of incidence on the surface is $i = 2\theta$, and their angle of refraction is ϕ, the angle of observation, as shown in Figure 6.8. From Equation (6.33), there will be a wavelength change when the electrons pass back into the free-space region. Since the frequency does not change, from Snell's law,

$$\frac{\lambda_1}{\lambda_2} = \frac{\lambda_1\nu}{\lambda_2\nu} = \frac{w_1}{w_2} = \frac{\sin\phi}{\sin 28} \tag{6.47}$$

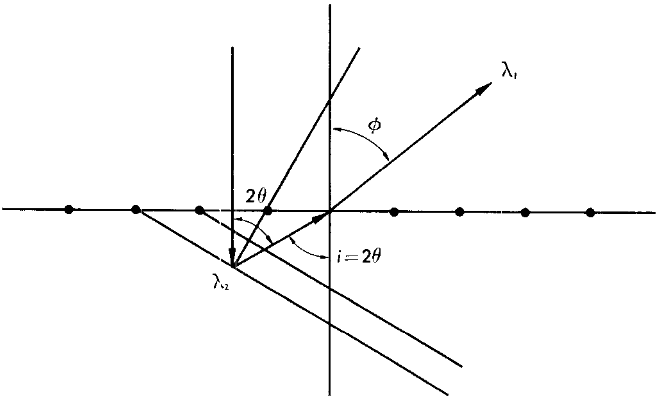


Figure 6.8. When the electron wave exits from the crystal, its angle of incidence is 26’ and the angle of refraction is ϕ, the angle of observation.

Eliminating λ_2 and θ from equations (6.46) and (6.47), we obtain

$$n\lambda_1 = D \sin \phi \tag{6.48}$$

Equation (6.48) can be used to experimentally determine the wavelength. The quantity λ_1 is the wavelength outside the crystal, i.e. it is the wavelength of the incident electrons. The angle ϕ is the angle of observation of the diffracted electron beam and n, which is the order of the diffraction peak, will be equal to 1 in this case.

In Figure 6.9 are the experimental results. The intensity is plotted for various accelerating voltages V (in volts) in polar coordinates. It is seen that a diffraction maximum occurs when V = 54 volts and ϕ = 50”. These results may be used to calculate the constant, $2\pi\hbar$. The lattice spacing D of nickel is known from x-ray diffraction analysis to be 2.15 Angstroms. Taking n = 1 in Equation (6.48) for the first order maximum, we find for the wavelength:

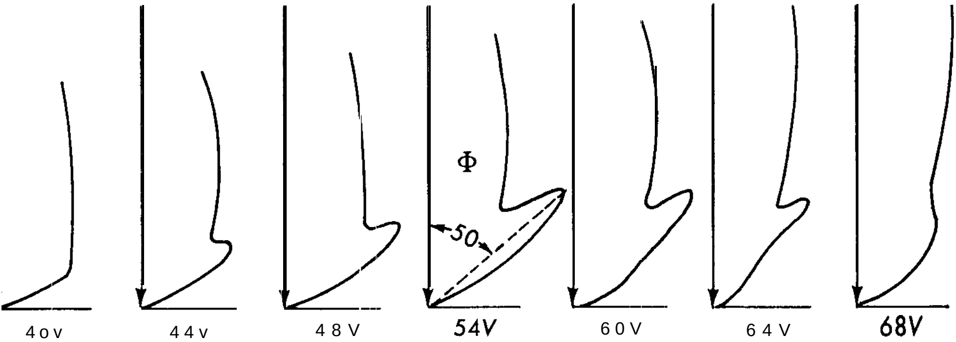


Figure 6.9. Curves, plotted in polar coordinates, showing the intensity of the scattered beam at different angles of scattering.

$$\lambda_1 = 1.65 \times 10^{-10} \text{ meters} \tag{6.49}$$

Next we calculate the momentum, knowing that the accelerating potential was 54 V. So the electron's energy was 54 eV, which is much smaller than the rest energy. Hence, we can use the nonrelativistic kinetic energy change to find the momentum:

$$\frac{p^2}{2m_0} = eV, \quad \text{or} \quad p = \sqrt{2m_0eV} \tag{6.50}$$

Using e = 1.6 x 10^{-19} coul, $m_0 = 9.11 \times 10^{-31}$ kg, the result is:

$$p \simeq 3.97 \times 10^{-24} \text{ kg m/sec} \tag{6.51}$$

The numerical value of $2\pi\hbar$ for this case is obtained from $p = \hbar k = 2\pi\hbar/\lambda$ or $\lambda p = 2\pi\hbar$, and we find:

$$\begin{aligned} 2\pi\hbar &= (3.97 \times 10^{-24}) \times (1.65 \times 10^{-10}) \text{ j-sec} \\ &= 6.55 \times 10^{-34} \text{ j-sec} \end{aligned} \tag{6.52}$$

Within experimental accuracy this value of $2\pi\hbar$ is equal to the value of $2\pi\hbar$ we would have obtained if we were dealing with photons where λp = h, Planck's constant. In their original experiment, Dovisson and Germer observed about 30 diffraction peaks under varying conditions of detector orientation and incident electron energy; these experiments, as well as others using neutrons, protons, electrons, etc., show the same numerical value for $2\pi\hbar$ as we obtaineol here. Thus, nature appears to be such that instead of several constants relating momentum and wavelength, there is only one universal constant, Planck's constant h. Hence, experimentally, in terms of Planck's constant,

$$\boxed{2\pi\hbar = h \qquad \text{Planck's constant}} \tag{6.53}$$

In fact, usually $\hbar$ is defined as an abbreviation for the symbol $h/2\pi$.

In terms of h, the wavelength of an electron can be computed from the de Broglie relation, $\lambda = h/p$, just as for a photon.

example 1. A particle has a mass of 1 kg and a speed of 30 m/sec, about like a softball. What is the wavelength of the de Broglie wave associated with the particle?

solution The momentum is mv = 30 kg-m/sec. Then the wavelength, using h = 6.63×10^{-34} j-sec, is

$$\lambda = \frac{h}{p} = 2.61 \times 10^{-34} \text{ meters}$$

A wavelength as small as 10^{-34} meters could never be measured in a direct experiment because the smallest diffraction gratings available are crystals, which have a grating space of about 10^{-10} meters.

example 2. Neutrons have a mass of 1.675 x 10^{-27} kg. Slow neutrons coming out of a nuclear reactor have kinetic energies of about T = 0.0466 eV. What is the wavelength of such a thermal neutron?

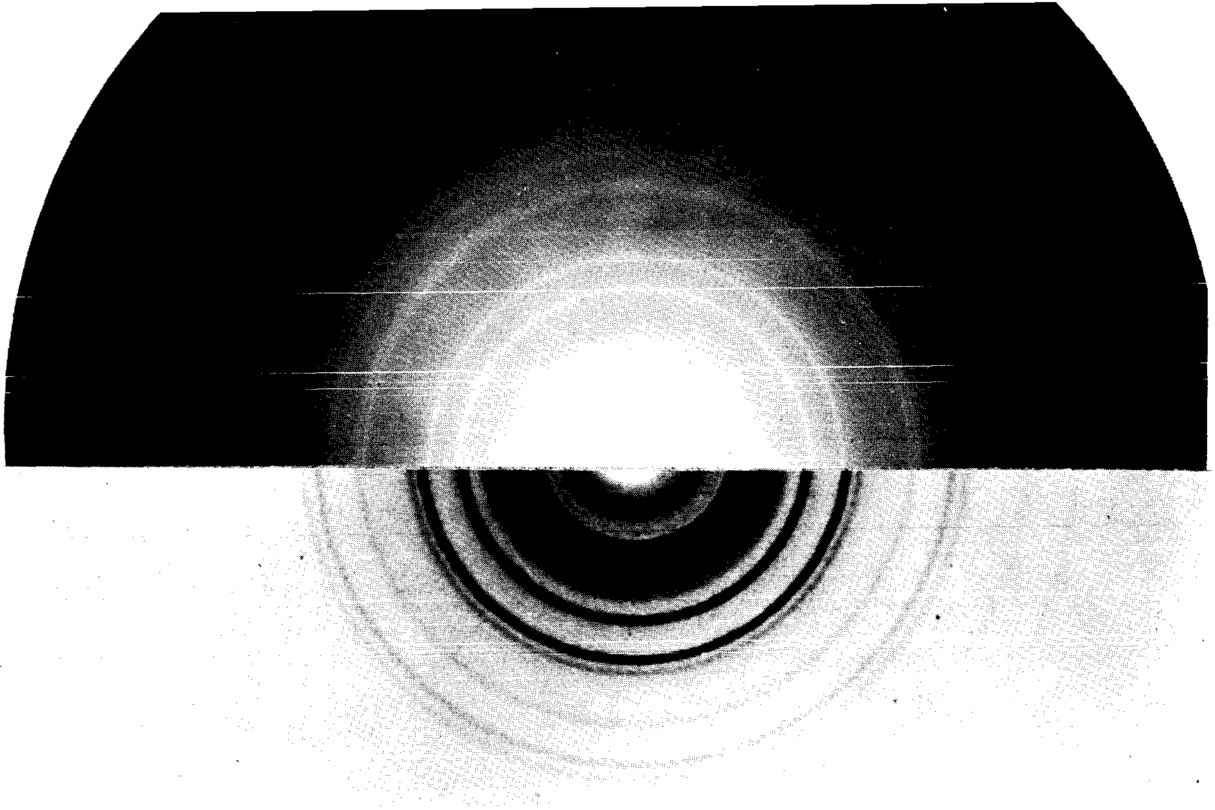


Figure 6.10. Superposition of two photographs of diffraction patterns produced by beams of particles passing through polycrystalline aluminum. The upper half of the photograph is the pattern produced by diffraction of a monoenergetic electron beam; the lower half is the pattern produced by x rays. The appearance of diffraction rings of similar radius is a direct demonstration of the wave nature of electrons. The slight discrepancies in the radii of the rings results from the use of electrons and x rays of different wavelengths.

solution The nonrelativistic expression for kinetic energy may be used, hence $p = \sqrt{2m_0T} = 5.00 \times 10^{-24}$ j-sec. Then

$$\lambda = \frac{h}{p} = 1.33 \text{ Å}$$

This wavelength is comparable to crystal atom spacings, and could therefore be observed.

6.11 UNCERTAINTY PRINCIPLE FOR PARTICLES

We have seen how particles of energy E and momentum p have associated with them waves of frequency ν and wavelength λ. Hence, one could measure the energy of a particle by measuring ν, or one could measure p by measuring λ. When we discussed light waves earlier, we saw that in a single measurement which lasted over a time Δt, an inevitable uncertainty $\Delta\nu$ in the measured frequency would be present. This uncertainty was such that, to within an order of magnitude, $\Delta\nu\Delta t \simeq 1$. Since $E = h\nu$, in terms of the uncertainty of energy, ΔE, the product of ΔE and Δt must be $\Delta E\Delta t \simeq h$. Similarly, for a measurement of momentum in a single measurement which takes place over a spatial interval Δx, the uncertainty in momentum Δp for a light wave is given by

$$\Delta p\Delta x \simeq \frac{\hbar}{2} \qquad (15.54)$$

These considerations were based principally on the wave nature of light and did not depend on the wave speed. In a similar way, particles have de Broglie waves associated with them, with energy related to frequency, and momentum related to wavelength in just the same way as for light. So we would expect an uncertainty principle for matter waves similar to that for light.

6.12 UNCERTAINTY AND SINGLE-SLIT DIFFRACTION

Due to their wavelike nature, particles can undergo diffraction. To illustrate the uncertainty principle for particles, imagine, for example, a beam of particles represented by a plane wave propagating in the $+x$ direction, as in Figure 6.11.

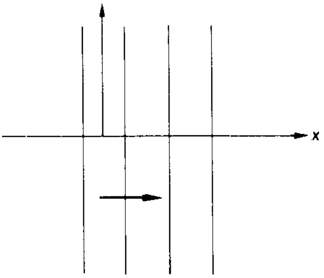


Figure **6.11.** A beam of particles traveling in the x direction is represented by a plane wave propagating in the x direction.

In this plane wave, the amplitude or wavefunction, by definition, does not depend on y or z, so the particles in the wave all have y components of momenta equal to zero. However, since the wavefunction does not depend on y, one knows nothing about the y coordinates of the particles. There is just as likely to be a particle at y = + 1 lm as at y = Om. So if the uncertainty in the y position of the particle is Δy, $\Delta y = \infty$. The y momentum, however, is definitely known: $p_y = 0$, so the uncertainty in y momentum is $\Delta p_y = 0$.

Let us imagine making a measurement of y position. This we could do by putting a slit of width a in the path of the beam of particles, as in Figure 6.12. Then

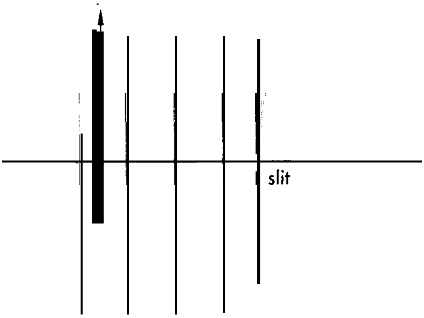


Figure **6.12. A slit placed in the path of the particle beom causes the particles passing through the slit to have their y positions measured to an accuracy of $\Delta y \cong$ the slit width.**

only those particles will get through whose y positions are somewhere inside the slit. Thus, all particles passing through have had their y coordinates measured to within an accuracy equal to a, the width of the slit. For these particles, the uncertainty Δy is then roughly,

$$\Delta y \cong a \qquad \textbf{(6.55)}$$

On passing through the slit, the particles will be diffracted due to their wavelike character. Experimentally, it is found that upon using a beam of many electrons, a single-slit diffraction peak is observed which has the same form as that observed for light. Most of the particles will go into the central diffraction peak as illustrated in Figure 6.13. Thus, in order to account for the particles going other than in the straightforward direction, we must assume that the particles will have acquired some indefinite amount of y momentum in passing through the slit. To make a rough estirnate of the uncertainty in this momentum, Δp_y, let us assume that all the particles go into the central diffraction peak. Then the maximum magnitude of the momentum p_y, such that a particle goes into this region, is roughly equal to the uncertainty Δp_y in y momentum. From the diagram, if $p = h/\lambda$, and θ is the position of the first diffraction minimum, it follows that, in terms of θ,

$$p_{y_{max}} = \frac{h}{\lambda} \sin\theta \qquad (6.56)$$

and so,

$$\Delta p_y \cong \frac{h \sin\theta}{\lambda} \qquad \textbf{(6.57)}$$

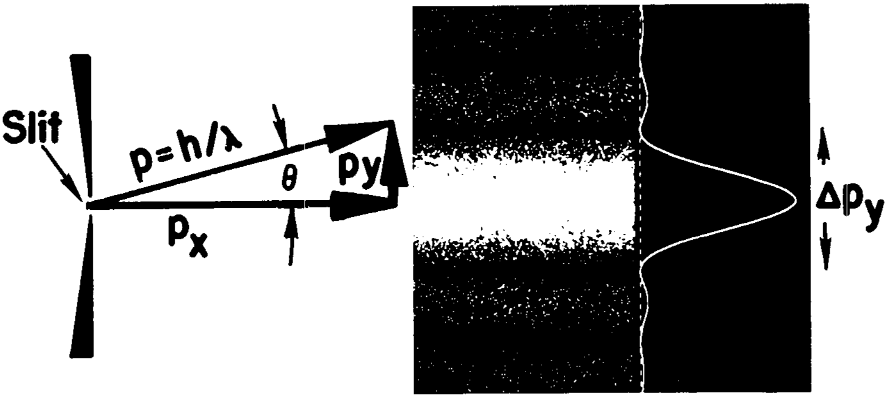


Figure 6.113. A beam of particles passing through a slit gives rise to a single-slit diffraction pattern.

But from the study of single-slit diffraction, it is known that the first diffraction minimum occurs at

$$\tfrac{1}{2}\lambda = a\sin\theta \quad\text{or}\quad a = \frac{\lambda}{2\sin\theta} \tag{6.58}$$

Thus, combining this result with Equation (6.57), we find that

$$\Delta p_y \cdot a \cong \frac{h\sin\theta}{\lambda}\cdot\frac{\lambda}{2\sin\theta} \simeq \frac{h}{2} \tag{6.59}$$

Since a is the uncertainty in y position, $a \simeq \Delta y$, we obtain the following rough uncertainty relation:

$$\Delta p_y \Delta y \simeq \frac{h}{2}$$

which is of the order of magnitude of li.

In this hypothetical measurement of y position of a particle, an uncertainty in y momentum is introduced by the measurement process. More rigorous calculations show that the correct uncertainty relation is

$$\Delta p_y \Delta_y \geq \frac{\hbar}{2}$$

In general, it can be shown that there is one such relation for each coordinate of a particle, so we also have for the uncertainties, Δp_z and Δz, the relation $\Delta p_z\, \Delta z \geq$ ½ A, and similarly for Δp_x and Δx. As in the uncertainty principle for light, the uncertainties, Δx, Δp_x, etc. are defined to be the root mean square deviations from the mean. In our discussion above we used only order of magnitude values for Δy and Δp_y. Analyses of other kinds of measurements always show that there are uncertainties in momentum and position connected by the above relations.

13 UNCERTAINTY IN BALANCING AN OBJECT

To illustrate one effect of the uncertainty principle, consider the problem of balancing an icepick on its point. Let the icepick be an ideal one **consisting of a single** particle of mass m concentrated at the position of the center of mass of the icepick, with its point a distance ℓ away. (Reasonable values for m and ℓ are m = 100 g, and ℓ = 20 cm.) Classically, to balance the icepick one has to place the particle exactly **above the point** of contact of the point with the tabletop, and one also has to place the particle at rest. If the particle is not at rest, the icepick will fall over because of the initial velocity. If the particle is not exactly over the point of contact, gravity will make it fall over. This means that to balance an icepick, both the position and momentum of the particle must be exactly determined. However, according to the uncertainty principle, both the position and the momentum cannot be determined precisely at the same time, so if the position of the particle is such that the particle lies exactly over the point, then $\Delta p \simeq \hbar/2\Delta x \simeq \hbar/0$. The uncertainty in momentum of the particle will become very large; and hence the momentum will likely be large, so the icepick will fall over. If the particle is exactly at rest, then the position of the particle is undetermined, so gravity will make the icepick fall over. (See Figure 6.14.) Thus, it is impossible to balance an icepick on its point! It is not too hard to calculate roughly the average time one can expect to keep the icepick on its point if one starts with the smallest possible $\Delta x \Delta p$; it is approximately

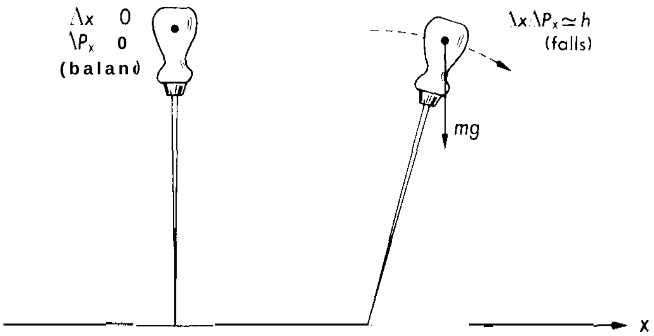


Figure 6.14. The uncertainty principle implies that an icepick cannot be balanced on its point, for both position and momentum of the center of moss would then have to be definitely known, which contradicts the uncertainty principle.

$$\frac{1}{4}\sqrt{\frac{\ell}{g}}\ \ln\left(\frac{m^2 g \ell^3}{\hbar^2}\right)$$

or about 5 seconds with the reasonable choice of ℓ and m **given above (see** Problem 6.15).

4 ENERGY-TIME UNCERTAINTY

It is also ordinarily true for particles, as well as for light waves, that $\Delta E \Delta t \simeq \hbar$. One way to interpret this is as follows. Suppose a wavetrain, illustrated in Figure

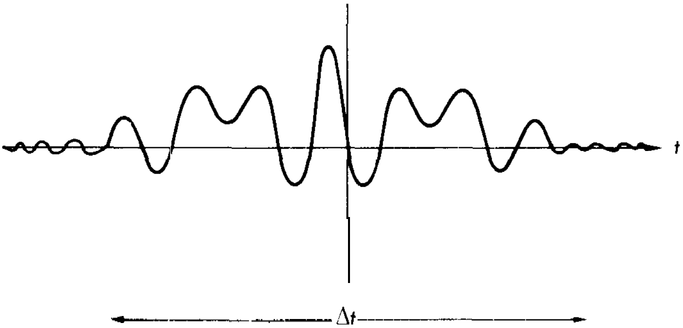


Figure 6.15. Amplitude of a wave train passing an observer in time Δt.

6.15, passes the position of the observer, and that the wave train lasts for a time Δt. Then it is impossible to associate a definite frequency with that wave train, since it lasts only for a finite time. The train can be thought of as a superposition of waves of many frequencies and the spread in frequencies $\Delta\nu$ is roughly given by $\Delta\nu\Delta t \simeq 1/2\pi$. Since the corresponding spread in energies is $\Delta E = h\Delta\nu$, then to within an order of magnitude, $\Delta E\Delta t \simeq h$. For example, nuclear interactions may sometimes be thought of as due to an exchange of π mesons. If the mesons exist only for a time 10^{-23} sec, then for $\Delta E\Delta t \cong \hbar/2$, the uncertainty in their energy would be roughly 5×10^{-10} joules, or in electron volts, 3×10^{9} eV.

example If a hydrogen atom with a diameter of about 10^{-10} m moves at about 10^{3} m/sec, considered as a wave train, it takes about 10^{-13} sec to pass by an observer; then the spread in frequencies of the wave train is in order of magnitude about 10^{13} sec^{-1}. The uncertainty in energy is roughly,

$$\frac{\hbar}{10^{-13}} = \frac{10^{-34}}{10^{-13}} = 10^{-21} \text{ joules}$$

In electron volts, this uncertainty in energy is $10^{-21}/1.6 \times 10^{-19} = 0.006$ eV. This uncertainty may be compared to the average thermal energy of an atom in a gas of hydrogen atoms at room temperature, around 293 K, which is k_BT, with $k_B = 1.38 \times 10^{-23}$ j/K. The uncertainties are about the same to within an order of magnitude.

6.15 PROBABILITY INTERPRETATION OF WAVE FUNCTIONS

Since particles have waves associated with them, one might expect a wavefunction ψ to exist which could be used to describe whatever quantity it is in a particle which is wavelike. One should be able to describe such phenomena as diffraction through a slit in terms of this wave function. If one performs a single slit diffraction experiment with a beam of electrons, in which the intensity of the beam is so low that only one electron should go through the slit system at a time, then the electrons as they pass through seem to go randomly in various directions. Thus, it appears that we cannot predict exactly where any one electron will go. However, it is found experimentally that after observing many electrons, the probability with which they go into some small range of directions is just proportional to the calculated diffraction intensity for waves. For light waves, the same thing happened; the diffraction intensity was found experimentally to be proportional to the probability of finding a photon in the small range of angles. In that case, if ψ is the wavefunction describing the light wave at the screen, the intensity is proportional to $|\psi|^2$. It is thus natural to assume that for a particle there exists a wavefunction ψ such that $|\psi|^2$ is proportional to the probability of finding a particle near a point.

Thus, one cannot predict the position of any one particle, but with the wave amplitude, ψ, one can say that the squared magnitude $|\psi(\theta)|^2$ times some range $d\theta$ of the continuous variable θ is proportional to the probability of finding a particle in the range of positions $d\theta$. Therefore, ψ for particles is called a *probability* amplitude. No better interpretation has ever been found for ψ.

Suppose we had a double slit set up so that, as in Figure 6.16 at the observation point P at θ, the probability amplitude for finding a particle is ψ_1 when

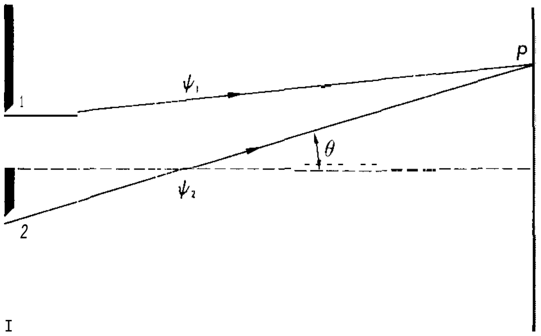


Figure 6.16. Wavefunctions ψ_1 and ψ_2 from two sources add at P.

slit 1 only is open, and ψ_2 when slit 2 only is open. When both slits are open, it is observed experimentally that if the beam intensity is high, so that there are many particles incident on the slits, then the usual double-slit intensity pattern is seen. If the beam intensity is so low that only one particle at a time can go through the slits, then the individual particles passing through go off in various directions. However, after observing for a long time, it is found that the probability with which they go into some range of directions $d\theta$ is just proportional to the calculated diffraction intensity for waves. We may conclude that these waves obey Huygen's principle, and that they obey the principle of superposition. Then to explain mathematically the double-slit diffraction pattern which is actually observed when both slits are opened, the total probability amplitude at P must be

$$\psi = \psi_1 + \psi_2 \tag{6.24}$$

and the probability for finding a particle in $d\theta$ will be, in terms of ψ_1 and ψ_2, proportional to $|\psi_1 + \psi_2|^2 d\theta$. If we have a wavefunction or probability amplitude $\psi(x)$ which is a function of the single position variable x, then the wavefunction can be used to calculate the probability density, so that the probability of finding a particle in the range dx will be given by $|\psi|^2 dx$. Summarizing the properties of the wavefunction ψ which describes the wavelike properties of a particle, we can say:

(1) The wavefunction $\psi(x)$ is called a ***probability*** amplitude because the absolute magnitude squared of the wavefunction $|\psi(x)|^2$, times the differential dx, is proportional to the probability of finding a particle within the range of coordinates dx.

(2) The probability amplitude obeys the principle of superposition: e.g., if ψ_1 (x) and $\psi_2(x)$ are the wavefunctions when slit 1 only is open and when slit 2 only is open, respectively, then when both slits are open, the wavefunction is the sum ψ_1 (x) + $\psi_2(x)$, and the probability of finding a particle in ***dx*** is proportional to

$$|\psi_1(x) + \psi_2(x)|^2 dx$$

6.16 EIGENFUNCTIONS OF ENERGY AND MOMENTUM OPERATORS

Since particles have wavelike character, in effect, it is possible for a particle to go through both slits of a double slit system, and interfere with itself in doing so. This is a type of behavior which is impossible to explain on the basis of simple mechanical laws of the type, $\mathbf{F} = d\mathbf{p}/dt$. Therefore, we must find an equation which describes the behavior of these probability waves. This equation should be a wave equation of some kind, but in situations where $\hbar$ can be considered to be negligibly small, it should predict the same results as ordinary mechanics based on $\mathbf{F} = d\mathbf{p}/dt$. We shall now discuss this wave equation.

There are a number of criteria that the wave equation must satisfy, which will give us some clues as to what form the equation must have. For example, the equation must be consistent with the previously discussed wave properties of particles moving through free space and passing into a refractive medium. Also, it must agree with Newtonian mechanics in some limit. We will obtain the wave equation by analogy with the equations of motion of ordinary mechanics.

Let us first try to find a wavefunction ψ which corresponds to a beam of particles of exactly known momentum. This function will be called a momentum ***eigenfunction,*** and the corresponding value of momentum will be called the momentum *eigenvalue.* Thus, consider a wavefunction describing a beam of particles which are traveling with exactly known momentum in the positive x direction. In this hypothetical situation, the uncertainty in x momentum is zero; so by the uncertainty principle, the uncertainty Δx in the x positions of the particles is infinite. Hence, the particles are spread out all along the x axis. If there are no spatial boundary conditions such as reflecting walls, which could make some x coordinates preferred over others, and if the particle beam is prepared so that it is of uniform intensity, then there should be a completely uniform distribution of particles along the x axis. Thus, the particles must be distributed with equal probability everywhere along the x axis, and the square of the wavefunction, $|\psi(x,t)|^2$, must be a constant, independent of x.

This means, for example, that $\psi(x,t)$ could not be of the form of a sine or cosine function, because then $|\psi(x,t)|^2$ would be a varying function of x. However, $\psi(x,t)$ could be of a complex exponential form, say:

$$\psi = Ae^{i\Phi(x,t)} \tag{6.60}$$

where A is a constant. This satisfies $|\psi|^2 = |A|^2 =$ constant. If this function is to describe a wave with phase speed w traveling in the positive x direction, the phase $\Phi(x,t)$ must be of the form:

$$\Phi(x,t) = f(x - wt) \tag{6.61}$$

where, so far, *f* is some arbitrary function. Therefore,

$$\psi = Ae^{if(x-wt)} \tag{6.62}$$

We also know that the particle speed must be equal to the group speed of this wave. Then, if the function ψ corresponds to an exactly known group speed, the momentum will be known exactly. In Chapter 1 the expression $v_g = d\omega/dk$, for group speed, was derived for a packet of sinusoidal waves grouped closely about a central frequency, $\nu = \omega/2\pi$. The expression $v_g = d\omega/dk$ becomes exact in the limit as the frequency spread approaches zero. Hence, for a packet of known momentum, we need to consider a wave of definite frequency, but with zero frequency spread. A phase $f(x - wt) = kx - \omega t = 2\pi(x/\lambda - \nu t)$ would then correspond to an exactly known group speed and hence to an exactly known momentum. Let us check that this group speed is correct. Since $\omega^2 - k^2c^2$ is a constant, using $E = \hbar\omega$, $p = \hbar k$, we have

$$v_g = \frac{d\omega}{dk} = \frac{kc^2}{\omega} = \frac{\hbar kc^2}{\hbar\omega} = \frac{pc^2}{E} = \frac{mVc^2}{mc^2} = V \tag{6.63}$$

for a particle with energy mc^2 and momentum mV. The wavefunction then takes the form:

$$\psi = Ae^{i(kx-\omega t)} \tag{6.64}$$

Since the connection between momentum and wavelength is $p = h/\lambda$, and that between energy and frequency is $E = h\nu$, the above wavefunction could be written in terms of momentum p and energy E as follows:

$$\psi = Ae^{i(2\pi/h)(px-Et)} \tag{6.65}$$

or

$$\psi = Ae^{i(px-Et)/\hbar} \tag{6.66}$$

This wavefunction represents a wave of definite wave length, traveling in the x direction, which means that the x component of momentum is definitely known.

We see that the wavefunction $\psi = Ae^{i(px-Et)/\hbar}$ satisfies all the requirements for it to represent a beam of particles of definite x momentum. Only a complex wavefunction of this form can have the correct probability interpretation— that $|\psi|^2$ is a constant representing particles whose positions are completely unknown. Also, the frequency is definite, which means that the particle velocity V, which equals the group speed v_g , has a definite value.

6.17 EXPECTATION VALUES FOR MOMENTUM IN A PARTICLE BEAM

In practice, waves will usually consist of superpositions of perhaps many different frequencies, and hence many different momenta. We might be interested in the average value, or expectation value, of the momentum. To see how this may be calculated, suppose there were two sources of particles, as in Figure 6.17, each producing uniform beams traveling in the x direction, with ψ_1 the wavefunction from source 1 when source 2 is off, and ψ_2 the wavefunction from source 2 when source 1 is off. Then the total wavefunction ψ_T when both sources 1 and 2 are on is, by the principle of superposition,

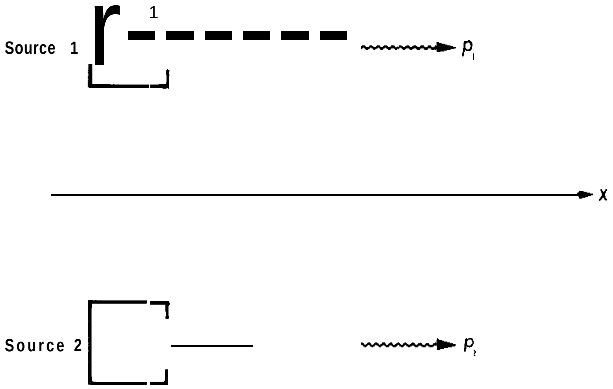


Figure 6.17. Consideration of the superposition of two beams of particles of different momenta gives rise to differential operators representing observable physical quantities.

$$\psi_T = \psi_1 + \psi_2 \tag{6.67}$$

The probability of finding a particle in dx with both sources turned on would be equal to

$$|\psi_1 + \psi_2|^2 dx$$

This interpretation must still be valid, even when the sources do not produce electron beams of the same momentum. So let us assume the individual wavefunctions are:

$$\psi_1 = A_1 e^{i(p_1x-E_1t)/\hbar}, \quad \psi_2 = A_2 e^{i(p_2x-E_2t)/\hbar} \tag{6.68}$$

where A_1 and A_2 are constants. Then $|A_1|^2 dx$ would be the probability of finding a particle of momentum p_1 in dx when source 2 is turned off. Similarly, $|A_2|^2 dx$ is the probability of finding a particle of momentum p_2 in dx when source 1 is turned off. The total probability of finding a particle in some interval $0 \le x \le L$ when both sources are on would be proportional to

$$\int_0^L |\psi_1 + \psi_2|^2 dx = \int_0^L dx\{|\psi_1|^2 + |\psi_2|^2 + \psi_1^*\psi_2 + \psi_2^*\psi_1\} \tag{6.69}$$

In this expression, the asterisks mean complex conjugates. Consider these integrals one at a time. In calculating $|\psi_1|^2$, all the x and t dependence goes out, because $|e^{i(p_1x-E_1t)/\hbar}|^2 = 1$. So,

$$\int_0^L dx\,|\psi_1|^2 = |A_1|^2 L \tag{6.70}$$

Similarly,

$$\int_0^L dx\,|\psi_2|^2 = |A_2|^2 L \tag{6.71}$$

However, when calculating an integral like:

$$\int_0^L dx\,\psi_1^*\psi_2 = \int dx A_1^* A_2 \exp\left[\frac{i(-p_1 + p_2)x}{\hbar} + \frac{i(E_1 - E_2)t}{\hbar}\right] \tag{6.72}$$

if we assume L to be large and p_1 is not equal to p_2, then the exponential will oscillate so that on the average the x integral will be zero. (This is in agreement with the general considerations in Appendix 2.) We shall assume this happens here. Then, for large L, we have:

$$\int_0^L dx\{\psi_1^*\psi_2 + \psi_2^*\psi_1\} = 0 \tag{6.73}$$

Thus the total probability of finding a particle in the interval $0 \le x \le L$ is equal to

$$\int_0^L |\psi_T|^2 dx = L(|A_1|^2 + |A_2|^2) \tag{6.74}$$

This is just the sum of the probabilities for finding particles of the two momenta in the interval, as we might have expected.

Since $|A_1|^2$ is the probability of finding a particle of momentum p_1 in the interval, and $|A_2|^2$ is the probability of finding a particle of momentum p_2 in the interval, then the average value, or expectation value, of the momentum of this beam of electrons should be:

$$\langle p \rangle = \frac{p_1|A_1|^2 L + p_2|A_2|^2 L}{|A_1|^2 L + |A_2|^2 L} \tag{6.75}$$

In the above expression, the factors L all cancel out, so the expectation value of momentum reduces to:

$$\langle p \rangle = \frac{p_1|A_1|^2 + p_2|A_2|^2}{|A_1|^2 + |A_2|^2} \tag{6.76}$$

independent of the interval considered, provided it is sufficiently large.

6.18 OPERATOR FORMALISM FOR CALCULATION OF MOMENTUM EXPECTATION VALUES

Now we shall demonstrate a simple formal way to calculate expectation values which agree with the expression in Equation (6.76), using the wavefunction ψ. Consider the wavefunction ψ_1 , which has a definite momentum p_1 . Let us differentiate the exponential function $\psi_1 = A_1 \exp [i(p_1 x \quad E_1 t)/\hbar]$ with respect to x, keeping t constant. Since for any constant a, we have

$$\frac{\partial}{\partial x} e^{ax} = a e^{ax} \tag{6.77}$$

it follows that

$$\frac{\partial}{\partial x} \psi_1 (x, t) = \frac{i p_1}{\hbar} \psi_1 (x, t) \tag{6.78}$$

We may write this last equation as

$$\frac{\hbar}{i} \frac{\partial}{\partial x} \psi_1 (x, t) = p_1 \psi_1 (x, t) \tag{6.79}$$

The constants h/i, multiplied by the x derivative of ψ, have the effect of multiplying ψ by a number equal to the x component of momentum. If $\frac{\hbar}{i}\frac{\partial}{\partial x}\psi_1 = p_1\psi_1$, where p_1 has exactly the same numerical value for all values of x and t, then we can say that the wavefunction represents a state of definite momentum. If the effect of the differential operator $(\hbar/i)(\partial/\partial x)$ on the wavefunction were to give something other than $p_1 \psi_1$, then we could not say that the x momentum had the value p_1.

The operator $(\hbar/i)(\partial/\partial x)$ is ordinarily called the p_x operator, or momentum operator, or $p_{x_{op}}$. When this operator acts on a function and gives a constant times the ***same function,*** the function is called an ***eigenfunction*** of the momentum operator. The constant is called an ***eigenvalue.***

example Which of the following functions are eigenfunctions of $p_{x_{op}}$, and what are the corresponding eigenvalues? (a) $\psi_a = \sin kx$; (b) $\psi_b = \exp(-6\pi ix/L)$; (c) $\psi_c = \ln(x/L)$.

solution Only ψ_b is a momentum eigenfunction:

$$\frac{\hbar}{i}\frac{\partial \psi_b}{\partial x} = \frac{\hbar}{i}\left(-\frac{6\pi i}{L}\right)\psi_b = -\frac{6\pi\hbar}{L}\psi_b$$

So the eigenvalue is $p_b = -6\pi\hbar/L$. ψ_a and ψ_b are not eigenfunctions, because when differentiated they do not yield a constant times the same wavefunction:

$$\frac{A}{i}\frac{\partial \psi_a}{\partial x} = \frac{\hbar k}{i} \cos kx \neq \text{const.} \times \psi_a$$

$$\frac{\hbar}{i}\frac{\partial\psi_c}{\partial x} = \frac{1}{x} \neq \text{const.} \times \psi_c$$

The eigenvalues p_a and p_b corresponding to ψ_a and ψ_b therefore, do not exist.

In the case of Figure 6.17, with superimposed beams of different momenta, if the momentum operator acts on the total wavefunction,

$$\psi_T = \psi_1 + \psi_2 = A_1 e^{i(p_1x-E_1t)/\hbar} + A_2 e^{i(p_2x-E_2t)/\hbar} \tag{6.80}$$

then it does not give just a number times ψ_T; instead, the effect is:

$$p_{x_{op}}\psi_T = \frac{\hbar}{i}\frac{\partial}{\partial x}(\psi_1 + \psi_2) = p_1\psi_1 + p_2\psi_2 \tag{6.81}$$

Hence $\psi_1 + \psi_2$ is not a momentum eigenfunction. Now, multiplying the above equation on the left by ψ_T^* and integrating from 0 to L, we get:

$$\int_0^L dx\psi_T^* p_{x_{op}}\psi_T = \int_0^L dx\{p_1|A_1|^2 + p_2|A_2|^2 + \psi_1^* p_2\psi_2 + \psi_2^* p_1\psi_1\} \tag{6.82}$$

When we integrate over some large length l, the righthand side of this equation has two terms which average to zero, because if $p_1 \neq p_2$, they oscillate sinusoidally with changing x. Then the remaining two terms give:

$$\int_0^L dx\psi_T^* p_{x_{op}}\psi_T = L(p_1|A_1|^2 + p_2|A_2|^2) \tag{6.83}$$

Thus, from Equation (6.26), we have:

$$\frac{\int_0^L dx\psi_T^* p_{x_{op}}\psi_T}{\int_0^L dx\psi_T^*\psi_T} = \frac{p_1|A_1|^2 + p_2|A_2|^2}{|A_1|^2 + |A_2|^2} \tag{6.84}$$

This is just the expectation value of momentum given in Equation (6.76). Thus, expectation values may be written concisely in terms of operators. The procedure would still hold if the total wavefunction ψ were a superposition of many momenta rather than just two. Thus, in general, the average x component of momentum per particle for particles in the interval $0 \leq x \leq L$ is:

$$\langle p_x\rangle = \frac{\int_0^L \psi^* p_{x_{op}}\psi dx}{\int_0^L \psi^*\psi dx} \tag{6.85}$$

6.19 ENERGY OPERATOR AND EXPECTATION VALUES

Energy eigenfunctions con be discussed in a similar way. The wavefunction $\psi = \exp(ipx - iEt)/\hbar$ is a wavefunction representing particles of definite known energy. On differentiating partially with respect to time, keeping x constant, we get:

$$\frac{\partial}{\partial t}\psi = \left(\frac{-iE}{\hbar}\right)\psi \tag{6.86}$$

This equation could be written as:

$$i\hbar\frac{\partial}{\partial t}\psi = E\psi \tag{6.87}$$

Since this is true for all x and t, the wavefunction represents particles of definite energy E. We could define an energy operator on the basis of the above equation. It would be:

$$E_{\text{op}} = i\hbar\frac{\partial}{\text{at}} \tag{6.88}$$

A function is said to be an eigenfunction of an operator if the effect of the operator acting on the function is to give a constant-the eigenvalue—multiplying the function. An eigenfunction of the energy operator $i\hbar\partial/\partial t$ would be $Ae^{-iEt/\hbar}$.

Just as an expectation value of momentum could be written in terms of momentum operators, so can an expectation value of energy be written in terms of E_{op}. The expectation value of energy for particles in the region $0 \leq x \leq L$ when L is large, if the wavefunction is ψ and the energy operator is $i\hbar\partial/\partial t$, is given by:

$$\langle E\rangle = \int_0^L \psi^* i\hbar\frac{\partial}{\partial t}\psi\,dx \bigg/ \int_0^L \psi^*\psi\,dx \tag{6.89}$$

Clearly, if ψ is an eigenrtate of the energy operator, then the expectation value of E is equal to the corresponding eigenvalue. An expression such as (6.89) can be interpreted in terms of probabilities; if $P(x)dx$ is the probability of finding a particle in dx, then the average of some property f(x) is just

$$\langle f\rangle = \frac{\int P(x)f(x)dx}{\int P(x)dx} \tag{6.90}$$

In this case, $\int P(x)dx$ is analogous to $\int\psi^*\psi dx$, so P(x) is analogous to $\psi^*\psi$. Also, if f(x) is represented by some operator f,,, then $P(x)f(x)$ is analogous to $\psi^* f_{\text{op}}\psi$.

These rules for computation of expectation values of a physical quantity have shown that the combination of quantities $\psi^* f_{\text{op}}\psi$ should be used rather than some other combination, (For example, $f_{\text{op}}(\psi^*\psi)$ would be incorrect.)

We have defined differential operators for momentum and energy, given by Equations (6.79) and (6.88). Similarly, for y and z components of momentum, we could write:

$$p_{y_{op}} = \frac{\hbar}{i}\frac{\partial}{\partial y}; \quad p_{z_{op}} = \frac{\hbar}{i}\frac{\partial}{\partial z} \tag{6.91}$$

In summary, when an operator acting on a function has the effect of multiplying that function by a constant, this constant is said to be the eigenvalue of the operator, and the function is said to be an eigenfunction of the operator. The wavefunction $e^{+i(p_x x - Et)/\hbar}$ represents a beam of particles of definitely known momentum p_x, and definitely known energy E. It is also an eigenfunction of the operators $p_{x_{op}}$ and E_{op}. The eigenvalues are just the physical volues of the momentum and energy, respectively, for this particular beam of particles.

When the wavefunction is not an eigenfunction of $p_{x_{op}}$, the expectation value (average value) of the x component of momentum may conveniently be calculated in terms of Equations (6.85) and (6.89). These mathematical expressions are important, because there are many times when we are interested in particles not having definite momentum or energy. Then the operators allow us to compute expectation values.

20 SCHRÖDINGER EQUATION

Now that the energy and momentum operators have been introduced, we can attempt to find a wave equation that the wave function of a particle should satisfy. Suppose we consider a number of regions separated by parallel planes with a constant potential energy in each region. If a particle moves perpendicular to the separating planes, we need consider only the dimension parallel to the particle's motion. Calling this the x direction, we then have the potential energy graph shown in Figure 6.18, where regions I, II, III are the constant potential energy regions. In any of these regions, it should be possible to have a wavefunction which is a momentum and an energy eigenfunction. That is, in terms of momentum p_x and energy E_T,

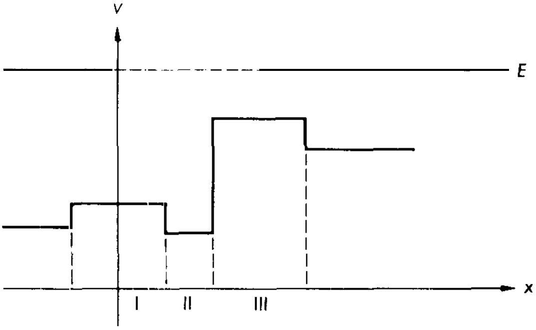


Figure 6.18. Graph of a potential energy curve which consists of a number of constant potentiol energy regions.

$$\psi_T = e^{i(p_x x - E_T t)/\hbar}. \tag{6.92}$$

In the expression for ψ we have now written E_T for energy to imply total energy including rest energy. Thus, $E_T = m_0c^2 + E$, where E is the part of the energy not including rest energy. That is, for low-energy particles, E is the total energy in the nonrelativistic sense, kinetic energy plus potential energy. Let a wavefunction be written in the form $\psi_T = \psi(x,t) \exp(-im_0c^2t/\hbar)$. It is convenient to use $\psi(x,t)$ here instead of ψ_T, because then the rest energy need not be considered explicitly. This is ordinarily done in non-relativistic quantum mechanics. The energy operator acting on ψ_T gives:

$$i\hbar\frac{\partial\psi_T}{\partial t} = \left(i\hbar\frac{\partial\psi}{\partial t} + m_0c^2\psi\right)\exp\left(\frac{-im_0c^2t}{\hbar}\right) = (E + m_0c^2)\psi\exp\left(\frac{-im_0c^2t}{\hbar}\right) \tag{6.93}$$

After cancellation of the terms in m_0c^2 and the phase factor $\exp(-im_0c^2t/\hbar)$, the above equation can be written as:

$$i\hbar\frac{\partial\psi}{\partial t} = E\psi \tag{6.94}$$

Since $i\hbar\,\partial/\partial t$ acting on ψ_T is the operator for total energy, the operator $i\hbar\,\partial/\partial t$ acting on ψ can be interpreted as the operator corresponding to the nonrelativistic total energy, $i\hbar\,\partial/\partial t = E_{op}$.

Now we are in a position to obtain a nonrelativistic wave equation. A wave function ψ which is an eigenfunction of $p_{x_{op}}$ and E_{op}, with eigenvalues p_x and E, is given by

$$\psi = Ae^{i(p_xx-Et)/\hbar} \tag{6.95}$$

It should therefore be possible to find a solution of this form, of the general wave equation, in each region of constant potential energy (Figure 6.18). Of course, p_x varies from region to region, while E must remain constant if energy is conserved. The nonrelativistic relationship between p_x, E and V for a particle of mass m is

$$\frac{p_x^2}{2m} + V = E \tag{6.96}$$

We shall assume that this same relationship holds in quantum mechanics if V is constant. Using $p_{x_{op}}$ and E_{op}, a differential equation which leads to this relationship for the wavefunction of Equation (6.95) is:

$$\frac{1}{2m}(p_{x_{op}})^2\psi + V\psi = E_{op}\psi \tag{6.97}$$

or writing out the differential operators in full,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = i\hbar\frac{\partial\psi}{\partial t} \tag{6.98}$$

Here the operator $\left(\frac{\partial}{\partial x}\right)^2$ means that the function upon which this operator acts is differentiated partially twice with respect to x:

$$\left(\frac{\partial}{\partial x}\right)^2 \psi \equiv \frac{\partial^2 \psi}{\partial x^2} \tag{6.99}$$

Thus, for example,

$$\frac{1}{2m_0}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 e^{ip_x x/\hbar} = \left(\frac{p_x^2}{2m_0}\right) e^{ip_x x/\hbar} \tag{6.100}$$

Suppose next that ψ were a combination of energy-momentum eigenfunctions, corresponding to different energies E_i, such as

$$\psi = \sum A_i e^{i(p_{xi}x - E_i t)/\hbar} \tag{6.101}$$

Each and every term in this superposition satisfies the differential equation, Equation (6.98), in the constant potential energy region, provided

$$\frac{p_{xi}^2}{2m} + V = E_i \tag{6.102}$$

Therefore, any wavefunction describing motion of a particle in a constant potential energy region should satisfy the differential equation, Equation (6.98).

.21 SCHRÖDINGER EQUATION FOR VARIABLE POTENTIAL

We shall assume that for a continuously variable potential energy, V(x), the differential equation still holds. This is reasonable but not rigorous, since in a certain sense, a continuous potential energy can be thought of as a large number of narrow constant potential energy regions.

In three dimensions, the relation between energy and momentum is:

$$\frac{p^2}{2m} + V = \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right) + V = E \tag{6.103}$$

By the same line of argument which led to Equation (6.98), the differential equation arising from this would be:

$$\frac{1}{2m}\left(p_{x_{op}}^2 + p_{y_{op}}^2 + p_{z_{op}}^2\right)\psi + V\psi = E_{op}\psi \tag{6.104}$$

or

$$\boxed{-\frac{\hbar^2}{2m}\left(\frac{\partial\psi^2}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + V\psi = i\hbar\frac{\partial\psi}{\partial t} \quad \text{Schrodinger equation}} \tag{6.105}$$

This is called the Schrödinger equation, after Erwin Schrodinger who first proposed it. While our discussion makes Equation (6.105) appear to be a reasonable wave equation, the equation's correctness depends on whether or not it predicts the experimental results. As will be seen, it agrees with experiment to a high degree of accuracy; examples of this will be given in Chapter 8, on the hydrogen atom.

In the Schrödinger equation, the operator,

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)$$

has the physical significance of the kinetic energy operator. In three dimensions, the wavefunction ψ is a function of x, y, z and t, and the probability of finding a particle in the volume element dxdydz is $\psi\;^2 dxdydz$. Hence, extending the formalism for calculation of expectation values, for example, we would expect that if the wavefunction is normalized to unity, the expectation value of the kinetic energy would be

$$-\int \psi^* \frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)dxdydz$$

If more than one particle is present, the relationship between the momenta and the total energy is

$$\frac{\mathbf{p}_1^2}{2m_1}+\frac{\mathbf{p}_2^2}{2m_2}+\cdots+\frac{\mathbf{p}_n^2}{2m_n}+V=E \qquad (6.106)$$

and the Schrödinger equation is obtained by the following prescription:

$$\text{Replace } \mathbf{p}_1^2 \text{ by } -\hbar^2\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial y_1^2}+\frac{\partial^2}{\partial z_1^2}\right);$$

$$\mathbf{p}_2^2 \text{ by } -\hbar\left(\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial y_2^2}+\frac{\partial^2}{\partial z_2^2}\right);$$

$$\cdots\cdots\cdots$$

$$\mathbf{p}_n^2 \text{ by } -\hbar^2\left(\frac{\partial^2}{\partial x_n^2}+\frac{\partial^2}{\partial y_n^2}+\frac{\partial^2}{\partial z_n^2}\right);$$

$$E \text{ by } i\hbar\frac{\partial}{\partial t}$$

and let all these terms operate on the wavefunction ψ, which is a function of all the variables:

$$\psi=\psi(x_1, y_1, z_1, x_2, y_2, z_2, \ldots, x_n, y_n, z_n, t) \qquad (6.1107)$$

Similarly, to find a relativistic wave equation for one particle, we can use the relativistic relationship between energy, potential energy and momentum. This is

$$\mathbf{p}^2c^2+m_0^2c^4=(E_T-V)^2 \qquad (6.108)$$

Here E_T includes the rest energy, m_0c^2. The corresponding wave equation is

$$-\hbar^2c^2\left(\frac{\partial^2\psi_T}{\partial x^2}+\frac{\partial^2\psi_T}{\partial y^2}+\frac{\partial^2\psi_T}{\partial z^2}\right)+m_0^2c^4\psi_T$$

$$=\left(i\hbar\frac{\partial}{\partial t}-V\right)^2\psi_T=-\hbar^2\frac{\partial^2\psi_T}{\partial t^2}-2\,i\hbar V\frac{\partial\psi_T}{\partial t}+V^2\psi_T \qquad (6.109)$$

if V does not depend on t. This is called the Klein-Gordon ***equation.*** It does not have spin (intrinsic angular momentum) appearing in it, and it applies to spinless particles. Another relativistic wave equation, called the *Dirac* ***equation,*** which has spin included, applies tc relativistic electrons. We shall consider in detail only the Schrödinger equation.

The wave equation, Equation (6.105), describing the propagation of matter waves, is the equation we obtained from considerations of conservation of energy. After elimination of the rest energy, the equation in one dimension takes the form of Equation (6.98). Although Equation (6.98) was shown to be true in a region where V is constant, as already noted, it is also true when V is varying. If the consequences of this equation turn out to agree with experiment, then we can be satisfied that the Schrödinger wave equation is valid. In the next sections we shall study some simple properties and consequences of Schrödinger's equation.

.22 SOLUTION OF THE: SCHRÖDINGER EQUATION FOR A CONSTANT POTENTIAL

Let us consider a state of definite energy E, so that

$$i\hbar\frac{\partial\psi}{\partial t}=E_{\rm op}\psi=E\psi \qquad (6.110)$$

Here E is the total kinetic + potential energy. The equation

$$i\hbar\frac{\partial\psi}{\partial t}=E\psi \qquad (6.111)$$

must have a solution of the form:

$$\psi=\Phi(x)e^{-iEt/\hbar} \qquad (6.112)$$

When this is put back into the Schrödinger equation, all time dependence will cancel out, and the equation will be one for the spatial part of the wavefunction,

$$-\frac{\hbar^2}{2m}\frac{d^2\Phi(x)}{dx^2}+V\Phi(x)=E\Phi(x) \qquad (6.113)$$

This is a second order differential equation, which cnn be written in the form:

$$\frac{d^2\Phi(x)}{dx^2}+\left[\frac{2m(E-V)}{\hbar^2}\right]\Phi(x)=0 \qquad (6.114)$$

In this form, it is very similar to the differential equation for simple harmonic motion, which, for a displacement $\Phi(t)$, is:

$$\frac{d^2\Phi}{dt^2} + \omega^2\Phi = 0 \tag{6.115}$$

In our case, however, $E - V$ may not always be a constant, since the potential may vary with x. So in general, the solutions may be difficult to find. Suppose, however, that in some range of x, V is constant. Then we can put

$$k^2 = \frac{2m(E - V)}{\hbar^2} \tag{6.116}$$

and k will be a constant. We can then solve the Schrödinger equation by analogy, for the general solution of Equation (6.115) can be written in either the form:

$$\Phi = a \sin \omega t + b \cos \omega t \tag{6.117}$$

with a, b arbitrary constants, or in the exponential form:

$$\Phi = Ae^{i\omega t} + Be^{-i\omega t} \tag{6.118}$$

where A, B may be complex constants. This latter form is allowed in our case, because the wavefunction $\Phi(x)$ may be complex.

By analogy, then, in terms of

$$k = \sqrt{\frac{2m(E - V)}{\hbar^2}} \tag{6.119}$$

for k constant, a general solution for the wavefunction Φ (x) is:

$$\Phi(x) = Ae^{ikx} + Be^{-ikx} \tag{6.120}$$

This is simply a superposition of momentum eigenfunctions discussed previously, with $k = p_x/\hbar$.

Thus, when $E > V$, we expect oscillatory solutions in space. What happens when $E < V$? Although this case would appear to violate our intuitive feeling that kinetic energy should be positive, it is still possible to find a wavefunction which satisfies the wave equation in a region of such high potential energy. The quantity $k = \sqrt{2m(E - V)/\hbar^2}$ defined in the previous frame becomes pure imaginary: $k = i\kappa = i\sqrt{2m(V - E)/\hbar^2}$. Then $\pm ik = \mp\kappa$, and the general solutions are of the form of increasing or decreasing exponentials:

$$\Phi(x) = Ae^{\kappa x} + Be^{-\kappa x} \tag{6.121}$$

where the arbitrary constants are A and B.

6.23 BOUNDARY CONDITIONS

The arbitrary constants which appear in these solutions are determined by means of boundary conditions, which are special conditions placed on the wavefunction due to the particular physical situation in which the particles find themselves. Suppose, for example, that the system is set up so that it is impossible for a particle to be found in the range of positions $x > x_0$. Then the probability, $\psi^2 = \Phi^2$, of finding a particle in the range of $x > x_0$ must be zero, and so we would conclude that:

$$\Phi = 0 \quad \text{for} \quad x > x_0 \tag{6.122}$$

Next, let us consider the behavior of ψ in a transition region where V is changing very rapidly from some value V_1 to some other value V_2. Suppose, for simplicity that the boundary of these regions is at x = 0, as in Figure 6.19. In region I, V = V_1, the wavefunction will be of the form $\Phi_I = Ae^{ik_1x} + Be^{-ik_1x}$, a superposition of momentum eigenfunctions. In region II, where V = V_2 and the corresponding wavenumber is k_2, the wavefunction will be of the form:

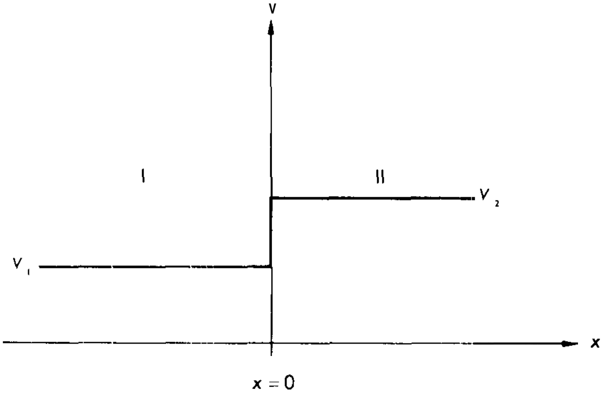


Figure 6.19. Potential energy curve for $V(x) = V_1 =$ const. x 0; $V(x)$ = const. x 0.

$$\Phi_{II} = Ce^{ik_2x} + De^{-ik_2x} \tag{6.123}$$

The value of the wavefunction at x = 0 in region II is related to the value of the wavefunction at x = 0, in region I, just on the other side of the boundary, by two boundary conditions which give us two relations, between the constants A, B, C, D. The two boundary conditions are:

(1) The wavefunction is continuous across the boundary:

$$\psi_I \Big|_{x=0} = \psi_{II} \Big|_{x=0} \tag{6.124}$$

or

$$\Phi_I \Big|_{x=0} = \Phi_{II} \Big|_{x=0} \tag{6.125}$$

and

(2) The derivative of the wavefunction is continuous across the boundary:

$$\frac{\partial \psi_I}{\partial x} \Big|_{x=0} = \frac{\partial \psi_{II}}{\partial x} \Big|_{x=0} \tag{6.126}$$

or

$$\frac{\partial \Phi_I}{\partial x} \Big|_{x=0} = \frac{\partial \Phi_{II}}{\partial x} \Big|_{x=0} \tag{6.127}$$

To understand the reasons for these two conditions, suppose ψ changed nearly discontinuously across the boundary. This would be the same as having a slope which is arbitrarily large at the boundary, as in Figure 6.20. The sudden increase in the slope, $\partial\psi/\partial x$, would in turn mean that $\partial^2\psi/\partial x^2$ would have to be very large. Likewise, if the slope were discontinuous at the point, $\partial^2\psi/\partial x^2$ would be so large as to be undefined at the point. However, if the potential energy and ψ do not become large at the point, Schrödinger's equation tells us that $\partial^2\psi/\partial x^2$ does not become large at the point. Thus, if the wave equation is to be satisfied, ψ and $\partial\psi/\partial x$ must be continuous.

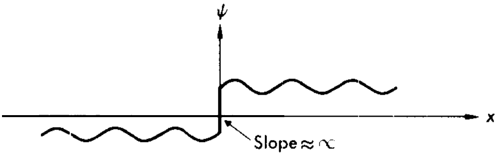


Figure 6.20.

A useful analogy might be to consider two strings of different mass per unit length, tied together and sustaining wave motion while under tension. It is obvious that the displacements of the strings on opposite sides of the knot would be the same. This is analogous to continuity of the wavefunction representing "displacement" of a matter wave. Also, it is easy to see that the slopes of the two strings on each side of the knot would have to be equal (if the knot is massless); otherwise, there would be an unbalanced component of tension acting on the knot and producing an infinite acceleration. This is analogous to continuity of slopes of the wavefunction.

Since the one dimensional Schrödinger equation is of second order in the derivative with respect to x, if the values of ψ and $\partial\psi/\partial x$ are specified at one point, and there are no discontinuities, a unique solution can be found by integration. So then a given physical situation can be represented uniquely by a wavefunction.

Another condition on the wavefunction is that, as x, y, z go to infinity, ψ must not approach infinity. Otherwise, $|\psi|^2$ would give infinite particle densities, or else lead to infinite total probability. In fact, for particles which are restricted to a limited region by some binding force, the wavefunction approaches zero at infinity. A number of examples of these ideas will be studied in the next chapter.

summary

PROPERTIES OF PLANE WAVES

A plane wave may be represented by a wavefunction of the form $e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$; the phase $\mathbf{k}\cdot\mathbf{r}-\omega t$ is a relativistic invariant. It follows that the propagation vector **k** and frequency ω satisfy the following transformation equations between inertial systems:

$$k'_x = \frac{1}{\sqrt{1 - v^2/c^2}}\left(k_x - \frac{v\omega}{c^2}\right) \qquad k'_y = k_y$$

$$\omega' = \frac{1}{\sqrt{1 - v^2/c^2}}(\omega \quad vk_x) \qquad k'_z = k_z$$

These equations imply that $\omega^2 - k^2/c^2$ is a relativistic invariant, and hence that the equation wV = c^2 is invariant. Here, w is the phase speed of the matter wave w = w/k, and V = $d\omega/dk$ is the group speed of the particle with which the wave is associated. V is identical to the particle velocity.

DE BROGUE RELATIONS

The momentum, propagation vector, and wavelength of a particle (de Broglie waves) are related by

$$p = \hbar k = \frac{h}{\lambda}$$

and energy and frequency are related by

$$E = \hbar\omega = h\nu$$

where $\hbar$ = h/2x; h is Planck's constant.

DAVISSON-GERMER EXPERIMENT

In the Davisson-Germer experiment, electrons were scattered off nickel. The existence of diffraction peaks showed that a wavelength was associated with the electron, and the position of the peaks showed that the wavelength was consistent with λ = h/p, where h is Planck's constant.

UNCERTAINTY PRINCIPLE FOR PARTICLES

In any experiment in which both the x component of position and momentum are measured simultaneously, the uncertainties Ax in position and Δp_x in momentum satisfy the inequality,

$$\Delta p_x \Delta x \geq \hbar/2$$

where Δp_x and Ax are rms deviations from the mean. Similarly, in a measurement of energy which lasts for a time At,

$$\Delta E \Delta t \simeq \hbar$$

PROBABILITY INTERPRETATION OF WAVEFUNCTION

Associated with a material particle is a wavefunction ψ. In one dimension, $|\psi|^2 dx$ is proportional to the probability of finding the particle in the range dx. If ψ_1 is the probability amplitude, or wavefunction,. for particles from source 1 alone, and ψ_2 is that for source 2 alone, then when both sources are on, the total wavefunction is obtained by superposition of the individual contributions, and is $\psi_1 + \psi_2$. The total probability of finding a particle in dx is then proportional to $|\psi_1 + \psi_2|^2 dx$.

ENERGY AND MOMENTUM OPERATORS

The momentum p_x of a particle can be represented by the differential operator:

$$p_{x_{op}} = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

The energy operator is:

$$E_{op} = i\hbar\frac{\partial}{\partial t}$$

When an operator acts on a function to give a constant multiplied by that same function, the function is said to be an eigenfunction of that operator and the constant is called the eigenvalue. The function $\psi = Ae^{i(p_x x - Et)/\hbar}$ is an eigenfunction of both p_{op} and E_{op}, with eigenvalues p_x and E, respectively. For any state of indefinite momentum or indefinite energy, the average value or expectation value of the momentum may conveniently be calculated in terms of operators as follows:

$$\langle p_x \rangle = \frac{\int \psi^* p_{x_{op}} \psi\, dx}{\int \psi^* \psi\, dx}$$

$$\langle E \rangle = \frac{\int \psi^* E_{op} \psi\, dx}{\int \psi^* \psi\, dx}$$

SCHRÖDINGER EQUATION

After eliminating the rest energy, the nonrelativistic: wave equation satisfied by the wavefunction $\psi(x, y, z, t)$, describing a particle having a potential energy $V(x, y, z)$, is obtained from the conservation of energy equation:

$$E = \left(\frac{p^2}{2m}\right) + V$$

by replacing all the quantities by their corresponding operators and allowing them to operate on the wavefunction. In one dimension, the wave equation is:

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{dx}\right)^2\psi + V\psi$$

BOUNDARY CONDITIONS

(1) The wavefunction is continuous across a boundary at, for example, $x = 0$:

$$\psi_1\Big|_{x=0} = \psi_2\Big|_{x=0}$$

(2) **The** derivative of the wavefunction is continuous across the boundary:

$$\frac{\partial\psi_1}{\partial x}\Bigg|_{x=0} = \frac{\partial\psi_1}{\partial x}\Bigg|_{x=0}$$

(3) The wavefunction remains finite or goes to zero as the coordinates go to infinity.

problems

1. Use Equation (6.22) to derive the general Doppler effect; assume that in one frame, light of frequency ν is propagating at angle θ relative to the positive x axis. Show that in another frame, moving at velocity v along the x axis relative to the first frame, the frequency observed is

$$\nu' = \frac{1 - v\cos e/c}{\sqrt{1 - v^2/c^2}}\nu$$

Use $w = 2\pi\nu = kc$.

2. If the group speed, $v_g = d\omega/dk$, and phase speed, $w = w/k$, are related by $v_g w = c^2$, where c^2 is a constant, find the most general relationship between ω and k.

Answer: $\omega^2 = c^2k^2$ + constant.

3. Suppose that in the free particle wave function, $\psi = e^{i(kx-\omega t)} = e^{i(px\ \ E_T t)/\hbar}$, the nonrelativistic kinetic: energy, $\frac{1}{2}mv^2 = p^2/2m$, *were* incorrectly used for E_T What would be the relationship between the momentum p and the group speed? Find the relationship between the group speed and phase speed, w.

Answer: $p = mv_g$; $w = \frac{1}{2}v_g$.

4. An electron (mass = .91 × 10^{-30} kg) moves at a speed of 2 x 10^8 m/sec in a region where the potential energy is zero. It hits the plane boundary of a region where its potential energy is − 4.1 1 x 10^{-14} joules at an angle of incidence of 60 Find its angle of refraction.

Answer: 30'.

5. What are the phase speed and wavelength of a proton moving at a particle speed, (a) 100 m/sec (b) 2×10^8 m/sec?
   Answer: (a) 9×10^{14} m/sec, 3.96×10^{-9} m;
   (b) 4.5×10^8 m/sec, 1.477×10^{-15} m.
6. An electron is accelerated through 50,000 volts in an electron microscope. What is the smallest distance between objects that could possibly be observed?
   Answer: 5×10^{-10} cm.
7. What is the kinetic energy in electron volts of electrons in a beam incident at an angle of 30” relative to a crystal surface, reflected coherently from planes 2 angstroms apart? Assume this is the fourth order reflection, that the planes are parallel to the surface, and that no wavelength change is suffered upon passage into the crystal.
   Answer: 201 eV.
8. Electrons hitting a metal target produce X rays with a minimum wavelength of 1 angstrom. What is the electron wavelength?
   Answer: 1.1×10^{-9} cm.
9. What is the ratio between the wavelengths of 10^9 eV electrons and 10^9 eV photons?
   Answer: $1 + 1.3 \times 10^{-7}$.
10. For $-\ell \leq x \leq \ell$, the wavefunction of a particle is $\psi = a(\ell^2 \quad x^2)e^{ikx-i\omega t}$. If $|\psi|^2$ is a probability density, find a. Find the expectation value of the x component of momentum.
    Answer: $\frac{1}{4}\sqrt{\frac{15}{\ell^5}}$; $\hbar k$.
11. For the wavefunction of Problem 10, find $\Delta x \Delta p_x$, where Δx and Δp_x are rms deviations from the mean.
    Answer: $\hbar\sqrt{\frac{5}{14}} = 0.5986 > \hbar/2$.
12. An electron gun in a TV tube has an opening of diameter a. Electrons come out with a speed v of 100 m/sec, and the distance to the screen is $L = 1$ meter. What should the diameter a be in order to minimize the size of the spot on the screen if there is no focussing? Take into account that uncertainties in the position of electrons at the screen arise both from uncertainties in the initial position of the electrons within the gun and from diffraction.
    Answer: $a \simeq \sqrt{\frac{\hbar L}{mv}} = 0.11$ cm.
13. What is the minimum possible kinetic energy, consistent with the uncertainty principle, of a proton confined to a region of size 5×10^{-15} meters, which is the approximate size of a nucleus?
    Answer: About 0.83 MeV.
14. A particle of mass m moves along a vertical wire in the gravitational field of the earth above a rigid impenetrable floor, which is at height $x = 0$. Hence, the particle's height is always greater than zero and its potential energy is mgx. Using the uncertainty principle, estimate the lowest possible energy of the particle. Do you think this energy is observable?
    Answer: $\frac{3}{2}m^{1/3}(g\hbar)^{2/3}$.
15. An ideal icepick of mass $m = 100$ g concentrated at its center of mass, which is a distance $r = 25$ cm from the point of the icepick, is set on its point and an attempt is made to balance it. This is impossible, of course, because to balance it, the center of mass must be both directly over the point $(\Delta x = 0)$ and at rest (Ap, = 0). If sin 0

$\simeq \theta$, show that the Newtonian equation of rotational motion is

$$\frac{d^2\theta}{dt^2} = \frac{g}{r}\theta$$

with the solution $r\theta = \frac{1}{2}(\Delta x - \Delta p/m\sqrt{r/g})e^{-\sqrt{g/r}t} + \frac{1}{2}(\Delta x + \Delta p/m\sqrt{r/g})e^{\sqrt{g/r}t}$, with Δx and Δp the initial displacement and momentum. For $t \gg \sqrt{r/g}$, the negative exponential can be neglected. Use the uncertainty principle to estimate the maximum time, on the average, during which the center of mass of the icepick moves the distance $\frac{1}{2}r$ sideways in falling, i.e. the time for the best balance you can expect.

Answer: $t \sim \sqrt{\frac{r}{16g}}\ ln\left(\frac{m^2gr^3}{16\hbar^2}\right) \sim 6$ sec.

16. A particle of mass m has a wavefunction,

$$\psi = A\exp\left(-\frac{1}{2}\frac{m\omega x^2}{h} + ik_yy + ik_zz - i\frac{Et}{\hbar}\right),$$

where ω is an angular frequency. Find the potential energy of this particle as a function of x, and find the total energy for this state.

Answer: $\frac{1}{2}m\omega^2x^2$, $E = \frac{1}{2}\hbar\omega + \frac{(k_y^2 + k_z^2)\hbar^2}{2m}$

17. The wavefunction of a two particle system with masses m_1, m_2 and position vectors $\mathbf{r}_1$, $\mathbf{r}_2$ is

$$\psi = A\exp\left[ik\left(\frac{m_1x_1 + m_2x_2}{m_1 + m_2}\right) - \frac{m_1m_2e^2}{4\pi\epsilon_0\hbar^2(m_1 + m_2)} \times \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2} - i\frac{Et}{\hbar}\right]$$

where $e^2/4\pi\epsilon_0$ is a constant. Find the potential energy and the total energy. What is the physical meaning of this state?

Answer: $\left[\frac{-e^2}{4\pi\epsilon_0\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}}\right]$;

$$-\frac{1}{2}\frac{m_1m_2}{m_1 + m_2}\frac{e^4}{(4\pi\epsilon_0\hbar)^2} + \frac{\hbar^2k^2}{2(m_1 + m_2)}.$$

7 examples of the use of Schrödinger's equation

In this chapter several examples will be presented to illustrate the use of the Schrodinger equation and the application of boundary conditions. In the process of studying these examples, the physical meaning of the wavefunction should become clearer. For simplicity, all the examples will be done only in one dimension.

7.1 FREE-PARTICLE GAUSSIAN WAVE PACKET

In Chapter 6 we saw that the nonrelativistic timedependent Schrodinger equation for free particles moving in one dimension is:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = i\hbar\frac{\partial\psi}{\partial t} \tag{7.1}$$

and that a typical solution is a wavefunction of the form

$$\psi = Ae^{i(px-Et)/\hbar} \tag{7.2}$$

where $E = E(p) = p^2/2m$ is the nonrelativistic kinetic energy. Physically, this solution might correspond to a beam of particles uniformly distributed along the x axis, moving with definite particle velocity, $v = p/m$, and with definite energy $E = E(p)$. The solution in Equation (7.2) is thus both a momentum eigenfunction and an energy eigenfunction.

By superposition of such eigenfunctions corresponding to different values of momentum (and energy), we can build up interesting solutions of the free-particle Schrodinger equation. For example, as was also discussed in Chapter 6, the wavefunction

$$\psi = A_1 \exp\left[\frac{i(p_1x - p_1^2t/2m)}{\hbar}\right] + A_2 \exp\left[\frac{i(p_2x - p_2^2t/2m)}{\hbar}\right] \tag{7.3}$$

with $p_1 \neq p_2$, is likewise a solution to Equation (7.2), but it is no longer a momentum or energy eigenfunction.

We now wish to discuss the quantum-mechanical description of a free particle, which corresponds more closely to our intuitive notion of a particle as being well localized in space. The solution in Equation (7.2) is certainly not well localized, because there is no information at all in this wavefunction about the x coordinate of the particle; all x coordinates are equally probable. A wavefunction describing a localized particle, with some small uncertainty Δ x in position, must have a large uncertainty in momentum according to the uncertainty principle, $\Delta x \Delta p_x \geq \frac{1}{2}\hbar$. To obtain a localized wave packet, we will consider a more general superposition of free-particle momentum eigenfunctions of many different momenta. This superposition has the form:

$$\psi(x, t) = \sum A_i \exp\left[\frac{i(p_i x - p_i^2 t/2m)}{\hbar}\right] \tag{7.4}$$

where the numbers A, are any constant coefficients. Since each term in Equation (7.4) satisfies the Schrödinger equation, which is a linear differential equation, the sum satisfies it.

We can also consider the superposition of wavefunctions with a continuous distribution of momenta by passing from the summation in Equation (7.4) to an integration:

$$\psi(x,t) = \int_{-\infty}^{\infty} dpA(p) \exp\left[\frac{i(px - p^2t/2m)}{\hbar}\right] \tag{7.5}$$

where A(p) is any function of p.

Now to obtain a function which is localized in space, we shall consider the superposition in Equation (7.5), with *A(p)* chosen to give a distribution of momenta about some central value, p_0. If the momenta (appearing in the integral in Equation (7.5) are distributed symmetrically about the value p_0, we would expect the particle to move with an average momentum $p_0 = mv_0$. Furthermore, if there is a large spread in momenta, i.e. if Δp is large, we would expect it to be possible to have Δx small. We shall choose a distribution of momenta given by a gaussian, as follows,:

$$A(p) = \sqrt{\frac{\sigma}{2\pi\sqrt{\pi}\hbar^2}} \exp\left[\frac{-\frac{1}{2}\sigma^2(p - p_0)^2}{\hbar^2}\right] \tag{7.6}$$

While this is only one of an infinite number of choices, the choice in Equation (7.6) is particularly interesting for several reasons and is not too difficult to handle mathematically. The constants in front of the exponential in Equation (7.6) make the function $\psi(x, t)$ a normalized one, so that the total probability is unity. Thus, we shall study the wave ***packet:***

$$\psi(x,t) = \sqrt{\frac{\sigma}{2\pi\sqrt{\pi}\hbar^2}} \int_{-\infty}^{\infty} \exp\left[\frac{-\frac{1}{2}\sigma^2(p - p_0)^2}{\hbar^2}\right] \exp\left[\frac{i(px - p^2t/2m)}{\hbar}\right] dp \tag{7.7}$$

7.2 PACKET AT $t = 0$

Consider first the resulting description of the particle at time $t = 0$:

$$\psi(x, t = 0) = \sqrt{\frac{\sigma}{2\pi\sqrt{\pi}\hbar^2}} \int_{-\infty}^{\infty} \exp\left[\frac{-\frac{1}{2}\sigma^2(p - p_0)^2}{\hbar^2}\right] \exp\left(\frac{ipx}{\hbar}\right) dp \qquad (7.8)$$

The integral may be performed with the help of Table 7.1, after changing $e^{ipx/\hbar}$ to $e^{ip_0x/\hbar}e^{i(p-p_0)x/\hbar}$ and introducing a new integration variable by the substitution $y = p - p_0$:

$$\psi(x, t = 0) = \frac{1}{\sqrt{\sqrt{\pi}\,\sigma}} \exp\left(\frac{-x^2}{2\sigma^2}\right) \exp\left(\frac{ip_0x}{\hbar}\right) \qquad (7.9)$$

Clearly, at this time the wavefunction is localized in space, near the origin at $x = 0$. The probability density is

$$|\psi|^2 = \frac{1}{\sqrt{\pi}\,\sigma} \exp\left(\frac{-x^2}{\sigma^2}\right) \qquad (7.10)$$

which is a normalized gaussian distribution centered at $x = 0$. Thus at $t = 0$, $\langle x \rangle = 0$. To calculate Δx at this time, we need

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \left[\int_{-\infty}^{\infty} dx\, x^2 \,|\psi|^2\right]^{1/2}$$

$$= \left[\int_{-\infty}^{\infty} dx\, x^2 \frac{1}{\sqrt{\pi}\,\sigma} \exp\left(-\frac{x^2}{\sigma^2}\right)\right]^{1/2} = \frac{\sigma}{\sqrt{2}} \qquad (7.11)$$

from Table 7.1. Thus, σ is a measure of the distance within which the particle is initially localized.

TABLE 7.1 Some Integrals Involving Complex Exponentials

$$\int_{-\infty}^{\infty} \exp\left(-\frac{y^2}{a^2} + iby\right) dy = \sqrt{\pi}\, a \exp\left[-\left(\frac{ab}{2}\right)^2\right], \text{ Real part of } a^2 > 0$$

$$\int_{-\infty}^{\infty} \exp\left(-\frac{y^2}{a^2}\right) y^2\, dy = \frac{1}{2} a^3 \sqrt{\pi}$$

$$\int_{-\infty}^{\infty} y \exp\left(-\frac{y^2}{a^2}\right) dy = 0$$

The oscillating factor $\exp(ip_0x/\hbar)$, which multiplies the gaussian in Equation (7.9), corresponds to the fact that the particle has an overall momentum p_0, because, calculating the expectation value of momentum, we have:

$$\langle p\rangle = \int_{-\infty}^{\infty} \psi^* \frac{\hbar}{i}\frac{\partial\psi}{\partial x}\,dx = \frac{1}{\sqrt{\pi}\,\sigma}\int_{-\infty}^{\infty} \exp\left(-\frac{x^2}{\sigma^2}\right)\left(-\frac{\hbar}{i}\frac{x}{\sigma^2}+p_0\right)dx = p_0 \tag{7.12}$$

Thus the wavefunction corresponds to a particle with average velocity, $v_0 = p_0/m$. The rms deviation from the mean momentum, or uncertainty in momentum, is:

$$\begin{aligned}\Delta p &= \left[\int_{-\infty}^{\infty} \psi^*\left(-\hbar^2\frac{\partial^2\psi}{\partial x^2}\right)dx - p_0^2\right]^{1/2}\\ &= \left\{\int_{-\infty}^{\infty}\frac{1}{\sqrt{\pi}\,\sigma}\exp\left(-\frac{x^2}{\sigma^2}\right)\left[-\frac{\hbar^2x^2}{\sigma^4}+2i\frac{\hbar x p_0}{\sigma^2}+p_0^2+\frac{\hbar^2}{\sigma^2}\right]dx - p_0^2\right\}^{1/2}\\ &= \left[-\frac{1}{2}\frac{\hbar^2}{\sigma^2}+0+p_0^2+\frac{\hbar^2}{\sigma^2}-p_0^2\right]^{1/2} = \frac{\hbar}{\sqrt{2}\sigma}\end{aligned} \tag{7.13}$$

Note that at $t = 0$ the uncertainty product is the minimum allowed by the uncertainty principle,

$$\Delta p\Delta x = \frac{\hbar}{\sqrt{2}\sigma}\cdot\frac{\sigma}{\sqrt{2}} = \frac{\hbar}{2} \tag{7.14}$$

Thus, at first the gaussian wave packet is actually a minimum uncertainty packet; this is one of the reasons the gaussian packet is of particular interest.

Summarizing our results so far, we have, at $t = 0$,

$$\langle x\rangle = 0,\ \Delta x = \frac{\sigma}{\sqrt{2}} \tag{7.15}$$

$$\langle p\rangle = p_0,\ \Delta p = \frac{\hbar}{\sqrt{2}\,\sigma} \tag{7.16}$$

.3 PACKET FOR t > 0

Next, we shall calculate the expectation values and uncertainties at any later time t. We would expect that the average momentum and uncertainty in momentum would not change with time, since there are no forces to modify the momentum distribution. This could be verified by detailed calculation using the ψ in Equation (7.18) below. To calculate $\langle x\rangle$ and Δx, we need the wavefunction $\psi(x, t)$ at an arbitrary time and hence must perform the p integral in Equation (7.7) at an arbitrary time. This may be done in a straightforward way, using the integrals in Table 7.1, although the algebra is a little messy. The integral may be written as:

$$\psi(x,t) = \sqrt{\frac{\sigma}{2\pi\sqrt{\pi}\hbar^2}}\ \exp\left[\frac{i(p_0x - p_0^2t/2m)}{\hbar}\right] \times$$

$$\int dp \exp\left[-(p - p_0)^2\left(\frac{\sigma^2}{2\hbar^2} + \frac{it}{2m\hbar}\right) + i(p \quad \mathrm{PO})\left(\frac{x}{\hbar} \quad \frac{p_0t}{m\hbar}\right)\right] \tag{7.17}$$

The first integral in Table 7.1 then gives us:

$$\psi(x,t) = \sqrt{\frac{\sigma}{\sqrt{\pi}(\sigma^2 + i\hbar t/m)}}\ \exp\left[-\frac{1}{2}\frac{(x - p_0t/m)^2}{\sigma^2 + i\hbar t/m} + \frac{i}{\hbar}\left(p_0x - \frac{p_0^2t}{2m}\right)\right] \tag{7.18}$$

This wave function leads to a probability density of

$$\psi^*\psi = |\psi|^2 = \frac{\sigma}{\sqrt{\pi}\sqrt{\sigma^4 + \hbar^2t^2/m^2}}\ \exp\left[\frac{-\sigma^2(x - p_0t/m)^2}{(\sigma^4 + \hbar^2t^2/m^2)}\right] \tag{7.19}$$

This distribution is centered about the point x = p_0t/m, corresponding to an average particle speed of p_0/m. This agrees with the result (p) of Equation (7.12). The distribution center, p_0 t/m, is, of course, also the expectation value of x. The rms deviation of x from its mean is:

$$\Delta x = \sqrt{\left\langle\left(x - \frac{p_0t}{m}\right)^2\right\rangle}$$

$$= \left\{\int_{-\infty}^{\infty} \frac{\sigma}{\sqrt{\pi}\sqrt{\sigma^4 + \hbar^2t^2/m^2}}\left(x - \frac{p_0t}{m}\right)^2 \exp\left[\frac{-\sigma^2(x - p_0t/m)^2}{(\sigma^4 + \hbar^2t^2/m^2)}\right] dx\right\}^{1/2}$$

$$= \frac{\sqrt{\sigma^2 + h^2t^2/m^2\sigma^2}}{\sqrt{2}} \tag{7.20}$$

This Ax is least at t = 0 and increases thereafter. This is because of the possible presence of momenta greatly different from p_0 within the momentum distribution, resulting in the possibility that the particle may be moving with velocities greater or less than the average, p_0/m, and thus the possibility of the particle being farther and farther from (x) as time progresses. If the particle is very sharply localized in space initially, that is if σ is very small, then from Equation (7.20) it is seen that the wave packet will spread very rapidly, because at large times, Ax $\sim$ tit/ma. This is due to the complementary presence of very high momenta, which must be present in order that Ap be large, Ap $\geq \hbar/2\Delta x$. If the particle is not very well localized initially, (large a), the wave packet spreads slowly. We could expect that at sufficiently large times, the spread of the packet would be on the order of Avt = $\Delta pt/m = \hbar t/2\sigma m$. The uncertainty Ax in Equation (7.20) is of this order of magnitude for large t. The uncertainty principle is satisfied at all times, since from Equations (7.12) and (7.20)

$$\Delta p\Delta x = \frac{1}{2}\hbar\sqrt{1 + \frac{\hbar^2t^2}{m^2\sigma^2}} \geq \frac{1}{2}\hbar \tag{7.21}$$

Let us put some numbers in, to see how long we can expect a particle to remain reasonably well localized. Suppose we consider an electron with mass of about 10^{-30} kg. If it has a few electron volts kinetic energy, such as it might pick up in a low voltage vacuum tube, it is moving with a speed of around 10^6 m/sec. Also, if in an experiment the electron is initially localized to within a distance Δx of 0.01 cm, then the spread in velocities, $\Delta v = \Delta p/m = \hbar/(2\Delta x m)$, is on the order of 1 m/sec, very small compared to the speed. Now, from Equation (7.20) the spread in the distribution will be multiplied by $\sqrt{2}$ when $\hbar t/m = \sigma^2$. Since σ is of the order of 0.01 cm, this time is of the order of 10^{-4} sec. While this may not seem a long time, with a speed of 10^6 m/sec, the electron will have gone 10^2 meters, or about 300 feet, in that time. During this displacement, the packet will spread only about 40% in width. Thus, for most macroscopic experiments, we do not have to worry about the electrons' becoming nonlocalized. For a macroscopic object, such as a stone of 100 gm mass, the time required for Δx to increase by a factor of $\sqrt{2}$ is around 10^{25} sec, or about 10^{18} years. This indicates why quantum mechanics is ordinarily unimportant for the description of macroscopic bodies. The spreading and motion of a gaussian wave packet is illustrated in Figure 7.1.

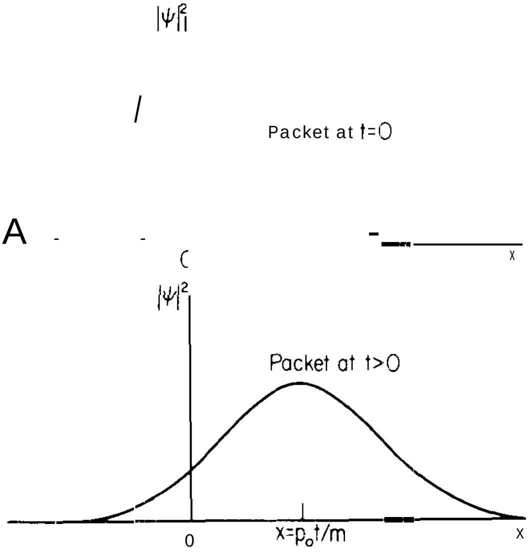


Figure 7.1. Graph of probability density in a Gaussian wave packet. The wave packet spreads in space as time progresses.

STEP POTENTIAL; HIGH ENERGY $E > V_0$

The first example involving the matching of boundary conditions will involve the one dimensional potential energy shown in Figure 7.2. This is called a ***step*** potential, and corresponds to the particle experiencing a very large force over a very small distance when going from region I to region II. In region I the potential energy is zero, and in region II it is the constant V_0.

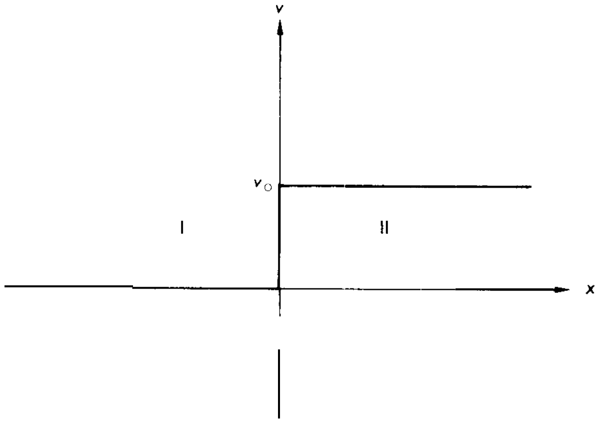


Figure 7.2. Step potential such that $V = 0$, $x < 0$; $V = V_0$ x 0

If the nonrelativistic wavefunction is of the form

$$\psi(x, t) = \Phi(x)e^{-iEt/\hbar} \tag{7.22}$$

then the one dimensional differential equation for the spatial part of the wavefunction $\Phi(x)$, for a particle of mass m, is:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Phi}{\partial x^2} + V\Phi = E\Phi \tag{7.23}$$

In region I, since $V = 0$, the equation is:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Phi_I}{\partial x^2} = E\Phi_I \tag{7.24}$$

The equation can be rearranged by multiplying through by $2m/\hbar^2$:

$$\frac{\partial^2\Phi_I}{\partial x^2} + \frac{2mE}{\hbar^2}\Phi_I = 0 \tag{7.25}$$

or, with

$$k = +[2mE/\hbar^2]^{1/2} \tag{7.26}$$

$$\frac{\partial^2\Phi_I}{\partial x^2} + k^2\Phi_I = 0 \tag{7.27}$$

In this form, it resembles the harmonic oscillator equation of classical mechanics, $\ddot{x} + \omega^2 x = 0$, and has solutions which are oscillating in space,

$$\Phi_I = Ae^{ikx} + Be^{-ikx} \tag{7.28}$$

where A and B are constants.

In region II, the differential equation is:

$$\frac{\hbar^2}{2m}\frac{\partial^2\Phi_{II}}{\partial x^2} + V_0\Phi_{II} = E\Phi_{II} \tag{7.29}$$

or

$$\frac{\partial^2 \Phi_{II}}{\partial x^2} + \frac{2m(E - V_0)}{\hbar^2}\Phi_{II} = 0 \tag{7.30}$$

Since we are assuming $E > V_0$, the solutions are of a form similar to those in Equation (7.18); putting $\alpha = +[2m(E - V_0/\hbar^2]^{1/2}$, we have:

$$\Phi_{II} = Ce^{i\alpha x} + De^{-i\alpha x} \tag{7.31}$$

where C and D are constants.

7.5 BEAM OF INCIDENT PARTICLES

The constants A, B, C, and D in Equations (7.28) and (7.31) are determined by the imposition of physical boundary conditions. As an example, we shall consider what happens when a beam of particles of energy E is incident on the step potential from the left. The incident beam corresponds to a nonzero value of A in Equation (7.31); i.e., since the momentum operator is $p_x = -i\hbar\partial/\partial x$, the term Ae^{ikx} corresponds to a beam of positive x momentum, $p_x = \hbar k$. The term Be^{-ikx} would correspond to a beam of particles in region I traveling to the left, such as could occur if the step could cause particles to be reflected. In Equation (7.31), the term $Ce^{i\alpha x}$ corresponds to a beam of particles traveling to the right, due to particles transmitted through the potential barrier, while $De^{-i\alpha x}$ corresponds to particles incident on the barrier from the right. If the experiment is set up so that a source of particles is far to the left, then we have to allow for a transmitted beam in region II; but there is no source for particles incident on the step from the right. Hence, we must have $D \equiv 0$ in Equation (7.31). Thus, for this particular problem,

$$\Phi_{II} = Ce^{i\alpha x} \tag{7.32}$$

Now let us apply boundary conditions at x = 0 to find B and C in terms of A. We must satisfy the conditions:

$$\Phi_I \big|_{x=0} = \Phi_{II} \big|_{x=0} \tag{7.33}$$

and

$$\left.\frac{\partial \Phi_I}{\partial x}\right|_{x=0} = \left.\frac{\partial \Phi_{II}}{\partial x}\right|_{x=0} \tag{7.34}$$

With the substitution, $x = 0$, the first of these conditions gives us:

$$A + B = C \tag{7.35}$$

The second condition leads to:

$$ikA \quad ikB = i\alpha C \tag{7.36}$$

If the two equations, Equations (7.35) and (7.36), are used to find B in terms of A, the result is:

$$B = \frac{1 - (\alpha/k)}{1 + (\alpha/k)}A \tag{7.37}$$

Likewise, the solution for C gives us:

$$C = \frac{2}{1 + (\alpha/k)}A \tag{7.38}$$

Then the wavefunctions are:

$$\Phi_I = A\left[e^{ikx} + \frac{1 - (\alpha/k)}{1 + (\alpha/k)}e^{-ikx}\right] \tag{7.39}$$

$$\Phi_{II} = A\frac{2}{1 + (\alpha/k)}e^{\alpha x} \tag{7.40}$$

Thus, incoming particles in region I moving in the positive x direction are partially reflected and partially transmitted into region II.

7.6 TRANSMISSION AND REFLECTION COEFFICIENTS

An interesting relationship is obtained if Equations (7.35) and (7.36) are multiplied together and the resulting equation is multiplied by $\hbar/im$. Then

$$\frac{\hbar k}{m}A^2 = \frac{\hbar k}{m}B^2 + \frac{\hbar\alpha}{m}C^2 \tag{7.41}$$

This equation has a very simple physical interpretation. We shall, for convenience, assume that A is real, ard thus from Equations (7.37) and (7.38), B and C must also be real. In general, ψ^2 is proportional to the probability density of particles. Then, in the function $\Phi_I = Ae^{ikx} + Be^{-ikx}$, A^2 is proportional to the number of particles of momentum $\hbar k$ per unit length along the x axis. Let us assume that A is normalized, so that A^2 is exactly the number of incoming particles per unit length. Since $\hbar k$ is the momentum, $\hbar k/m$ is the particle speed, and the term, $\hbar kA^2/m$, in Equation 7.40 is the speed times the number of incoming particles per unit length. This is equal to the number of incoming particles arriving at $x = 0$ per unit time. Likewise, $\hbar kB^2/m$ is the number of particles per unit time reflected back into region I by the step at $x = 0$. Similarly, $\hbar\alpha C^2/m$ is the number of particles transmitted through the step $x = 0$ into region II, per unit time. Thus, the overall meaning of Equation (7.41) is that the number of particles reaching x = 0 per unit time equals the total number leaving that point per unit time; i.e. the total number of particles is conserved.

One can define a reflection coefficient R to be the fraction of incident particles reflected, or the ratio of the number of particles going back into region I to the number of incident particles at $x = 0$. Thus, from Equation (7.37),

$$R = \frac{(\hbar kB^2/m)}{(\hbar kA^2/m)} = \frac{(1 - \alpha/k)^2}{(1 + \alpha/k)^2} \tag{7.42}$$

Likewise, the transmission coefficient T is defined as the fraction of incident particles which are transmitted, or the ratio of the number of particles going into region II to the number of incident particles:

$$T = \frac{(\hbar\alpha C^2/m)}{(\hbar k A^2/m)} = \frac{4\alpha/k}{(1 + \alpha/k)^2} \tag{7.43}$$

We see that $T + R = 1$; this is another form of the conservation of particles equation. As the energy E becomes very large compared to the potential height V,, we would expect the potential to be less and less important, so the transmission coefficient should approach unity. Since a/k approaches one in this limit, Equation (7.43) shows that this is indeed the case. When $E = V_0$, $\alpha = 0$. Then the transmission coefficient is zero and all the particles are reflected. If the particles obeyed Newtonian mechanics rather than quantum mechanics, T would be equal to unity for all energies $E > V_0$, and there would be no particles reflected. Thus, the wave properties of the particles cause reflections that would not occur classically.

7.7 ENERGY LESS THAN THE STEP HEIGHT

Suppose that $E < V_0$ for the same potential energy function, with a step height V_0. Then, in classical mechanics, no particles could go into region II where $V = V_0$, since there the kinetic energy would have to be negative, leading to imaginary speeds. Hence, Newtonian mechanics would say that all the particles are reflected. We shall see that quantum mechanics gives the same result. If $E < V_0$, we still have for the solution in region I,

$$\Phi_I = Ae^{ikx} + Be^{-ikx} \tag{7.44}$$

However, in region II, since E < V,, the solutions must involve real exponentials,

$$\Phi_{II} = Ce^{-\beta x} + De^{""} \tag{7.45}$$

where $\beta = \sqrt{2m(V_0 - E)}/\hbar$. As $x \to \infty$, $e^{+\beta x} \to +\infty$. Hence, if $D \neq 0$, there would be an infinitely large probability of finding particles infinitely far inside the classically forbidden region. This is not reasonable, so D must be zero. The remaining solution in region II is the same as the solution for $E > V_0$, but with α replaced by $i\beta$. If the boundary conditions are now applied at $x = 0$, the equations relating A, B and C are:

$$A + B = C \tag{7.46}$$

and

$$ik(A - B) = -\beta C \tag{7.47}$$

Then, in terms of A, the solutions for the coefficients are:

$$B = \frac{1 + (\beta/ik)}{1 - (\beta/ik)}A; \quad C = \frac{2}{1 - (\beta/ik)}A \tag{7.48}$$

In this case, even if A is real, B and C are both complex, and so the number of particles reflected back into region I per sec is

$$\frac{\hbar k}{m}|B|^2 = \frac{\hbar k B^*B}{m} \tag{7.49}$$

The reflection coefficient is then:

$$\begin{aligned} R &= \frac{(\hbar k BB^*/m)}{(\hbar k AA^*/m)} \\ &= \frac{[1+(\beta/ik)][1-(\beta/ik)]\,|A|^2}{[1-(\beta/ik)][1+(\beta/ik)]\,|A|^2} - , \end{aligned} \tag{7.50}$$

All the particles are therefore reflected.

Even though the transmission coefficient T is zero, this does not mean that a measurement would never show a particle in region II. In fact, the number of particles in region II per unit length is $|\Phi_{II}|^2 = |C|^2 e^{-2\beta x}$. The net particle current to the right is simply zero in that region. In Newtonian mechanics, the probability of finding a particle in region II would be zero. Thus, in quantum mechanics, particles can penetrate into a region which is forbidden classically.

7.8 TUNNELING FOR A SQUARE POTENTIAL BARRIER

One implication of this penetration effect is that if the higher potential region is not very wide, particles will have a possibility of tunneling through to the other side, and of being transmitted. Classically, this would be impossible.

To illustrate quantum mechanical tunneling, we will use the potential energy shown in Figure 7.3, with $V = V_0$, a constant, between $x = 0$ and $x = a$. We

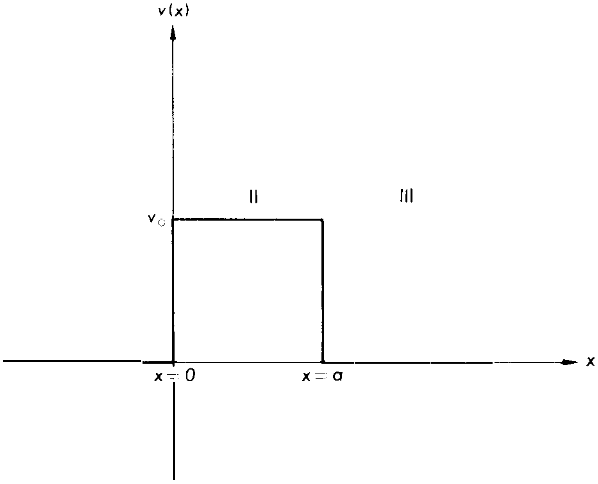


Figure 7.3. Square potential barrier used to illustrate quantum mechanical tunneling.

assume that elsewhere, V = 0. As was the case in the previous section, the solution in region I is now:

$$\Phi_I = Ae^{ikx} + Be^{-ikx}; \quad k = \frac{\sqrt{2mE}}{\hbar} \tag{7.51}$$

In region II, if E $< V_0$, the solution is:

$$\Phi_{II} = Ce^{-\beta x} + De^{\beta x}; \quad \beta = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \tag{7.52}$$

Here we cannot conclude that D = 0, since region II does not extend to x = $+\infty$. If the source of particles is to the left in region I, and there is no source far to the right, then we may allow for the possibility of particles tunneling through the barrier and continuing on to the right by taking the wavefunction in region III to be

$$\Phi_{III} = Fe'''' \tag{7.53}$$

As before, $\hbar k$ A $^2/m$ is the number of particles per unit time moving to the right in region I and hitting the potential barrier, $\hbar k \mid B \mid ^2/m$ is the number reflected, and $\hbar k$ $F \mid ^2/m$ is the number transmitted into region III. In this example, the particles in both regions I and III have momentum of magnitude Ak.

There are two boundary conditions at x = 0: continuity of the wavefunction and of its derivative; and there are two similar conditions at x = a. They give

$$\text{at } x = 0 \begin{cases} A + B = C + D \\ ik(A - 8) = \beta(-C + D) \end{cases} \tag{7.54}$$

$$\text{at } x = a \begin{cases} Ce^{-\beta a} + De^{\beta a} = Fe^{ika} \\ \beta(-Ce^{-\beta a} + De'''') = ikFe^{ika} \end{cases} \tag{7.55}$$

Solution of Equations (7.54) and (7.55), for *B*, C, *D* and *F*, in terms of A, gives us after some algebra,

$$B = \frac{[1 + (\beta/k)^2](1 - e^{-2\beta a})}{[1 - (\beta/k)^2](1 - e^{-2\beta a}) + 2i(\beta/k)(1 + e^{-2\beta a})} A \tag{7.56}$$

$$C = \frac{2[1 + i(\beta/k)]}{[1 - (\beta/k)^2](1 - e^{-2\beta a}) + 2i(\beta/k)(1 + e^{-2\beta a})} A \tag{7.57}$$

$$D = \frac{2[1 - i(\beta/k)]e^{-2\beta a}}{[1 \quad (\beta/k)^2](1 \quad e^{-2\beta a}) + 2i(\beta/k)(1 + e^{-2\beta a})} A \tag{7.58}$$

$$F = \frac{4i(\beta/k)e^{-(\beta + ik)a}}{[1 - (\beta/k)^2](1 - e^{-2\beta a}) + 2i(\beta/k)(1 + e^{-2\beta a})} A \tag{7.59}$$

While these results are somewhat involved, it is easy to substitute them into Equations (7.54) and (7.55) and to verify that they are solutions. Since the particle speed is the same in I and III, the transmission coefficient is simply $T = FF^*/AA^*$. It is

$$T = \frac{16(\beta/k)^2 e^{-2\beta a}}{[1 - (\beta/k)^2]^2(1 - e^{-2\beta a})^2 + 4(\beta/k)^2(1 + e^{-2\beta a})^2} \tag{7.60}$$

If βa is large compared to one, the exponentials in the denominator of Equation (7.60) are very small compared to one, and can be dropped. In this case,

$$T \simeq \left[\frac{4\beta/k}{1 + (\beta/k)^2}\right]^2 e^{-2\beta a} \tag{7.61}$$

Because the exponential, $e^{-2\beta a}$, rapidly becomes small with increasing βa, the fraction of particles getting through is very small when $\beta a = \sqrt{2m(V_0 - E)}a/\hbar$ is large. Thus, as the energy becomes smaller compared to V_0, or the width of the potential barrier becomes greater, fewer particles tunnel through. Of course, in Newtonion mechanics no particles would get through.

example 'I. When two materials are placed in contact, an electron often has to go through a potential barrier of a few electron volts to get from one material to the other. There are a number of solid state devices which are made this way deliberately. For electrons, $m = 9.1 \times 10^{-31}$ kg and $\hbar = 1.05 \times 10^{-34}$ j-sec. Take $V_0 - E = 1$ eV and $a = 3$ Angstroms, a reasonable distance between atom layers. Estimate the value of the exponential $e^{-2\beta a}$.

solution

$$2\beta a = \frac{2\sqrt{2m(V_0 - E)}\,a}{\hbar}$$

$$= \frac{2\sqrt{2(9.1 \times 10^{-31})(1.6 \times 10^{-19})}(3 \times 10^{-10})}{1.05 \times 10^{-34}} = 3.08.$$

Therefore, $e^{-2\beta a} = e^{-3.08} = 0.046$. So the tunneling is reasonably probable.

example 2. Hydrogen impurities in a solid might diffuse through it by tunneling of the hydrogen nucleus (the proton) from one lattice site to another. The proton mass is about 1836 times that of the electron. Take the other parameters to be the same as in part (1) of this Example. Find the exponential in this case.

solution Since the only change from Example 1 is in the mass, the exponent is increased by a factor of $\sqrt{1836}$. Then $e^{-2\beta a} = e^{-132} = 2 \times 10^{-57}$. The proton in oscillating about its equilibrium point in the solid might have a frequency of around 10^{13} per second. This is essentially how many times the proton hits the barrier per second. The product of 10^{13} and the exponential is a measure of the order of magnitude of the probability of a proton jump per second. This is of the order of 10^{-44}, completely negligible. If the quantity, V_0 E, were lowered by a factor of ten or more. this diffusion would begin to be more important.

7.9 PARTICLE IN A BOX

As a fourth illustration of the solutions of the one dimensional Schrödinger equation, we shall consider the case of a particle confined to a finite region, a one dimensional box of length L. By this we mean that the particle is definitely inside the box and is kept there by rigid impenetrable walls at the ends, $x = 0$ and $x = L$. This is illustrated in Figure 7.4. Since the particle is confined to a

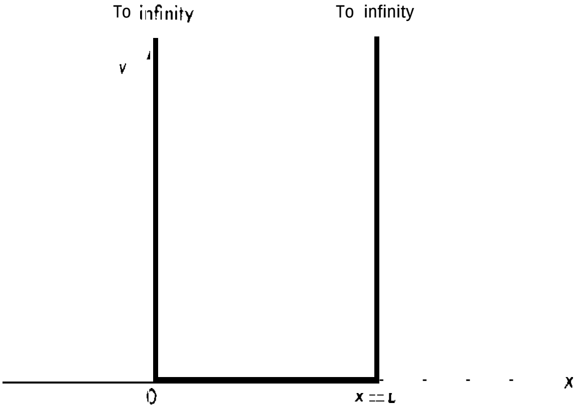


Figure 7.4. Potential energy function for a particle in a one dimensional box.

region of size L, the uncertainty in position Δx is about L, so the uncertainty Δp_x in momentum p_x should be about $\hbar/L$. Hence the particle cannot have a definite momentum. It can, however, still have a definite energy, as we shall see.

We still assume that the energy is definite, so $\psi = \Phi(x)e^{-iEt/\hbar}$, where $\Phi(x)$ is the spatial part of the wave function. Hence, inside the box, where $V = 0$, Φ satisfies the differential equation:

$$\frac{\hbar^2}{2m}\frac{d^2\Phi}{dx^2} = E\Phi \tag{7.62}$$

We expect this equation to tell us what $\Phi(x)$ is inside the box. The situation is somewhat analogous to the case of a stretched string held rigidly at both ends. In that case also, a wave may exist on the string, and solutions of definite frequencies arise only when an integral number of half wavelengths of the wave can fit into the length L of a string. This gives rise to standing waves on the string. A similar situation should hold for the de Broglie waves in the box of length L. If λ is the wavelength of a de Broglie wave, then in order for the wave not to interfere destructively with itself, an integral number n of half wavelengths should fit into the box, or:

$$\frac{n\lambda}{2} = L \tag{7.63}$$

The magnitude of the momentum would then be

$$p = \frac{h}{\lambda} = \frac{hn}{2L} \tag{7.64}$$

The kinetic energy would be

$$E = \frac{p^2}{2m} = \frac{(hn)^2}{8mL^2} \tag{7.65}$$

So only a discrete set of energies or frequencies would be allowed. These would be determined by values of the integer *n*.

7.10 BOUNDARY CONDITION WHEN POTENTIAL GOES TO INFINITY

Now let us see how this same situation would be treated using the Schrödinger equation, Equation (7.62). To solve a differential equation like this, we need to have boundary conditions, statements analogous to the requirement that the displacement at the ends of the stretched string must vanish. In our case, we know the particle is inside rather than outside the box. The reason that Φ is zero outside the box is that the walls are assumed to be perfectly rigid, so that all particles bounce elastically off the walls, or, equivalently, that the potential energy is infinite outside. The probability of finding a particle outside is therefore zero; so, for x outside the box, $|\Phi(x)|^2 = 0$. This implies that the value of Φ itself must be zero outside. Since the wavefunction must be continuous, the value of the wavefunction just inside the box must be zero at either end, so

$$\Phi(x = 0) = \Phi(x = l) = 0 \tag{7.66}$$

The slope of the wavefunction must also be continuous, and it might appear at first glance that both the wavefunction and its slope are zero at the endpoints; but this would mean the wavefunction would vanirh everywhere, an unreasonable solution. To see why the slope of the wavefunction can be finite at the endpoints, suppose the potential energy outside the box were not infinite, but had a large constant value. Then for x > L, $\Phi = Ce^{-\beta x}$, with β proportional to the square root of the potential energy. Outside, $d\Phi/dx = -\beta Ce^{-\beta x} = -\beta\Phi$. Hence, although Φ approaches zero as $V_0 \to \infty$, β approaches infinity and the product $\beta\Phi$ can remain finite. Indeed, $d\Phi/dx$ must be finite everywhere, both inside and just outside the box. The boundary conditions for the case of the particle in a box are therefore given by Equation (7.66), with no further available information on the slopes $d\Phi/dx$ at the endpoints, except that they are finite.

7.11 STANDING WAVES AND DISCRETE ENERGIES

We now have a differential equation, Equation (7.60), with boundary conditions. For ease in writing the equations, let

$$k = \frac{(2mE)^{1/2}}{\hbar} \tag{7.67}$$

Then the Schrödinger equation, Equation (7.32), becomes:

$$\frac{d^2\Phi}{dx^2} = -k^2\Phi \tag{7.68}$$

This equation is the same as that discussed in connection with the step potential, and has oscillatory solutions of the form of Equation (7.28). For the present application, however, it is more convenient to write the solutions in trigonometrical form, as a sum of a sine and a cosine:

$$\Phi(x) = A \cos kx + B \sin kx \tag{7.69}$$

where A and B are two arbitrary constants whose ratio is to be determined from the boundary conditions. One condition is $\Phi(x = 0) = 0$. This gives us:

$$\Phi(0) = A \cos(0) + B \sin(0) = 0 \tag{7.70}$$

or A = 0. The second boundary condition is $\Phi(x = L) = 0$. This gives us:

$$\Phi(L) = B \sin(kL) = 0 \tag{7.71}$$

This could be satisfied by setting $B = 0$, but then the whole wavefunction would vanish, which is not the desired solution. The other possibility is $\sin(kL) = 0$. The sine function has zeros at values of L such that:

$$kL = n\pi \tag{7.72}$$

where n is any integer not equal to zero. If $n = 0$, again the whole wavefunction would vanish, so this case is excluded. The possible wavefunctions are then:

$$\Phi_n(x) = B \sin\left(\frac{n\pi x}{L}\right) \qquad n = 1, 2, 3, \ldots \tag{7.73}$$

Only positive integers are taken, because negative integers just duplicate the same wavefunctions with an overall sign change; the overall sign, however, is not physically significant. The constant B can be determined by normalization. Thus, if the probability of finding the particle in the range dx is $\Phi_n{}^2 dx$, then for one particle in the box,

$$\int_0^L dx \, |\Phi_n(x)|^2 = 1 \tag{7.73}$$

Using the formula

$$\int_0^L dx \left\{\sin\left(\frac{n\pi x}{L}\right)\right\}^2 = \frac{1}{2} L \tag{7.74}$$

we find that

$$|B|^2 = \frac{2}{L} \tag{7.75}$$

If, for convenience, B is taken to be real, the final form of the eigenfunctions is:

$$\Phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \qquad n = 1, 2, 3, \ldots \tag{7.76}$$

The constant in front of the sine function is called the *normalization constant.*

Having solved the differential equation with boundary conditions, we can now find the allowed energies. From the definition of k, Equation (7.66), the energy is:

$$E = \frac{\hbar^2 k^2}{2m} \tag{7.77}$$

or

$$E = \frac{(n\pi\hbar)^2}{2mL^2} \tag{7.78}$$

This is the same as that obtained by analogy with a stretched string. The main point to be seen here is that because of the boundary conditions, only a discrete set of energies are possible; the energy is *quantized*. The smaller the size of the box L, the larger will be the spacings between allowed energies. Physically, it is the confinement of the electron to lie within a small region which gives rise to the discrete energy spacings. In classical mechanics, any energy would be possible for this mechanical situation.

7.12 MOMENTUM AND UNCERTAINTY FOR A PARTICLE IN A BOX

To investigate the momentum, the sine function can be written as a superposition of exponentials. For example, for n = 1, the ground state, the wavefunction is:

$$\Phi_1(x) = -\left(\frac{i}{\sqrt{2L}}\right)(e^{i\pi x/L} - e^{-i\pi x/L}) \tag{7.79}$$

The term involving $e^{i\pi x/L}$ by itself would correspond to a value of momentum given by:

$$p_x\Phi = \frac{\hbar}{i}\frac{d\Phi}{dx} \quad \text{or} \quad p_x = \frac{\hbar\pi}{L} \tag{7.80}$$

The term $e^{-i\pi x/L}$ would correspond to a value of momentum, $p_x = -\hbar\pi/L$. So appearance of these exponentials in Φ_1 with equal amplitudes corresponds to the motion of the particle in either direction with equal probability; the wavefunction Φ_1 is a superposition of waves of equal but opposite momenta. Thus the expectation value of the momentum is zero. This could be verified directly by calculating $\int_0^L dx\, \psi^*(\hbar/i)d\psi/dx$. The difference in the momenta of the superposed waves should give us a measure of the order of magnitude of the uncertainty in p_x. Thus, approximately,

$$\Delta p_x \cong \frac{\hbar\pi}{L} - \left(-\frac{\hbar\pi}{L}\right) = \frac{2\hbar\pi}{L} \tag{7.81}$$

Also, Δx is on the order of L, so $\Delta x \Delta p_x \cong$ h, in agreement with the uncertainty principle. A more careful calculation of the uncertainties using rms deviations from the means could easily be made, but the crude argument given above is sufficient to illustrate the uncertainty principle in this example.

7.13 LINEAR MOLECULES APPROXIMATED BY PARTICLE IN A BOX

Frequently, physicists represent energy levels by a diagram in which horizontal bars have a vertical spacing proportional to the energy spacing between levels. This allows one to see at a glance the energy structure of the system. In Figure 7.5 an energy level diagram is shown for the particle in a box, where the

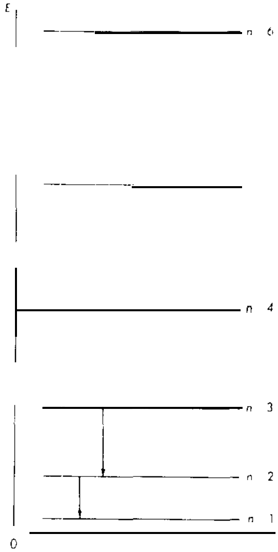


Figure 7.5. Energy level diagram and possible transitions for a particle in a one dimensional box.

energies are $E_n = n^2h^2/8mL^2$. Here the distance of the bars from the base line corresponding to the zero of energy is proportional to n^2. This is essentially a one dimensional plot of allowed energies with energy increasing upwards. The particle can exist in stationary states, states of definite frequency, only if the energies have these discrete values. If some external influence should disturb the particle, then it might change from one of these states to another. For example, if the particle started in the state labeled by the integer n_u, and ended up in the state n_ℓ (u for upper, ℓ for lower), then it would have to lose energy:

$$E_u - E_\ell = (n_u^2 - n_\ell^2)\left(\frac{h^2}{8mL^2}\right) \qquad (7.82)$$

This energy could be given up in the form of a photon The energy of the photon would be:

$$E = h\nu = E_u \quad E_\ell \qquad (7.83)$$

Therefore, the differences between levels in an energy level diagram are proportional to the light frequencies we might expect to see emitted from the system.

Physical systems for which the particle in the box is a good model are found in certain classes of long straight molecules of varying lengths L, which attract electrons in such a way that the electron moves back and forth between the ends of the molecule in a standing wave. The observed energies are closely approximated by those of the particle in a box, Equation (7.78). When the electron makes transitions between these energy states, absorption and emission of photons are observed. If the upper state is the $n = 2$ state, and the lower state is the $n = 1$ state, then for a molecule of length L the frequency of the photon should be:

$$\nu = \frac{3h}{8mL^2} \tag{7.84}$$

The wavelength of the photon would be given by:

$$\lambda = \frac{c}{\nu} = \frac{8mL^2c}{3h} \tag{7.85}$$

For the electron, $m = 9.11 \times 10^{-31}$ kg. Then, for a molecule of length $L = 7$ Angstroms, this wavelength is in the visible region:

$$\lambda \; \frac{8(9.11 \times 10^{-31})(7 \times 10^{-10})^2(3 \times 10^8)}{[3(6.63 \times 10^{-34})]}$$

$$= 5.39 \times 10^{-7} \text{ m} = 5390 \text{ Angstroms} \tag{7.86}$$

7.14 HARMONIC OSCILLATOR

The final example to be studied in this chapter is the one dimensional harmonic oscillator. The study of the quantum mechanical harmonic oscillator is very important, because a number of physical systems can be considered to behave like a collection of harmonic oscillators. For small vibrations, particles in most potential wells have simple harmonic vibrations. For instance, a diatomic molecule has the energy levels of a one dimensional harmonic oscillator (along with rotational and atomic levels). Also, quantized sound waves (phonons) and light waves (photons) can be represented as harmonic oscillators.

The Schrödinger equation for a one dimensional harmonic oscillator must first be obtained. For a particle of mass m with displacement x from equilibrium, the kinetic energy operator is $-(\hbar^2/2m)\partial^2/\partial x^2$. The total energy operator is $i\hbar\partial/\partial t$. Also, for a spring constant K, the harmonic oscillator potential is $V = \frac{1}{2}Kx^2$. These operators lead to the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}Kx^2\psi = i\hbar\frac{\partial\psi}{\partial t} \tag{7.87}$$

If, again, a stationary state with definite energy is assumed, so that $\psi = \Phi(x)e^{-iEt/\hbar}$, the equation for Φ is:

$$\frac{\hbar^2}{2m}\frac{d^2\Phi}{dx^2} + \frac{1}{2}Kx^2\Phi = E\Phi \tag{7.88}$$

Since in microscopic systems, frequency is more easily measurable than spring constants, it is desirable to eliminate **K** by expressing it in terms of the angular frequency for a harmonic oscillator from Newtonian mechanics, $\omega = \sqrt{K/m} = 2\pi\nu$. Then, in terms of ω,

$$-\frac{\hbar^2}{2m}\frac{d^2\Phi}{dx^2} + \frac{1}{2}m\omega^2x^2\Phi = E\Phi \tag{7.89}$$

Let us verify that for the proper choice of α, an energy eigenfunction is:

$$\Phi_0 = a_0e^{-1/2\alpha x^2} \tag{7.90}$$

where a_0 is a normalization constant. The first term in the differential equation, Equation (7.89), contains:

$$\frac{d^2\Phi}{dx^2} = a_0\frac{d}{dx}\left(\frac{de^{-1/2\alpha x^2}}{dx}\right) = a_0e^{-1/2\alpha x^2}(\alpha^2x^2 \quad \alpha) \tag{7.91}$$

The differential equation then becomes:

$$a_0e^{1/2\ \alpha x^2}\left(-\frac{h^2\alpha^2}{2m}x^2 + \frac{\hbar^2\alpha}{2m} + \frac{1}{2}m\omega^2x^2\right) = a_0e^{-1/2\alpha x^2}E \tag{7.92}$$

Since this must hold for any arbitrary x, in order to have a solution the sum of the coefficients of x^2 must be zero. Thus, $-\hbar^2\alpha^2/2m + \frac{1}{2}m\omega^2 = 0$, and this leads to a value for α,

$$\alpha = \frac{m\omega}{\hbar} \tag{7.93}$$

Then for the remainder of the equation to be satisfied, the energy eigenvalue must be:

$$E = E_0 = \frac{1}{2}\omega\hbar \tag{7.94}$$

Note that the probability density $\Phi_0|^2$ for this solution to the Schrödinger equation is gaussian in form. One might suspect that for this case the uncertainty product $\Delta p\Delta x$ would be a minimum. Comparison of the wavefunction of Equation (7.90) with the free-particle gaussian packet, Equation (7.9), indicates that $\frac{1}{2}\alpha = \frac{1}{2}\sigma^2$, so for this case,

$$\langle x\rangle = 0 \tag{7.95}$$

$$\Delta x = \frac{1}{\sqrt{2}}\sqrt{\frac{1}{\alpha}} = \frac{1}{\sqrt{2\alpha}} \tag{7.96}$$

$$\langle p\rangle = 0 \tag{7.97}$$

$$\Delta p = \frac{\hbar}{\sqrt{2}}\cdot\sqrt{\alpha} = \hbar\sqrt{\frac{\alpha}{2}} \tag{7.98}$$

Hence, again, $\Delta x\Delta p = \hbar/2$. In fact, it is because of the uncertainty principle that the minimum possible energy of the oscillator is greater than zero. Classically, the minimum energy state of an oscillator would occur when the mass was at rest ($p = 0$) at the position of zero displacement ($x = 0$). Then both kinetic and potential energies would vanish, and $E_{min} = 0$. This is not possible in quantum mechanics, because then both position and momentum would be known, with $\Delta x = \Delta p = 0$ violating the principle of uncertainty.

Since $\langle x \rangle = (p) = 0$ for the oscillator, $\Delta p^2 = (p')$ and $\Delta x^2 = \langle x^2 \rangle$. The average value for the energy in the ground state is thus:

$$\langle E \rangle = \frac{1}{2m}(p') + \frac{1}{2}K(x') = \frac{1}{2m}\Delta p^2 + \frac{1}{2}K\Delta x^2$$

$$= \frac{1}{2m}\,\frac{\hbar^2\alpha}{2} + \frac{1}{2}\,\frac{K}{2\alpha} \tag{7.99}$$

Since $\alpha = m\omega/\hbar$,

$$\langle E \rangle = \frac{1}{2m}\,\frac{\hbar^2 m\omega}{2\hbar} + \frac{1}{2}K\frac{\hbar}{2m\omega} = \frac{1}{4}\hbar\omega + \frac{1}{4}\hbar\omega = \frac{1}{2}\hbar\omega \tag{7.100}$$

Thus, in a sense, the uncertainty principle requires both $\langle p^2 \rangle$ and (x') to be positive, and forces the ground state energy to have a positive value.

7.15 GENERAL WAVEFUNCTION AND ENERGY FOR THE HARMONIC OSCILLATOR

The general solution of the one dimensional harmonic oscillator Schrodinger equation which satisfies the boundary condition, $\Phi \rightarrow 0$ as $x \rightarrow \pm\infty$, is, for $\alpha = m\omega/\hbar$,

$$\Phi_n(x) = \sum_{\ell=0}^{1/2\,n} a_\ell\, x^{2\ell} e^{-1/2\,\alpha x^2}, \quad \text{for n an even integer} \tag{7.101}$$

$$\Phi_n(x) = x\sum_{\ell=0}^{1/2(n-1)} a_\ell\, x^{2\ell} e^{-1/2\,\alpha x^2} \quad \text{for n an odd integer} \tag{7.102}$$

By substituting into the Schrodinger equation, Equation (7.63), one may find the coefficients a_ℓ in terms of a,,, and determine the energy eigenvalues. The general expression for the energy is found to be:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n = 0, 1, 2, 3, \ldots \tag{7.103}$$

The first five of the eigenfunctions are given in Table 7.2, along with their energy eigenvolues. The lowest (energy, ½$\hbar\omega$, belongs to the state described by the wavefunction Φ_0 already discussed. This is ‘called the zero ***point energy.*** The five lowest possible energy eigenfunctions of Table 7.2 are graphed in Figures 7.6 through 7.10, along with their probability densities, $\Phi_n{}^2$.

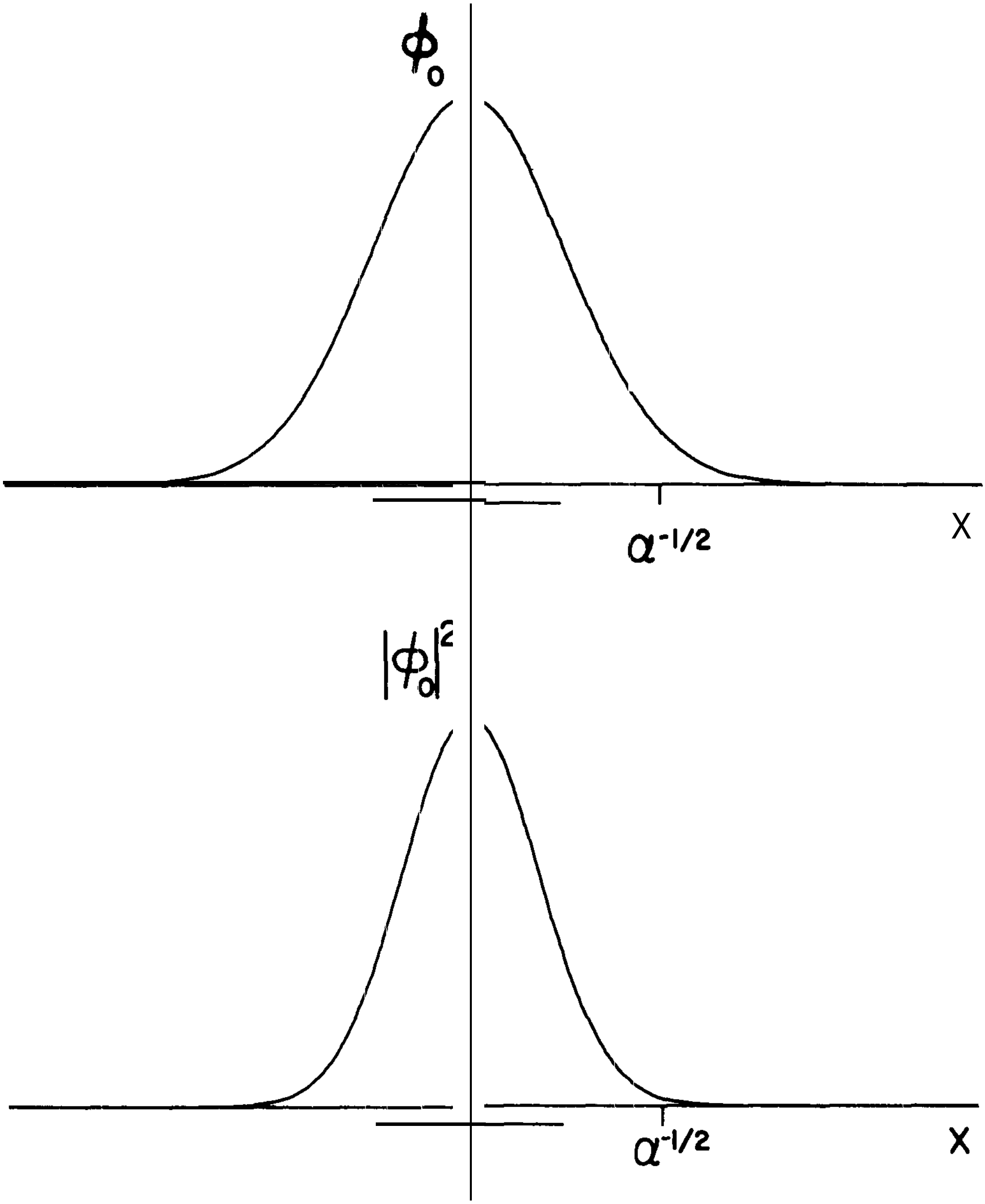


Figure 7.6. Wavefunction and probability density for the ground state (n = 0) of the harmonic oscillator. The horizontal bar beneath the origin indicates the range of possible positions for classical motion with the same energy.

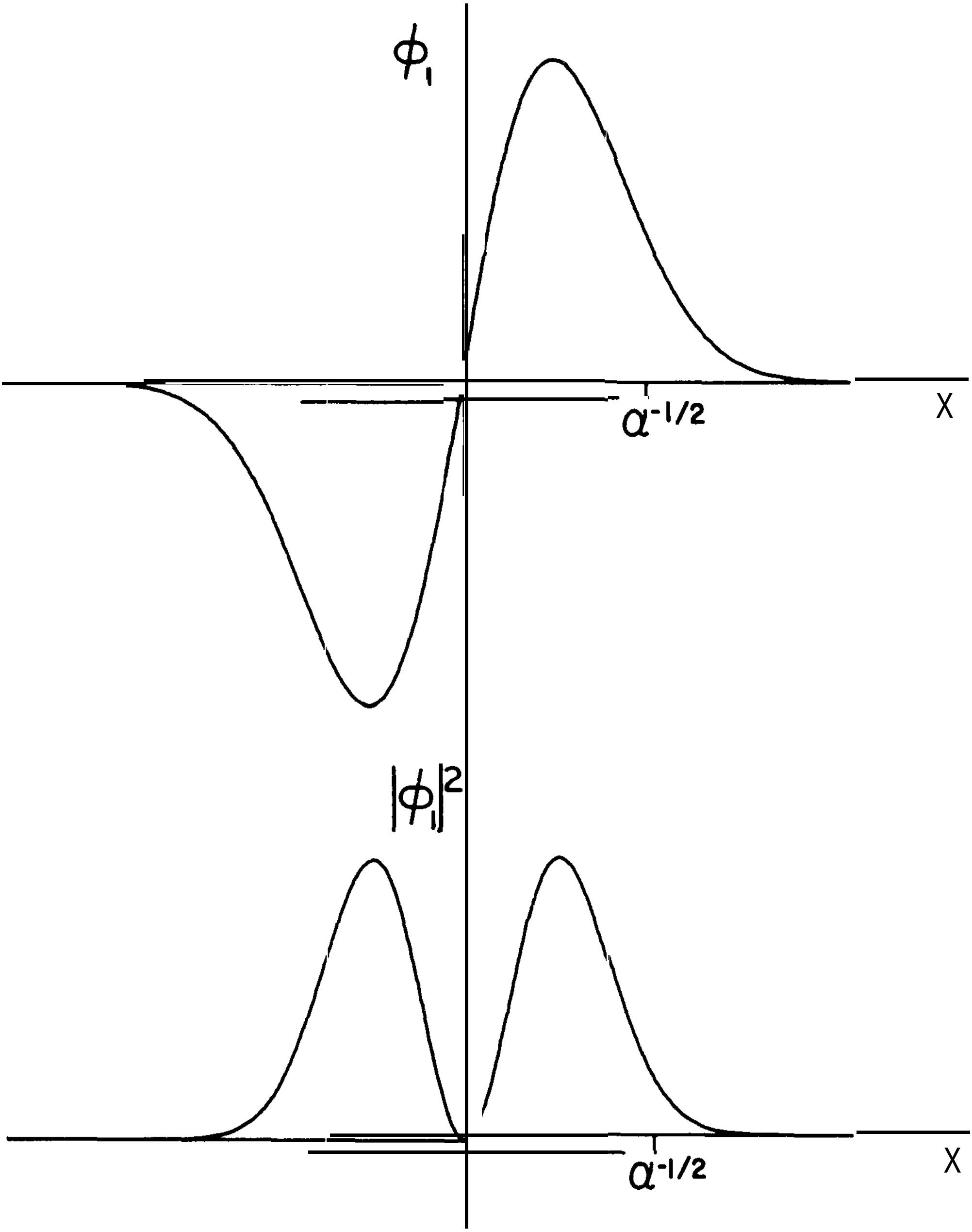


Figure 7.7. Wavefunction and probability density for the harmonic oscillator state with n = 1.

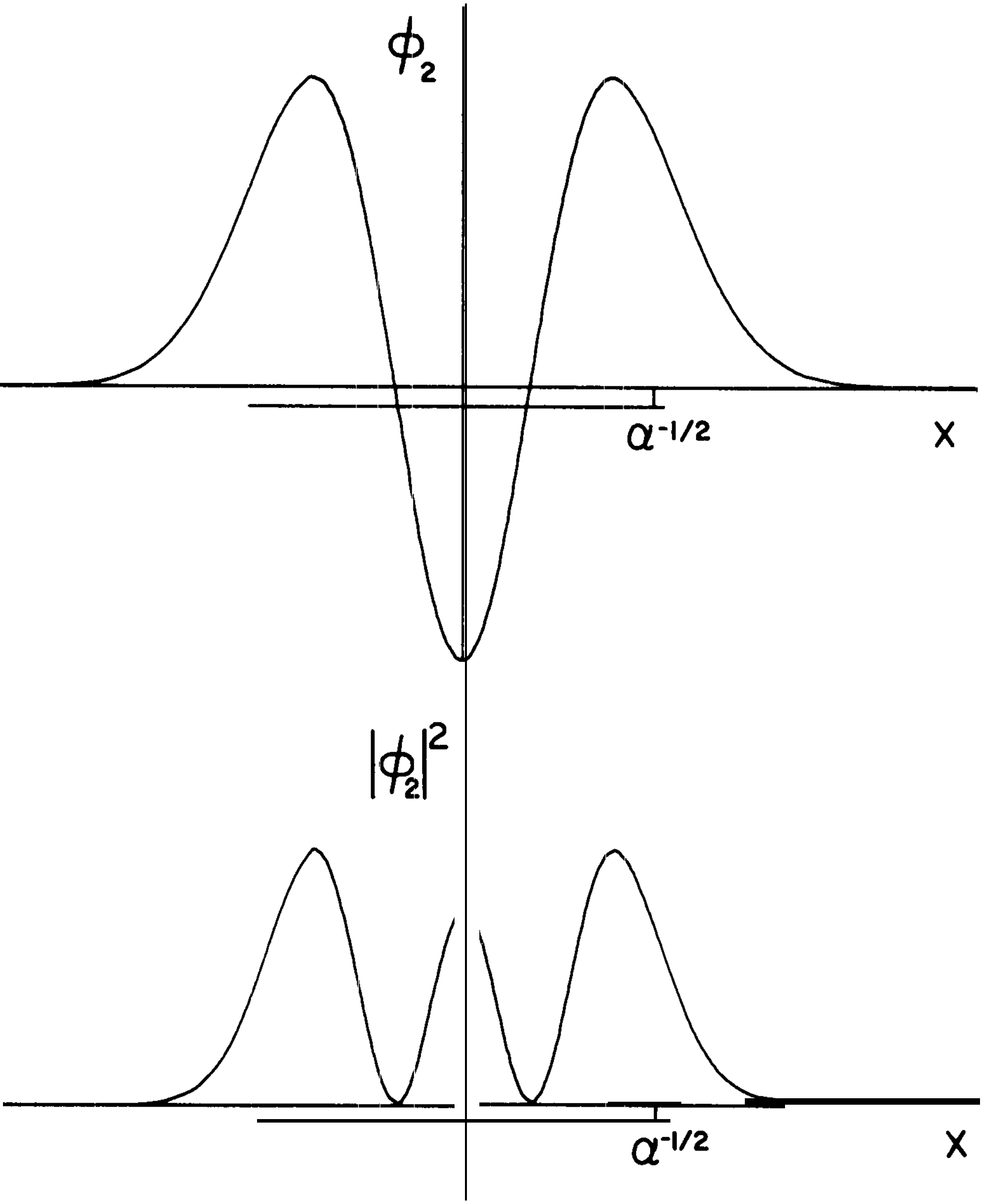


Figure 7.8. Wavefunctian and probability density for the harmonic oscillator state with $n = 2$.

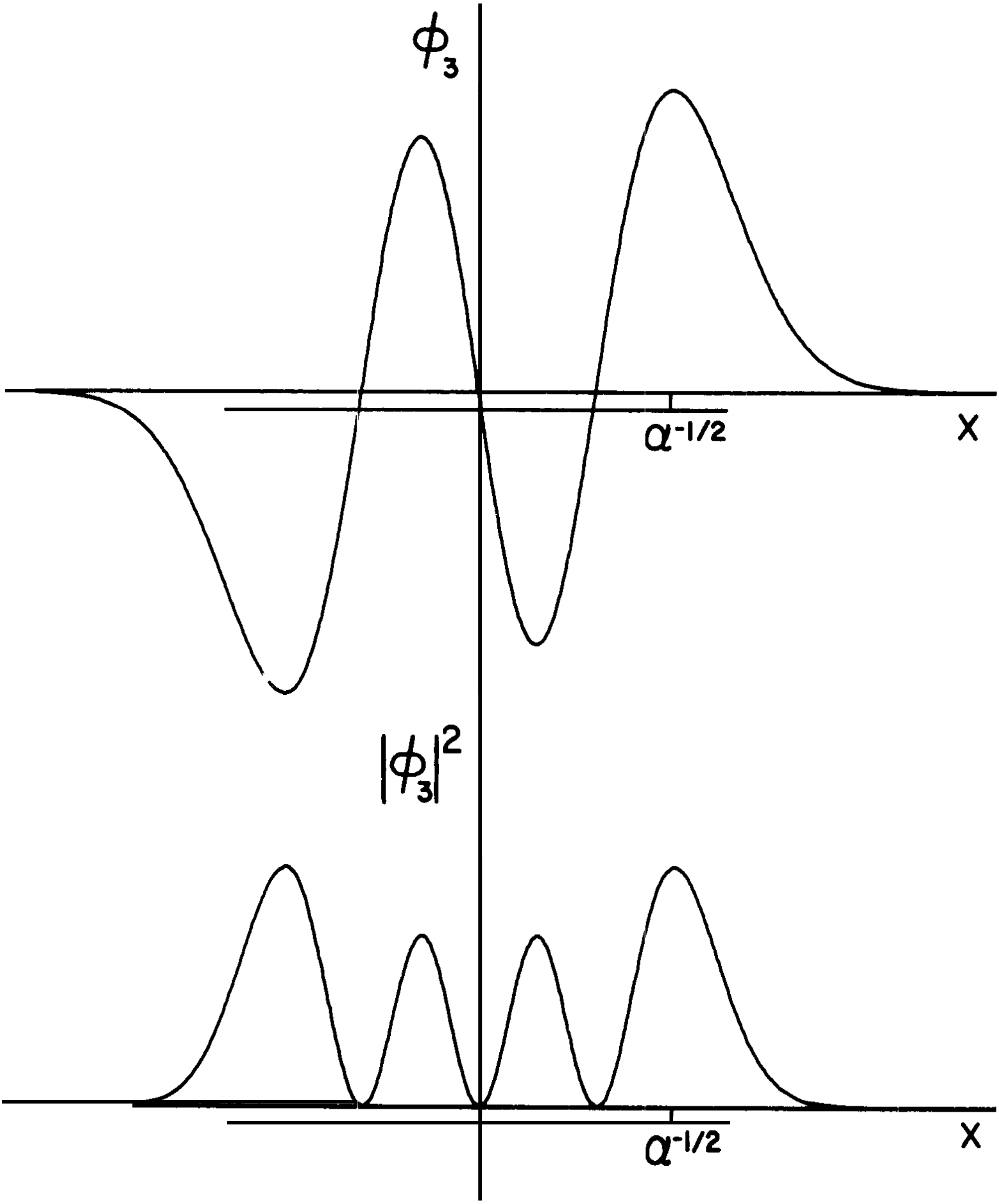


Figure 7.9. Wavefunction and probability density for the harmonic oscillator state with $n = 3$.

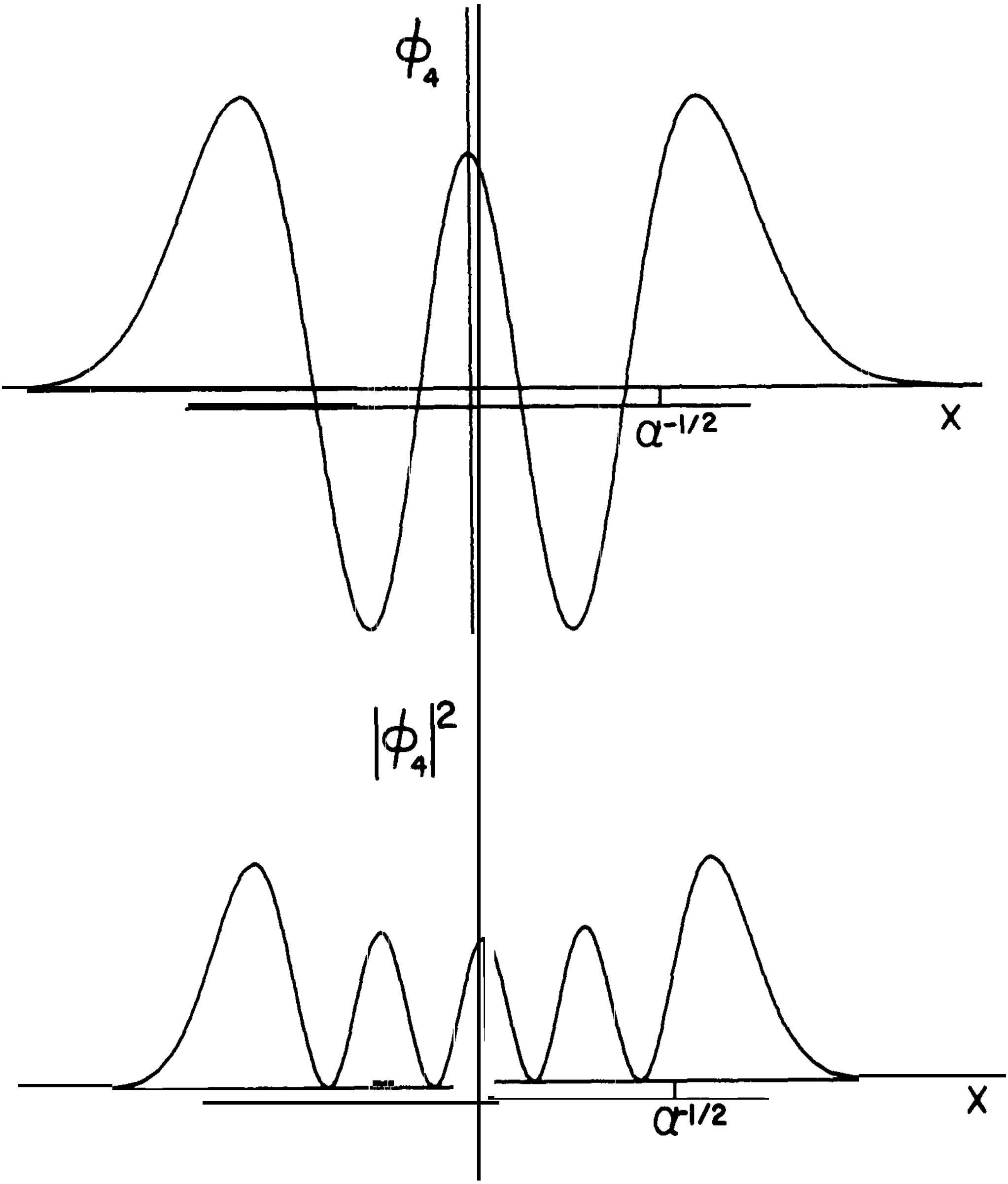


Figure 7.10. Wavefunction and probability density for the harmonic oscillator state with $n = 4$.

TABLE 7.2 Eigenvalues and Eigenfunctions for First Five Simple Harmonic Oscillator States

Quantum Number n	Wavefunction Φ_n	Energy Eigenvalue E_n
0	$\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-1/2\,\alpha x^2}$	$\frac{1}{2}\hbar\omega$
1	$\left(\frac{4\alpha^3}{\pi}\right)^{1/4} x\, e^{-1/2\,\alpha x^2}$	$\frac{3}{2}\hbar\omega$
2	$\left(\frac{\alpha}{4\pi}\right)^{1/4}(1-2\,\alpha x^2)e^{-1/2\,\alpha x^2}$	$\frac{5}{2}\hbar\omega$
3	$\left(\frac{9\alpha^3}{\pi}\right)^{1/4} x\left(1-2\alpha\frac{x^2}{3}\right)e^{-1/2\,\alpha x^2}$	$\frac{7}{2}\hbar\omega$
4	$\left(\frac{9\alpha}{64\pi}\right)^{1/4}\left(1-4\alpha x^2+4\alpha^2\frac{x^4}{3}\right)e^{-1/2\,\alpha x^2}$	$\frac{9}{2}\hbar\omega$

The coefficient a_0, in the case of each eigenfunction Φ_n, may be found by requiring that the total probability of finding a particle be unity. Thus, for Φ_0, the probability density is, from Equation (7.90),

$$\Phi_0{}^*\Phi_0 = |a_0|^2 e^{-\alpha x^2} \tag{7.104}$$

and the total probability is:

$$1 = \int_{-\infty}^{\infty} |a_0|^2 e^{-\alpha x^2} dx = \sqrt{\pi}\frac{|a_0|^2}{\sqrt{\alpha}} \tag{7.105}$$

from Table 7.1. Therefore, assuming it is real and positive, the value of a_0 for this state is $(\alpha/\pi)^{1/4}$, as shown in Table 7.2. A similar integration must be done to determine a_0 for each state.

7.16 COMPARISON OF QUANTUM AND NEWTONIAN MECHANICS FOR THE HARMONIC OSCILLATOR

It is of interest to compare the probability distribution from quantum mechanics to that from Newtonian mechanics for a state of high n. If in Newtonian mechanics the position of the particle is measured at arbitrary times, one would expect that the probability of finding it in dx is inversely proportional to the speed,. i.e. proportional to the time $dt = dx/(dx/dt)$ that the particle spends in the range of positions dx. In Problem 21 of Chapter 2 it was found; that the probability is then:

$$p\,dx = \frac{dx}{\pi\sqrt{x_0^2 - x^2}} \tag{7.106}$$

for an amplitude x_0. The classical amplitude x_0 for a given energy is found by equating the maximum potential energy to the total energy:

$$E = \frac{1}{2} m\omega^2 x_0^2 \quad \text{or} \quad x_0^2 = \frac{2E}{m\omega^2}$$

The probability density, $1/(\pi\sqrt{x_0^2 - x^2})$, is plotted in Figure 7.11 as the dotted curve for $E = 41/2\ \hbar\omega$, corresponding to n = 20. The quantum density, $\Phi^*\Phi$,

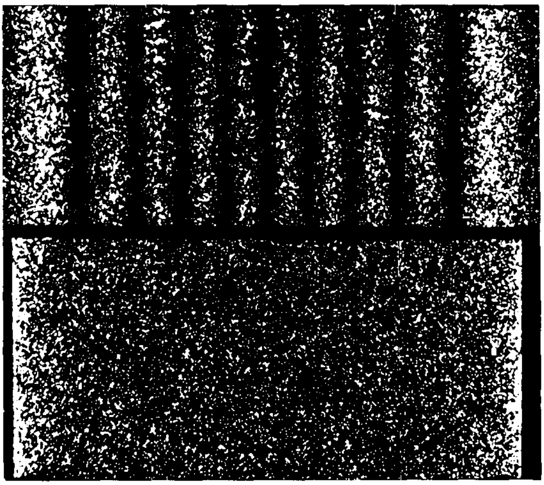


Figure 7.11. Comparison **of classical (dotted) and quantum mechanical (solid) distribution functions for the one dimensional harmonic oscillator with n = 20.**

is the corresponding solid curve for n = 20. Between $-x_0$ and x_0 the main differences are the oscillations and zeros in the quantum curve. Outside this range of x, the Newtonian probability density is exactly **zero**; the particle cannot go into a region in which the kinetic energy would be negative. There is a tail to the quantum curve in those regions, however, indicating a possibility for the particle to be found there.

In Figure 7.12 are given probability density plots for a harmonic oscillator with n = 10, together with the corresponding classical density. These plots correspond to a particle which is free to move in the vertical direction but is bound by the oscillator potential in the horizontal direction. If several thousand measurements of position of the oscillator were made and plotted on a graph, the resulting plot would have the appearance of the Figure.

The connection with Newtonian mechanics may be seen more easily by considering a gaussian wave packet similar to that discussed for the free particle ot the beginning of this chapter. The reader may verify by substituting into Equation (7.87) that the Schrödinger equation is satisfied by:

$$\psi(x,t) = \left(\frac{\alpha}{\pi}\right)^{1/4} \exp\left[-\frac{1}{2}\alpha(x - x_0 \cos\omega t)^2 - i\left(\frac{1}{2}\,\omega t + \alpha x x_0 \sin\omega t - \frac{1}{4}\,\alpha x_0^2 \sin 2\omega t\right)\right] \tag{7.107}$$

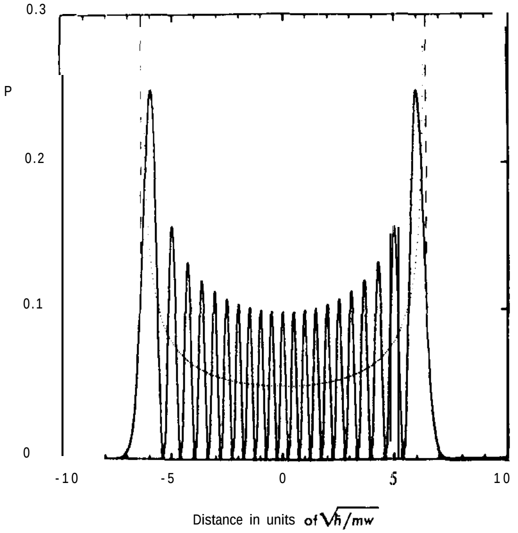


Figure 7.12. Density of points is proportional to the probability density for the harmonic oscillator with n = 1; quantum mechanical density at the top of the diagram, classical density below.

This function is a superposition of many stationary states $\Phi_n \exp(-iE_nt/\hbar)$, and thus does not correspond to a definite energy. The probability density is:

$$|\psi|^2 = \sqrt{\frac{\alpha}{\pi}} \exp[-\alpha(x \quad x_0 \cos \omega t)^2] \tag{7.108}$$

This is a wave packet of constant characteristic width I/da = $\sqrt{\hbar/m\omega}$, with its center moving with the Newtonian simple harmonic motion, x = x_0 cos wt. For a macroscopic mass of 1 kg and a spring frequency of 1 cycle/sec, the characteristic width of the gaussian is around 10^{-17} m. Therefore, for all practical purposes, the position is known with negligible error.

What about the energy spread? The expectation value of the energy operator, $i\hbar\partial/\partial t$, is easily found with the help of Table 7.1 to be:

$$(E) = \frac{1}{2} m\omega^2 x_0^2 + \frac{1}{4} \hbar\omega \tag{7.109}$$

This is the Newtonian energy plus one-half the zero point energy. Since the zero point energy for a frequency of 1 cycle/sec is approximately 10^{-34} j, one can forget about it for macroscopic bodies. The rms deviation of the energy from its mean is:

$$\Delta E = \left[\left\langle\left(i\hbar \frac{\partial}{\partial t}\right)^2\right\rangle - \langle E\rangle^2\right]^{1/2} = \sqrt{2}\sqrt{\frac{1}{2} m\omega^2 x_0^2}\sqrt{\frac{1}{2} \hbar\omega} \tag{7.110}$$

This is $\sqrt{2}$ times the square root of the Newtonian energy times the zero point energy. For a macroscopic body, ΔE is negligible compared to E; it is about 10^{-17} j if E is approximately a joule. On the other hand, ΔE is very large compared to the zero point energy. So we conclude that for macroscopic bodies, as closely as we can measure, quantum and Newtonian mechanics agree for the harmonic oscillator. Of course, for microscopic bodies this is not true. In particular, as the maximum classical displacement x_0 approaches zero, the wavefunction, Equation (7.44), approaches the ground state wavefunction and E approaches the zero point energy. Also, ΔE approaches zero as one would expect for the stationary ground state.

17 CORRESPONDENCE PRINCIPLE IN QUANTUM THEORY

The above discussions of the classical and quantum descriptions of a simple harmonic oscillator and of a gaussian wave packet far a free particle provide illustrations of the application to quantum theory of the correspondence principle, which was discussed in (Chapter 3, in connection with special relativity. According to this principle, the quantum theory should give essentially the same results as the classical theory—Newtonian mechanics--in situations where the classical theory is known to hold, such as in situations involving bodies of macroscopic mass and size. It was seen, for example, that a wave packet describing a particle of macroscopic mass had negligible spreading, and, similarly, that a well-localized oscillator having negligible spread could be obtained for an oscillator of macroscopic mass.

These situations almost always involve the superposition of an extremely large number of stationary states, leading to large quantum numbers. Hence, another way of stating the correspondence principle is that the classical theory must be an appropriate limit of the quantum theory involving extremely large quantum numbers. For example, in order for a particle of mass 1 g, in a one dimensional box of length 1 cm, to have a kinetic energy of 1 erg (1 0^{-7} joules), the quantum number n must be determined through Equation (7.38), and so:

$$n \simeq \frac{(8)(10^{-3})(10^{-2})^2(10^{-7})}{(6.63 \times 10^{-34})^2} \qquad (7.111)$$

or

$$t\ \mathrm{l} \simeq 10^{27} \qquad (7.112)$$

As another example, the classical 'oscillator has an energy of order $m\omega^2 x_0^2$; for this to be described by a packet or superposition of quantum oscillators, which have energy of order $n\hbar\omega$, we must have:

$$n\hbar\omega \simeq m\omega^2 x_0^2 \qquad (7.113)$$

or form = 1 g, w = 1 sec^{-1}, x_0 = 1 cm,

$$n \simeq \frac{m\omega x_0^2}{\hbar} = \frac{(10^{-3})(1)(10^{-2})^2}{10^{-34}} \simeq 10^{27} \qquad (7.114)$$

So in these examples n is indeed large.

One can actually show rigorously that if the oscillator wave packet, Equation (7.107), is expressed in terms of a superposition of oscillator wavefunctions,

$$\psi(x,t) = \sum_{n=0}^{\infty} A_n \Phi_n(x) \exp\left(\frac{-iE_n t}{\hbar}\right) \qquad (7.115)$$

then to describe a macroscopic particle, the majority of quantum numbers n which contribute to the above sum are given approximately by Equation (7.113) above, and are hence very large.

Numerous additional examples of this correspondence between quantum and classical theories in the limit of large quantum numbers will be discussed in later chapters, in connection with statistical mechanics, lattice vibrations in solids, and the hydrogen atom.

summary

FREE PARTICLE

A free-particle wavefunction with properties similar to those of a Newtonian particle may be formed with an initial gaussian distribution. Subsequently, the wavefunction is also gaussian, with the characteristic spatial width increasing with time due to the uncertainty in the momentum. For macroscopic cases, Newtonian and quantum mechanics agree.

STEP POTENTIAL

If $E > V_0$, the wavefunctions are simple oscillating exponentials in the two regions separated by the step. By using the conditions that the wavefunction and its derivative are continuous at the step, one may find the amplitudes of the reflected and transmitted waves. The particle current is proportional to the magnitude of the amplitude squared times the speed. The ratio of the transmitted current or reflected current to the incoming current is the transmission or reflection coefficient, respectively. The sum of these coefficients is unity, expressing conservation of number of particles. For energies below the top of the step, $E < V_0$, the reflection coefficient is unity.

SQUARE POTENTIAL BARRIER

For a square potential barrier of height V_0, some of the incident particles may tunnel through to the other side even if $E < V_0$. The fraction tunneling through is of order $e^{-2\beta a}$, where a is the barrier width and $\beta = \sqrt{2m(V_0 - E)}/\hbar$

PARTICLE IN A BOX

A particle confined in a finite region can have only discrete energies. This is illustrated by the discrete energy eigenvalues of the particle in the one dimensional box. At the boundaries of the box, where the potential energy suddenly goes to infinity, the wavefunction must be zero. These boundary conditions lead to standing waves with the discrete energies, $E_n = h^2n^2/8mL^2$, with n a non-negative integer for a box of length L. The lowest energy is greater than zero.

HARMONIC OSCILLATOR

Many physical systems approximate the harmonic oscillator potential for small vibrations, i.e. for low energies. This is another system in which there are only discrete energies. In this case, the levels are evenly spaced; $E_n = (n + \frac{1}{2})\hbar\omega$, where ω is the angular frequency which the harmonic oscillator would have in Newtonian mechanics. Again in this case, a solution may be found which is of gaussian shape and moves like a Newtonian particle. Here, the uncertainty in the momentum does not increase the gaussian width because the particle is bound. For macroscopic systems, Newtonian and quantum mechanics are equivalent.

problems

1. Consider a particle of mass 10^{-6} kg inside a one dimensional box of length 3 cm. Suppose it is in a state such that its speed is about 1 cm/sec, to within 0.1%. What is the corresponding quantum number n, and the corresponding uncertainty in the quantum number?

   Answer: 9×10^{23}; 9×10^{20}—so quantization of E is unimportant.

2. A simple harmonic oscillator consists of a particle of mass m with a potential energy of $\frac{1}{2}kx^2$, where **k** is a constant. Estimate the minimum energy which the particle may have consistent with the uncertainty principle, i.e. by assuming $\Delta p_x = \sqrt{\langle p^2\rangle} \simeq \hbar/2\Delta x$ and minimizing the energy. (Use the exact form $\Delta p_x\Delta x \geq \hbar/2$) If $\sqrt{k/m} \sim 10^{15}$ per sec, what is the magnitude of the energy in eV?

   Answer: $E_{\min} \simeq \frac{1}{2}\hbar\sqrt{\frac{k}{m}}$; 0.3 eV.

3. Write the one dimensional Schrödinger equation for a mass m with a potential energy corresponding to that of (a) the gravitational field near the earth's surface; (b) the interaction of an electron with a fixed point positive charge, q.

4. Let φ be the angle relative to the x axis of the position of a particle in the xy plane. Thus, in terms of x and y, $\varphi = \tan^{-1}(y/x)$. Show that $\psi = e^{in\varphi}$ satisfier, the two dimensional Schrödinger equation, with V = 0 for a particle constrained to move in a circular path where $x^2 + y^2 = R^2$ is a constant. $\hbar^2/2m(\partial^2\psi/\partial x^2 + \partial^2\psi/\partial y^2 + E\psi = 0$. What is the energy, E, in terms of the constants, n and R? If the wave function can have only one value for a given φ, find the possible values that n can have.

   Answer: $\dfrac{\hbar^2n^2}{2mR^2}$; $n = 0, \pm 1, \pm 2, \ldots$

5. The rigorous definition of Δx is the root mean square deviation from the average of x, or:

$$\Delta x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle} = \sqrt{\int \psi^*(x - \int \psi^* x \psi dx)^2 \psi dx}$$

similarly for Δp. Find Δx, Δp_x and $\Delta x \Delta p_x$ for the lowest-energy level of o particle of mass m in a one dimensional box of width ℓ.

Answer: $\frac{\ell}{\pi}\sqrt{\frac{(\pi^2 - 6)}{12}}, \frac{\pi\hbar}{\ell}, \hbar\sqrt{\frac{(\pi^2 - 6)}{12}} = 0.567\hbar > \frac{1}{2}\hbar$, the minimum possible.

6. Using the exact time-dependent gaussian wave packet for a localized free particle given in Equation (7.18), calculate (p,) and Δp_x, and verify that these expectation values do not change in time.

7. A one dimensional potential is $V = V_0 > 0$ for $x < 0$ and $x > L$, and is $V = 0$ for $0 < x < L$. Show that if $V_0 > E > 0$, the energy E must satisfy $\tan(kL) = 2\beta k/(k^2 \ \beta^2)$ where $k = \sqrt{2mE}/\hbar$ and $\beta = \sqrt{2m(V_0 - E)}/\hbar$.

8. For the wave function of Equation (7.9), $\Delta x \Delta p = \frac{1}{2}\hbar$ when $t = 0$. Also for $t = 0$, show that $(E) = (p_0^2/2m) + \frac{1}{4}\hbar^2/m\sigma^2$, the Newtonian energy, plus a quantum term associated with the wave packet due to the momentum distribution. Find ΔE where $\Delta E = \sqrt{\langle (E - \langle E \rangle)^2 \rangle}$. In addition to the integrals given in Table 7.1, use $\int_{-\infty}^{\infty} x^4 e^{-\alpha x^2} dx = \frac{3}{4}\sqrt{\pi/\alpha^5}$. These results are independent of time.

Answer: $\sqrt{\frac{p_0^2\hbar^2}{2m^2\sigma^2} + \frac{1}{8}\frac{\hbar^4}{m^2\sigma^2}}$

9. If ψ_1 and ψ_2 are the normalized wavefunctions for the two lowest-energy wavefunctions for a particle in a one dimensional box, normalize $\psi_1 + 2\psi_2$ and find the expectation value of the energy.

Answer: $\frac{9\hbar^2\pi^2}{2\sqrt{5}mL^2}$.

10. For the wavefunction of Problem 9, find the expectation value of the momentum as a function of time.

Answer: $-\frac{32\hbar}{15L}\sin\left(\frac{3\hbar\pi^2 t}{2mL^2}\right)$.

11. Show that the function $\psi = A \sin(k_x x) \sin(k_y y) \sin(k_z z)$ satisfies the three dimensional Schrödinger equation,

$$\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + E\psi = 0$$

If this is the wavefunction in a box of dimensions a,b,c, in the x,y,z directions, find the possible values for k,, k,, k,, and find the possible energies E.

Answer: $\frac{n_x\pi}{a}, \frac{n_y\pi}{b}, \frac{n_z\pi}{c}, \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$ for $n_x, n_y, n_z = 1, 2, 3, \ldots$

12. If the potential energy is $V = V_0 > 0$ for $0 < x < a$ and $V = 0$ elsewhere, find the transmission coefficient for $E > V_0$. Show thot this approaches one for large E. What would this transmission coefficient be for Newtonian mechanics?

Answer: $$\frac{8(\alpha/k)^2}{\left[1+6\left(\frac{\alpha}{k}\right)^2+\left(\frac{\alpha}{k}\right)^4\right]-\left[1-2\left(\frac{\alpha}{k}\right)^2+\left(\frac{\alpha}{k}\right)^4\right]^2\cos(2\alpha a)},$$ where

$k = \sqrt{\frac{2mE}{\hbar}}$ and $\alpha = \frac{\sqrt{2m(E-V_0)}}{\hbar}$

13. For particles inside a spherical container of radius r, V = 0 for $r = \sqrt{x^2+y^2+z^2} < R$, the wave function is zero at $r = R$. For a particle of mass m, show that there are solutions of the three dimensional wave equation of the form: $\psi = a\sin(kr)/kr\, e^{-iEt/\hbar}$. What are the possible values of k and E?

Answer: $k = \frac{n\pi}{R}$, $E = \frac{(n\pi\hbar)^2}{2mR^2}$, $n = 1, 2, 3, .$

14. For the particle in the spherical box of Problem 13, show that there are solutions of the form:

$$\psi = a\left[\frac{\sin(kr)}{(kr)^2} - \frac{\cos(kr)}{kr}\right]e^{-iEt/\hbar}\cos\theta$$

where θ is the angle relative to the z axis, $\cos\theta = z/r$. Write the transcendental equation, the solutions of which would give the possible values of k. How are k and E related? What is the probability of finding the particle at $z = 0$?

Answer: $\tan(kR) = kR$; $E = \hbar^2k^2/2m$; zero.

15. In three dimensions, the potential energy a particle sees is V = 0 for $r = \sqrt{x^2+y^2+z^2} < R$ and $V = V_0 > 0$ for $r \geq R$. The solution $\psi = a\sin(kr)/kr\; e^{-iEt/\hbar}$ is given for $r < R$. For $r \geq R$ and $E < 0$, show that a solution is $\psi = b\frac{e^{-\beta r}}{\beta r}e^{-iEt/\hbar}$, where $\beta = \sqrt{2m(V_0 - E)}/\hbar$. This ψ satisfies the boundary condition, $\psi \to 0$ as $r \to \infty$. From the boundary conditions at $r = R$, find a relationship between β and k. This leads to the possible values of E.

Answer: $\tan(kR) = -k/\beta$.

16. Two particles of masses m_1 and m_2, constrained to move on the x axis, are connected by a spring, so that $V = \frac{1}{2}k(x_2 - x_1)^2$. Thus, the Schrödinger equation becomes:

$$-\frac{\hbar^2}{2}\left(\frac{1}{m_1}\frac{\partial^2\Phi}{\partial x_1^2} + \frac{1}{m_2}\frac{\partial^2\Phi}{\partial x_2^2}\right) + \frac{1}{2}k(x_2 - x_1)^2\Phi = E\Phi$$

Now let $x = x_2 - x_1$, the relative coordinate, and $X = (m_1x_1 + m_2x_2)/(m_1 + m_2)$, the center of mass coordinate. Use $\partial/\partial x_1 = \partial x/\partial x_1(\partial/\partial x) + \partial X/\partial x_1(\partial/\partial X)$ and a similar expression for $\partial/\partial x_2$ to obtain a differential equation in terms of x and X. Show that there is a solution of the form $\Phi = \Phi_n(x)e^{-ikX}$ with Φ_n, the one dimensional harmonic oscillator solutions. Verify that $E = E_n + k^2\hbar^2/2(m_1 + m_2)$ with the reduced mass, given by $\mu = m_1m_2/(m_1 + m_2)$, and with E_n, the harmonic oscillator energy, given by $E_n = (n + \frac{1}{2})\hbar\sqrt{k/\mu}$. What is the physical significance of the two parts of Φ and E?

17. Assume that the general solution of the one-dimensional harmonic oscillator equation is of the form $\Phi = f(x)e^{-1/2\,ax^2}$, with $a = m\omega/\hbar$. Show that $(\hbar^2/2m)\,d^2f/dx^2 - \hbar\omega x\,df/dx + (E - \frac{1}{2}\hbar\omega)\,f = 0$. Assume that $f = \sum_{\ell=0}^{\infty} a_\ell x^{2\ell}$. Substitute into the differential equation and find a relationship between a_ℓ and $a_{\ell+1}$ by setting the coefficient of each power of x to zero. Show that $a_\ell = 0$ for $\ell > n/2$ if

$E - \frac{1}{2}$ ho = nhw with n an even integer. Thus, f is a polynomial with a finite number of ter Similar results occur for: $f = \sum_{\ell=0}^{\infty} a_\ell x^{2\ell+1}$ Then n is an odd integer.

18. By comparison with the one dimensional simple harmonic oscillator Schrbdinger equation, show that:

$$(1)\quad -\frac{\hbar^2}{2m}\left(\frac{d}{dx} + \frac{m\omega}{\hbar}x\right)\left[\left(\frac{d}{dx} - \frac{m\omega}{\hbar}x\right)\Phi_n\right] = \left(E_n + \frac{1}{2}\hbar\omega\right)\Phi_n;\ \text{and}$$

$$(2)\quad \frac{\hbar^2}{2m}\left(\frac{d}{dx} - \frac{m\omega}{\hbar}\right)\left[\left(\frac{d}{dx} + \frac{m\omega}{\hbar}x\right)\Phi_n\right] = \left(E_n - \frac{1}{2}\hbar\omega\right)\Phi_n.$$

By operating on Equation (1) on both sides with $d/dx - m\omega/\hbar\, x$ and comparing the result with Equation (2), show that $(d/dx - m\omega/\hbar\, x)\Phi_n = \Phi_{n+1}$ where Φ_{n+1} is an eigenfunction with $E = E_{n+1} = E_n + \hbar\omega$. This shows that if $E_0 = \frac{1}{2}\hbar\omega$, there are energies $E_n = (n + \frac{1}{2})\hbar\omega$. Starting with $\Phi_0 = ae^{-1/2\,\alpha x^2}$ with $\alpha = m\omega/\hbar$, find Φ_1 and Φ_2 by this method.

19. Verify that the expectation values for the energy and its uncertainty ΔE given in Equations (7.109) and (7.110) are correct for the harmonic oscillator wave packet, Equation (7.107).

20. Show that the expectation value of the momentum is the same as the Newtonian momentum, $p = mV = -m\omega x_0 \sin \omega t$ for the simple harmonic oscillator wave packet, Equation (7.107)

21. Find the potential energy in the one dimensional Schrödinger equation that is satisfied by the wave function:

$$\psi(x,t) = \frac{\sqrt{\sigma}}{\pi^{1/4}\sqrt{\sigma^2 + i\hbar t/m}} \exp\left\{\frac{1}{2}\frac{[x - (p_0t/m) - \frac{1}{2}gt^2]^2}{\sigma^2 + i\hbar t/m} + i\left[\frac{mgt + p_0}{\hbar}x - \frac{(mgt + p_0)^3}{6m^2gh}\right]\right\}$$

Show that the probability density is:

$$\psi^*\psi = \frac{\sigma}{\sqrt{\pi}\sqrt{\sigma^4 + \hbar^2t^2/m^2}} \exp\left[-\sigma\frac{\frac{1}{2}gt^2)^2\ p_0t/m}{(\sigma^4 + \hbar^2t^2/m^2)}\right]$$

What is the meaning of this density?

Answer: $V = -mgx$.

22. Show that for the wavefunction of Problem 21, the expectation value of the momentum is the Newtonian value, $\langle p_x\rangle = p_0 + mgt$, for the potential energy $V = -mgx$.

hydrogen atom and angular momentum

We have seen how electrons can behave like waves when traveling from one point to another, such as when they pass through crystals and are diffracted just like x rays. In this chapter it will be shown how the wavelike character of electrons,. as described by the Schrödinger equation, can be used to explain many of the observed properties of hydrogen atoms. A hydrogen atom at rest is to be pictured as consisting of a negatively charged electron and a much more massive, positively charged proton. The attractive Coulomb force between the oppositoly charged particles keeps the electron bound to the heavy proton, which remains nearly at rest while the electron probability waves may oscillate in many different ways in the nearby neighborhooo of the proton. The states of oscillation, having a definite energy-or definite frequency--are quite stable and are called stationary *states.* Transitions between these stationary states give rise to the emission or absorption of photons of discrete frequencies, and hence to a discrete spectrum.

The positions of the stationary state energy levels were first calculated by Bohr using some very simple postulates, a number of years before the Schrödinger wave equation was discovered. Although Bohr's theory was not entirely correct, when the wave equation was solved for the hydrogen atom the energy levels were found to lie at exactly the positions calculated by Bohr. The problem of the hydrogen atom, because it involves only two particles, is one of the very few problems for which the Schrödinger equation is exactly soluble in terms of simple functions. The solution of this problem and its agreement with observation has been one of the most spectacular successes of quantum theory.

We shall first briefly discuss the Bohr theory of hydrogen. We shall then see how the wave equation leads to quantization of energies and will discover, as well, that the wave equation implies that the atom's angular momentum is quantized.

1 PARTICLE IN A BOX

Before discussing the theory of hydrogen in detail, it will be useful to recapitulate some of the ideas used in Chapter 7 in the quantum mechanical description of a particle in a one dimensional box. There it was seen that a discrete set of stationary state energy levels arose due to the confinement of the particle within the box of finite size. The smaller the box, the more widely spaced were the energy levels.

The energy levels of the particle in the one dimensional box may be represented in the energy level diagram in Figure 8.1, where energy is plotted upwards, with the horizontal lines representing the allowed values of the energy. These are the stationary states of the system, and if the system is perturbed slightly, it may make transitions between states and conserve energy by emitting or absorbing a photon. If, for example, the transition goes from an upper state of energy E_u to a lower state E_ℓ, the frequency of the emitted photon will be given by:

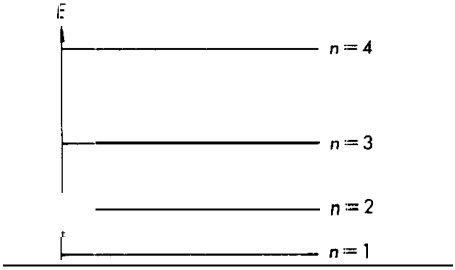


Figure 8.1. Energy level diagram for the particle in a one dimensional box

$$h\nu = E_u \quad E_\ell = \frac{hc}{\lambda} \tag{8.1}$$

Since the energies are discrete, the possible frequencies ν are discrete, and the spectrum will also be discrete.

Atoms are systems in which electrons are confined to a small volume, known to be of dimensions on the order of a few angstroms. In this case, the potential energy is negative, and is due to the attractive Coulomb force between electrons and nucleus. Although the particle in a box has zero potential energy, and moves in one dimension rather than in three as do the electrons in atoms, we should be able to get a rough idea of the energy level spacing in atoms, arising from confinement of the electrons, by comparing the lower energy level spacings of a particle in a box whose size is roughly that of an atom.

For example, let us calculate the wavelength of light given off in the transition from the state with n = 2 to that for n = 1 for a length L of the box equal to three Angstroms. The energies for the particle in the box are given by:

$$E_n = \frac{(nh)^2}{8mL^2}, \quad n = 1,2,3,\ldots \tag{8.2}$$

Then for the 2 → 1 transition,

$$E_2 - E_1 = \frac{3}{8}\frac{h^2}{mL^2} = h\nu = \frac{hc}{\lambda} \tag{8.3}$$

Therefore, using form the mass of the electron, 9.11 $\times 10^{-31}$ kg,

$$\lambda = \frac{8mL^2c}{3h} \quad \frac{8(9.11 \times 10^{-31})(3 \times 10^{-10})^2(3 \times 10^8)}{3(6.63 \times 10^{-34})}$$

$$\simeq 10^{-7}m = 1000 \text{ Angstroms.} \tag{8.4}$$

This is comparable to the wavelengths emitted by atoms for transitions between the lower states, which strongly suggests that the wavelike character of the electrons in the atom is responsible for the observed discrete spectra.

It should be noted that the reciprocal of the wavelength of the emitted light is given by a simple formula, involving a difference between the energies of two stationary states:

$$\frac{1}{\lambda} = \frac{1}{hc}(E_u - E_\ell) \tag{8.5}$$

8.2 BALMER'S EXPERIMENTAL FORMULA FOR THE HYDROGEN SPECTRUM

We shall now consider in detail the lightest and simplest element, hydrogen. The spectrum of hydrogen contains many discrete lines. By fitting the experimental data, Balmer showed in 1885 that the values of the wavelengths in this spectrum can be expressed by the following formula:

$$\frac{1}{\lambda} = R_H\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right); \quad n_1 = 1,2,3,\ldots; \; n_2 = n_1 -- 1,\ n_1 + 2,\ldots \tag{8.6}$$

The Rydberg constant R_H has been measured with great accuracy by spectroscopists. It has the value:

$$R_H = 10{,}967{,}758.1\ m^{-1} \tag{8.7}$$

The fact that, as in the case of the particle in a box, I/X is proportional to a difference of terms suggests that the hydrogen atom has stationary states of definite energies, and that transitions between these states give rise to the discrete spectral lines. For a transition from some energy level E_u down to a lower level E_ℓ, the values of I/X would be given by Equation (8.5) above. In the case of hydrogen, when the electron and proton are separated on infinite distance, the potential energy is defined to be zero. The potential energy in the actual atom must therefore be negative. The magnitude of the potential energy must be larger than the kinetic energy in order for the system to remain confined in a bound state, Then the nonrelativistic energy levels should be negative. Upon comparison of Equation (8.5) with the experimental result in Equation (8.6), we see that apart from an additive constant, the values of the hydrogen atom energy levels must be given by:

$$E_n = \frac{R_H hc}{2}; \quad n = 1,2,3,\ldots \tag{8.8}$$

8.3 SPECTRAL SERIES FOR HYDROGEN

The energies $E_n = -R_H hc/n^2$ can be represented by the energy level diagram in Figure 8.2. The lowest-lying level is labeled $n = 1$. As n takes on larger and larger integral values, the energies E_n approach zero. In electron volts:

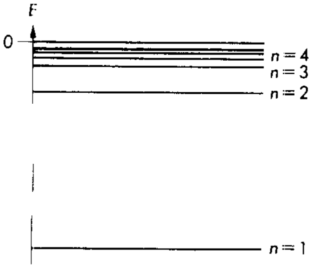


Figure 8.2. Energy level diagram for the electron in atomic hydrogen. The zero of energy is at the top of the diagram.

$$E_1 = -R_H hc = -\frac{(1.097 \times 10^7)(6.63 \times 10^{-34})(3 \times 10^8)}{1.6 \times 10^{-19}\ \mathrm{J/eV}}$$

$$= -13.6\ \mathrm{eV} \tag{8.9}$$

The value of E_2 is one-fourth of this or -3.4 eV. A transition from the $n = 2$ to the $n = 1$ state would then correspond to a photon of (energy $-3.4-(-13.6)$ eV or 10.2 eV, with a wavelength of 1216 angstroms in the ultraviolet. Transitions down to a given state from all higher states give rise to series of spectral lines which have been given the names of the scientists who first observed them experimentally. Thus, for example, the various transitions $n = 2 \to n = 1$, $n = 3 \to n = 1$, etc., down to the lowest (ground) state, correspond to a series of ultraviolet lines known as the *Lyman series.* The 1216 angstrom line calculated above is the line having the longest wavelength in this series. The transitions leading to the Lyman series are depicted schematically in the energy level diagram, Figure 8.3. The names of the various series of lines *are* given in Table 8.1. Within each series, the lines are labeled $\alpha, \beta, \gamma, \delta, \ldots$ in order of decreasing wavelength (increasing energy). The $\alpha, \beta, \gamma, \delta$ lines of the Balmer series lie in the visible.

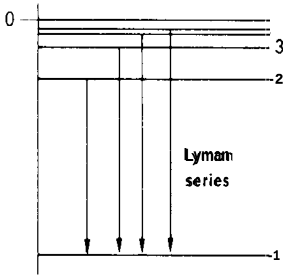


Figure 8.3. Energy level diagram showing the series of transitions down to the ground level which give rise to the Lyman series of spectral lines.

TABLE 8.1 Names of the Series of Spectral lines observed in Hydrogen.

$n = 2, 3, \ldots$	$\rightarrow n = 1$	**Lyman series**
$n = 3, 4, \ldots$	$\rightarrow n = 2$	**Balmer series**
$n = 4, 5, \ldots$	$\rightarrow n = 3$	**Paschen series**
$n = 5, 6, \ldots$	$\rightarrow n = 4$	**Brackett series**
$n = 6, 7, \ldots$	$\rightarrow n = 5$	**Pfund series**
Etc.		**unnamed**

mple What is the energy in eV of a photon in the β line of the Lyman series?

ution The β line of the Lyman series corresponds to a transition from the n = 3 state to then = 1 state. The energy is:

$$E = R_H hc\left(1 - \frac{1}{9}\right) = \frac{(1.097 \times 10^7)(6.63 \times 10^{-34})(3 \times 10^8)(8/9)}{1.6 \times 10^{-19}\ \mathrm{J/eV}} = 12.1\,\mathrm{eV}$$

8.4 BOHR MODEL FOR HYDROGEN

We have inferred from the experimental data that there exists a series of energy levels in hydrogen. This is a compact way of describing the experimental data, and is certainly consistent with the previous discussion of de Broglie waves. Let us now approach the bound electron-proton system from the point of view of theory, and see if we can predict or explain mathematically why the energy levels, in hydrogen have the values they do have. We will first discuss the theory of Bohr, in which the electron is pictured as moving in an orbit described by Newtonian mechanics, but with an additional condition on the orbit circumference due to the wave properties of the electron. This theory is not correct. However, because it agreed with experimental energies so well, it did cause people to think more about the wave properties of particles and eventually to find the correct theory. Also, it gives an intuitive, although incorrect, feeling for the quantization of the orbits.

We first consider those aspects of the Bohr model of hydrogen which can be treated using Newtonian mechanics. In Bohr's model, an electron orbits around a proton under the action of electrostatic forces. We will initially assume that the proton mass is so large that the proton can be treated as being at rest. Also we shall assume the electron moves in a circular orbit of radius r. The Newtonian force equation **F** = ma, means that the electron mass times the centripetal acceleration in the circular orbit is equal to the electrostatic force of attraction. Thus, if the electron's speed is v,

$$m\left(\frac{v^2}{r}\right) = \frac{Ze^2}{4\pi\epsilon_0 r^2} \qquad (8.10)$$

where e is the electronic charge and Z is the number of protons in the nucleus. (For hydrogen, Z = 1. However, with Z = 2,3, . . . , one would have the Bohr model for singly ionized helium, doubly ionized lithium, etc.) The energy we desire to find is, according to Newtonian mechanics, the kinetic energy plus the electrostatic potential energy:

$$E = \frac{1}{2} mv^2 - \frac{Ze^2}{4\pi\epsilon_0 r} \tag{8.11}$$

The speed may be eliminated between Equations (8.10) and (8.11) to find that the total energy is:

$$E = -\frac{1}{2} \frac{Ze^2}{4\pi\epsilon_0 r} \tag{8.12}$$

which is one-half the potential energy.

8.5 QUANTIZATION IN THE BOHR MODEL

Next we may use the wave nature of the electron to obtain quantization conditions on the orbits of the electron which will lead to a discrete set of energy levels. The de Broglie wavelength is Planck's constant divided by the momentum, or:

$$\lambda = \frac{h}{mv} \tag{13.13}$$

Imagine the electron de Broglie wave propagating around in the circular orbit. In order for it not to interfere destructively with itself after many revolutions, the wave amplitude must fit continuously onto itself after each revolution. This would mean that the circumference of the orbit is an integral number of wavelengths, so that as the electron goes around the orbit, the wave is periodically repeated. This condition is

$$m_\varphi \lambda = 2\pi r; \quad m_\varphi = 1, 2, 3, \ldots \tag{8.14}$$

This equation may be rewritten from the expression for the de Broglie wavelength as:

$$mvr = \left(\frac{h}{\lambda}\right) \cdot \left(\frac{m_\varphi \lambda}{2\pi}\right) = \frac{m_\varphi h}{2\pi} = m_\varphi \hbar \tag{13.15}$$

Since mvr is the angular momentum, Equation (8.15) states Bohr's original rule for the postulated quantization of angular momentum. This quantization rule was generalized by Bohr and Sommerfeld to apply to elliptical orbits, but we shall discuss only the circular case. The speed may be eliminated between the quantization condition, Equation (8.15), and the Newtonian force equation, Equation (8.10). The result, after solving for r, is:

$$r = \frac{4\pi\epsilon_0 m_\varphi^2 \hbar^2}{Ze^2 m} \tag{8.16}$$

Finally, this radius may be substituted into the energy equation, Equation (8.6). This gives the Bohr formula for the energy levels:

$$E_n = -\frac{1}{2}\frac{Z^2 e^4 m}{(4\pi\epsilon_0\hbar)^2}\frac{1}{m_\varphi^2} \tag{8.17}$$

This result says that the energy levels of the electron in hydrogen are negative, corresponding to a bound state, and are inversely proportional to the square of an integer. Thus the energy level diagram will look just like that of Figure 8.2 from experiment.

The quantization arises in Bohr's theory from a condition, Equation (8.15), on the allowed values of orbital angular momentum. Physically, this can arise from a boundary condition which, stated mathematically, takes the form of a periodicity condition. For a particle moving in a circular orbit, the particle's position is described by an angle φ. This is quite different from the case of a particle in a box, because the circle is endless. The wave, rather than bouncing back from the ends, just keeps on going. If the wavefunction at the angle φ has the value $\psi(\varphi)$, then as φ increases, $\psi(\varphi)$ will change in some fashion; if φ increases by 2π, so that the wave has come around to the same physical point, the wavefunction is $\psi(\varphi + 2\pi)$, and this should be the same as $\psi(\varphi)$ itself. Otherwise, the wavefunction would not have *a* unique ‘value at a given physical point. Hence, instead of a boundary condition, we have a periodicity condition:

$$\psi(\varphi + 2\pi) = \psi(\varphi) \tag{8.18}$$

This equation is the mathematical analogue of the requirement that the circumference of the orbit must contain an integral number of wavelengths.

We can now see if the energies obtained in Equation (8.17) have the correct magnitude. In analogy with Equation (8.8), the energy derived from the Bohr theory may be written as:

$$E = \frac{-R_\infty hc}{m_\varphi^2} \tag{8.19}$$

where, since Z = 1 for hydrogen,

$$R_\infty = \frac{1}{2}\frac{1}{h/mc}\left(\frac{e^2}{4\pi\epsilon_0\hbar c}\right)^2 = \frac{\alpha^2}{2\lambda_c} \tag{8.20}$$

The subscript ∞ on R_∞ denotes that we treated the proton as a particle of infinite mass, since we assumed it was at rest. This constant R_∞ has been written in terms of two basic physical constants; the Compton wavelength, $\lambda_c = h/mc$, which was discussed in connection with Compton scattering of photons by electrons; and the physically dimensionless ***fine structure constant*** $\alpha \equiv e^2/4\pi\epsilon_0\hbar c$. The fine structure constant is an extremely important fundamental constant in physics and occurs in many places, such as in small corrections to atomic energy levels due to relativistic and intrinsic angular momentum effects. The Compton wavelength is $\lambda_c = 2.4263 \times 10^{-12}$ m; the fine structure constant has the value $\alpha =$

1/137.036. Therefore, R_∞ can be evaluated, and is found to have the value:

$$R_\infty = 1.09738 \times 10^7 \mathrm{m}^{-1} \tag{13.21}$$

8.6 REDUCED MASS

The value of R_∞ differs from the experimental value of R_H of Equation (8.7) starting in the fourth significant figure. The reader might well think that this agreement is close enough. However, it can be made even closer. The fractional error in the theoretical Rydberg constant R_∞ is:

$$\frac{R_\infty - R_H}{R_H} = \frac{6.0 \times 10^3}{1.0968 \times 10^7} = \frac{1}{1830} \tag{8.22}$$

We may also observe that the mass of the proton is just 1836 times the mass of the electron, which suggests that we may be able to arrive at even closer agreement if we take into account the motion of the proton.

In a two-particle system, one particle does not move around the other, but both move around the common center of mass. The position of the center of mass is given by:

$$\mathbf{r}_c = \frac{(\mathbf{r}_e m_e + \mathbf{r}_p m_p)}{(m_e + m_p)} \tag{8.23}$$

where the subscripts e and p refer to electron and proton, respectively. Also, the position of the electron relative to the proton is:

$$\mathbf{r}_r = \mathbf{r}_e - \mathbf{r}_p \tag{8.24}$$

The force between electron and proton depends only on the relative displacement $\mathbf{r}_r$. If Equations (8.23) and (8.24) are solved for $\mathbf{r}_e$ and $\mathbf{r}_p$ in terms of $\mathbf{r}_c$ and $\mathbf{r}_r$ and substituted into the Newtonian force equations $\mathbf{F} = m\mathbf{a}$ for the two particles, then two equations result, one for $\mathbf{r}_c$ alone and one for $\mathbf{r}_r$ alone. The equation for $\mathbf{r}_c$ simply states that the center of mass of the system is not accelerated. The equation for $\mathbf{r}_r$ gives a radial equation similar to Equation (8.10) but with r replaced by the relative distance r_r and m replaced by $\mu = m_e m_p/(m_e + m_p)$. The quantity μ is called the reduced mass. Likewise, the total orbital angular momentum of the atom, including a small contribution from motion of the nucleus, depends only on μ and r_r. It is $\mu v r_r$, where v is the speed of the electron relative to the proton. If the total angular momentum is set equal to $m_\varphi \hbar$ in analogy with Equation (8.15), all the theory is as before but with μ replacing m in the energy. Thus the energy levels are

$$E_n = -\frac{1}{2}\frac{\mu e^4}{(4\pi\epsilon_0\hbar)^2}\frac{1}{m_\varphi^2} \tag{8.25}$$

Thus, when the slight motion of the proton is taken into account, the predicted value of the Rydberg constant for hydrogen is

$$R_H = \frac{1}{2}\frac{1}{(h/\mu c)}\left(\frac{e^2}{4\pi\epsilon_0\hbar c}\right)^2 \tag{8.26}$$

TABLE 6.2 Experimental Values of the Rydberg Constant for Some Multiply-Ionized Atoms

Atom	Rydberg Constant m^{1}
$_1H^1$	10,967,758.1
$_1H^2$	10,970,741.9
$_1H^3$	10,971,734.8
$_2He^3$	10,971,734.4
$_2He^4$	10,972,226.4
$_3Li^6$	10,972,729.5
$_3Li^7$	10,972,872.3
$_4Be^9$	10,973,062.3
$_5B^{11}$	10,973,183.5
$_6C^{12}$	10,973,228.6
$_7N^{14}$	10,973,300.4
$_8O^{16}$	10,973,353.9

This agrees with experiment to seven significant figures. The Rydberg constants for other similar systems such as singly ionized helium, doubly ionized lithium, etc., which also have hydrogen-like spectra, may be found by putting in the reduced mass for the nucleus-electron system and by multiplying by the square of the nuclear charge number Z^2, as in Equation (8.17). These agree equally well with experiment. A list of some observed Rydberg constants for multiply ionized atoms is given in Table 8.2. The Bohr model thus gives a simple and compact explanation of an enormous amount of experimental data.

The characteristic size or "radius" of the hydrogen, atom for the ground state may be found from Equation (8.16) using $m_\varphi = 1$ and $Z = 1$. In terms of the fine structure constant and the Compton wavelength, this is (neglecting reduced mass corrections),

$$r_1 = \frac{\lambda_c}{2\pi\alpha} = 0.529 \times 10^{-10}\text{m} = 0.529 \text{ Angstroms} \qquad (8.27)$$

The speed of the electron in its orbit may be found by substituting the radius r of Equation (8.9) into Equation (8.8). 'The result is

$$\frac{v}{c} \quad \frac{\alpha}{m_\varphi} \qquad (8.28)$$

Then, for the ground state of the hydrogen atom, v/c is about $^1/_{137}$, much less than unity. This justifies the nonrelativistic treatment in the theory.

SCHRÖDINGER EQUATION FOR HYDROGEN

We have discussed a simple picture of the hydrogen atom which agrees well with experiment as far as the energy levels are concerned. However, this model cannot be used in finding the probability of a transition from one state to another with emission or absorption of a photon. It also cannot be applied successfully to more complicated atoms such as a neutral helium atom with two electrons. Furthermore, although with the Bohr theory the quantum number in the energy expression is proportional to the orbital angular momentum, the correct theory to be discussed next shows that the energy is actually not dependent on this angular momentum.

The correct way to approach these problems is by means of the three dimensional Schrödinger equation. If for the hydrogen atom the two-particle wave equation is used, it may be separated into a part describing the center of mass motion and another part describing relative motion. The part giving the relative motion is found to be similar to the Schrödinger equation obtained when the mass of the proton is assumed to be infinite. The only difference is that in place of the electron mass m, the reduced mass μ appears. Let us then, for simplicity, temporarily assume the proton is infinitely massive and is placed at the origin. After deriving the energy levels, we can then introduce the small corrections due to motion of the nucleus about the center of mass by making the replacement $m \rightarrow \mu$.

The electron is at position (x, y, z) a distance $r = (x^2 + y^2 + z^2)^{1/2}$ from the proton. In three dimensions, the kinetic energy operator is:

$$\frac{p_{op}^2}{2m} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \qquad (8.29)$$

The potential energy for the hydrogen atom, where $Z = 1$, is:

$$V = \frac{-e^2}{4\pi\epsilon_0 r} \qquad (8.30)$$

For a wave function of the form $\psi = \psi(\mathbf{r})e^{-iEt/\hbar}$, a stationary state, the Schrödinger equation in three dimensions is then:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) - \frac{e^2}{4\pi\epsilon_0 r}\psi = E\psi \qquad (8.31)$$

Because r is a moderately complicated function of x, y, and z, whereas the potential energy depends only on r, it is more convenient to work with spherical polar coordinates r, θ and φ. These coordinates are defined as follows: r is the distance from the origin to the electron as seen in Figure 8.4; φ is an angle in the xy plane, measured from the positive x axis to the projection of the vector r onto the xy plane; θ is the angle between r and the z axis. Thus the coordinate transformations are:

$$\begin{array}{lll} r = \sqrt{x^2 + y^2 + z^2} & & x = r\sin\theta\cos\varphi \\ \theta = \tan^{-1}\left(\dfrac{\sqrt{x^2 + y^2}}{z}\right) & \text{and} & y = r\sin\theta\sin\varphi \\ \varphi = \tan^{-1}\left(\dfrac{y}{x}\right) & & z = r\cos\theta \end{array} \qquad (8.32)$$

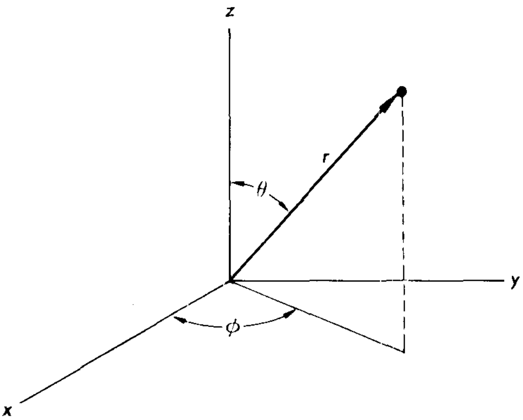


Figure 8.4. Spherical polar coordinates.

The kinetic energy operator expressed in spherical polar coordinates is derived in Appendix 1. The result of making the transformations to spherical polar coordinates is:

$$p_{\mathrm{op}}^2 = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} + \frac{1}{r^2 \tan\theta}\frac{\partial}{\partial \theta} + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial \varphi^2}\right) \qquad (8.33)$$

With this operator, the Schrödinger equation becomes:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2 \psi}{\partial r^2} + \frac{2}{r}\frac{\partial \psi}{\partial r} + \frac{1}{r^2}\frac{\partial^2 \psi}{\partial \theta^2} + \frac{1}{r^2 \tan\theta}\frac{\partial \psi}{\partial \theta} + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 \psi}{\partial \varphi^2}\right) - \frac{e^2\psi}{4\pi\epsilon_0 r} = E\psi$$

(8.34)

PHYSICAL INTERPRETATION OF DERIVATIVES WITH RESPECT TO r

The terms in Equation (8.34) involving only derivatives with respect to r have a very simple physical interpretation. Suppose we have a steady source of particles at the origin, which emits particles of definite energy that travel radially outward symmetrically in all directions. This corresponds to a stationary spherically symmetric de Broglie wave propagating radially outwards, which will be described by some wavefunction $\psi(r, t) = \Phi(r)e^{-iEt/\hbar}$. It is not difficult to guess what the form of the spatial part of the wavefunction must be. In order to have an outgoing spherical wave, $\Phi(r)$ must involve an exponential factor of the form $\exp(ip_r r)$, where p, is the radial component of momentum of the particles. This is analogous to a factor of the form $\exp(ip_x x)$ for a beam of particles, of momentum p_x propagating in the x direction.

In addition, if the system is to remain stationary so that particles do not pile up at any one radius, the number of particles to be found inside a spherical shell centered at the origin of radius r, area $4\pi r^2$ and thickness dr, must be the same for all r. Thus, $|\psi(r)|^2 \cdot 4\pi r^2 dr$ = constant, independent of r. The probability density $|\psi(r)|^2$ must be inversely proportional to the square of the radius. This is the quantum analogue of the well-known inverse square law for the intensity of outgoing spherical waves, found in classical physics. Since $\psi(r)|^2$ is proportional to $1/r^2$, the amplitude $\psi(r)$ itself must be inversely proportional to the radius itself, so we would expect the wavefunction to be given by:

$$\Phi(r) = \frac{Ae^{ip_r r/\hbar}}{r} \tag{13.35}$$

or

$$\psi(r,t) = \frac{Ae^{i(p_r r - Et)/\hbar}}{r} \tag{13.36}$$

We may now use this radial wavefunction $\Phi(r)$ to derive the form of the operator corresponding to p,, the radial component of momentum. Since E is definitely known, and $E = p_r^2/2m$, the radial momentum must be definitely known, and so $\Phi(r)$ must in fact be an eigenfunction of $p_{r_{op}}$ with eigenvalues p,. We might expect, by analogy with one dimensional wave motion, that p..$_{op}$ would involve a term of the form $\hbar/i(\partial/\partial r)$. However, if we differentiate $\Phi(r)$ using this operator, we find that

$$\frac{\hbar}{i}\frac{\partial}{\partial r}\Phi(r) = \frac{\hbar}{i}\frac{\partial}{\partial r}\left(\frac{Ae^{ip_r r/\hbar}}{r}\right) = \left(p_r - \frac{\hbar}{ir}\right)\Phi \tag{13.37}$$

because of the appearance of the factor r in the denominator of $\Phi(r)$. Thus Φ is not an eigenfunction of $\hbar/i(\partial/\partial r)$. However, the above equation can be rewritten as:

$$\frac{\hbar}{i}\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\Phi = p_r\Phi \tag{8.38}$$

Therefore, Φ is an eigenfunction of $-i\hbar(\partial/\partial r + 1/r)$, with eigenvalue p,. We can therefore identify the operator on the left of the above equation as:

$$p_{r_{op}} = \frac{\hbar}{i}\left(\frac{\partial}{\partial r} + \frac{1}{r}\right) \tag{8.39}$$

From this, the kinetic energy operator corresponding to radial motion can be obtained as:

$$\begin{aligned} T_{op}\psi = \frac{1}{2m}p_{r_{op}}^2\psi &= -\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\left(\frac{\partial\psi}{\partial r} + \frac{\psi}{r}\right) \\ &= -\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial r^2} - \frac{1}{r^2}\psi + \frac{1}{r}\frac{\partial\psi}{\partial r} + \frac{1}{r}\frac{\partial\psi}{\partial r} + \frac{\psi}{r^2}\right] \\ &= -\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial r^2} + \frac{2}{r}\frac{\partial\psi}{\partial r}\right] \end{aligned} \tag{8.40}$$

These are precisely the terms involving derivatives with respect to r in Equation (8.34), and thus may be interpreted as the contributions to kinetic energy due to radial motion.

The remaining terms, involving derivatives with respect to θ and φ, will be shown later to have a similar interpretation in terms of contributions to kinetic energy due to rotational motion.

SOLUTIONS OF THE SCHRÖDINGER EQUATION

It has been found that there exist energy eigenfunction solutions. of Equation (8.34) which may be written in the form of a product of functions, each factor in the product being a function of only one of the independent variables r, θ and φ. The solutions can be written as follows:

$$\Psi_{n\ell m_\varphi} = R_{n\ell}(r)\Theta_{\ell m_\varphi}(\theta)\Phi_{m_\varphi}(\varphi) \tag{8.41}$$

where $R_{n\ell}$ (r) is a function only of r; $\Theta_{\ell m_\varphi}(\theta)$ is a function only of θ; and Φ_{m_φ} is a function only of φ. The energy levels depend on n, a positive integer, but not on ℓ or m; ℓ is an integer associated with the total angular momentum such that $0 \le \ell < n$; and m_φ is a positive or hegative integer, or zero, associated with the z component of angular momentum such that $m_\varphi \le \ell$

The simplest of these solutions, corresponding to the ground state, is one in which the wavefunction depends only on r and not on θ or φ. In this case, the Schrödinger equation, Equation (8.34), reduces to:

$$-\frac{\hbar^2}{2m}\left(\frac{d^2\psi}{dr^2} + \frac{2}{r}\frac{d\psi}{dr}\right) - \frac{e^2}{4\pi\epsilon_0 r} = E\psi \tag{8.42}$$

and the simplest solution is:

$$\psi_{100} = \sqrt{1/\pi a^3}\, e^{-r/a} \tag{8.43}$$

where the constant a is the Bohr radius, equal to 0.529 angstroms for hydrogen, and given by:

$$a = \frac{4\pi\epsilon_0\hbar^2}{me^2} \tag{8.44}$$

The labels on the wavefunction ψ_{100} mean $n = 1$, $\ell = 0$, $m_\varphi = 0$, as will be seen. The function is normalized so that the integral of the probability density $\psi^*\psi$ over all space ($0 \le r < \infty$, $0 \le \theta \le \pi$, $0 \le \varphi < 2\pi$) is unity. We can show that this is a solution by direct substitution into Equation (8.34) or (8.4.2). Differentiation with respect to r gives us:

$$\frac{d(e^{-r/a})}{dr} = -\frac{1}{a}e^{-r/a} \tag{8.45}$$

so that the second term in Equation (8.42), $-(\hbar^2/2m)(2/r)d\psi_{100}/dr$, cancels the potential energy term, $-(e^2/4\pi\epsilon_0 r)\psi_{100}$. Two derivatives of ψ_{100} are equivalent to multiplying by a factor of $1/a^2$, so the energy must be:

$$E_1 = -\frac{\hbar^2}{2m}\cdot\frac{1}{a^2} = -\frac{me^4}{2(4\pi\epsilon_0\hbar)^2} \tag{8.46}$$

This is identical to the ground state energy given by the Bohr theory.

In fact, solutions to this three dimensional equation, Equation (8.42), exist which satisfy the boundary conditions, provided the energies have only the values given by the Bohr theory formula:

$$E_n = \frac{-me^4}{2(4\pi\epsilon_0\hbar n)^2} \tag{8.47}$$

However, the integer n, which is called the principal ***quantum number,*** has nothing to do with angular momentum. For a given value of the integer, there are n^2 solutions which differ in their dependence on the angular variables θ and φ. All these solutions have the same energy E_n; they are said to be ***degenerate.*** In Table 8.3 are given all the wave functions for n = 1, 2 and 3.

TABLE 8.3 Normalized Wavefunctions for Low-Lying States of Hydrogen.

$n = 1$	$\psi_{100} = \sqrt{\frac{1}{\pi a^3}}\, e^{-r/a}$
$n = 2$	$\psi_{200} = \frac{1}{\sqrt{8\pi a^3}}\left(1 - \frac{1}{2}\frac{r}{a}\right)\exp\left(-\frac{1}{2}\frac{r}{a}\right)$
	$\psi_{210} = \frac{1}{4\sqrt{2\pi a^3}}\frac{r}{a}\exp\left(-\frac{1}{2}\frac{r}{a}\right)\cos\theta$
	$\psi_{21,\pm1} = \frac{1}{8\sqrt{\pi a^3}}\frac{r}{a}\exp\left(-\frac{1}{2}\frac{r}{a}\right)\sin\theta\, e^{\pm i\varphi}$
$n = 3$	$\psi_{300} = \frac{1}{3\sqrt{3\pi a^3}}\left(1 - \frac{2}{3}\frac{r}{a} + \frac{2}{27}\frac{r^2}{a^2}\right)\exp\left(-\frac{1}{3}\frac{r}{a}\right)$
	$\psi_{310} = \frac{4}{27}\frac{1}{\sqrt{2\pi a^3}}\frac{r}{a}\left(1 - \frac{1}{6}\frac{r}{a}\right)\exp\left(-\frac{1}{3}\frac{r}{a}\right)\cos\theta$
	$\psi_{31,\pm1} = \frac{2}{27}\frac{1}{\sqrt{\pi a^3}}\frac{r}{a}\left(1 - \frac{1}{6}\frac{r}{a}\right)\exp\left(-\frac{1}{3}\frac{r}{a}\right)\sin\theta\, e^{\pm i\varphi}$
	$\psi_{320} = \frac{1}{81}\frac{1}{\sqrt{6\pi a^3}}\frac{r^2}{a^2}\exp\left(-\frac{1}{3}\frac{r}{a}\right)(1 - 3\cos^2\theta)$
	$\psi_{32,\pm1} = \frac{1}{81}\frac{1}{\sqrt{\pi a^3}}\frac{r^2}{a^2}\exp\left(-\frac{1}{3}\frac{r}{a}\right)\sin\theta\cos\theta\, e^{\pm i\varphi}$
	$\psi_{32,\pm2} = \frac{1}{162}\frac{1}{\sqrt{\pi a^3}}\frac{r^2}{a^2}\exp\left(-\frac{1}{3}\frac{r}{a}\right)\sin^2\theta\, e^{\pm 2i\varphi}$

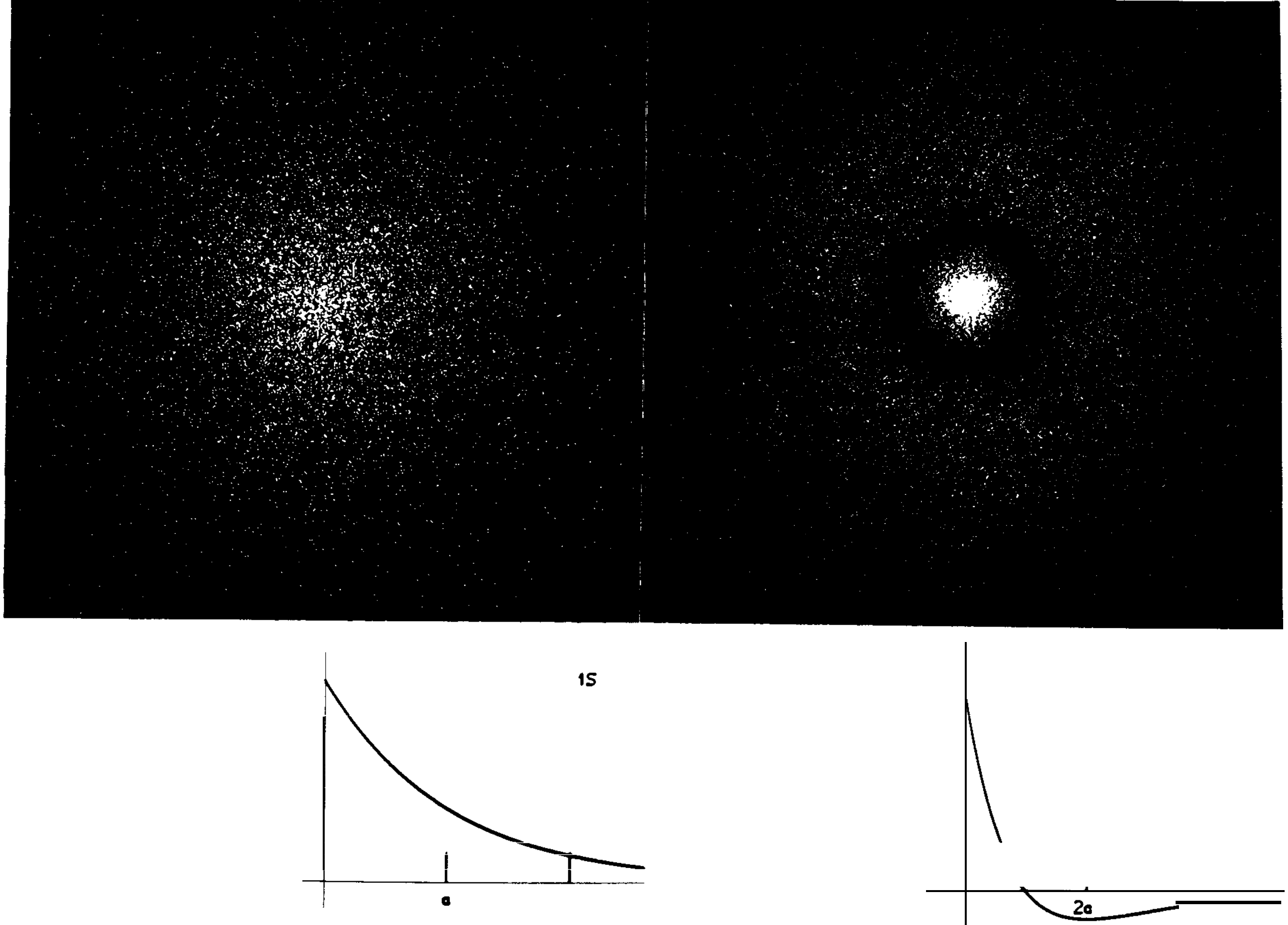


Figure **8.5.** Computer-generated probability density plots of the 1*s* and 2*s* hydrogen wavefunc he curves below a $|\psi(r)|^2$ for comparison.

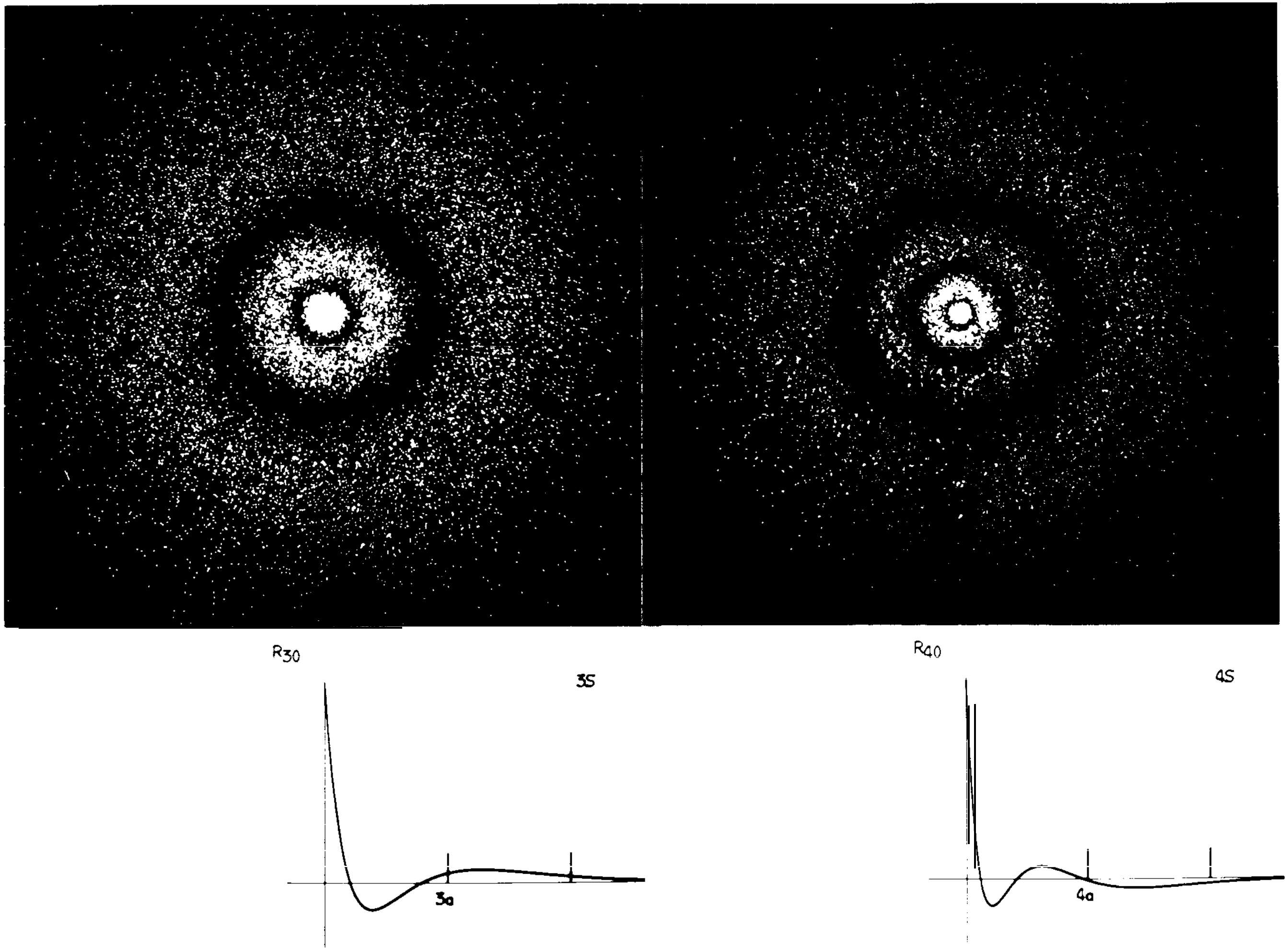


Figure 8.6. Squares of 3s and 4s hydrogen wavefunctions.

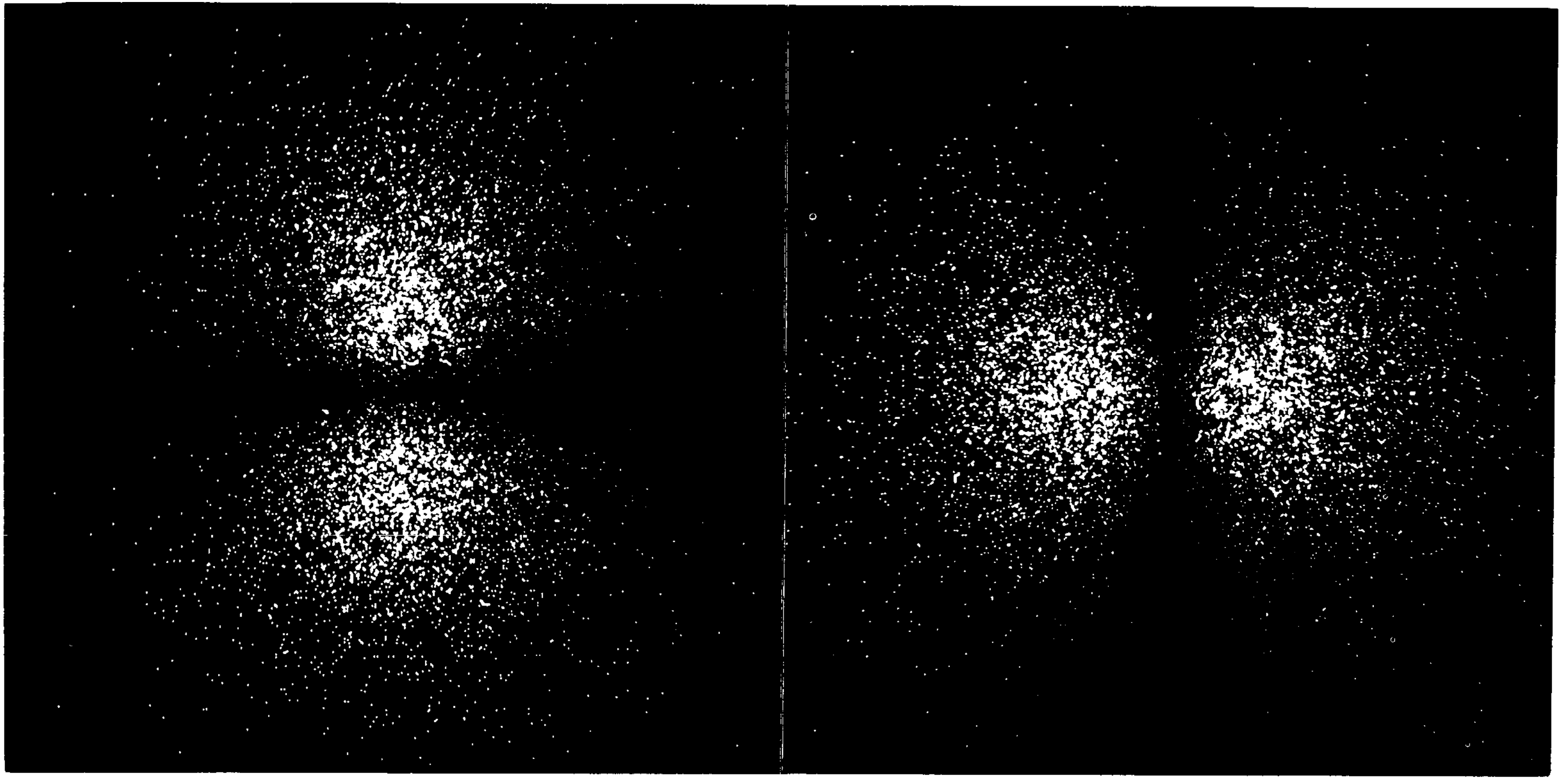


Figure **8.7**. From left to right, squares of hydrogen wavefunction for $2p$ states with $m = 0, m = +1$. The plots are the same except for a 90° rotation.

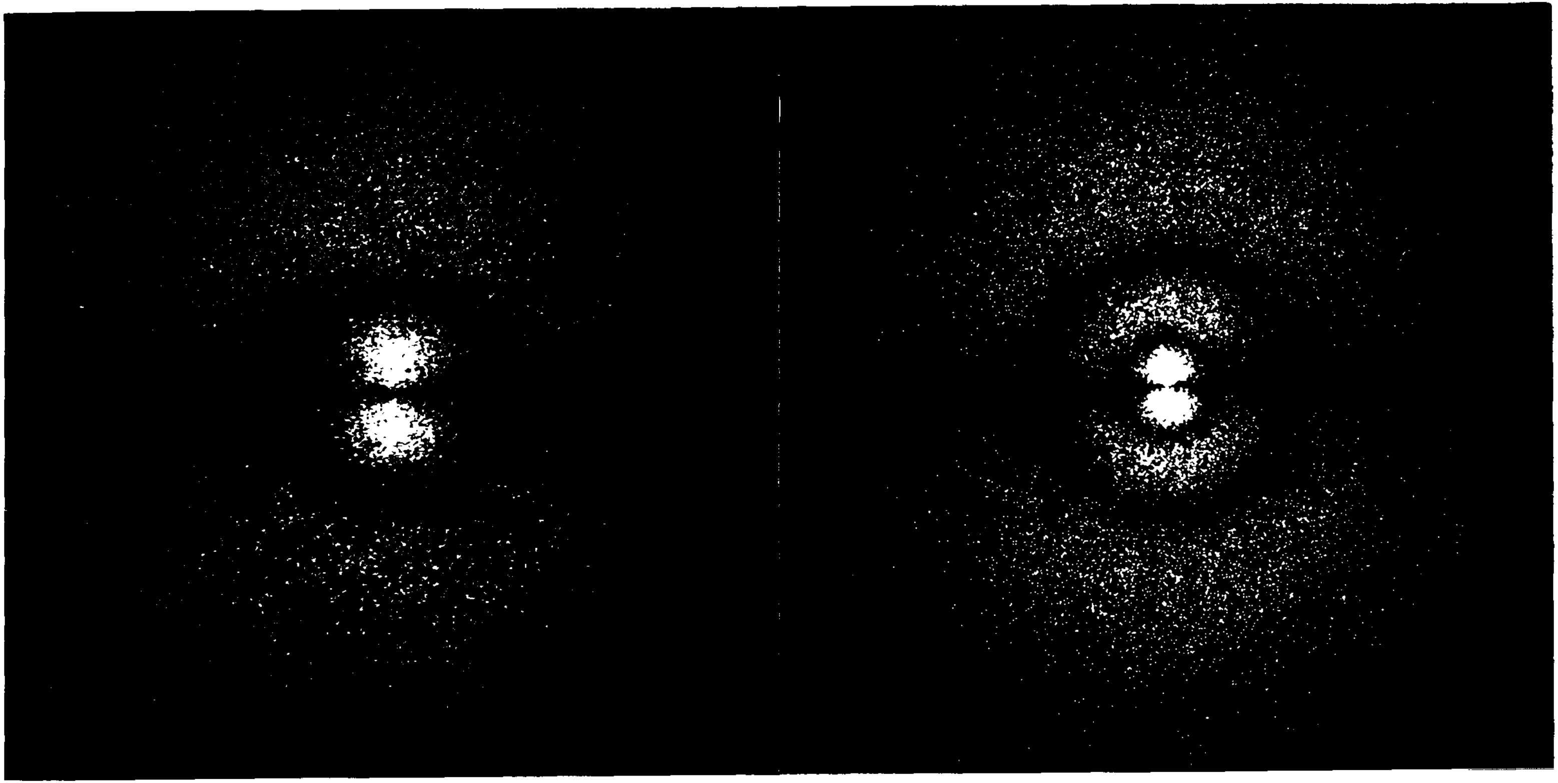


Figure **8.8.** From left to right, squares of hydrogen wavefunctions for $3p(m = 0)$ and $4p(m = 0)$ states.

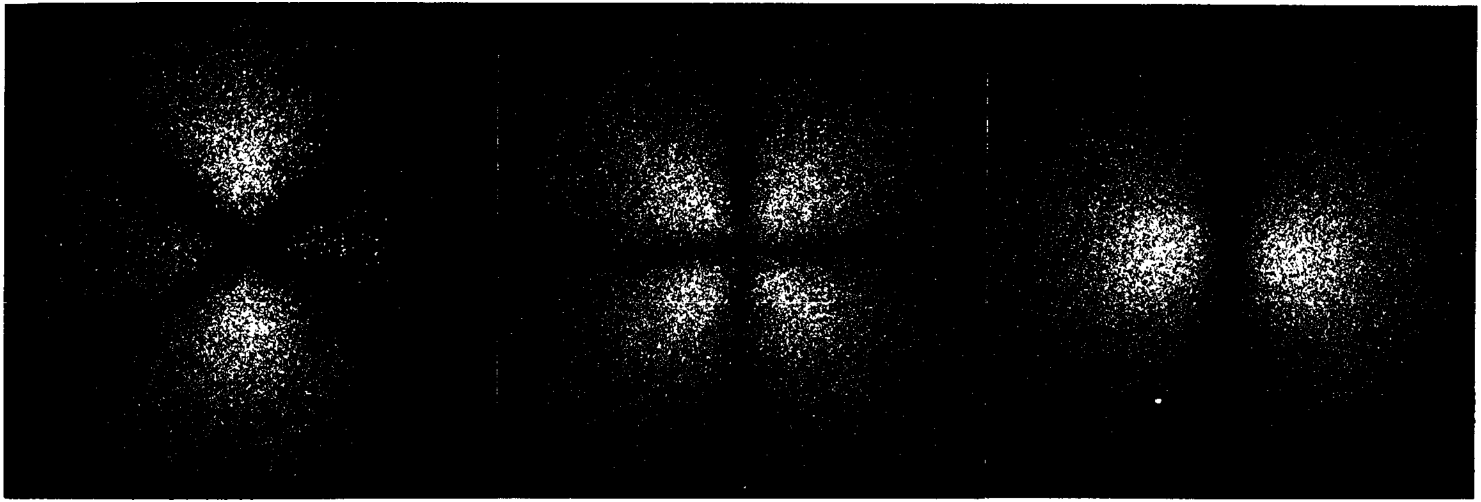


Figure 8.9. Squares of hydrogen wavefunctions for 3d states with $m = 0, \pm 1, \pm 2$.

Figure 8.10. Squares of hydrogen wavefunctions for $4d$ states with $m = 0, \pm 1, \pm 2$.

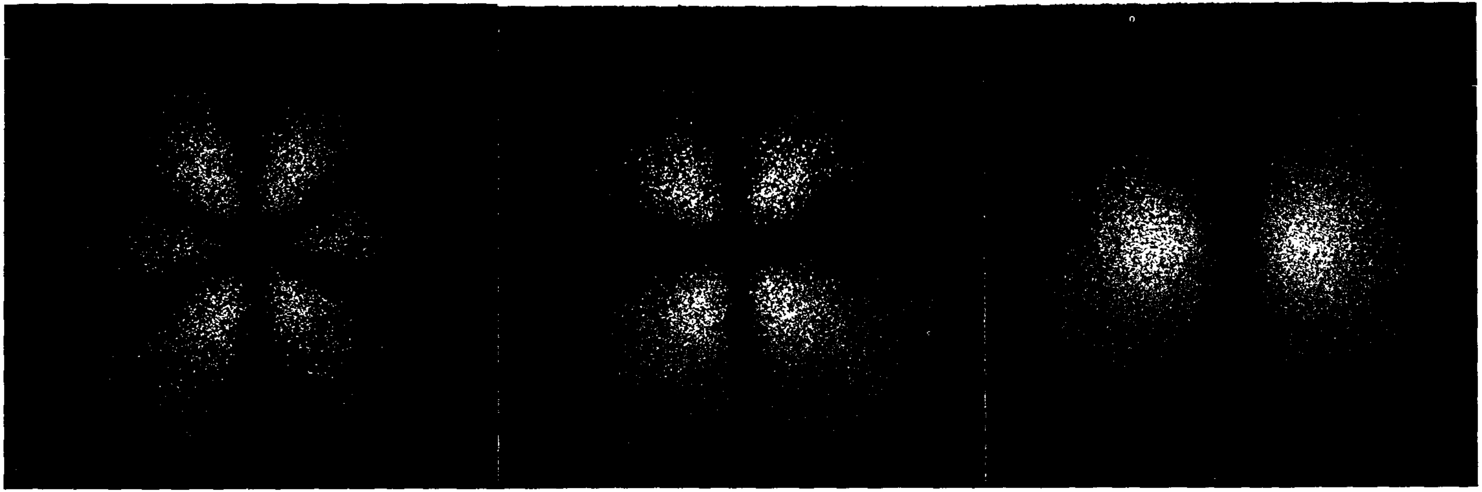


Figure **8.11.** Squares of wavefunctions for *4f* states with $m = \pm 1, \pm 2, \pm 3$.

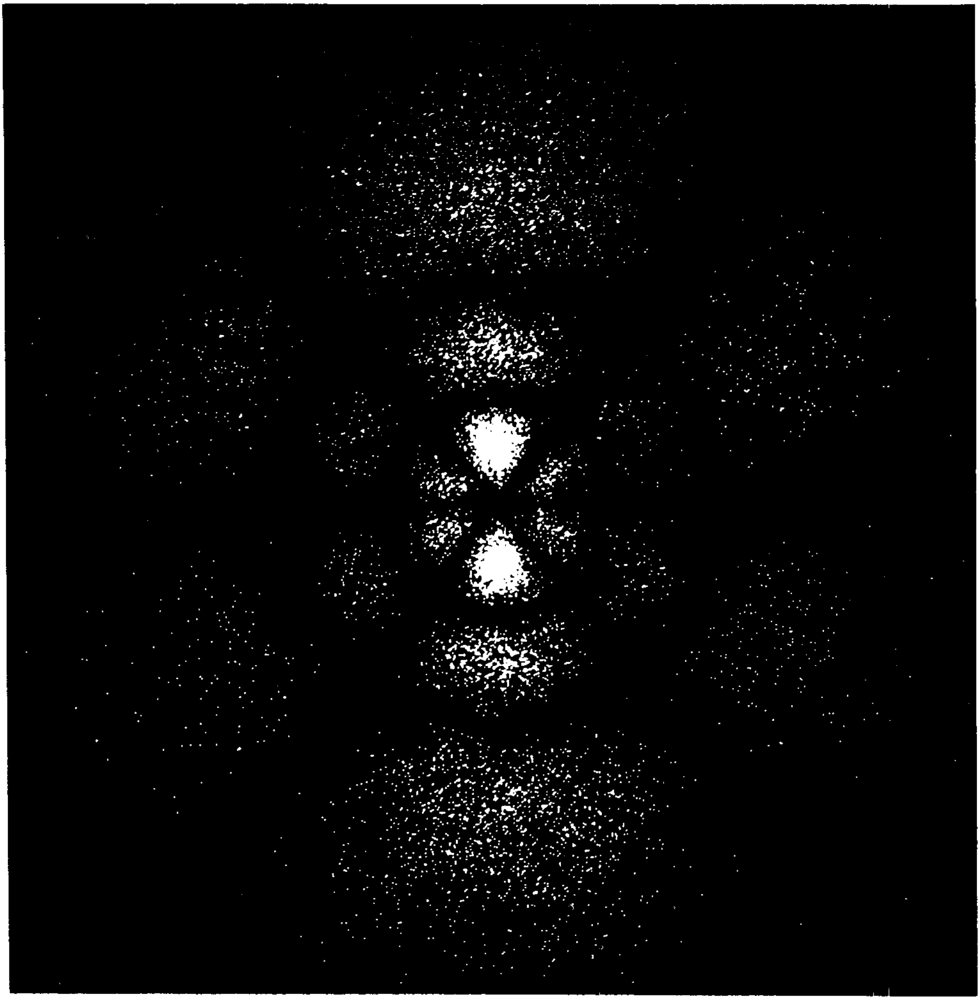


Figure 8.12. Square of 6f (m = 0) hydrogen wavefunction.

Figures 8.5 through 8.12 are probability density pictures of the squares of some of these wavefunctions. These pictures have been drawn in such a way that, if one were to make a few thousand measurements of position of the electron in the given state, and then plot all those positions as dots on polar graph paper with r versus θ, the density of dots would appear as in the pictures. The density of dots is thus proportional to the probability of finding the electron at the plotted r and θ.

The reader may verify that the wavefunctions given in Table 8.3 satisfy Equation (8.34) with the proper energies, by direct substitution into the equation. In general, the functions, $R_{n\ell}$, are of the form of an exponential $e^{-r/na}$, times a polynomial in r; the functions, $\Theta_{\ell m_\varphi}$ are of the form $(\sin \theta)^{|m_\varphi|}$ times a polynomial in cos θ, and $\Phi_{m_\varphi}(\varphi)$ is proportional to $e^{im_\varphi \varphi}$. These wavefunctions satisfy the general orthogonality properties discussed in Appendix 2:

$$\int dV\, \psi^*_{n\ell m_\varphi}\, \psi_{n'\ell' m'_\varphi} = 0 \quad \text{unless } n = n',\ \ell = \ell',\ m_\varphi = m'_\varphi \tag{8.48}$$

8.10 BINDING ENERGY AND IONIZATION ENERGY

We will frequently be interested in systems in which the constituent particles have negative energies due to the attractive forces which bind them together. Such particles might be electrons in atoms, protons in a nucleus, or water molecules in a drop of water. To remove any one of the particles from the system requires the addition of a positive amount of ***energy,*** which is called ***binding energy.*** In other words, the term, *binding* energy, refers to the positive amount of energy which must be added to a system of particles bound together by attractive forces, in order to separate the system into its constituent particles and place them at rest an infinite distance away from each other. Sometimes, the term is used for the amount of energy required to remove just one of several bound particles of a system out of the range of the attractive forces; then the specific particle to which the term refers should be made clear from the context. For example, the binding energy of the hydrogen atom in the ground state is 13.6 eV, since this is the energy which would have to be added to the atom in order to separate the electron from the nucleus. The binding energy of an electron in an excited state of hydrogen is less than this, since less additional energy is required to separate the electron from the nucleus. Thus, the binding energy depends on the specific state which the system is in initially.

The *ionization energy* of an electron in an atom is the energy required to remove that electron, when in its ground state, from the atom. The ionization energy is thus the same as the binding energy when the electron is in its ground state.

8.11 ANGULAR MOMENTUM IN QUANTUM MECHANICS

In Newtonian mechanics, a radial force, such as the Coulomb force, exerts no torques about the origin, and thus angular momentum is conserved. By investigating the meaning of angular momentum in quantum mechanics, we will be able to see the quantum analogue of the conservation of angular momentum. We will find that the angular part of the wavefunction, which is $\Theta_{\ell m_\varphi}(\theta)\Phi_{m_\varphi}(\varphi)$, corresponds to an eigenfunction of the total orbital angular momentum operator, and that $\Phi_{m_\varphi}(\varphi)$ is an eigenfunction of the operator corresponding to the z component of the angular momentum. Thus, the total angular momentum and the z component of the angular momentum of the atom are definite numbers independent of time.

Just as momentum itself is represented by a differential operator in quantum mechanics, so is angular momentum. In Newtonian mechanics, in terms of **r** and the momentum **p**, the vector angular momentum of a particle is given by:

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}$$

The same definition is used in quantum mechanics, but with the momentum operator inserted for **p**. Thus, for example, the z component of the angular momentum operator is:

$$L_z = xp_y \quad yp_x = -i\hbar\left(x\frac{\partial}{\partial y} - - \quad y\frac{\partial}{\partial x}\right) \tag{8.49}$$

.12 ANGULAR MOMENTUM COMPONENTS IN SPHERICAL COORDINATES

It is desirable to **express** this operator in terms of spherical polar coordinates. This could be done by straightforward coordinate transformations; however, it is easier to note that since only first derivatives occur in Equation (8.49), in spherical coordinates I, must be some linear combination of the derivatives with respect to r, θ and φ:

$$L_z = A\frac{\partial}{\partial r} + B\frac{\partial}{\partial \theta} + C\frac{\partial}{\partial \varphi} \tag{8.50}$$

where A, B and C can be functions of the coordinates. The coefficients A, B and C can easily be determined by comparing the effect of the two expressions for L_z when differentiating some simple functions. If the latter operator acts on the function, $r = \sqrt{x^2 + y^2 + z^2}$, it gives A. But the form, Equation (8.49), operating on r gives:

$$-i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)r = i\hbar\left(\frac{xy}{r} - \quad - \quad \frac{yx}{r}\right) = 0 \tag{8.51}$$

Therefore, A = 0. Likewise, L_z operating on cos θ = z/r gives $-B$ sin θ = $-B(x^2 + y^2)^{1/2}/r$. The form, Equation (8.49), operating on z/r gives zero since, as we have seen, it gives zero when operating on a function of r and there is no derivative with respect to z appearing in Equation (8.49). Therefore, B = 0. When L_z operates on tan φ = y/x, it gives C $\sec^2\varphi = C(x^2 + y^2)/x^2$. The form, Equation (8.49), then gives

$$-i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\left(\frac{y}{x}\right) = -i\hbar\left(1 + \frac{y^2}{x^2}\right) \tag{8.52}$$

Therefore, C is $-i\hbar$, and the operator for the z component of angular momentum is:

$$L_z = -i\hbar\frac{\partial}{\partial\varphi} \tag{8.53}$$

In a similar way, we could show that

$$L_x = i\hbar\left(\sin\varphi\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right)$$

$$L_y = i\hbar\left(-\cos\varphi\frac{\partial}{\partial\theta} + \frac{\sin\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right) \tag{8.54}$$

When any of these angular momentum operators act on a function of r only, the result is zero, since there is no derivative with respect to r involved. Thus, the ground state wavefunction and, in general, wavefunctions for which $\ell = 0$ and which depend only on r, not on θ or φ, correspond to states of zero angular momentum. This is in contrast to the Bohr model, where the ground state had an angular momentum of $\hbar$.

8.13 EIGENFUNCTIONS OF L_z AND AZIMUTHAL QUANTUM NUMBER

Using the L_z operator of Equation (8.53), we may give a rigorous interpretation to the number m_φ. In the wavefunction $\psi_{n\ell m_\varphi}$, the φ dependence is contained in the factor

$$\Phi_{m_\varphi}(\varphi) = e^{im_\varphi\varphi} \tag{8.55}$$

Therefore, this is an eigenfunction of the L_z operator, because

$$L_z e^{im_\varphi\varphi} = -i\hbar\frac{\partial}{\partial\varphi}e^{im_\varphi\varphi} = m_\varphi\hbar\, e^{im_\varphi\varphi} \tag{8.56}$$

Hence, such a state can be said-to possess a definite value for the z component of angular momentum.

These values must be quantized. Since the probability density $|\psi|^2$ must be single-valued in space, a reasonable condition on Φ_{m_φ} is that it has the same value at $\varphi = 0$ as at $\varphi = 2\pi$. This means that $e^{im_\varphi(2\pi)} = 1$, or that m_φ is an integer, which could be positive or negative,, or zero. This argument is really the same as that used in discussing the Bohr model, in which it was necessary that the wave amplitude fit onto itself after one revolution in order that the de Broglie wave not interfere destructively with itself. Mathematically, this is expressed by the periodicity condition $\Phi_{m_\varphi}(\varphi) = \Phi_{m_\varphi}(\varphi + 2\pi)$, which can be satisfied only if m_φ is an integer. m_φ is called the azimuthal quantum number.

Thus, the z component of angular momentum has the possible values $\hbar m_\varphi$, where m_φ is a positive or negative integer, or zero. The functions given in Table 8.3 have z components of angular momentum, varying from -(n $-$ 1)$\hbar$ to $+(n-1)\hbar$ for a given n. These are zero for n = 1; zero and $\pm\hbar$ for n = 2; and zero, $\pm\hbar$ and $\pm 2\hbar$ for n = 3. No solutions exist for values of m_φ outside the range $m_\varphi \;| \leq (n-1)\hbar$.

It is also possible to find sums of the wavefunctions $\psi_{n\ell m_\varphi}$ such that L_x or L_y yield an integer times h. For instance, the reader may verify, using Table 8.3 and Equation (8.54), that:

$$\psi'_{310} = \frac{1}{\sqrt{2}}(\psi_{31,-1} + \psi_{31,+1})$$

and

$$\psi'_{31,\pm1} = \frac{1}{2}(\psi_{31,-1} - \psi_{31,+1}) \pm \frac{1}{\sqrt{2}}\psi_{310} \qquad \textit{(8.57)}$$

are eigenfunctions of L_z. However, except when ℓ = 0, for any single wavefunction $\psi_{n\ell m_\varphi}$, the x and y components do not have such definite quantized values.

.14 SQUARE OF THE TOTAL ANGULAR MOMENTUM

Another operator exists which does yield a definite quantized value; this is the square of the angular momentum, $L^2 = L_x^2 + L_y^2 + L_z^2$. The meaning of the square of L_x is, for instance, just the differential operator L_x applied twice: $L_x^2\psi = L_x(L_x\psi)$, and L^2 is the sum of three such terms. In Appendix 1 it is shown that:

$$L^2\psi = -\hbar^2\left(\frac{\partial}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)\psi. \qquad (8.58)$$

It is interesting to note that this same combination of operators occurs in the kinetic energy operator in Equation (8.34). Thus, the kinetic energy operator can be written in terms of L^2 *as* follows:

$$\frac{p_r^2}{2m} + \frac{L^2}{2mr^2}$$

The contribution to kinetic energy arising from the L^2 term makes sense; in classical mechanics, an object of moment of inertia I and angular momentum L has a kinetic energy $L^2/2I$, due to rotation. In this case, the moment of inertia of the electron is mr^2, and the total kinetic energy can thus be written as the sum of a contribution due to radial motion and a contribution due to rotational motion. Since the only angular dependence in the Schrödinger equation, Equation (8.34), is in the L^2 term, and the wavefunction is the product of a part depending only on r and a part depending only on the angles, the energy eigenfunctions, $\psi_{n\ell m_\varphi}$, must also be eigenfunctions of L^2.

8.15 LEGENDRE POLYNOMIALS

We next consider the eigenfunctions of the square of the total angular momentum, L^2, in the special case in which the z component is zero, or $m_\varphi = 0$. Then there is no dependence on φ and the operator effectively depends only on θ:

$$L^2\psi = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta}\right)\psi \tag{8.59}$$

Let us look for wavefunctions P_ℓ (cos θ), finite at $\theta = 0$ and $\theta = \pi$, such that

$$L^2P_\ell = (\text{constant}) \times P_\ell \tag{8.60}$$

The function P_ℓ here is the same as $\Theta_{\ell 0}(\theta)$ in the hydrogen $m_\varphi = 0$ functions, $\psi_{n\ell 0}$. The constant on the right of this equation resulting from the action of L^2 is the eigenvalue, or a possible value of the square of the total angular momentum. One solution is $P_0(\cos\theta) = 1$, a constant. This corresponds to a state of total angular momentum zero, as was the case for the $\ell = 0$ states of the hydrogen atom in which the wavefunctions did not depend on θ or φ. A second solution is $P_1(\cos\theta) = \cos\theta$. The eigenvalue for his function is found by letting L^2 act on it:

$$\frac{d(\cos\theta)}{d\theta} = -\sin\theta; \quad \frac{d^2(\cos\theta)}{d\theta^2} = -\cos\theta \tag{8.61}$$

Then, from Equation (8.59),

$$L^2\cos\theta = \hbar^2\left(\cos\theta + \frac{\sin\theta}{\tan\theta}\right) = 2\hbar^2\cos\theta \tag{88.62}$$

In general, the functions $P_\ell(\cos\theta)$ are polynomials in cos θ, called *Legendre polynomials*, in which only even or only odd powers of cos θ appear for a given ℓ. The highest power of cos θ in the ℓth polynomial is $(\cos\theta)^\ell$. The Legendre polynomials are given in Table 8.4 for $\ell = 0, 1, 2, 3, 4$, along with the corresponding eigenvalues. The general equation for the eigenvalues is $\ell(\ell + 1)\hbar^2$; $\ell = 0, 1, 2, \ldots$.

TABLE **8.4** Some Eigenfunctions of L^2 for $m_\varphi = 0$.

Function	Eigenvalue of L^2
$\ell = 0$: $P_0 = 1$	$0 = \hbar^2 0(0 + 1)$
$\ell = 1$: $P_1 = \cos\theta$	$2\hbar^2 = \hbar^2 1(1 + 1)$
$\ell = 2$: $P_2 = 2\cos^2\theta - \frac{1}{2}$	$6\hbar^2 = \hbar^2 2(2 + 1)$
$\ell = 3$: $P_3 = 2\cos^3\theta - \frac{3}{2}\cos\theta$	$12\hbar^2 = \hbar^2 3(3 + 1)$
$\ell = 4$: $P_4 = \frac{35}{8}\cos^4\theta \quad \frac{15}{4}\cos^2\theta + \frac{3}{8}$	$20\hbar^2 = \hbar^2 4(4 + 1)$

Note that the total angular momentum squared is *not* the square of an integer times $\hbar^2$.

The above states all correspond to $m_\varphi = 0$. For states in which m_φ is not zero, it can be shown that L^2 has the same eigenvalues $\ell(\ell + 1)\hbar^2$.

Since the square of the z component of a vector can never be greater than the square of the vector, $(\hbar m_\varphi)^2 \leq \hbar^2 \ell(\ell + 1)$. Hence, the maximum value of the magnitude of m_φ must be $m_\varphi| = \ell$. If it were assumed that the maximum value of $|m_\varphi$ were $\ell + 1$, instead of ℓ, then L_z^2 would be $[\ell(\ell + 1) + \ell + 1]\hbar^2$, which is greater than $\ell(\ell + 1)\hbar^2$. This is not possible. Thus, actually the square of the z component, L_z^2, can never be as great as L^2. The remaining contributions to L^2 arise from x and y components squared; the individual values of L_x and L_y remain unknown.

There are then $2\ell + 1$ possible values for the z component of the angular momentum for a given orbital angular momentum quantum number ℓ:

$$m_\varphi \hbar = 0, \pm\hbar, \pm 2\hbar, \ldots, \pm\ell\hbar$$

By letting L^2 and L_z act on the various functions in Table 8.3, the reader may verify the properties discussed for these functions.

16 SUMMARY OF QUANTUM NUMBERS FOR HYDROGEN ATOM

Detailed analysis of the complete wavefunctions,

$$\psi_{n\ell m} = R_{n\ell}(r)\Theta_{\ell m_\varphi}(\theta)\Phi_{m_\varphi}(\varphi) \tag{8.63}$$

shows that the total energy depends only on the principal quantum number n:

$$E_n = \frac{-\frac{1}{2} m e^4}{(4\pi\epsilon_0 \hbar n)^2}; \quad n = 1, 2, 3, \ldots \tag{8.64}$$

The energy does not depend on ℓ or m,, as it does (incorrectly) in the Bohr model. In order to satisfy the condition that the wavefunction goes to zero as r goes to infinity, it can be shown to be necessary that ℓ be less than n. Thus,

$$\ell = 0, 1, 2, \ldots, n \quad 1 \tag{8.65}$$

The three quantum numbers:

n — principal quantum number; $n = 1, 2, 3, \ldots$
ℓ — orbital angular momentum quantum number; $\ell = 0, 1, 2, \ldots, n \quad 1$
m_φ -- azimuthal quantum number; $m_\ell = -\ell, -\ell + 1, \ldots 0, \ldots, +\ell$

give a complete description of the possible states of a point electron moving in the Coulomb field of a massive nucleus, neglecting the intrinsic angular momentum of the electron. For a given n or given energy, there are n^2 distinct angular momentum states, so we say the energies are n^2-fold degenerate. When relativistic effects and the spin or intrinsic angular momentum of the electron are taken into account, the energies are changed slightly and the degeneracy is less.

Also, as mentioned at the start of the discussion, the reduced mass, $\mu = m_e m_p/(m_e + m_p)$, should be used in the various equations rather than the electron mass, to incorporate the effect of motion of the nucleus.

8.17 ZEEMAN EFFECT

The angular momentum (quantum numbers can be made observable in one way by placing the atom in a magnetic field. A charged particle which has some angular momentum also has a magnetic dipole moment. This magnetic moment interacts with the field and causes a slight splitting of the energy levels into additional levels. To see how this comes about, consider a classical negatively charged electron, going around in a circle of radius r with speed v, as depicted in Figure 8.13. The angular momentum is $L = mvr$. If the electron carries the

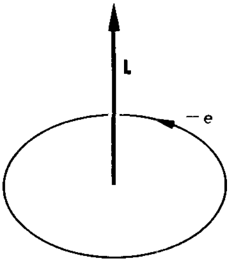


Figure 8.13. A classical point charge moving in a circular orbit with angular momentum **L** has an orbital magnetic moment which is proportional to **L**.

charge $-e$, then the current, or charge per second, passing a given point is the charge times the number of times per second the charge goes around. The number of revolutions per second is $v/2\pi r$, so the current is $-ev/2\pi r$. It is known that a plane current I enclosing area A has a magnetic moment IA. Therefore, in this case, the magnetic moment μ_m is:

$$\mu_m = -\frac{ev}{2\pi r}\pi r^2 = -\frac{1}{2}evr \tag{8.66}$$

This can be expressed in terms of angular momentum $L = mvr$. In this case,

$$\mu_m = -\frac{e}{2m}L \tag{8.67}$$

This equation holds as a vector equation in quantum mechanics:

$$\boldsymbol{\mu}_m = -\frac{e}{2m}\mathbf{L} \tag{8.68}$$

where $-e$ and m are the charge and mass of the electron, and **L** is the angular momentum operator.

Now when a magnetic field **B** is present, there is an energy of interaction between the field and the dipole:

$$E_{mag} = -\boldsymbol{\mu}_m\cdot\mathbf{B} = -B(\mu_m)_z \tag{8.69}$$

if the z axis is chosen in the direction of the field. But $(\mu_m)_z$ is related to the z component of angular momentum: hence, in terms of $L_z = -i\hbar\partial/\partial\varphi$,

$$E_{mag} = \frac{eB}{2m} L_z \tag{8.70}$$

Further, in the hydrogen atom, L_z is quantized and has only the values $\hbar m_\varphi$. Therefore, the energy due to the magnetic field interacting with the magnetic moment can take on only the values:

$$E_{mag} = \frac{e\hbar}{2m} B m_\varphi \tag{8.71}$$

The constant $e\hbar/2m$ is called the Bohr **magneton**, and is denoted by β; $\beta = 0.927 \times 10^{-23}$ joule/weber/m^2.

Now let us return to the Schrödinger equation, to see what happens to the energy levels. The total energy of the electron will be comprised of kinetic energy, plus potential energy due to Coulomb interaction, plus potential energy due to magnetic interaction with the applied field. Hence, the Schrödinger equation would be:

$$E\psi = \left[\frac{p^2}{2m} + V(r)\right]\psi + E_{mag}\psi \tag{8.72}$$

Using a wavefunction $\psi_{n\ell m_\varphi}$, which gives the ordinary energy levels E_n of hydrogen, it is seen that the net energy will just be:

$$E = E_n + E_{mag} \tag{8.73}$$

So the magnetic energy is an additive contribution, provided that the magnetic field is not so large that the wavefunctions are changed appreciably by the field.

Actually, a large magnetic field can itself cause radical changes in the orbital motion of the electron, so these considerations hold only if B is small enough that $E_{mag} \ll E_n$. Let us estimate the magnitude in electron volts of E_{mag} for a typical field of $B = 1.0$ weber/m^2 and $m_\varphi = 1$. This will be:

$$E_{mag} = \frac{e\hbar}{2m}\cdot B = \frac{(0.927 \times 10^{-23})(1.0)}{1.6 \times 10^{-19}\ \text{j/eV}}$$
$$= 5.8 \times 10^{-3}\ \text{eV} \tag{8.74}$$

So this contribution is very small compared to the atomic level spacings, which are on the order of several electron volts.

.18 SPLITTING OF LEVELS IN A MAGNETIC FIELD

Let us consider what happens to an atomic energy level when the atom is placed in a magnetic field. For example, consider an $n = 5$, $\ell = 2$ level, as shown on the left in Figure 8.14. In the absence of a magnetic field, there are $2\ell + 1 = 5$ degenerate states,, described by $m_\varphi = 0, \pm 1, \pm 2$, which all lie together and

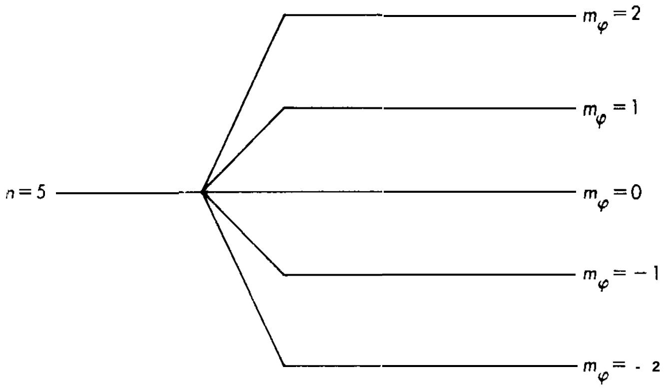
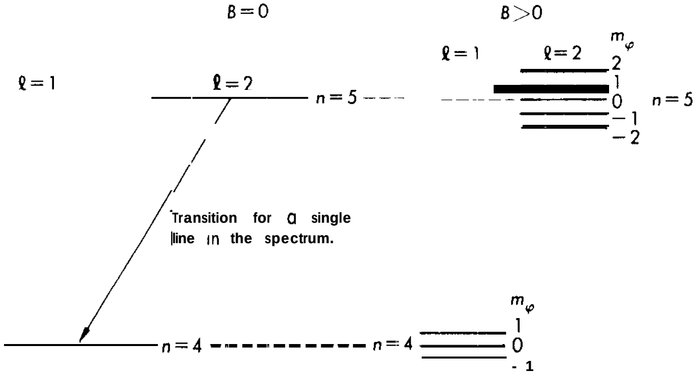


Figure 8.14. Splitting of a $5d$ level into $2l + 1 = 5$ components in an externally applied magnetic field.

appear as a single level, as shown. But when B is different from zero, this level will be replaced by a number of levels of energies, $E_n + E_{mag}$. Since E_{mag} is proportional to m_φ, the number of these levels will be equal to the number of values of m_φ for a given ℓ, $2\ell + 1$. In this example with $\ell = 2$, the five levels are shown at the right of Figure 8.14. In a similar way, an $\ell = 1$ level would be split into three levels. So if we had an energy level diagram looking like the left side of Figure 8.15, at zero field, it would look like the right side of the figure



Transition for a single line in the spectrum.

Figure 8.15. Energy level diagram showing the splittings of $4p$ and $5d$ levels in an applied magnetic field.

when the field is turned on. Thus, in place of a transition yielding a photon with a single frequency, a number of different transitions are possible.

8.19 SELECTION RULES

It appears at first that in Figure 8.15 there are 5 x 3 or 15 possible transitions. However, not all transitions have the same probability. From the theory of transition probabilities, which will not be discussed in this book, it is found that only transitions for which the change $\Delta\ell$ in ℓ is ± 1, and the changes $\Delta m_\varphi = \pm 1, 0$ in m_φ have sufficiently high probability to be readily observed. This is related to the fact that the solutions of Maxwell's classical electromagnetic equations for spherical light waves are eigenfunctions of the operator L^2 with possible quantum numbers $\ell = 1,2,3,\ldots$, but a solution for $\ell = 0$ is impossible. This means that the photon itself has a minimum angular momentum corresponding to the quantum number $\ell = 1$. Only the $\ell = 1$ case occurs with appreciable probability for most transitions. Since the photon carries off one unit of angular momentum, the angular momentum of the atom must change by one unit, in order for angular momentum to be conserved. Therefore, A $\ell = \pm 1$; and Am, $= \pm 1, 0$ for the atom. We shall not prove these rules here, but only state the so-called

$$\text{Selection rules:}\quad \Delta\ell = \pm 1$$

$$\text{Am,} \quad = \pm 1 \text{ or } 0 \qquad (8.75)$$

Thus, a transition from $m_\varphi = 2$ to $m_\varphi = 1$ is probable, but a transition from $m_\varphi = 2$ to $m_\varphi = 0$, → 1 has negligible probability.

.20 NORMAL ZEEMAN SPLITTING

The selection rules are satisfied for the change in ℓ in Figure 8.15, $\ell = 2$ to $\ell = 1$. Table 8.5 shows the values of m_φ for the various lower states with $\ell = 1$ for the allowed transitions corresponding to the various possible values of m_φ in the upper state with $\ell = 2$. Altogether, there are nine allowed transitions. Furthermore, these nine transitions give rise to only three rather than nine spectral lines, because the spacings between the splittings are equal. The transitions are indicated in Figure 8.16. If ΔE_0 is the energy difference between the levels before the field is turned on, then for the Am, = 0 transition, the energy difference after the field is turned on is still:

TABLE 8.5 Allowed Transitions for o $5d \rightarrow 4p$ Transition.

Upper state $\ell = 2$, value of m_φ	**Lower state** $\ell = 1$ values of m_φ **for allowed** transitions
2	1
1	1,0
0	1,0,−1
−1	0,−1
−2	−1

$$\text{AE} = \text{AE,} \qquad (8.76)$$

For the Am $= \pm 1$ transitions, the energy difference with the field on is:

$$\Delta E = \Delta E_0 \mp \frac{e\hbar}{2m} B \qquad (8.77)$$

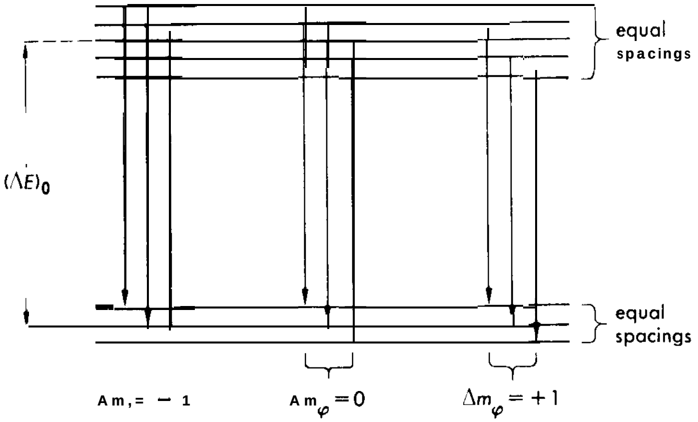


Figure 8.16. **Allowed** transitions for 5d → 4p lines which are split into components by a magnetic field.

Thus a line will be split into three lines; the magnitude of the splitting is proportional to the magnetic field. This phenomenon is observed in some lines of calcium and mercury, and is called the normal Zeeman effect. Usually, however, various elements show splittings with different magnitudes, and also with more or fewer than the three lines predicted here. This is called the anomalous Zeeman effect, and is due to electron spin.

8.21 ELECTRON SPIN

In explaining the anomalous Zeeman effect and other effects to be discussed later, it is necessary to consider the possibility that the electron can have an internal property. The electron is charged, and if it has internal angular momentum or intrinsic spin, it may also have an intrinsic magnetic dipole moment. This dipole moment could then interact with magnetic fields which are present, either externally applied fields or atomic fields, and contribute to the energy of the system. The observation of such energies would give evidence of the existence of internal angular momentum.

Let us call this intrinsic angular momentum spin, and denote the corresponding operator by $\mathbf{S}$. The eigenvalues of $\mathbf{S}^2$ should be $\hbar^2 s(s+1)$, just as for the orbital angular momentum, where s is a spin quantum number. We would expect, then, that the magnetic moment would be proportional to S, and that if this magnetic moment is placed in a magnetic field, it can contribute to the energy. If S_z is the z component of the spin, then the number of different values of S_z should be 2s + 1. This implies that there would also be 2s + 1 magnetic energy terms, or that a level would split into 2s + 1 levels in a magnetic field.

8.22 SPIN-ORBIT INTERACTION

Now so far as the electron in an atom is concerned, it is always in a type of internal magnetic field which leads to a splitting of energy levels, called fine structure splitting. To understand this, consider the Bohr model of the atom, where the electron moves in an orbit through the electric field produced by the nucleus. If the electron has velocity v small compared to c, and moves in an electric field E, we know from electricity theory that in the instantaneous rest frame of the electron there is a magnetic field of $\mathbf{B} = -\mathbf{v} \times \mathbf{E}/c^2$. Then there is an interaction energy between the electron's magnetic moment μ_m and this magnetic field given by $-\boldsymbol{\mu}_m \cdot \mathbf{B}$. If E is pointing radially outward, as is approximately the case in atoms, it is of the form $\mathbf{E} = \mathbf{r} f(r)$, and therefore,

$$\mathbf{B} = [\mathbf{r} \times (m\mathbf{v})]\frac{f(r)}{mc^2} = \frac{\mathbf{L} f(r)}{mc^2} \tag{8.78}$$

Since $\boldsymbol{\mu}_m$ is proportional to the spin S, the energy is proportional to $\mathbf{S} \cdot \mathbf{L}$; this is called ***spin-orbit*** interaction. In place of one level, there will then ordinarily be 2s + 1 levels due to this splitting. In the $\ell = 0$ states there is no such splitting. This is because with no orbital angular momentum there is no component of velocity perpendicular to E in the Bohr picture. Thus there would be no B in the electron's rest frame with which to interact. So if the upper level is split into 2s + 1 levels and there are transitions to a lower $\ell = 0$ level which is not split, one would expect to see 2s + 1 spectral lines due to the splitting.

In hydrogen, there is such a splitting; the magnitude of the splitting can be calculated theoretically and has been observed with special instruments. The splittings are much too small to be observed with a simple diffraction grating or prism spectrometer.

In the alkali metals which consist of an electron orbiting a core of other electrons bound tightly to the nucleus, the splittings are much larger. The observations show that the lines consist of very closely spaced ***pairs*** of lines. For example, in sodium vapor the bright yellow color comes from a pair of yellow lines at 5895.92 Angstroms and 5889.95 Angstroms. The fact that there is a pair of lines or a doublet shows that 2s + 1 should be equal to 2, and therefore the spin quantum number is

$$s = \frac{1}{2} \tag{8.79}$$

.23 HALF-INTEGRAL SPINS

If the spin quantum number is $s = \frac{1}{2}$, then the magnitude of the square of the angular momentum of the electron should be $s(s+1)\hbar^2 = \frac{3}{4}\hbar^2$. In discussing orbital angular momentum, we found that the z component of angular momentum, was always integral. This resulted from the condition that the wavefunction be single-valued, so that it is the same for $\varphi = 0$ and $\varphi = 2x$. If we had said that the function becomes its ***negative*** when φ changes by 2π, the probability density, which depends on the square of the wavefunction, would still be single valued. This would have led to half-integral quantum numbers. While this is not the case for orbital wavefunctions, half-integral spins do occur for intrinsic angular momenta of certain particles, and the spin wavefunctions do change into their negatives upon rotation by 2π.

For a half-integral spin, the maximum magnitude of s_z is still the total angular momentum quantum number, s. Also, neighboring spin states are separated in the z component of angular momentum by $\hbar$. Thus, for a spin $\frac{3}{2}\hbar$ system, the possible values of s_z are $-\frac{3}{2}\hbar, \frac{1}{2}\hbar, \frac{1}{2}\hbar, \frac{3}{2}\hbar$. For the electron, with $s = \frac{1}{2}$, the possible values of s_z are $-\frac{1}{2}\hbar$ (spin down) and $\frac{1}{2}\hbar$ (spin up). Particles have been observed with various integral and half-integral spins. The more fundamental particles such as electrons, protons, neutrons and muons, have intrinsic angular momenta corresponding to $\frac{1}{2}\hbar$. Other fundamental particles such as photons and some mesons have angular momenta corresponding to 0 or $\hbar$.

8.24 STERN-GERLACH EXPERIMENT

An experiment was performed by 0. Stern and W. Gerlach in 1921, which demonstrated directly that $s = \frac{1}{2}$ for the electron. They passed a beam of silver atoms through a strong inhomogeneous magnetic field. Such a field exerts a force on a magnetic dipole which depends on the orientation of the dipole relative to the field. Silver contains 47 electrons, an odd number. Inside the atom the electrons tend to pair off so that their magnetic moments cancel in pairs, except for one left-over electron, with $s = \frac{1}{2}$ and a magnetic moment, $\boldsymbol{\mu}_m$. If the direction of the field **B** is taken to define the z axis, the potential energy of the electron in the magnetic field is:

$$E_{mag} = \boldsymbol{\mu}_m \cdot \mathbf{B} = -\mu_{mz} \cdot B_z \tag{8.80}$$

The magnetic field is constructed so that B_z varies as a function of z; thus the potential energy varies with z, and there will be a z component of force:

$$F = \frac{-\partial E_{mag}}{\partial z} = t\text{-}\mu_{mz}\frac{\partial B_z}{\partial z} \tag{8.81}$$

on the electron and hence on the atom. Because the magnetic moment is proportional to **S**, it can take on only 2s + 1 orientations, giving 2s + 1 possible distinct forces on the particles in the beam. This would split the beam into 2s + 1 beams. When the experiment was performed, the experimenters found the beam to be split into two. Hence again, 2s + 1 = 2, so that $s = \frac{1}{2}$.

8.25 SUMS OF ANGULAR MOMENTA

In general, when treating (angular momenta in quantum mechanics, there are the two types, integral and half-integral. If a system consists of parts which have various angular momenta, such as several particles each of which has intrinsic and orbital angular momenta, the vector sum of the various angular momenta gives the total angular momentum. This total is ordinarily denoted by J. Thus, for a single particle with spin operator S and orbital angular momentum operator, **L**,

$$\mathbf{J} = \mathbf{L} + \mathbf{S} \tag{8.8'2}$$

Combinations of spin and orbital wavefunctions may be found that yield eigenfunctions of the total angular momentum operator squared, $\mathbf{J}^2$, and of the z component of the total angular momentum, J_z. Thus,, acting on these functions the operators yields:

$$\mathbf{J}^2 \rightarrow j(j+1)\hbar^2 \tag{8.83}$$

$$J_z \rightarrow m_j\hbar \tag{8.84}$$

Here j is the total angular momentum quantum number and m_j is the z component quantum number. There are $2j + 1$ possible values of m_j:

$$m_j = -j, -j+1, \ldots, +j \tag{8.85}$$

The j and m_j may either be integral or half-integral, depending on the individual angular momenta which combine to give the total.

26 ANOMALOUS ZEEMAN EFFECT

Let us now return to the discussion of the anomalous Zeeman effect, where an atomic electron in an external magnetic field shows splittings different from those based on orbital angular momentum alone. This anomalous effect arises primarily because the relationship between spin and magnetic moment is different from that for orbital angular momentum. In the orbital case [Equation (8.68)],

$$\boldsymbol{\mu}_m = -\frac{1}{2}\frac{e}{m}\mathbf{L} \tag{8.86}$$

However, for the electron spin, it has been found that:

$$\boldsymbol{\mu}_m = -\frac{e}{m}\mathbf{S} \tag{8.87}$$

These equations differ by a factor of two. This factor of two is predicted by a relativistic wave equation which was discovered by Dirac in 1933.

When treating the splitting of spectral lines in a magnetic field, we must consider the total angular momentum of an electron $\mathbf{J} = \mathbf{L} + \mathbf{S}$. Then the states of the electron are described by quantum numbers j and m_j. If the relation between magnetic moment and angular momentum were the same for the spin and orbital parts, the splittings would be given in terms of m_j, just as in the normal Zeeman case they are given in terms of m_l. One would then always see the normal case. However, because of the difference in the magnetic moment relations, the magnetic moments of the resulting states of definite j and m_j are somewhat complicated. This gives rise to various kinds of splitting of the spectral lines in a magnetic field. By carrying out the analysis in detail using these ideas, one may explain the anomalous Zeeman effect completely.

The idea of angular momentum is important in quantum mechanics for the same reason it was important in Newtonian mechanics; it is conserved relative to a point if the potential energy does not lead to a torque about that point. The conservation of angular momentum has been observed in an enormous number of different experiments.

8.27 RIGID DIATOMIC ROTATOR

In classical mechanics a rigid symmetric top rotating freely about an axis of symmetry through the center of mass has the kinetic energy $L^2/2I$, where I is the moment of inertia about the rotation axis, and L^2 is the square of the angular momentum vector. Certain quantum systems have a kinetic energy operator of the same form, where L^2 is the angular momentum operator given in Equation (8.58). An example of such a system is a linear diatomic molecule such as H_2, N_2 or $HC\ell$, in which the atoms themselves are treated as point masses, separated by a fixed distance. If we imagine a coordinate system placed at the molecule's center of mass, then the position of the line of centers connecting the two atoms may be completely specified by the angles θ and φ defining the direction of the line of centers. Equation (8.58) then gives the operator corresponding to the square of the total angular momentum. The moment of inertia is $I = \mu r^2$, where μ is the reduced mass of the molecule and r the fixed atomic separation distance. If there were a third particle in the molecule not on the line of centers, an additional angle would be needed to specify completely the orientation of the molecule, and there would be additional contributions to the angular momentum and to the energy.

If we consider only linear diatomic molecules, the Schrödinger equation for the stationary states will take the form:

$$E\psi(\theta,\varphi) = \frac{L^2}{2I}\psi(\theta,\varphi) \tag{8.88}$$

Hence, eigenstates of L^2 are also energy eigenstates. We have already seen that the possible eigenvalues of L^2 are of the form $\hbar^2\ell(\ell+1)$; in the case of the rigid rotor it is customary to introduce the symbol J for the quantum number instead of ℓ. Thus,

$$L^2\psi(\theta,\varphi) = \hbar^2 J(J+1)\psi(\theta,\varphi) \tag{8.89}$$

where J is a nonnegative integer. The energies due to rotation of the diatomic molecule are then:

$$E_J = \frac{\hbar^2 J(J+1)}{2I} \tag{8.90}$$

An energy level diagram for these rotational energy levels is given in Figure 8.17.

Transitions between these rotational states are governed by the selection rule $\Delta J = \pm 1$, analogous to the selection rule on ℓ for atomic transitions. Thus, in a

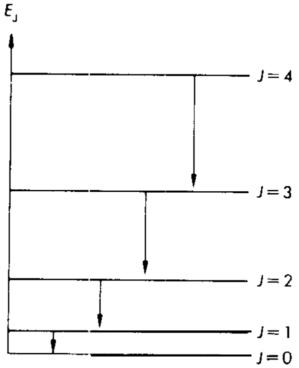


Figure 8.17. Energy level diagram **for the rigid rotator,** $E_J = \hbar^2 J(J+1)/2I$. **The allowed** transitions are governed by the selection rule $\Delta J = \pm 1$.

transition from a rotational state characterized by the quantum number $J+1$, down to the next lower level J, if the atomic electrons do not also change their state, a photon of frequency ν will be emitted, with:

$$\begin{aligned} \hbar\nu &= E_{J+1} \quad E, \\ &= \frac{\hbar^2}{2I}[(J+1)(J+2) - J(J+1)] \\ &= \frac{\hbar^2}{I}(J+1) \qquad (8.91) \end{aligned}$$

The resulting rotational spectrum will therefore consist of lines equally spaced, separated in frequency by $\Delta\nu = \hbar/2\pi I$. Measurements on these spectra thus yield information on the moment of inertia and hence on the interatomic spacing.

To estimate the frequency region in which these lines will be seen, consider a nitrogen molecule N_2 with reduced moss 7 atomic mass units, **and interatomic** spacing $\cong$ 2 Angstroms. The wavelengths will be comparable to

$$\frac{2\pi cI}{\hbar} = \frac{2\pi c\mu r^2}{\hbar} \qquad (8.92)$$

or a few centimeters, in the microwave region. The energy for $J = 0$ is $E = \hbar^2/I \cong 2 \times 10^{-4}$ eV, or about 10^{-4} times smaller than typical atomic electron energies.

Actually, diatomic molecules are not rigidly bound together at a fixed separation distance, but can vibrate slightly back and forth along their line of centers. This vibration is a quantum mechanical simple harmonic oscillation, and the vibrational energies are quantized as well. In Chapter 7 it was seen that the energies are $E_n = \hbar\omega(n + \frac{1}{2})$, where n is a positive integer and ω is proportional to the square root of the effective spring constant. In most diatomic molecules, the interatomic spacings stay quite close to their equilibrium or average values, which means the spring constant is rather large; usually, the spacings between vibrational levels are roughly 100 times the rotational level spacings, or around 0.01 eV; hence the molecular vibrational spectra lie in the far infrared. These vibrational and rotational energy levels give rise to band spectra, consisting of lines spaced so closely together that the spectrum appears to be practically continuous. These bands result from the molecules' changing from one vibrational state to another, while at the same time many different rotational transitions occur. Thus, near one vibrational line could be grouped many lines corresponding to many possible different initial and final rotational levels, which are relatively close together in frequency.

summary

SPECTRUM OF HYDROGEN

The wavelengths of the observed lines in the spectrum of hydrogen are given by the Balmer formula:

$$\frac{1}{\lambda} = R_H\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right), \quad n_1 = 1,2,3,\ldots$$

$$n_2 = n_1 + 1, n_1 + 2, \ldots$$

where the Rydberg constant R_H has the experimental value:

$$R_H = 10{,}967{,}758.1\ m^{-1}$$

The spectrum of the hydrogen atom can be interpreted in terms of an energy level diagram where the discrete energies are:

$$E_n = \frac{-R_H hc}{n^2} \quad n = 1,2,3,\ldots$$

BOHR THEORY OF THE HYDROGEN ATOM

Bohr postulated that the stationary states within the hydrogen atom could be characterized by a quantized value $m_\varphi \hbar$ of the orbital angular momentum. This can also be understood qualitatively by assuming that an integral number of wavelengths of the de Broglie electron waves must fit into a circular orbit. Thus, the tangential component of momentum is given by:

$$mvr = m_\varphi \hbar \quad m_\varphi = 1,2,3,\ldots$$

where r is the radius of the orbit and v is the speed. In addition, the centripetal force necessary to bind the electron in the circular orbit is that due to the

Coulomb attraction between electron and nucleus, or:

$$\frac{mv^2}{r} = \frac{e^2}{4\pi\epsilon_0 r^2}$$

For hydrogen, the total kinetic plus potential energy of the electron is then:

$$E = \frac{-R_\infty hc}{m_\varphi^2}$$

where

$$R_\infty = \frac{mc}{2h}\left(\frac{e^2}{4\pi\epsilon_0\hbar c}\right)^2 = 1.09738 \times 10^7 m^{-1}$$

While this formula agrees well with the observed levels, it is conceptually incorrect, because the exact theory shows that the energy depends on the radial quantum number, n, and not at all on m_φ.

When the motion of the nucleus of mass M is taken into account as well, the energy levels are given by:

$$E = \frac{-R_H hc}{m_\varphi^2}$$

where

$$R_H = \frac{m}{1 + m/M}\frac{1}{2hc}\left(\frac{e^2}{4\pi\epsilon_0\hbar}\right)^2$$

and where

$$\frac{m}{1 + m/M}$$

is called the reduced mass.

SCHRÖDINGER EQUATION FOR HYDROGEN ATOM

In terms of momentum operators, the Schrödinger equation for the hydrogen atom of an infinite-mass nucleus is:

$$\begin{aligned}
E\psi &= \frac{\mathbf{p}^2}{2m}\psi - \frac{e^2}{4\pi\epsilon_0 r}\psi \\
&= -\frac{\hbar^2}{2m}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)\right. \\
&\quad \left. + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}\right\} - \frac{e^2}{4\pi\epsilon_0 r}\psi
\end{aligned}$$

This was obtained by calculating $\mathbf{p}^2$ in spherical polar coordinates in Appendix 1.

The solution to the Schrödinger equation for the ground state is:

$$\psi = \text{const} \times \exp\left(\frac{-me^2}{4\pi\epsilon_0\hbar^2}\right) r$$

In general, the solutions are of the form:

$$\psi_{n\ell m_\varphi} = R_{n\ell}(r)\Theta_{\ell m_\varphi}(\theta)\Phi_{m_\varphi}(\varphi)$$

where $R_{n\ell}(r)$ is a function only of r, $\Theta_{\ell m_\varphi}$ (19) is a function only of θ, and $\Phi_{m_\varphi}(\varphi)$ is a function only of φ. The energies depend only on the principal quantum number n and are given by $E_n = -R_\infty hc/n^2$.

ANGULAR MOMENTUM

The orbital angular momentum operator $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ can be calculated in terms of spherical polar coordinates when the momentum operator is known in terms of those coordinates. The z component of orbital angular momentum is:

$$L_z = \frac{\hbar}{i}\frac{\partial}{\partial\varphi}$$

and the wavefunctions,

$$\Phi_{m_\varphi}(\varphi) = e^{im_\varphi\varphi}$$

with $m_\varphi = -\ell, \ldots 0, \ldots \ell - 1, \ell$, are eigenfunctions of L_z with eigenvalues $m_\varphi\hbar$. The total angular momentum operator is given by:

$$L^2\psi = -\frac{\hbar^2}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) - \frac{\hbar^2}{\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}$$

and the wavefunctions $\Theta_{\ell m_\varphi}(\theta)\Phi_{m_\varphi}(\varphi)$ are eigenfunctions of L^2 with the possible eigenvalues $\hbar^2\ell(\ell + 1)$, where $\ell = 0, 1, 2, \ldots n - 1$. Thus the stationary states of the hydrogen atom, corresponding to the wavefunctions $\psi_{n\ell m}(r, \theta, \varphi)$, are described by three quantum numbers. The principal quantum number n determines the energy. The orbital angular momentum number ℓ is a positive integer $\leq n - 1$, and the azimuthal quantum number m_φ is an integer such that:

$$-\ell \leq m_\varphi \leq +\ell$$

NORMAL ZEEMAN EFFECT

An electron of orbital angular momentum $\mathbf{L}$ has a magnetic dipole moment:

$$\mu_m = -\frac{e}{2m}\mathbf{L}$$

and interacts with an external magnetic field $\mathbf{B}$ along the z axis with the energies:

$$\mathbf{E} = -\mu_m \cdot \mathbf{B} = \frac{eB}{2m}L_z = \frac{eB}{2m}m_\varphi\hbar = m_\varphi\beta B$$

where the Bohr magneton β is

$$\beta = \frac{e\hbar}{2m} = 0.927 \times 10^{-23}\ \mathrm{j/w/m^2}$$

This additional energy causes a splitting of a level corresponding to some value of ℓ into $2\ell + 1$ levels, and transitions between levels occur restricted by the selection rules $\Delta\ell = \pm 1$, $\Delta m_\ell = \pm 1, 0$. In the normal Zeeman effect, only orbital angular momentum is important, and spectral lines are split into three components.

ELECTRON SPIN

Electrons possess internal angular momentum, or spin, S, characterized by a quantum number $s = ½$ such that:

$$S^2\psi = \hbar^2 s(s+1)\psi = \frac{3}{4}\hbar^2\psi$$

The intrinsic magnetic moment of the electron is given by:

$$\mu_s = -\frac{e}{m}\mathbf{S}$$

The total angular momentum of an electron is then $J = \mathbf{L} + \mathbf{S}$, and the electron states are described by quantum numbers j and m_j, where j is half an odd integer. The eigenvalues of total angular momentum are:

$$J^2\psi = \hbar^2 j(j+1)\psi$$

The z component of total angular momentum has the eigenvalues:

$$J_z\psi = \hbar m_j\psi, \quad m_j = \pm\frac{1}{2}, \pm\frac{3}{2}, \ldots \pm j$$

RIGID ROTATOR

A diatomic molecule has rotational energy levels given by:

$$E = \frac{\hbar^2 J(J+1)}{2I}, \quad J = 0, 1, 2, \ldots$$

where I is the moment of inertia of the molecule about the center of mass.

problems

1. **Estimate the ratio of the gravitational attraction at a given distance between the electron and proton in hydrogen, to the Coulomb attraction.**
   Answer: $4\pi\epsilon_0 GmM/e^2 \cong 4 \times 10^{-40}$.
2. **The energy of the electron in the hydrogen atom is $p^2/2m - e^2/4\pi\epsilon_0 r$. Assume this is a one dimensional problem with $\Delta p\Delta r \geq \hbar$, and find the radius r corresponding to the minimum possible energy, by taking $p^2 \sim (\Delta p)^2 \sim (\hbar/\Delta r)^2$,**

$r \sim \Delta r$, and minimizing the resulting expression for energy. Compare with the first Bohr radius.

Answer: $4\pi\epsilon_0\hbar^2/me^2 = 5.28 \times 10^{-11}$ meters.

3. Show that the wavefunction ψ_{300} of Table 8.2 is a solution of the Schrödinger equation for the hydrogen atom, and find the corresponding energy.

   Answer: E_3

4. Calculate the shortest and longest possible wovelengths of lines in the Balmer series of hydrogen.

   Answer: 3647 Angstroms, 6563 Angstroms.

5. Doubly ianized lithium has three protons in its nucleus and a spectrum very similar to that of hydrogen. Calculate the energy of the lowest state in eV, and the wavelength of the spectral line arising from an $n = 2$ to $n = 1$ transition in this ion.

   Answer: $E = -122.7$ eV; $\lambda = 135$ Angstroms.

6. Calculate the reduced mass of five times ionized carbon,: the mass of the neutral carbon atom is 12.000 amu = 19.929×10^{-27}kg. Calculate the effective Rydberg constant for this system. 'The experimentally observed value is $10{,}973{,}228.6\ m^{-1}$.

7. Verify the correctness of the expression for the x component of the angular momentum operator in Equation (8.22).

8. Verify that the functions in Equation (8.23) are eigenfunctions of L_x with the indicated eigenvalues.

9. Find the wavelength of a photon emitted when the 'electron in a hydrogen atom makes a transition from then = 3 state to the $n = 1$ state.

   Answer: 1026 Angstroms.

10. A photon is given off by hydrogen in the trahsition $n = 3$ to $n = 1$. The work function for silver is 4.73 eV. What is the maximum kinetic energy an electron can have if knocked out of silver by this photon?

    Answer: 7.36 eV.

11. For two particles of mosses m and M and positions r_2 and r_1, the Schrödinger equation is:

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial y_2^2}+\frac{\partial^2}{\partial z_2^2}\right)-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial y_1^2}+\frac{\partial^2}{\partial z_1^2}\right)\right]\psi + V\psi = E\psi$$

Let $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$ and $\mathbf{r}_c = (m\mathbf{r}_2 + M\mathbf{r}_1)/(M + m)$, the center of mass position vector. If k is a constant vector and V depends only an the relative vector $\mathbf{r}$, show that a solution for ψ is of the form $\psi = f(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}_c}$, where $f(r)$ satisfies the equation:

$$-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)f + Vf = \left[E - \frac{h^2k^2}{2(M+m)}\right]f$$

with the reduced mass, $\mu = mM/(M + m)$. What is the physical interpretation of this form?

12. The positron is a particle identical in mass, ***m,*** to the electron with charge equal and opposite to that of an electron. The electron and positron can form a hydrogen-like combination called positronium. Using the result in the previous problem, find an expression for the energy levels of positronium.

    Answer: $E = -\frac{1}{4}\, me^4/(4\pi\epsilon_0)^2\hbar^2 n^2$

13. The electric field an electron in a hydrogen atom sees is $e\mathbf{r}/4\pi\epsilon_0 r^3$. Using $\mathbf{B} = -\mathbf{v} \times \mathbf{E}/c^2$ and the fact that the magnetic moment of an electron is $\mu_s = -e/m\ \mathbf{S}$,

show that the spin-orbit coupling energy is $(e^2/4\pi\epsilon_0 m^2c^2)\mathbf{S}\cdot\mathbf{L}/r^3$. (Actually, this is a factor of 2 too large, due to relativistic effects associated with the rotating rest frame of the electron). Using the orders of magnitude: S $\sim \hbar$, $L \sim$ ii, $r \sim$ Bohr radius, show that the spin-orbit splitting is comparable to the hydrogen atom energy times α^2, where $\alpha = e^2/4\pi\epsilon_0\hbar c \cong 1/137$ is the fine structure constant. Since the hydrogen atom energy is on the order of -- 10 eV, what is the order of magnitude of the spin-orbit or fine-structure splitting?

Answer: 10^{-3}eV.

14. The relativistic kinetic energy is $T = \sqrt{p^2c^2 + m_0^2c^4} - m_0c^2$. For pc << mc^2 this is $T \cong (\frac{1}{2}p^2/m)(1 - \frac{1}{4}p^2/m^2c^2)$. The first term is of the order of the hydrogen atom energy when it is used for the kinetic energy part of the hydrogen atom Schrödinger equation. Use this ta show that the next term is of order α^2 times the hydrogen atom energy, where $\alpha = e^2/4\pi\epsilon_0\hbar c \cong 1/137$ is the fine structure constant. From the results in the previous problem, thiris also the order of magnitude of the spin-orbit coupling energy.

15. Write the Schrödinger equation for a free particle in spherical coordinates. Show that two solutions are:

$$\psi_0 = \frac{[\sin(kr)]}{kr}$$

and

$$\psi_1 = \left[\frac{\cos(kr)}{kr} - \frac{\sin(kr)}{(kr)^2}\right]\cos\theta$$

where k is a constant. What is the energy in terms of k?

16. For a particle in a spherical box of radius r_0, what are the conditions on the k's in ψ_0 and ψ_1 of the previous problem? Which of the two solutions could give the wavefunction for a hemispherical box?

Answer: $\sin(kr_0) = 0$ or $k = \frac{n\pi}{r_0}$ for ψ_0

$\tan(kr_0) = kr_0$ for ψ_1; ψ_1 .

17. The operator, L^2 is given in Equation (8.24). Assume that there exist eigenfunctions of the form $\psi = \sum_n a_n \cos^n\theta$. Substitute into the equation $L^2\psi = \lambda\psi$. By using the condition that the coefficient of a given power of cos θ on the left side of this equation must equal that on the right, find a relationship between a_{n+2} and a_n. Determine the values of λ such that the series is actually a polynomial, i.e. that $a_n = 0$ for some n. Assume that $a_0 = 1$ and $a_1 = 0$, or $a_0 = 0$ and $a_1 = 1$.

Answer: $\lambda = \hbar^2 \ell(\ell + 1)$ with $\ell = 1, 2, 3, \ldots$.

18. Verify that the following are eigenfunctions of the operator, L^2:

$$\psi_0 = 1;\quad \psi_1 = \cos\theta;\quad \psi_2 = \frac{3}{2}\cos^2\theta - \frac{1}{2};\quad \psi_3 = \frac{5}{2}\cos^3\theta - \frac{3}{2}\cos\theta$$

The volume element in spherical coordinates is: $r^2 dr \sin\theta\, d\theta d\Phi$. Find what constant each wavefunction ψ_ℓ must be multiplied by to make:

$$\int_0^{2\pi} d\varphi \int_0^{\pi} \psi_\ell^2 \sin\theta\, d\theta = 1$$

19. Verify that the angular functions in ψ_{311}, ψ_{321}, ψ_{322} of Table 8.2 are eigenfunctions of L^2.

20. An angular momentum eigenfunction for the rigid rotator is given by $\sin\theta \times (5\cos^2\theta \;\; 1)e^{i\phi}$. What are the eignvalues of L^2 and L_z?

Answer: $12\hbar^2, \hbar$.

21. The three $\ell = 0$ wavefunctions for the hydrogen atom in Table 8.2 are:

$$\psi_{100} = \text{const.} \times e^{r/a}\ ; \quad \psi_{200} = \text{const.} \times e^{-r/2a}\left(1 - \frac{1}{2}\frac{r}{a}\right);$$

$$\psi_{300} = \text{const.} \times e^{-r/3a}\left(1 - \frac{2r}{3a} + \frac{2}{27}\frac{r^2}{a^2}\right)$$

The volume element in spherical coordinates is $r^2 dr \sin\theta\, d\theta\, d\varphi$. Find by what constant each wavefunction must be multiplied so that:

$$4\pi \int_0^\infty |\psi_n\ {}^2 r^2\,dr = 1$$

22. Find the expectation value of r for the ground state, ψ_{100} = const. x $e^{-\gamma r}$ with $\gamma = me^2/4\pi\epsilon_0\hbar^2$, of the hydrogen atom. Compare with the Bohr radius, a = 0.53×10^{-10} meters.

Answer: $\langle r\rangle = \dfrac{3}{(2\gamma)} = \left(\dfrac{3}{2}\right)a$

23. Find the expectation value of the potential energy, $-e^2/(4\pi\epsilon_0 r)$, and the kinetic energy,

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{1}{r^2}\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)$$

for the state, $\psi_{100} = (\text{const})e^{-\gamma r}$ with $\gamma = me^2/4\pi\epsilon_0\hbar^2$. Compare the two results.

Answer: $\langle V\rangle = -2\langle T\rangle = -27.2$ eV.

24. Calculate the frequency shifts in sec^{-1} for a line exhibiting the normal Zeeman effect when the applied magnetic field is 1.72 w/m^2.

Answer: $2.4 \times 10^{12}/\text{sec}$.

25. Calculate the maximum component of the spin magnetic moment of the electron along the direction of an applied magnetic field.

Answer: 0.927×10^{-23} joule/(weber/m^2).

26. Show that for wavefunctions that are eigenfunctions of J^2, L^2, S^2, and J_z where $\mathbf{J} = \mathbf{L} + \mathbf{S}$,

$$\langle \mathbf{L}\cdot\mathbf{J}\rangle = \frac{1}{2}\,[j(j+1) + \ell(\ell+1) - s(s+1)]\hbar^2$$

27. Suppose two particles of orbital angular momentum quantum numbers $\ell_1 = 2$ and $\ell_2 = 3$ combine to form a single system. Then the total angular momentum quantum number can have the values j = 5, 4, 3, 2, or 1 with a maximum and a minimum value, just as if we added two vectors vectorially of lengths 2 and 3. Show that the total number of possible states when the particles are specified by the combination of ℓ, m_{φ_1} and ℓ_2, m_{φ_2} is the same as when specified by j and m_j.

28 The experimentally observed frequency spacing between two successive rotational lines observed in the spectrum of the HCl molecule is $6.3502 \times 10^{11}\ \text{sec}^{-1}$. Using this information, calculate the distance between the hydrogen atom and the chlorine atom which make up the diatomic molecule.

Answer: 1.803 Angstroms.

9 Pauli exclusion principle and the periodic table

We have seen how the hydrogen atom, and hydrogen-like atoms, may be pictured as very small, positively charged nuclei surrounded by "clouds" of negative electricity due to the electron. In fact, a similar picture is valid for more complicated atoms containing many electrons. In the hydrogen atom the charge cloud is around an Angstrom in diameter and the energy differences involved when the electron changes its state are a few electron volts. Similarly, in many-electron atoms, from experimental studies of spectra, chemical reactions, formation of crystals, etc., it can be concluded that the charge clouds are of the order of a few Angstroms in size, and that energy changes are also of the order of a few electron volts. For example, when a sodium atom and a chlorine atom combine to form NaCl, the total energy given up per molecule formed is 4.24 eV and the NaCl distance is 2.36 Angstroms.

When two atoms are brought close together, the electronic charge clouds will begin to overlap, and ii is to be expected that the features of the interaction between atoms will be largely determined by the structure of the electronic cloud, or in other words, by the states of the electrons in the atoms. Some atoms tend to give up an electron and form positive ions, such as the alkali metals sodium, potassium, rubidium, cesium. Some atoms tend to attract an extra electron and form negative ions, such as the halogens, fluorine and iodine. Others are chemically nearly inert, such as helium and neon. Because of the great variety of chemical behavior we would not expect the electronic states of all atoms to be similar, but important differences must exist among them.

In studying the mathematical solution of the hydrogen atom problem by means of Schrödinger's equation, it has been seen how the various states of the electron can be labeled by a set of quantum numbers. The spectrum of light emitted by hydrogen can then be understood by saying that the electron makes a transition from one state to another, emitting a photon in order to conserve energy. Although in more complicated atoms the energy levels do not have the same numerical values as in hydrogen, still the state's may be labeled by the same set, or a very similar set, of quantum numbers as are used for hydrogen.

In addition to the fact that other nuclei have larger charges than does the proton in hydrogen, the complications due to electron-electron interactions shift the energy levels around somewhat.

From a study of the spectrum of an atom, it is possible to determine the various energy levels and their quantum numbers. It is observed experimentally that in the spectra of atoms having two or more electrons, certain lines are missing. For example, in lithium there are no transitions from $n = 2$ states to $n = 1$ states. In explaining these and related phenomena, Pauli proposed the **exclusion *principle.*** Loosely stated, this principle says that no two electrons in an atom can exist in the same quantum state. This remarkably simple principle can also be used to explain the structure of the periodic table of the elements and the chemical behavior of the atoms of each element. Let us begin by reviewing the nomenclature used in describing atomic energy levels.

.1 DESIGNATION OF ATOMIC STATES

In solving the Schrödinger equation for the isolated hydrogen atom, it was found that the wavefunctions were labeled by the quantum numbers: **n,** ℓ, and m_ϕ, and spin quantum numbers. The energies were degenerate and depended only on the principal quantum number, n. While in the previous chapter m_ϕ with subscript was used to avoid confusion with the symbol **m** for mass, no such confusion should occur in this chapter. Therefore, we will from here on use m for the azimuthal quantum number, as is usual in physics. The second quantum number ℓ is called the orbital angular momentum quantum number. It can have the possible values $\ell = 0, 1, 2, \ldots, (n - 1)$. Thus for a given value of n, there are n values of ℓ. If a state is described by a value ℓ for the orbital angular momentum quantum number, then the square of the orbital angular momentum is $L^2 = \hbar^2 \ell(\ell + 1)$.

The various ℓ states are also denoted by letters. States for which $\ell = 0$ are also referred to as s states; $\ell = 1$ are **p** states. In various applications, these letters may be either capital or small. The designation is given in Table 9.1.

TABLE 9.1 Alphabetic designations of states for different orbital angular momentum quantum numbers ℓ.

ℓ value	alphabetical designation
0	s
1	p
2	d
3	f
4	g
The rest in alphabetical order.	

An $\ell = 5$ state would be an h state. All s states have zero orbital angular momentum, and the wavefunctions depend only on r. So the probability density $|\psi_{n00}|^2$ has spherical symmetry. If $n = 3$, the states s, p, d are possible corresponding to the ℓ values, 0, 1, 2. States are sometimes designated by writing an integer and then a letter: 3p, 1s, 2p, etc. The integer refers to the value of n and the letter refers to the value of ℓ. Thus a 4p state has $n = 4$, $\ell = 1$. If $n = 5$, the possible states are 5s, 5p, 5d, 5f, 5g. In the hydrogen atom, all these $n = 5$ states are approximately degenerate and have the same energy.

9.2 NUMBER OF STATES IN AN n SHELL

The azimuthal quantum number m can have positive or negative integral values or zero. Since $m\hbar$ is the z component of orbital angular momentum, the maximum magnitude of m is equal to ℓ. Thus, m can vary in integral steps from a minimum value of $-\ell$ to a maximum value of ℓ. This gives $2\ell + 1$ values of m for a given ℓ. Thus, for example, for a 5p state there are three possible m values, and for a 3d state there are five. If there are $2\ell + 1$ values of m for a given ℓ, and n values of ℓ ($\ell = 0, 1, \ldots n - 1$) for a given n, then for a given n the total number N_n of states of the electron in a hydrogen atom is equal to:

$$N_n = \sum_{\ell=0}^{n-1} (2\ell + 1) \tag{9.1}$$

The arithmetic series formula gives us:

$$\sum_{\ell=0}^{n-1} \ell = \frac{n(n-1)}{2} \tag{9.2}$$

so the number N_n in terms of n is $N_n = 2[n(n \quad 1)/2] + n = n^2$. This means that in hydrogen the energy degeneracy is n^2. These n^2 states are different because the dependence of $\psi_{n\ell m}$ on (r, θ, Φ) changes as ℓ and m change, i.e. as the angular momentum changes.

The specification of electronic states in terms of n, ℓ and m is not quite complete, because in addition to these quantum numbers the electron has internal quantum numbers, i.e. spin angular momentum numbers, with values $s = ½$ and $m_s = \pm ½$. The number s is the total spin angular momentum quantum number; and the z component of spin angular momentum has eigenvalues of $m_s\hbar$. Thus, including the effect of spin, to completely specify the state of an electron we need five quantum numbers, n, ℓ, m, s, m_s. However, for an electron, s is always equal to ½ So if we keep this fact in mind, we only need to use the four quantum numbers n, ℓ, m and m_s. Since for a given n, ℓ and m, there are two possible values of m_s, the degeneracy of the electron in the hydrogen atom is actually not n^2, but $2n^2$. Also, in addition to the spatial coordinate r describing position of an electron, there is another coordinate describing spin, so in general an electronic wavefunction will be a function of the form $\psi_{n\ell mm_s}(\mathbf{r}, \mathbf{S})$ where $\mathbf{S}$ is a ***spin coordinate.***

9.3 INDISTINGUISHABILITY OF PARTICLES

The above considerations are valid when we have one electron in a state in a hydrogen-like atom. If we have a many-electron atom, then the energy levels will in general be shifted, so that they may depend on ℓ as well as n. This is because the outer electron wavefunctions penetrate the cloud of inner electrons to different extents depending on ℓ, leading to different 'average potential energies. Also, since total angular momentum $(\mathbf{L} + \mathbf{S})$ is quantized, it may be more useful in some cases to label states by total angular momentum quantum numbers j, m_j, rather than ℓ and m. We shall not need to do this here, however.

Consider an atom, such as helium, which has two electrons. The wavefunction ψ will then depend on two sets of variables: $\mathbf{r}_1, \mathbf{S}_1$ for one electron and $\mathbf{r}_2, \mathbf{S}_2$ for the other. So the wavefunction could be written $\psi(\mathbf{r}_1, \mathbf{S}_1; \mathbf{r}_2, \mathbf{S}_2)$, where the labels before the semicolon refer to the values of the coordinates of electron 1 and the labels after the semicolon refer to values of the coordinates of electron 2. Suppose the coordinates of the electrons are interchanged; that is, the electron 2 is given coordinates $\mathbf{r}_1, \mathbf{S}_1$, and electron 1 is given coordinates $\mathbf{r}_2, \mathbf{S}_2$. The resulting wavefunction will be $\psi(\mathbf{r}_2, \mathbf{S}_2; \mathbf{r}_1, \mathbf{S}_1)$. It is of importance to consider this hypothetical "exchange" of electrons, because it has been found that electrons are indistinguishable from each other. In classical mechanics it was assumed that all particles-even identical particles--could be given labels to distinguish one from another. In quantum mechanical systems of identical particles, this is not possible. If

$$dp_{12} = |\psi(\mathbf{r}_1, \mathbf{S}_1; \mathbf{r}_2, \mathbf{S}_2)|^2 dV_1 dV_2 \tag{9.3}$$

is the probability of finding electron 1 in $dV_1 = dx_1 dy_1 dz_1$ and electron 2 in $dV_2 = dx_2 dy_2 dz_2$, then since the particles are indistinguishable, this must be the same as the probability of finding electron 2 in dV_1 and electron 1 in dV_2; which electron we call 1 and which we call 2 should make no difference. But the probability of finding electron 2 in dV_1 and electron 1 in dV_2 is:

$$dp_{21} = |\psi(\mathbf{r}_2, \mathbf{S}_2; \mathbf{r}_1, \mathbf{S}_1)|^2 dV_2 dV_1. \tag{9.4}$$

Indistinguishability of particles requires that the two probabilities in Equations (9.3) and (9.4) be equal. Thus, $|\psi(\mathbf{r}_1, \mathbf{S}_1; \mathbf{r}_2, \mathbf{S}_2)|^2 dV_1 dV_2 = |\psi(\mathbf{r}_2, \mathbf{S}_2; \mathbf{r}_1, \mathbf{S}_1)|^2 dV_2 dV_1$, or:

$$|\psi(\mathbf{r}_1, \mathbf{S}_1; \mathbf{r}_2, \mathbf{S}_2)|^2 = |\psi(\mathbf{r}_2, \mathbf{S}_2; \mathbf{r}_1, \mathbf{S}_1)|^2 \tag{9.5}$$

When the magnitudes of two numbers are equal, the numbers themselves must be equal, except possibly for a phase factor, $e^{i\Phi}$, since $|e^{i\Phi}| = 1$. Thus, the most general conclusion which can be drawn from equation (9.5) is that:

$$\psi(\mathbf{r}_2, \mathbf{S}_2; \mathbf{r}_1, \mathbf{S}_1) = e^{i\Phi}\psi(\mathbf{r}_1, \mathbf{S}_1; \mathbf{r}_2, \mathbf{S}_2) \tag{9.6}$$

where $e^{i\Phi}$ is some unknown phase factor.

The phase factor Φ is actually a constant, independent of coordinates. While a completely rigorous demonstration of this fact is rather difficult, the constancy of Φ can be seen to be quite reasonable, by considering1 the expectation value of a quantity such as the x component of momentum; this involves an integral of the form:

$$\langle p_x \rangle = \int \psi^*(\mathbf{r}_1, \mathbf{S}_1; \mathbf{r}_2, \mathbf{S}_2)\left(\frac{\hbar}{i}\frac{\partial}{\partial x_1} + \frac{\hbar}{i}\frac{\partial}{\partial x_2}\right)\psi(\mathbf{r}_1, \mathbf{S}_1; \mathbf{r}_2, \mathbf{S}_2)\, dV_1 dV_2 \tag{9.7}$$

which must remain unchanged if the particles are interchanged:

$$\langle p_x\rangle = \int \psi^*(\mathbf{r}_2,\mathbf{S}_2;\mathbf{r}_1,\mathbf{S}_1)e^{-i\Phi}\left(\frac{\hbar}{i}\frac{\partial}{\partial x_1}+\frac{\hbar}{i}\frac{\partial}{\partial x_2}\right) e^{i\Phi}\psi(\mathbf{r}_2,\mathbf{S}_2;\mathbf{r}_1,\mathbf{S}_1)\,dV_2\,dV_1 \qquad (9.8)$$

Hence the operator $e^{-i\Phi}(p_{1_{x_{op}}} + p_{2_{x_{op}}})e^{+i\Phi}$ must be equivalent to the operator $p_{1_{x_{op}}} + p_{2_{x_{op}}}$. More generally, for any differential operator O_{op} representing a physical quantity,

$$e^{-i\Phi}O_{op}e^{i\Phi} = O_{op} \qquad (9.9)$$

which can be true for all differential operators only if Φ is a constant.

After exchanging two particles, the new wavefunction is equal to the old, multiplied by e”. If we carry out a second exchange of the same two particles, the same thing will happen, so in addition to Equation (9.6), we have:

$$\psi(\mathbf{r}_1,\mathbf{S}_1;\mathbf{r}_2,\mathbf{S}_2) = e^{i\Phi}\psi(\mathbf{r}_2,\mathbf{S}_2;\mathbf{r}_1,\mathbf{S}_1) \qquad (9.10)$$

Substituting Equation (9.10) into Equation (9.6), we conclude that $\psi(\mathbf{r}_2,\mathbf{S}_2;\mathbf{r}_1,\mathbf{S}_1) = e^{2i\Phi}\psi(\mathbf{r}_2,\mathbf{S}_2;\mathbf{r}_1,\mathbf{S}_1)$, and therefore $e^{2i\Phi} = 1$. If $e^{2i\Phi} = 1$, then there are two possibilities for the phase factor $e^{i\Phi}$. They are $e^{i\Phi} = +1$ or -1. Thus we have two possibilities upon exchanging identical particles:

$$\psi(\mathbf{r}_2,\mathbf{S}_2;\mathbf{r}_1,\mathbf{S}_1) = (\pm 1)\psi(\mathbf{r}_1,\mathbf{S}_1;\mathbf{r}_2,\mathbf{S}_2) \qquad (9.11)$$

Exchanging two particles has the effect of either leaving the wavefunction unchanged or changing it into its negative. Wavefunctions which have the property $\psi(\mathbf{r}_2,\mathbf{S}_2;\mathbf{r}_1,\mathbf{S}_1) = +\psi(\mathbf{r}_1,\mathbf{S}_1;\mathbf{r}_2,\mathbf{S}_2)$ are said to be symmetric under particle exchange. When $\psi(\mathbf{r}_2,\mathbf{S}_2;\mathbf{r}_1,\mathbf{S}_1) = -\psi(\mathbf{r}_1,\mathbf{S}_1;\mathbf{r}_2,\mathbf{S}_2)$ so that the minus sign applies, the wavefunctions are said to be *antisymmetric* under exchange. Both of these possibilities are found in nature. Experimentally, the $+1$ arises when dealing with identical particles of integral spin, called *bosons.* The minus sign arises when exchanging particles of half-integral spin, called fermions. Since an electron has spin ½ and it is a fermion, upon interchanging two electrons the wavefunction will be multiplied by -1.

9.4 PAULI EXCLUSION PRINCIPLE

Suppose we ask whether two electrons can have equal r and S, that is, can we have $\mathbf{r}_1,\mathbf{S}_1 = \mathbf{r}_2,\mathbf{S}_2 = \mathbf{r},\mathbf{S}$? Since the wavefunctions describing electrons are antisymmetric, we start with a wavefunction $\psi(\mathbf{r},\mathbf{S};\mathbf{r},\mathbf{S})$, then after exchanging two electrons, we find $\psi(\mathbf{r},\mathbf{S};\mathbf{r},\mathbf{S}) = -\psi(\mathbf{r},\mathbf{S};\mathbf{r},\mathbf{S})$. It follows that the probability of finding two electrons at the same place with the same spin must be zero.

Suppose we assumed that two electrons can each be described by quantum numbers $n\ell m m_s$, with $n_1\ell_1m_1m_{s1}$ for electron 1 and $n_2\ell_2m_2m_{s2}$ for electron 2; and suppose we tried to write an overall wavefunction as a product of single-particle hydrogen-like wavefunctions:

$$\psi(\mathbf{r}_1, \mathbf{S}_1; \mathbf{r}_2, \mathbf{S}_2) = \psi_{n_1\ell_1m_1m_{s1}}(\mathbf{r}_1, \mathbf{S}_1)\psi_{n_2\ell_2m_2m_{s2}}(\mathbf{r}_2, \mathbf{S}_2) \tag{9.12}$$

We would find that this simple product function is not antisymmetric, and hence does not satisfy the condition of indistinguishability of particles, Equation (9.5). We can, however, construct a wavefunction describing a state of the same energy by taking a linear combination:

$$\psi(\mathbf{r}_1\mathbf{S}_1; \mathbf{r}_2\mathbf{S}_2) = \frac{1}{\sqrt{2}}[\psi_{n_1\ell_1m_1m_{s1}}(\mathbf{r}_1, \mathbf{S}_1)\psi_{n_2\ell_2m_2m_{s2}}(\mathbf{r}_2, \mathbf{S}_2)$$

$$-\psi_{n_1\ell_1m_1m_{s1}}(\mathbf{r}_2, \mathbf{S}_2)\psi_{n_2\ell_2m_2m_{s2}}(\mathbf{r}_1, \mathbf{S}_1)] \tag{9.13}$$

Upon interchange of the coordinates $\mathbf{r}_1$, $\mathbf{S}_1$ and $\mathbf{r}_2$, $\mathbf{S}_2$, the above function is easily seen to be antisymmetric.

So a linear combination of single-particle product wavefunctions with opposite signs for the two terms gives us a correctly "antisymmetrized" overall wavefunction. The factor $1/\sqrt{2}$ is for correct normalization. The first term could be interpreted by saying that electron 1 is in state $n_1\ell_1m_1m_{s1}$ and electron 2 is in state $n_2\ell_2m_2m_{s2}$, while the second term could be interpreted by saying that electron 2 is in state $n_1\ell_1m_1m_{s1}$ and electron 1 is in state $n_2\ell_2m_2m_{s2}$. Thus, because of the indistinguishability of electrons and the related fact that the wavefunction must be antisymmetric, the two electrons are both partially in the states $n_1\ell_1m_1m_{s1}$ and $n_2\ell_2m_2m_{s2}$. Suppose that both states were identical, however: $n_1 = n_2$, $\ell_1 = \ell_2$, $m_1 = m_2$ and $m_{s1} = m_{s2}$. Then, from an inspection of the antisymmetric wavefunction in Equation (9.13), it is immediately seen that $\psi = 0$ -an impossibility.

Although we have been discussing the situation for electrons in an atom, a similar situation holds no matter what system is being considered. Thus, for two electrons in a one dimensional box, the individual single-particle wavefunctions are described by values of $k_n = n\pi/L$, and apart from spin the wavefunctions are $\psi_n(x) = \sqrt{2/L}\sin(n\pi/L)x$. With spin, the wavefunctions would be denoted by ψ_{nm_s} (x, S). Then, if two noninteracting particles were in the box with wavefunctions $\psi_{n_1m_{s1}}$ and $\psi_{n_2m_{s2}}$, one could write the antisymmetric wavefunction as:

$$\psi(x_1\mathbf{S}_1; x_2\mathbf{S}_2) = \frac{1}{\sqrt{2}}[\psi_{n_1m_{s1}}(x_1, \mathbf{S}_1)\psi_{n_2m_{s2}}(x_2, \mathbf{S}_2)$$

$$-\psi_{n_1m_{s1}}(x_2, \mathbf{S}_2)\psi_{n_2m_{s2}}(x_1, \mathbf{S}_1)] \tag{9.14}$$

Then in this case also, if the two states are the same: $n_1 = n_2$, $m_{s1} = m_{s2}$, we find:

$$\psi(x_1, \mathbf{S}_1; x_2, \mathbf{S}_2) = 0 \tag{9.15}$$

Thus, it is impossible for the two electrons to be in the same single-particle state. This leads to the statement of the Pauli exclusion principle for states in which the electron wave function is approximately an antisymmetric linear combination of products of single-particle wavefunctions. No two electrons in an atom can exist in the same quantum state. In other words, if the wavefunction is to be non-vanishing, the two electrons must be in different quantum states. This means that in an atom at least one of the quantum numbers n, ℓ, m, m_s for the two electrons must be different.

9.5 EXCLUSION PRINCIPLE AND ATOMIC ELECTRON STATES

The above discussion of the exclusion principle applies to any two electrons in a system no matter how many there are, except that when there are more than two electrons, the overall wavefunction depends on more variables. In an atom, where the four quantum numbers, n, ℓ, m, m_s are used to describe the electron states, then every single-particle wave function will have a set $n \ell m m_s$ which is different from that of every other single-particle wave function. Since there is a tendency for isolated systems in nature to seek the lowest possible energy state, we would expect that the electrons in an atom would arrange themselves so that the overall atomic energy will be a minimum. Thus, in a hydrogen atom, for example, the single electron would ordinarily be found in a state of n = 1. This is the case unless the atom is put in contact with matter, such as in a gas discharge, where the electron can be excited to higher states. We shall discuss here only atoms as normally found in nature-in their ground state, or state of lowest energy.

For hydrogen, since the ground state (also called ***normal*** state) is a state of $n = 1$, the orbital angular momentum quantum number ℓ and the magnetic quantum number m must both equal zero. However, to a very good approximation, the energy does not depend on the spin, which means that the energy does not depend on the quantum number m,. The quantum number m_s has the possible values $\pm \frac{1}{2}$; so in hydrogen there are actually two possible states of lowest energy, labeled by $n = 1$, $\ell = 0$, $m = 0$, $m_s = +\frac{1}{2}$ and $n = 1$, $\ell = 0$, $m = 0$, $m_s = -\frac{1}{2}$. We shall represent states of $m_s = +\frac{1}{2}$ by an arrow pointing up: ↑, and $m_s = -\frac{1}{2}$ by an arrow pointing down: ↓. The ground state of hydrogen could be represented in an energy level diagram, Figure 9.1, in two ways corresponding to the two spin orientations. In these diagrams, the presence of the arrow indicates which level the electron occupies.

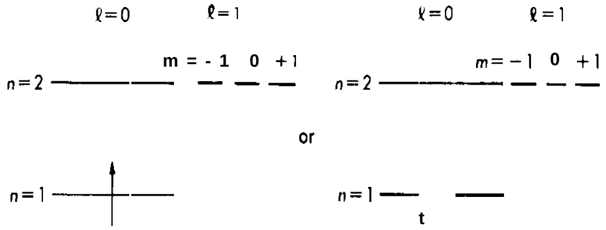


Figure 9.1. **Diagram** indicating the lower levels of the electron in a hydrogen atom. Presence of an arrow up or an arrow down, represents an electron occupying that state with $m_s = +\frac{1}{2}$ or $m_s = -\frac{1}{2}$, respectively.

Now consider helium, which has two electrons. If we assume that the hydrogen quantum numbers can be used approximately, the state of lowest energy would be that state for which both electrons had $n = 1$. Then $\ell = 0$, $m = 0$; and to satisfy the exclusion principle, if one electron has $m_s = +\frac{1}{2}$ (spin up), the other electron must have $m_s = -\frac{1}{2}$ (spin down). This state is illustrated in the energy level diagram of Figure 9.2. Having two electrons in the n = 1 state, with spin

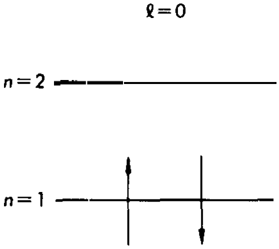


Figure 9.2. Illustration at helium ground state.

up and spin down, completely exhausts all the possibilities for different sets of quantum numbers with n = 1. We then say that the n = 1 shell is filled, or closed.

In lithium, which has three electrons, the lowest energy state is one in which the n = 1 shell is filled and the third electron goes into a state of next lowest energy, which is an n = 2 state. Since helium has two electrons in a closed $n = 1$ shell, and lithium has one more electron outside a closed shell, we would expect the chemical properties of lithium to be quite different from those of helium. Because the n = 2 electron is less tightly bound than n = 1 electrons, it takes less energy to remove the $n = 2$ electron than the n = 1 electron. So it should be relatively easy to add enough energy to the Li atom to remove the electron in the n = 2 state. The remaining atom would then be an ion with a net positive charge. In chemistry, it is known that Li forms positive ions and tends to give up one electron in chemical reactions; it has a valence of + 1. After one electron is removed from Li, the ground state of the remaining ion has two electrons in the n = 1 state. This is similar to helium. Since the n = 1 electrons are very tightly bound, it should be much more difficult to remove an electron in He, and in fact helium is one of the gases which are known as inert gases. Likewise, it is difficult to remove another electron from the Li ion. The possible energy level diagrams for lithium, which has three electrons, are shown in Figure 9.3, with the third

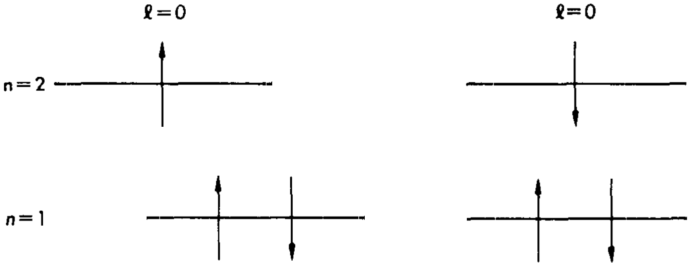


Figure 9.3. Lithium ground state.

electron in a 2s state. It does not matter whether the third electron is drawn ↑ or ↓ since here we are neglecting magnetic interactions. In such an approximation, 2s states with spin up or spin down are degenerate.

In the next most complicated atom, beryllium, there are four electrons. The 2p levels lie slightly above the 2s levels, so the ground state has two electrons in 1s states, two in 2s states, and none in 2p states. The energy level diagram for beryllium in the ground state is shown in Figure 9.4.

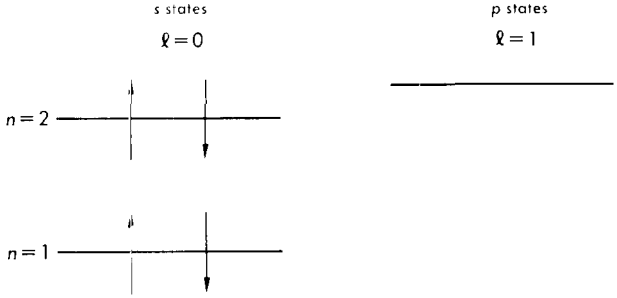


Figure 9.4. Beryllium ground state.

9.6 ELECTRON CONFIGURATIONS

The electronic configuration of atoms in their ground state is sometimes indicated symbolically as follows: hydrogen: $1s$; helium: $1s^2$; lithium: $1s^2 2s$; beryllium: $1s^2 2s^2$. Thus a sequence of symbols of the form $n\ell^N$ is written, where the first symbol n is an integer denoting the value of the principal quantum number, the second symbol ℓ is a letter representing the value of orbital angular momentum quantum number ℓ, ard the third symbol is a superscript equal to the number of electrons in the $n\ell$ state. Thus, in beryllium, $1s^2$ means that in the $1s$ state there are two electrons. The symbol $2s^2$ means that there are two electrons in the n = 2, $\ell = 0$ state.

The next element is boron, with five electrons. In the ground state of this atom, there will be two electrons in the $1s$ states, two in the 2s states, and one left over which has to go into the next higher energy state, which is a $2p$ state. Thus, the ground state of the entire atom would be represented by $1s^2 2s^2 2p^1$. The state $2p$ is a state of orbital angular momentum quantum number $\ell = 1$, so the magnetic quantum number m can have the three values ± 1 or 0. For each of these values of m, there are two different possible m_s values. So the total number of different $2p$ states is six. An atom in which the $2p$ state is completely filled would be represented by the symbols: $1s^2 2s^2 2p^6$. This would be an atom having a total of ten electrons. For an atom with 10 electrons, the n = 2 shell is completely closed, and closed shells tend to be exceptionally stable configurations in nature. Just as the atom with n = 1 shell closed (helium) is an inert gas, so the atom with the n = 2 shell closed (neon) is chemically inert.

The atom with nine electrons, flourine, has the configuration $1s^2 2s^2 2p^5$, with only five electrons in the $2p$ subshell. If one electron were added to a flourine atom, the result would be an ion with a negative charge, and the extra electron could go into the $2p$ state to form a closed shell. So flourine in chemical reactions should accept one electron and have a valence of -1.

The atom with 11 electrons, sodium, is chemically very similar to lithium; it has a valence of $+1$ and gives up one electron in chemical reactions. According to the exclusion principle, the first 10 of these 11 electrons go into the lowest energy states with two in the $1s$, two in the 2s and six in the $2p$ level. The eleventh electron goes into the 3s level; so the electronic configuration of sodium could be written as $1s^2 2s^2 2p^6 3s^1$. In the energy level diagram of Figure 9.5 the sodium

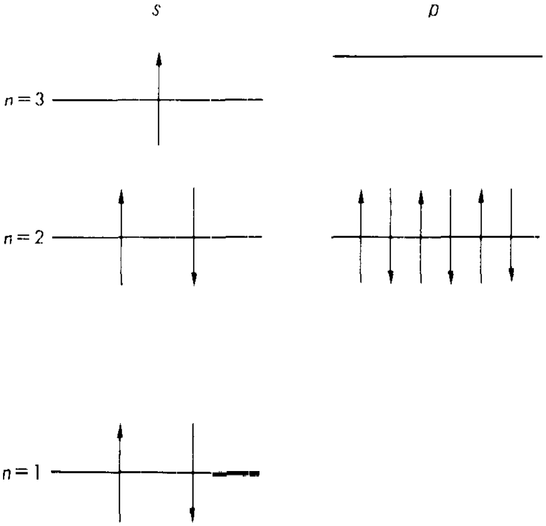


Figure 9.5. Sodium atom in its lowest state.

atom in its lowest state is represented. Sodium has one extra electron outside a closed n = 3 shell. Since closed shells tend to form exceptionally stable configurations, one would expect sodium to form positive ions.

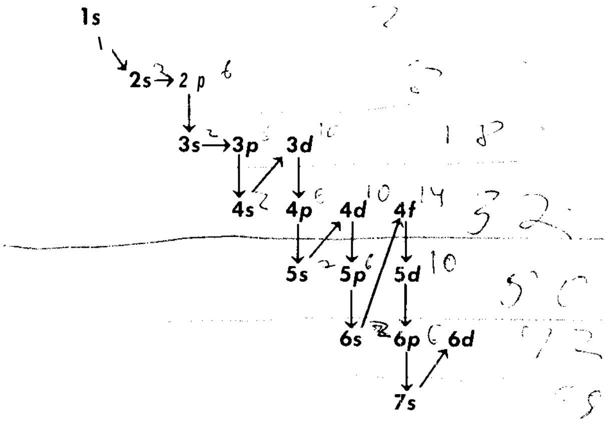
.7 INERT GASES

The next level after the 3s level which fills up with electrons as we go higher in the periodic table is the $3p$ level. It takes six electrons to fill the $3p$ level by itself, and two electrons to fill the 3s level. So for an atom with the configuration $1s^2 2s^2 2p^6 3s^2 3p^6$, there are eighteen electrons. The element argon has 18 electrons, and is an inert gas. So in this case, an inert gas is formed when the $3p$ subshell is filled, before any of the ten 3d states is filled. It is found experimentally that every tirne a p level is completely filled up, an inert gas is formed. The reason this occurs is that the nd levels lie so much higher in energy in many-electron atoms. In general, because of the (complicated electron-electron repulsive forces, the positions of the energy levels are very difficult to calculate, but their sequence can be determined from experiment. Using the fact that higher closed p levels give rise to inert gases, and the experimental fact that the general order in which the electron subshells are filled up is given in Table ‘9.2, we can predict the numbers of electrons in the inert **gases:**

Helium	**2 electrons**	$(1s^2)$
Neon	**10 electrons**	$(1s^2 2s^2 2p^6)$
Argon	**18 electrons**	$(1s^2 2s^2 2p^6 3s^2 3p^6)$
Krypton	**36 electrons**	$(1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6)$
Xenon	**54 electrons**	$(1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6)$
Radon	**86 electrons**	$(1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6$ $6s^2 4f^{14} 5d^{10} 6p^6)$

In a closed 1*s* shell, there are two electrons whose spins point in opposite directions. The total angular momentum (**L** + S) of this closed shell is equal to zero. Also, the contribution to the total magnetic moment of the electrons in a closed 1*s* shell will be zero. Similarly, in any closed subshell of the type we have been considering, the total number of electrons is even and there are just as many electrons with spin up as with spin down; so the contribution to total intrinsic magnetic moment from electrons in any closed subshell should be zero. Also, since all positive and negative m states are filled for each ℓ occurring, the orbital magnetic moments cancel. So the electronic magnetic moments of all the intert gases should be zero.

TABLE 9.2



This diagram provides an easy way of remembering the order in which the levels fill. The resulting order is:

1*s*, 2*s*, 2*p*, 3*s*, 3*p*, 4*s*, 3*d*, 4*p*, 5*s*, 4*d*, 5*p*, 6*s*, 4*f*, 5*d*, 6*p*, 7*s*, 6d

.8 HALOGENS

Let us next consider the group of elements which need one more electron in order to fill up a *p* subshell; these have one fewer electron than the inert gases. Since the inert gases have 10, 18, 36, 54 and 86 electrons, the elements with one fewer electron are those with 9, 17, 35, 53 and 85 electrons. These elements are called ***halogens.*** They are fluorine, chlorine, bromine, iodine and astatine. Hydrogen, which has one less electron than helium, is also sometimes classed as a halogen. Since the halogens, in order to complete their subshells, need one electron, they tend to form ions of negative charge and have a valence of − 1 in chemical reactions.

.9 ALKALI METALS

Consider those elements which have one extra electron, outside a closed *p* subshell. These elements are called ***alkali metals.*** Hydrogen, which just has one electron, is also usually classed as an alkali. Apart from hydrogen, the alkalis have the following numbers of electrons: 3, 11, 19, 37, 55, 87. The corresponding names of the alkali metals are: lithium, sodium, potassium, rubidium, cesium and francium. These elements tend to have valence + 1 since the extra electron outside the closed subshell has a relatively low binding energy and is easily removed. Also, the electrons in lower subshells tend to screen out the nuclear charge, so that the spectra of the alkali metals are very similar to that of hydrogen. Figures 9.6 and 9.7 are the energy level diagrams for outermost electrons of lithium and sodium, which illustrate their similarity to that of hydrogen.

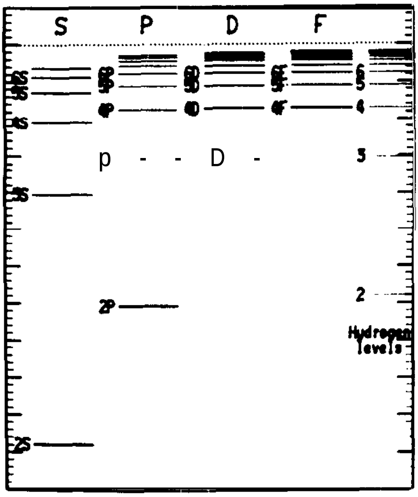


Figure 9.6. Energy levels of lithium

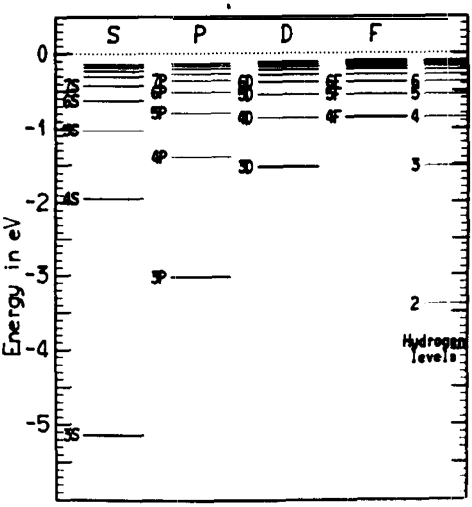


Figure 9.7. Energy levels of sodium.

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9.10 PERIODIC TABLE OF ELEMENTS

In Table 9.3 the periodic table of the elements is shown,. with elements of similar chemical properties arranged in columns. The alkali metals are put in the first column, the inert gases in the last column; number of electrons (atomic number) increases to the right. In the second column are the metals beryllium, magnesium, calcium, strontium, barium and radium. These elements have two electrons outside a closed p subshell. They should usually have a valence of $+2$. The elements oxygen and sulphur occur in the third column from the right and need two electrons to form a closed shell, leading to a valance of -2. It is seen from Table 9.3 that, starting with scandium, which has an atomic number $Z = 21$, the ten 3d states are beginning to fill up, after the 4s states. The corresponding ten elements are called transition elements; their chemical properties are largely determined by their two outer 4s electrons, but the inner incomplete *3d* subshell gives rise to some nonzero magnetic moments of the atoms. Thus, many of the transition elements have interesting magnetic properties. Iron, one of the most magnetizable of all substances, lies near the middle of the transition group at $Z = 26$. In this group, elements 24 (Cr) and 29 (Cu) have only one 4s electron.

In the heavier atoms, particularly in the rare earth group $Z = 57$ to $Z = 70$, the order in which electrons go into the various states is somewhat irregular. The actual order in which the states are filled up is given in detail in Table 9.4; numbers starred there are not known precisely. In these elements the outermost electrons are 6s electrons. The chemical behavior of these elements is largely determined by the outermost electrons, and so all these elements are chemically very similar.

Since it is total angular momentum rather than orbital or spin angular momentum which is conserved in atomic systems, the energy states of the electrons should, strictly speaking, be labeled by values of the total angular momentum quantum number j. Since the spin S can be either parallel to $\mathbf{L}$ or antiparallel to $\mathbf{L}$, for a single electron, either $j = \ell + \frac{1}{2}$ or $j = \ell - \frac{1}{2}$ when ℓ is greater than zero. For alkali metals in the ground state where $\ell = 0$, the total angular momentum quantum number is $j = \ell + \frac{1}{2} = \frac{1}{2}$. For the first excited state of sodium which is a *3P* state, there are two possibilities: $j = \frac{3}{2}$ or $j = \frac{1}{2}$. These states are usually denoted by subscripts: $3P_{3/2}$ and $3P_{1/2}$. These two states are separated slightly in energy due to the spin-orbit interaction which was discussed in the previous chapter. When the spin and orbital angular momenta are parallel as in the $3P_{3/2}$ state, the spin-orbit interaction is positive. In the other case, it is negative; hence the $3P_{3/2}$ state lies slightly above the $3P_{1/2}$ state in energy. The $3P_{3/2} \rightarrow 3S_{1/2}$ and $3P_{1/2} \rightarrow 3S_{1/2}$ transitions thus give rise to two closely spaced yellow lines.

When more than two electrons are present, the rules for adding angular momenta become quite complicated. The possible values of the total angular momentum quantum number may be obtained by considering all the possible ways in which spin $\frac{1}{2}$ and orbital angular momentum ℓ can be added or subtracted from each other to give integral or odd half-integral j. For example, if

TABLE 9.3 Periodic System of the Elements

1 H																															2 He
3 Li	4 Be																									5 B	6 C	7 N	8 0	9 F	10 Ne
11 Na	12 Mg																									13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca															21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr															39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 in	50 Sn	51 Sb	52 ie	53 i	54 Xe
55 Cs	56 Ba	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Em
87 Fr	88 Ra	09 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cl	99 Es	100 Fm	101 Md	102 No	103	104	105	106												

TABLE 9.4 Electron Configurations of the Elements

Element	Subshell													
	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f	5s	5p	5d	5f
1. H	1													
2. He	2													
3. Li	2	1												
4. Be	2	2												
5. B	2	2	1											
6. C	2	2	2											
7. N	2	2	3											
8. O	2	2	4											
9. F	2	2	5											
10. Ne	2	2	6											
11. Na				1										
12. Mg	Neon configrration- 10 electrons			2										
13. Al				2	1									
14. Si				2	2									
15. P				2	3									
16. S				2	4									
17. Cl				2	5									
18. Ar				2	6									
19. K						0	1							
20. Ca	Argon Configrration- 18 electrons					0	2							
21. Sc						1	2							
22. Ti						2	2							
23. V						3	2							
24. Cr						5	1							
25. Mn						5	2							
26. Fe						6	2							
27. Co						7	2							
28. Ni						8	2							
29. Cu						10	1							
30. Zn						10	2							
31. Ga						10	2	1						
32. Ge						10	2	2						
33. As						10	2	3						
34. Se						10	2	4						
35. Br						10	2	5						
36. Kr						10	2	6						
37. Rb									0	0	1			
38. Sr	Krypton Configuration— 36 electrons								0	0	2			
39. Y									1	0	2			
40. Zr									2	0	2			
41. Nb									4	0	1			
42. Mo									5	0	1			
43. Tc									5	0	2			
44. Ru									7	0	1			
45. Rh									8	0	1			
46. Pd									10	0	0			

TABLE 9.4 (Continued)

Element	4s	4p	4d	4f	5s	5p	5d	6s	6p	6d	7s
47. Ag				0	1						
48. Cd	Palladium configuration— 46 electrons			0	2						
49. In				0	2	1					
50. Sn				0	2	2					
51. Sb				0	2	3					
52. Te				0	2	4					
53. I				0	2	5					
54. Xe				0	2	6					
55. cs				0	2	6	0	1			
56. Ba				0	2	6	0	2			
57. La				0	2	6	1	2			
58. Ce				1*	2	6	1'	2*			
59. Pr				2"	2	6	1'	2*			
60. Nd				3*	2	6	1'	2*			
61. Pm				4*	2	6	1'	2*			
62. Sm				6	2	6	0	2			
63. Eu				7	2	6	0	2			
64. Gd				7	2	6	1	2			
65. Tb				a*	2	6	1'	2*			
66. Dy				9*	2	6	1'	2*			
67. Ho				10*	2	6	1'	2*			
68. Er				11*	2	6	1'	2*			
69. Tm				13	2	6	0	2			
70. Yb				14	2	6	0	2			
71. Lu							1	2			
72. Hf							2	2			
73. Ta	Shells 1 S to 5P filled—68 electrons						3	2			
74. w							4	2			
75. Re							5	2			
76. Os							6	2			
77. Ir							7	2			
78. Pt							9	1			
79. Au							10	1			
80. Hg							10	2			
al. Tl							10	2	1		
82. Pb							10	2	2		
83. Bi							10	2	3		
84. PO							10	2	4		
85. At							10	2	5		
86. Em							10	2	6		
87. Fr							10	2	6		1
88. Ra							10	2	6		2
89. Ac							10	2	6		2*
90. Th							10	2	6		2*
91. Pa							10	2	6		2*
92. U							10	2	6		2

*(Numbers starred are uncertain.)

for two n = 1 electrons, $\ell_1 = \ell_2 = 0$, the total spin $S = S_1 + S_2$ can be added to give two possible values; these are $j\hbar = (\frac{1}{2} + \frac{1}{2})\hbar = \hbar$ and $j\hbar = (\frac{1}{2} - \frac{1}{2})\hbar = 0$. However, because of the exclusion principle, only one of these values will occur. It is $j = 0$. Thus, the ground state of the helium atom should be a $j = 0$ state.

9.11 X RAYS

When we studied the quantum nature of light in Chapter 5, the continuous x-ray spectrum was discussed. This spectrum is produced by the deceleration of high energy electrons. The frequency distribution depends on the probability distribution of electron decelerations and on the probability distribution of frequencies for a given charged particle deceleration. The maximum x-ray frequency obtained is given by the Duane-Hunt law: $\nu_{max} = E/h$, where E is the electron kinetic energy. In addition to this continuous spectrum, there are often sharp peaks at certain energies. In this section we will discuss the discrete part of the spectrum.

Discreteness of photon energies ordinarily means that a particle makes a transition from one discrete energy level to another, giving off a photon.

The obvious levels to consider here are the lower levels of the bound electrons in the atoms. These are shown in the energy level diagram of Figure 9.8. The upper levels do not differ by enough energy to give the ‘observed x-ray energies. Ordinarily, photons corresponding to electrons going from one electron shell to another are not observed in many-electron atoms because the lower shells are already filled; and because of the exclusion principle, other electrons cannot go into them. However, if high-energy electrons are shot into a metal, such transitions do occur because the electrons knock other electrons out of the inner shells so that outer shell electrons can make transitions to the unoccupied holes. The innermost shell with $n = 1$ is called the K shell; the next with $n = 2$ is called the L shell; then the M, N, 0,. . . shells follow. There are two electrons in a closed K shell corresponding to $n = 1$, $\ell = 0$, and eight in a closed L shell with $n = 2$,

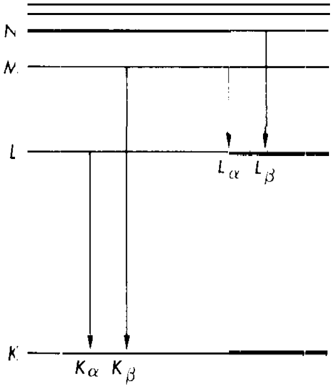


Figure 9.8. Series of x-ray lines result from transitions to unoccupied states in the inner shells.

ℓ = 0, or 1. If a K electron is knocked out by the electron beam, electrons in shells L, M, N, . . . can make transitions to the hole left behind. Likewise, M, N, O, . . . shells have electrons which could make transitions downward to a hole in the L shell. Thus, a series of x-ray lines is observed when a K electron is knocked out. These are called K_α, K_β, K_γ . . . , corresponding to transitions from the L, M, N, shells down to the K shell. Similarly, an L electron knocked out gives L_α, L_β, . . . lines, etc. The energies of the x rays can be estimated by (assuming that the electrons in the various shells have energies given by an equation similar to that for hydrogen, Equation (8.47). However, if Ze is the charge of the nucleus, the effective nuclear charge acting on an electron is less than Ze because of screening due to the presence of negative charge in the same and inner shells. The precise amount of screening is difficult to estimate; practically all of the electrons in shells inside a given shell are effective in screening out a portion of the nuclear charge. Also, some portion of the electrons in a given shell are effective in screening out the nuclear charge for other electrons in the same shell. The following simple model works well for the calculation of K_α series wavelengths: For an L electron with one electron knocked out of the K shell, the remaining electron in the K shell screens out one of the protons. Hence, an estimate of its energy would be:

$$E_L = -\frac{(Z-1)^2 me^4/2}{(4\pi\epsilon_0\hbar)^2} \times \frac{1}{2^2} \tag{9.16}$$

The energy, after falling to the K shell, is very roughly:

$$E_K = -\frac{(Z-1)^2 me^4/2}{(4\pi\epsilon_0\hbar)^2} \times \frac{1}{1^2} \tag{9.17}$$

These estimates of inner shell electron energies are fairly good for large Z, because the nuclear potential is large compared to that of electrons in the inner shells. The energy of the K_α x-ray line is then approximately:

$$E = E_L - E_K = \frac{(Z-1)^2 me^4/2}{(4\pi\epsilon_0\hbar)^2}\left(\frac{1}{1^2} - \frac{1}{2^2}\right) \tag{9.18}$$

The Lyman alpha line in the hydrogen spectrum, which arises from a similar transition, has a wavelength of λ_α = 1216 angstroms. The wavelength of the K_α line in terms of Z and λ_α should then be:

$$\lambda_{K_\alpha} = \frac{\lambda_\alpha}{(Z-1)^2} \tag{9.19}$$

For example, for Molybdenum, Z = 42. The K_α wavelength of Molybdenum should then be approximately 0.72 angstroms. The observed wavelength is 0.71 angstroms.

In 1913 Moseley was the first to recognize from experimental data that x-ray lines depended on Z in a simple fashion. He found that the expression $\lambda = \lambda_0/(Z-\gamma)^2$ agreed with experiment very well, where λ_0 and γ are constants depending on what line is observed. This is called Moseley's law. Moseley found experimentally that λ_0 = 1276 angstroms, and γ = 1.13 for K_α lines.

It is found experimentally that the K_α line actually consists of two closely spaced lines rather than one, due to energy splitting in the *L* shell. There are several causes of energy splitting in the *L* shell. One is due to the fact that the S electrons in the *L* shell have larger wave functions near the nucleus, as compared to the wave function for the *P* electrons. Thus, due to Coulomb forces, the S electrons will be more tightly bound. This gives an energy splitting between S and *P* subshells. Also, the six P electrons in the *L* shell are split into two levels. This is due to relativistic effects and spin-orbit splitting. The spin can be up or down, giving $j = \frac{1}{2}$ and $j = \frac{3}{2}$ states with different energies due to these effects. Only two closely spaced lines are seen rather than three, because the selection rule $\Delta \ell = \pm 1$ prevents transitions from the S states in the *L* shell to the *K* shell, which has only S states.

The three *L* shell levels can be seen in experiments when x rays are absorbed in materials. A continuous K-ray spectrum, when absorbed, has sudden jumps in absorption at frequencies where the energy is just sufficient to knock an electron in a particular shell state, out of the atom. Three such absorption edges are seen for the *L* shell. One would be seen for the K shell and five for the M shell. This behavior is seen in Figure 9.9 in lead.

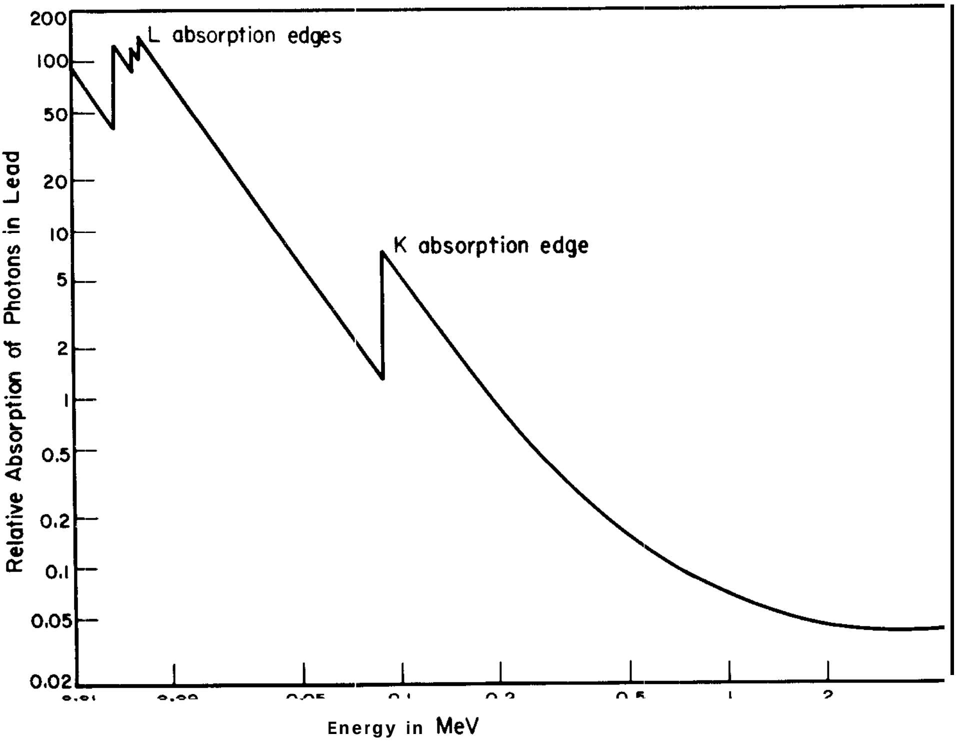


Figure 9.9. Mass absorption coefficient for lead showing K, *L* and M absorption edges.

.12 ORTHO- AND PARAHYDROGEN

The nuclei of hydrogen are protons which, like electrons, also are found to have spin ½ , and are indistinguishable particles. Hence, when a hydrogen molecule is formed, we have the intrinsic spin angular momentum of the nuclei, which must be added to the angular momenta of the rest of the system to give the total If we assume the two electrons go into their ground state in the molecule, with opposite spin and zero orbital angular momentum, then the total angular momentum of the molecule is due to the protons. Consider the angular momenta of the nuclear spins by themselves. The total angular momentum j_n of the two nuclear spins can be either $j_n = \frac{1}{2} + \frac{1}{2} = 1$ or $j_n = \frac{1}{2} - \frac{1}{2} = 0$. The $j_n = 1$ case occurs if the spins are parallel, and $j_n = 0$ occurs if the spins are antiparallel. If $j_n = 1$, the nuclear magnetic quantum number m_{j_n} can have the three values $\pm 1, 0$. There is only one $j_n = 0$ state. The total number of different spin states is four. Ordinarily, the hydrogen molecule is formed in a chemical reaction in which nuclear spins do not play any significant role. Hence, these four states all occur with equal probability. Then the states $j_n = 1$ should occur three times as often as the $j_n = 0$ states in nature The $j_n = 1$ state is called ***orthohydrogen,*** and the $j_n = 0$ state is called ***parahydrogen.*** It is found that orthohydrogen is three times as plentiful in nature as parahydrogen, as predicted. In the case of the $j_n = 1$ states, the spins are parallel, and the spin part of the wavefunction is symmetric under proton exchange. Thus the space part of the wavefunction must be antisymmetric. Likewise for parahydrogen, the spin is antisymmetric and the space part symmetric. This leads to the fact that the rotational quantum numbers, due to end-over-end tumbling of the molecule, must be even for parahydrogen and odd for orthohydrogen. Because of the different possible rotational states, quite different specific heats are observed at low temperature for the two kinds of hydrogen molecule. Since the lowest orbital angular momentum quantum number for orthohydrogen is 1, while it is 0 for parahydrogen, parahydrogen has a lower possible kinetic energy of rotation, and thus a lower energy ground state. When hydrogen molecules are formed on a platinum catalyst at very low temperatures, they form at the lowest energy, and almost pure parahydrogen results.

summary

EXCHANGE OF IDENTICAL PARTICLES

When two identical particles are exchanged, no measurement can tell the difference. Thus, the magnitude of the wavefunction must be unchanged and the wavefunction can at most be multiplied by a phase factor, $e^{i\Phi}$. Another exchange of the same two particles returns to the original state, so $e^{2i\Phi} = 1$ or $e^{i\Phi} = \pm 1$. For $e^{i\Phi} = -1$, we say that the wavefunction is antisymmetric under exchange of two particles; experimentally, this is found to be true for half-integral spin particles, fermions. For integral spin particles, bosons, the wave function is symmetric under exchange with $e^{i\Phi} = +1$.

PAULI EXCLUSION PRINCIPLE

If the Schrödinger equation is satisfied by a product of single-particle wavefunctions, an antisymmetric wavefunction under exchange can be generated by starting with such a product. If particles are exchanged in this product wavefunction two at a time, and the function is multiplied by minus one at each exchange, eventually all possible permutations of particles among the single particle products are obtained with a + or − sign in front of the function. The antisymmetric function is the sum of these. This sum is zero if any two of the single particle functions are the same. This results in the Pauli exclusion principle: No two identical fermions can exist in the same single-particle state.

ATOMIC ELECTRON CONFIGURATIONS

The hydrogen quantum numbers n, ℓ, m and m_s can approximately be used to describe electronic states in atoms. In the absence of magnetic fields, these states are closely degenerate in m and m_s. For a given ℓ, there are $2\ell + 1$ values of m, and m_s has two possible values. There are n values of ℓ for a given n. This leads to $2n^2$ states for a given n. The electronic energies for atoms other than hydrogen depend appreciably on n and ℓ. Thus energy shells are specified by $n\ell^N$, where N gives the number of electrons in a shell. By the Pauli exclusion principle, the maximum number of electrons in a shell is equal to the number of states in the shell. The electrons go to the lowest energy configuration, so that in the ground state, the lower energy inner shells become filled, generally leaving only the last few electrons in unfilled shells. When the number of electrons completely fills the P states in the lowest energy shells,. an inert gas results. These gases are very inactive chemically. If there are one or two electrons outside a closed shell, such as in sodium or calcium, these electrons are easily lost, and the atom has a valence of 1 or 2. If a shell is filled except for 1 or 2 electrons, such as in fluorine or oxygen, the atom acquires these electrons readily and has a valence of 1 or -2.

X RAYS

In addition to the continuous spectrum of x rays due to accelerated electrons, there are ordinarily sharp x-ray lines. Such a line results when an electron is knocked out of a low-lying shell in the atom and another electron falls into the resulting empty state, erritting a photon in the process. The inner shells are denoted by K, l, M, . , corresponding to n = 1, 2, 3,. . . . X-ray spectra are labeled by the shell into which the electron falls. The x-ray energy may be estimated by using the fact that the shell energies are approximately hydrogen-like:

$$E_n = -\frac{1}{2}\frac{(Z-p)^2 me^4}{(4\pi\epsilon_0\hbar)^2 n^2}$$

with Z the number of proton in the nucleus and p the total number of electrons in shells of smaller n. Differences in these energies give approximately the observed x-ray energies.

ORTHO- AND PARAHYDROGEN

An example where the exclusion principle affects a molecule occurs in the hydrogen molecule H_2, where the two protons are fermions. If the spins are parallel, $s = 1$ and $m_s = -1, 0, +1$ with the spin function symmetric, and thus the rest of the wave function is antisymmetric, under exchange. For $s = 0$, $m_s = 0$, and the opposite symmetries hold. Because rotational states have definite symmetries, this leads to different possible rotational states for the two kinds of hydrogen, and thus to different energies and specific heats.

problems

1. Suppose that three noninteracting identical electrons of spin ½ and ***mass m*** were sliding on a circular wire of radius a. What is the lowest possible energy consistent with the Pauli exclusion principle?

   Answer: $4\hbar^2/ma^2$

2. The particle-in-a-box wavefunctions for a single particle are: $\psi_n = \sqrt{2/L}\sin(n\pi x/L)$. If two noninteracting spinless bosons (integral spin) were placed in the box, in states n_1 and n_2, what would the overall symmetric wavefunction be? If a third particle were placed in the box in state n_3, what would the wavefunction be?

   Answer: $$\psi = \frac{1}{\sqrt{2}}[\psi_{n1}(x_1)\psi_{n2}(x_2) + \psi_{n1}(x_2)\psi_{n2}(x_1)];$$
   $$\psi = \frac{1}{\sqrt{6}}[\psi_{n1}(x_1)\psi_{n2}(x_2)\psi_{n3}(x_3) + \psi_{n1}(x_2)\psi_{n2}(x_1)\psi_{n3}(x_3) + \psi_{n1}(x_3)\psi_{n2}(x_2)\psi_{n3}(x_1) + \text{three more terms}]$$

3. Using the two-particle wavefunction of the previous problem, show that the wavefunction does not vanish if the particles are in the same state, so that both particles can have the same quantum numbers. If $n_1 = 1$, $n_2 = 3$, calculate the expectation value of the energy of the system.

   Answer: $E = E_1 + E_3$.

4. The four possible combinations of spin wave functions for two electrons are: $\uparrow_1\uparrow_2$, $\uparrow_1\downarrow_2$, $\uparrow_2\downarrow_1$, $\downarrow_1\downarrow_2$, where the arrows indicate m_s and the subscript indicates the particle. Show that the symmetric and antisymmetric functions under exchange are:

   $$\uparrow_1\uparrow_2, \frac{1}{\sqrt{2}}(\uparrow_1\downarrow_2 + \uparrow_2\downarrow_1), \downarrow_1\downarrow_2; \frac{1}{\sqrt{2}}(\uparrow_1\downarrow_2 - \uparrow_2\downarrow_1)$$

What are the total z components of angular momentum for these symmetrized and antisymmetrized spin functions?

5. For two electrons or protons, the square of the total spin angular momentum is: $S^2 = (\mathbf{S}_1 + \mathbf{S}_2)^2 = S_1^2 + S_2^2 + 2\mathbf{S}_1 \cdot \mathbf{S}_2$, where $\mathbf{S}_1 \cdot \mathbf{S}_2 = S_{1x}S_{2x} + S_{1y}S_{2y} + S_{1z}S_{2z}$. Now $S_1^2 \uparrow_1 = (\frac{1}{2})(\frac{1}{2} + 1)\hbar^2 \uparrow_1$, $S_{1z} \uparrow_1 = \frac{1}{2}\hbar \uparrow_1$, where $\uparrow_1$ is defined in the previous problem. Likewise, it can be shown that it is possible to choose S_{1x} and S_{1y} so that $S_{1x} \uparrow_1 = \frac{1}{2}\hbar \downarrow_1$, $S_{1x} \downarrow_1 = \frac{1}{2}\hbar \uparrow_1$, $S_{1y} \uparrow_1 = i\frac{1}{2}\hbar \downarrow_1$, $S_{1y} \downarrow_1 = -i\frac{1}{2}\hbar \uparrow_1$, where $i^2 = -1$. Similar equations hold for $\mathbf{S}_2$. Show that the symmetric states of the previous problem correspond to $s = 1$ or $S^2 = (1)(1 + 1)\hbar^2$, and the antisymmetric state corresponds to $s = 0$. This fact was used in discussing ortho- and para-hydrogen.

6. Imagine two electrons attached to the ends of a rigid rod, the system having a moment of inertia I about the center of mass. The kinetic energies of this system as it spins end-over-end are $\hbar^2 J(J + 1)/2I$, where J is the rotational angular momentum quantum number, Spatial exchange of the two electrons is equivalent to inversion of the system through the center of mass. Using the fact that the spatial wavefunctions ψ_J are changed by a factor $(-1)^J$ upon inversion, show that if the spins are parallel J must be odd.

7. Using the electronic configuration of aluminum ($Z = 13$), how would you explain the formation of the aluminum oxide molecule, Al_2O_3?

8. Discuss why the valence of carbon can be either $+4$ or -4.

9. Suppose the electron were spinless. What would the ground state configuration of "carbon" be? What would the C spectrum be like? Why?

Answer: $1S^6$, hydrogen-like.

10. If a series of spectral lines corresponds to a set of allowed transitions with the same final state, but with initial states all of the same ℓ and differing n, which spectral series of the Li and Na spectra have the same short-wavelength series limit?

11. If by some process, one 1S electron is knocked out of the sodium atom, discuss, using the Pauli exclusion principle, the various transitions which could occur afterwards.

12. Show that the total angular momentum of a closed p subshell is zero.

13. A certain atom of valence $+3$ in the ground state has its outer electron in the $4p$ state. Name the element.

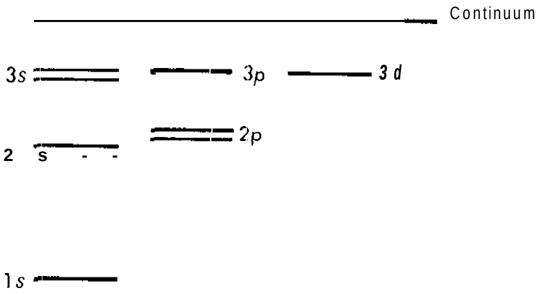
Answer: Gallium.

14. Write down the quantum numbers for each of the three outermost electrons of aluminum in its ground state, which is a state of $s = \frac{1}{2}$ ($Z = 13$) What quantum numbers n, ℓ and m_s would you expect for the lowest-lying excited-state of aluminum, neglecting magnetic interactions?

Answer: (1) $n = 3$, $\ell = 0$, $m_s = +\frac{1}{2}$;
(2) $n = 3$, $\ell = 0$, $m_s = -\frac{1}{2}$;
(3) $n = 3$, $\ell = 1$, $m_s = \pm\frac{1}{2}$.
Excited state, $n = 4$, $\ell = 0$, $j = \frac{1}{2}$

15. What should be the chemical properties and valences of the transuranic elements, $Z = 91$ to 102?

16. When a helium atom is singly ionized and an electron is subsequently captured, it may have either the same or opposite spin as the electron that stayed on the atom. There is a slightly different electron-electron interaction for the electrons, depending on whether their spins are parallel or antiparallel. This is because of the different symmetries of the spatial parts of the wavefunctions resulting from the exclusion principle. Assuming that when the captured electron goes from one state to another



there is negligible probability that its spin flips, what differences in the spectra of helium atoms with different captured electron spins would you expect?

17. Write the electronic configuration for rubidium (Z = 37) in terms of an energy level diagram with arrows.

18. Carbon has six electrons. Show that the electronic configuration of its ground state is $1s^2 2s^2 2p^2$.

19. What are the possible total angular momentum quantum numbers j of the $3p$ states of sodium?

Answer: $\frac{3}{2}, \frac{1}{2}$.

20. From the result of Problem 18, show that the possible values of the total spin s of the ground state of carbon are 0, 1 and the possible values of total orbital quantum number ℓ are 2, 1, 0. Thus, show that if the exclusion principle is ignored for these angular momenta, the total angular momentum quantum number j can be given the value 3 in one way, 2 in three ways, 1 in four ways, and 0 in two ways.

21. For two electrons, the $s = 1$ states are symmetric under particle exchange, and the $s = 0$ state is antisymmetric. Also, if they are both in p states, the $\ell = 2, 0$ stotes are symmetric and the $\ell = 1$ states are antisymmetric. Use these facts to show that some of the ways of getting j's for carbon in the previous problem are not possible because of the exclusion principle. In particular, show that the only possible states ore $s = 1$; $\ell = 1$, $j = 0, 1, 2$ or $s = 0$; $\ell = 2, 0$; $j = 2, 0$. The actual ground state of carbon is $s = 1$, $\ell = 1$, $j = 0$.

22. In nitrogen, with three outer electrons in p states, it is found experimentally that the ground state corresponds to a total spin quantum number of $s = \frac{3}{2}$, and total angular momentum quantum number of $j = \frac{3}{2}$. With three p electrons, the total angular momentum quantum number could be $\ell = 3, 2, 1$ or 0. Show, using the exclusion principle, that $\ell = 0$ is the only possibility here. (Saying that $j - s = 0$ is not sufficient.)

23. If $\psi_{1,m,m_s}(i)$ represents the single-particle function for the i^{th} particle with $\ell = 1$, $m = -1, 0$ or 1, and $m_s = \pm\frac{1}{2}$, multiply three such functions together to form an approximate solution of the Schrödinger equation for the three outer electrons of nitrogen in the previous problem. Add and subtract similar functions with i's interchanged to form the antisymmetric function.

Answer: $$\frac{1}{\sqrt{6}}[\psi_{1,1,1/2}(1)\,\psi_{1,0,1/2}(2)\,\psi_{1,-1,1/2}(3)$$
$$-\psi_{1,1,1/2}(2)\,\psi_{1,0,1/2}(1)\,\psi_{1,-1,1/2}(3)\,\psi_{1,0,1/2}(2)\,\psi_{1,-1,1/2}(1)$$
$+$ three other terms].

24. From the results of Problems 4, 5 and 6, show that the energy difference between the lowest two rotational states of parahydrogen is $^3/_5$ the energy difference for the two lowest rotational states of orthohydrogen. Which has the greatest specific heat at low temperatures?

25. From the information given in Problems 6 and 24 and in this chapter, what is the fraction of parahydrogen at equilibrium when the temperature is very low, and when it is very high?

Answer: 1, ¼

26. Show that the wavelength of the K_α line from a heavy element of atomic number Z is approximately $1.220 \times 10^{-7}/Z^2$ meters.

27. Find the energy in eV of a K_β x-ray photon given off by a lead atom.

Answer: **79,600** eV.

28. Show that the fractional change in mass of an atom emitting a K_α line is approximately $1.09 \times 10^{-8}Z^2/A$, where A is the atomic weight. Evaluate this for iron and uranium.

29. Find the minimum energy of electrons in a beam hitting tungsten to give (a) the K_β line; (b) the L_α line.

Answer: 72,500 eV; 18,100 eV.

30. How many closely spaced lines should be observed in the K_β x-ray emission line?

Answer: 2.

31. Estimate the wavelength of the K_β x-ray line for Molybdenum with $Z = 42$. The observed value is 0.63 angstroms.

Answer: 0.61 Angstroms.

32. An x-roy tube with a silver target must have 25.8×10^3 volts applied to it before the K_α x-ray lines of silver are observed. Calculate the approximate energy in eV of the *K* absorption edge of silver, and explain qualitatively why it is different from the energy of the K_α line as calculated from Moseley's law.

33. The bright yellow color in sodium is due to transitions of the outermost electron from $3P_{3/2}$ and $3P_{1/2}$ states down to the $2S_{1/2}$ state. There, lines exhibit an anomalous Zeeman effect, because the energy splittings of the $3P_{3/2}$, $3P_{1/2}$ and $3S_{1/2}$ levels ore different in a magnetic field. How many levels does each of the $3P_{3/2}$, $3P_{1/2}$ and $3S_{1/2}$ levels split in a magnetic field? Using the selection rules, how many lines will be seen in place of the $3P_{3/2} \rightarrow 3P_{1/2}$ line? How many lines will be seen in place of the $3P_{1/2} \rightarrow 3S_{1/2}$?

Answer: 4, 2, 2, 6, 4.

0 classical statistical mechanics

Many of the physical systems which we study are large enough to contain enormous numbers of particles. For example, a container of 22.4 liters of helium at 0°C and at atmospheric pressure is known to contain 6.023 x 10^{23} atoms. This gas, in addition to exerting pressure and storing energy, may also conduct heat from one point to another, may resist shearing motions (like molasses), may sustain sound waves, and in general may exhibit a variety of interesting phenomena. Other many-particle systems such as solids, liquids and plasmas may show similar effects.

Quite a bit is known about the microscopic properties of atoms in a gas such as helium. The atomic masses, sizes of atoms, interaction forces and other properties are known to a reasonable accuracy. The object of statistical mechanics is to use information about individual particles in constructing a theory which explains all the observed properties of a large system containing a great number of particles.

According to Newtonian mechanics, to describe the motion of a particle, one must solve the equation $F = ma$, where F is the total force on a particle due to its interactions with all other particles. In a system of 10^{23} particles, there would be 10^{23} such equations, and the solution of such a system of equations would be a practical impossibility. Furthermore, even if the solutions were known, they would not be very useful, since the properties of a system which can be observed macroscopically are usually very few in number-say on the order of 10 or 20. One would then need to know how to reduce the information contained in these 10^{23} solutions to about 20 numbers which could then be compared with experiment.

Statistical mechanics supplies the rules for treating many-particle systems in terms of a very few variables. It (accomplishes this by describing the system not in terms of definite positions and velocities of all the particles, but in terms of probabilities. In this chapter we will assume that the particle motions are governed by Newtonian mechanics. In the following chapter the effects of quantum mechanics will be discussed.

10.1 PROBABILITY DISTRIBUTION IN ENERGY FOR SYSTEMS IN THERMAL EQUILIBRIUM

One of the most important parameters used to describe large systems is temperature. This concept is based on the observed existence of states of a system called thermal equilibrium states. If two systems at different temperatures are placed in contact and left alone, they will eventually come into thermal equilibrium with each other. Their temperatures will then be equal. Two systems each in thermal equilibrium with a third system, will be in thermal equilibrium with each other.

The attainment of thermal equilibrium is accomplished by the exchange of heat energy through the systems contacting walls. Even after thermal equilibrium is established, these systems;, as long as they are in contact, could still continue exchanging energy. Then the amount given up by a system is balanced on the average by an equal amount received. At a particular instant, however, one system might have more energy than at some other instant. Thus, for a system in thermal equilibrium at a definite temperature, the energy does not have a definite value.

If we place a large number of identical systems all in contact and allow them to come into thermal equilibrium with each other (see Figure 10.1), then these systems will have various energies which can be described by a probability distribution or density P(E). It is usually assumed that this is the same as the distribution of energies of one particular system if observed repeatedly at different times. Although the energy is not definite, it is possible to find a simple expression for the probability P(E) that a particular system will be in a state of energy E. To find the mathematical form of this function P(E), we use the assumption that the systems are all in thermal equilibrium, at equal temperatures. Except for their thermal contact with each other, the systems are isolated, so they can not do work on each other, have chemical reactions with each other or interact in any other way. We will assume that the total momentum and angular momentum of each system is zero, and that the volume and number of particles in each system remain fixed. The only independent macroscopic quantity that can

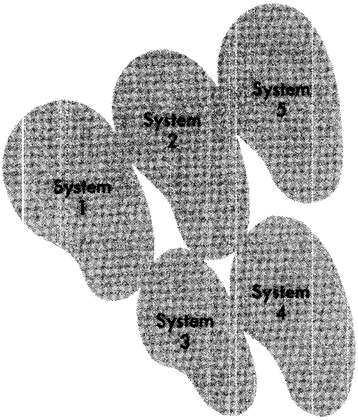


Figure 10.1. Identical systems in thermal contact.

be transferred from system to system is heat energy, and hence the energy may fluctuate in time in a particular system.

Thus we expect the probability that a system is found in a particular possible state, for a given volume and number of particles, will depend on the energy of the state of the system and also on the quantity which the systems have in common, the temperature.

0.2 THE BOLTZMANN DISTRIBUTION

Let us assume that systems 1 and 2 are identical in all respects so we can be sure that the probability functions are identical for the two systems when they have the same temperature T. We then define $P(E_1)$—which also depends on T—to be the probability that system 1 is in a particular state with energy E_1, and similarly, $P(E_2)$ is the probability of occurrence of a particular state with energy E_2 in system 2. In terms of these probabilities, we ask: What is the probability that, at the same time system 1 is in a particular state of energy E_1, system 2 is in a particular state of energy E_2? The net probability must be $P(E_1)\,P(E_2)$, by Equation (2.1).

Now, if we wish, we can think of systems 1 and 2 as a single, combined system. The probability that the combined system is in the given state of energy $E' = E_1 + E_2$ should, by the same reasoning as that used above, be a function only of the energy E' and the temperature T. Thus the probability should be a function of the form $P'(E_1 + E_2)$. Therefore, in terms of $P(E_1)$ and $P(E_2)$, for any E_1 and any E_2,

$$P'(E_1 + E_2) = P(E_1)\,P(E_2) \tag{10.1}$$

Here P' is not necessarily the same function of energy as P, because the combined system is not identical with the individual systems 1 and 2. What this equation tells us is that the function $P(E)$ must be such that the product $P(E_1)\,P(E_2)$ is a function of $E_1 + E_2$.

Equation (10.1) is sufficient to completely determine the dependence of P and P' on the energy variable E. It was obtained by assuming that the occurrence of the possible states of a system in thermal equilibrium with many other systems was described by a probability $f(E)$ depending on the energy E and the temperature. The probability of finding the combined system in a particular state of energy $E_1 + E_2$, with subsystem 1 in its particular state of energy E_1, and subsystem 2 in its particular state of energy E_2, must be equal to the product of the individual probabilities for these states.

The only function which satisfies an equation of the form of Equation (10.1) is an exponential:

$$P(E) = P(0)\,e^{-\beta E} \tag{10.2}$$

where P(0) is the value of $f(E)$ when $E = 0$, and β is a constant. One may verify that $P(E) = P(0)\,e^{-\beta E}$ is a solution to Equation (10.1), provided that:

$$P'(E_1 + E_2) = P(0)^2 e^{-\beta(E_1 + E_2)} \tag{10.3}$$

The quantities P(0) and β are constants independent of E but possibly dependent on the common temperature, volume and number of particles in the system. Since nothing has been said up to this point about the mechanics the particles in the systems satisfy, this result is equally valid for Newtonian and quantum systems.

If we consider an ideal gas in which the individual particles do not interact with each other, but where we allow the particles to interact with the container walls, then we can consider each particle as a system which is, on the average, in thermal equilibrium with the walls. The probability that a particle is in a particular state of energy E is then $P(E) = P(0)e^{-\beta E}$. Thus, the mathematical form of the energy distribution function is determined. However, we do not yet know the constants P(0) and β. These will be found in subsequent sections, by considering the ideal gas, a system which should already be familiar to the reader. In following sections we shall discuss in more detail what is meant by a "particular state" of a particle, and show how $P(E)$ is used.

10.3 PROOF THAT P(E) IS OF EXPONENTIAL FORM

We shall now give a proof that only an exponential function can satisfy Equation (10.1). This equation must be valid for all values of E_1 and E_2. In particular, if $E_1 = 0$ and $E_2 = E$, we obtain for any E:

$$P'(E) = P(E)P(0) \tag{10.4}$$

Substitution of $E = E_1 + E_2$ back into Equation (10.4) allows us to rewrite Equation (10.1) entirely in terms of P, by eliminating P'. The result is:

$$P(E_1 + E_2)P(0) = P(E_1)P(E_2). \tag{10.5}$$

Equation (10.5) is valid for any E_1 and E_2, and may be used to obtain a differential equation for $P(E)$. Put $E_1 = E$ and $E_2 = dE$, where dE is infinitesimally small. Then we get:

$$P(E + dE) = \frac{1}{P(0)}P(E)P(dE) \tag{10.6}$$

Subtracting $P(E)$ from both sides of this equation, and dividing by dE, one finds:

$$\frac{P(E + dE) - P(E)}{dE} = \frac{P(E)}{P(0)}\left[\frac{P(dE) - P(0)}{dE}\right] \tag{10.7}$$

or

$$\frac{dP(E)}{dE} = \frac{P(E)}{P(0)}\frac{dP(E = 0)}{dE} \tag{10.8}$$

Then, dividing both sides of the equation by $P(E)$, we get:

$$\frac{dP(E)/dE}{P(E)} \quad \frac{dP(E = 0)/dE}{pm} \tag{10.9}$$

The lefthand side of this equation is evaluated at any E, the righthand side is evaluated for the value $E = 0$, and is therefore a constant. Calling the constant $-\beta$ for convenience, we have:

$$\frac{dP(E)/dE}{P(E)} = -\beta \tag{10.10}$$

where β is a positive constant independent of E. This equation can be immediately integrated from $E = 0$ to E to obtain:

$$\ln f(E) \quad \ln P(0) = -\beta E \tag{10.11}$$

Here, $\ln P(0)$ is the constant of integration. Solving for $P(E)$, we find:

$$P(E) = P(0)\, e^{-\beta E} \tag{10.12}$$

Thus, the probability $P(E)$ is an exponential function of energy. Had we chosen the opposite sign for the constant β, the probability would not be normalizable.

3.4 PHASE SPACE

The *Boltzmann factor* $e^{-\beta E}$ gives the relative probability of finding a system, which is in thermal equilibrium, in a given state having energy E. The factor β depends in some way on the temperature, which we must determine. We are particularly interested in applying this result to a thermodynamic system containing a great many particles, such as a bottle of gas. The problem is to find some convenient way of specifying the state of such a complicated system.

To illustrate how this may be done, imagine a simple model of a gas in which the gas particles are represented by marbles of mass m which can roll in a long groove. The x axis is along the groove and the marbles all stay in the groove, so only the x_i coordinate, and not y_i or z_i coordinates, must be given in order to specify the i^{th} marble's position. To completely determine the state of one of the marbles using classical mechanics, one must at the same time give the momentum $p_{i_x} = m\dot{x}_i$ of the marble as well as its position, along the groove. Then, at the same time, we can represent the state of the marble by plotting (x_i, p_{i_x}) on a graph as in Figure 10.2. Of course, as time progresses, the point representing the state of the i^{th} particle will move and trace out some trajectory, which may have sharp kinks and bends in it due to collisions, as in Figure 10.3. If we have a large number of marbles in the groove, then we can represent the state of each marble by a different point on the p_x versus x graph, as in Figure 10.4. As time progresses, each point will move in some trajectory on the p, x graph. If we have an extremely large number of marbles, then there will be an extremely dense cloud of points in p_x, x space, as in Figure 10.5. As time progresses, the cloud may shift around, and fluctuate in density. If the position of each point in the cloud is known, then, of course, the state of the (entire system of marbles is known. However, if there are as many as 10^{23} particles in the system, as is common in thermodynamic systems, then there will be so many points that for

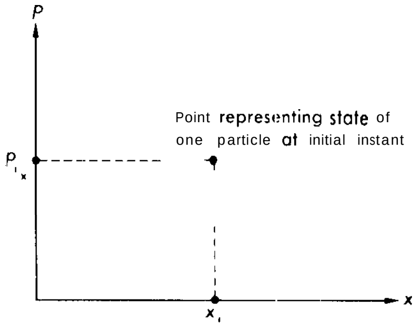


Figure 10.2. Phase space far a particle confined to move in the x direction.

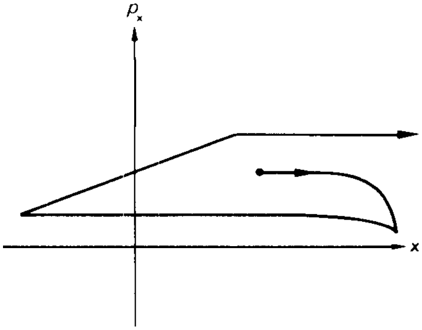


Figure 10.3. Motion of the representative point of one particle in phase space as time passes.

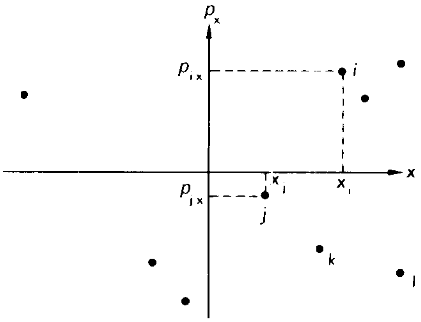


Figure 10.4. The representative points of any number of particles car be plotted in the same phase space.

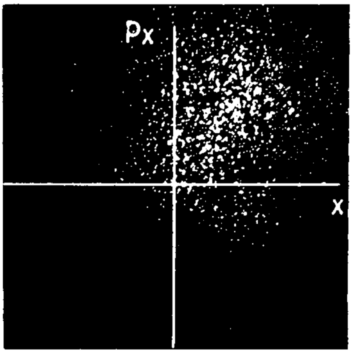


Figure 10.5. A cloud of representative points in phase space, for a system consisting of a large number of particles.

many purposes, only the average density of the cloud would be needed. This method of representing the state of a system turns out to be very useful, and can easily be applied to a more realistic gas of particles which move not only in the x, but in the x, y and z dimensions.

Let us consider a container of volume V, holding a gas of N particles. We shall assume that each particle has a mass m. In order to completely specify the state or condition of this gas, one would have to specify the position r and momentum p of every particle at some initial instant. A very convenient way to represent such information is to introduce a six dimensional space called phase space. This six dimensional space has three axes representing the spatial coordinates $\mathbf{r} = (x, y, z)$ of a particle, and three axes representing the momentum $p = (p_x, p_y, p_z)$ of the particle. The six numbers, (x, y, z, p_x, p_y, p_z) are then the coordinates of a single "point" in phase space, representing the state of one particle. Although it is difficult to visualize a space of six dimensions, one may think of all these coordinate axes as being orthogonal (at right angles) to each other. One may then plot the position r' and momentum p' of a second particle on the same coordinate axes, giving a second point in phase space representing the coordinates (r', p') of the second particle, and so on for all N particles. Then a system of N particles would correspond to a cloud of N points in six dimensional phase space.

In Figure 10.6 are two of the six axes in phase space. Consider the points of phase space which represent two particles with positions and momenta, given by:

$$x_1 = 3,\ y_1 = 4,\ z_1 = 2; \quad p_{x1} = 1,\ p_{y1} = 1,\ p_{z1} = 0;$$

and

$$x_2 = 0,\ y_2 = 1,\ z_2 = 1\ \ 2\ ; \quad \mathbf{p}_2 = 0$$

with lengths in meters, and momenta in kilogram-meters per second. These points are plotted as an example, in the part of phase space shown in Figure 10.6.

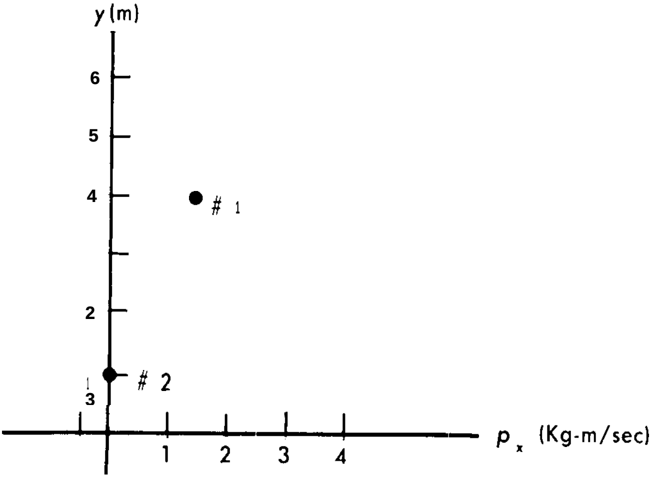


Figure 10.6. Exomple of representative points plotted along two axes in phose space.

If a particle moves with constant velocity v, the point in phase space representing it moves in a straight line, because r varies linearly with time, while p remains constant. For a particle moving in a circle in the xy plane with constant speed, the path of its representative point in the x, p_x plane would be elliptical in shape.

1.5 PHASE SPACE DISTRIBUTION FUNCTIONS

If we plot the N representative points of a macroscopic system of gas particles in phase space, as is illustrated in Figure 10.7, there will be so many of these points that they will be distributed almost continuously throughout phase space. Then we can define a continuous distribution function f (r, p, t) equal to the density of points in phase space. That is, f (r, p, t) is the number of points per unit volume of phase space at the position (r, p) = (x, y, z, p_x, p_y, p_z) at the time t. In a three dimensional space (x, y, z), the infinitesimal volume element is dxdydz. By analogy, in a six dimensional space (x, y, z, p_x, p_y, p_z) with orthog-

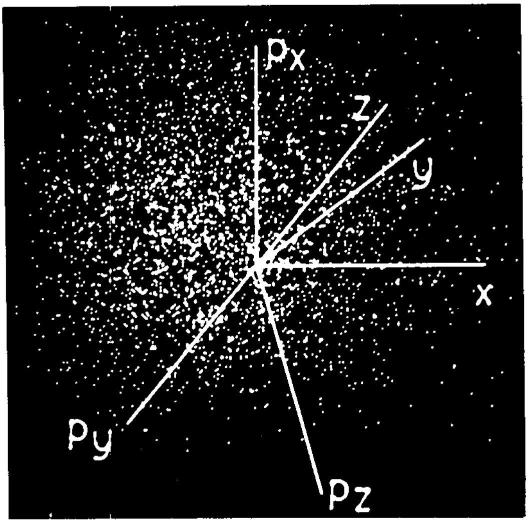


Figure 10.7. A macroscopic system of N particles is represented by a cloud of N points in six dimensional phase space; the axes are assumed to be mutually orthogonal.

onal Cartesian coordinates, the volume element can be assumed to be dxdydzdp, dp, dp,

So if the element of volume is $dxdydzdp_xdp_ydp_z$, and the density of points in phase space is $f(\mathbf{r}, p, t)$, then the number of points, dN, in the volume dxdydz • $dp_xdp_ydp_z$ is just:

$$dN = f(r, p, t)\, dxdydzdp_xdp_ydp_z \qquad (10.13)$$

Thus, f (r, p, t) is a distribution function in phase space, whose normalization is:

$$\int dN + \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dp_x \int_{-\infty}^{\infty} dp_y \int_{-\infty}^{\infty} dp_z f(\mathbf{r}, \mathbf{p}, t) = N \qquad (10.14)$$

-the total number of particles.

In writing such expressions, we regard the six variables x, y, z, p_x, p_y, p_z all as independent variables. This is because of the way the states of the particles are being represented on orthogonal axes in phase space. Although it is true that if x were known as a function of time, p_x could be calculated and so would depend on x, in phase space the positions and momenta are represented at one instant. A particle at x at some instant could have any value of p_x at that same instant; both x and p_x must be given at the same instant in order to specify the particle's state.

The integral $\int dN$ has been broken down in Equation (10.14) into a six-fold multiple integral which looks complicated; however, the idea is to integrate over the variable dN. In all cases which we shall consider,, the multiple integral is just a product of six single, independent integrals, which are performed in the ordinary way.

The quantity I/N f (r, p, t) could be interpreted as a probability distribution function, since its normalization would be unity. Thus, for example, the quantity

$$\frac{1}{N} f[x = 6 \text{ m}, y = 0, z = 0, p_x = 0, p_y = 2 \text{ kg-m/sec},$$

$$p_z = 3 \text{ kg-m/sec}, t = 1 \text{ sec}]\, dxdydzdp_xdp_ydp_z$$

is the probability of finding a particle in the element of volume $dxdydzdp_xdp_ydp_z$ surrounding the point whose x coordinate is 6 m, y coordinate is 0, p_y coordinate is 2 kg m/sec, etc., at the time t = 1 sec.

We shall henceforth assume that a knowledge of the continuous distribution function f, or of the probability density f/N, specifies the state of the macroscopic system.

6 MAXWELL-BOLTZMANN DISTRIBUTION

Imagine the cloud of points in phase space for a system in equilibrium. The density of the cloud of points should look the same 1 second or 10 seconds later on, so the density should not be changing significantly in time. Thus, if the system is in equilibrium, we could expect f to be a constant in time. Mathematically, this could be expressed by:

$$\frac{af}{\partial t} = 0 \qquad (10.15)$$

We shall henceforth consider only the equilibrium situation; then f (r, p, t) does not depend on time, and we can denote it more simply by f (r, p). Thus, as a whole, the cloud of points in phase space does not move. This does not mean that every point in phase space stays fixed, but only that on the whole, the number of points dN in any given volume element remain the same. For example, consider some volume element of phase space, denoted by:

$$d\,\Omega = dxdydzdp_xdp_ydp_z \qquad (10.16)$$

If some of the particles in $d\Omega$ have their velocities suddenly changed by collisions or other effects, so that their representative points go somewhere else in phase space, then on the average just as many points will come into $d\Omega$ from collisions and other effects in other regions of phase space. We conclude that although individual points may move about, an equilibrium situation is represented by a cloud of points in phase space whose density, on the average, remains constant in time, and that the quantity I/N f (r, p) $dxdydzdp_xdp_ydp_z$ is the probability of finding the point representing a particle inside the region $d\Omega$ = dxdydz • $dp_xdp_ydp_z$ in phase space.

In addition to r and p, the function f/N could depend on the temperature. However, in Equation (10.2) it was seen that the probability of finding a particle in a particular state of energy E was a function of energy and temperature, $P(E) = P(0)e^{-\beta E}$. Hence f/N and P(E) must be closely related. The quantity

$1/N\, f(\mathbf{r}, \mathbf{p})\, d\Omega$ is the probability of finding a particle in a range of states $d\Omega = dxdydzdp_xdp_ydp_z$. On the other hand, $f(E)$ is the probability of finding the particle in one particular state. Therefore, we need to know how many states there are in the phase space region $d\Omega$. There is no way to calculate this "number of states" using classical mechanics; there is, however, no reason to think there are more or fewer states inside a volume $d\Omega$ centered at (0,0,0,0,0,0) than for a $d\Omega$ centered at any other point; hence the question is answered by introducing the following postulate: The possible states are uniformly distributed in phase space. Thus, the number of states in the phase space region is taken to be $\rho d\Omega$, where ρ is some constant called the density of states. Then the number of states in the volume element $d\Omega$ is just equal to $\rho d\Omega$, and $P(E)\rho d\Omega$ is the probability of finding a particle in $d\Omega$. This is precisely the same quantity as $1/N\, f d\Omega$; so, in terms of $P(E)$,

$$\frac{1}{N} f(\mathbf{r}, \mathbf{p}) = \rho P(E) \tag{10.17}$$

and in terms of ρ and E,

$$\boxed{f(\mathbf{r}, \mathbf{p}) = \underbrace{NP(0)\rho}_{\substack{\text{constants}\\ \text{independent}\\ \text{of } E}} \times \underbrace{e^{-\beta E}}_{\substack{\text{important}\\ \text{factor}}} \qquad \text{Maxwell-Boltzmann distribution}} \tag{10.18}$$

We have thus obtained the general solution for the distribution function $f(\mathbf{r}, \mathbf{p})$ at equilibrium. The combination of factors $NP(0)\rho$ is just a normalization constant which can be determined for any particular physical system. We shall see how this is done for the ideal gas in Section 10.8. The most important dependence on the energy is in the exponent. This distribution is called the Maxwell-Boltzmann distribution, and is the basic result of this chapter. In deriving this, we have made use of the so-called fundamental postulate of statistical mechanics, which states that the possible states of a particle are uniformly distributed in phase space with a density of states ρ, which is a constant; this constant cannot be calculated using Newtonian mechanics, but can be determined using wave mechanics. (In Chapter 11 this will be shown to be $\rho = 1/h^3$, where h is Planck's constant.)

10.7 EVALUATION OF β

In Equation (10.18), the constants β and $P(0)\rho$ are unknown. To evaluate β we shall make use of a result found in discussions of the kinetic theory of the ideal gas, namely that if there are no internal energies within the particles of the gas, the average energy per particle is equal to:

$$\langle E \rangle = \frac{3}{2} k_B T \tag{10.19}$$

Here, k_B is Boltzmann's constant, 1.38 x 10^{-23} joules/degree Kelvin, and T is the absolute, or Kelvin temperature (centigrade temperature plus 273.2 K). The procedure is simply to calculate the average value of E, (E), using the distribution function we have just derived in Equation (10.18). Equating this to $\frac{3}{2}k_BT$, we will then determine the constant β.

For a distribution function f which depends only on one variable x, we saw in Chapter 2 that the expectation value of some quantity g (x) is (g) = $\int gf dx / \int f dx$, where the integral goes over the entire range of values of the variable. In our case, the distribution function depends on r and p, and the integral will go over the entire range of values of r and p, that is, over the entirety of six dimensional phase space. For example, we would indicate the integral of f (r, p), which is the distribution function itself, over all of phase space by:

$$\int f d\Omega = \int\!\!\int\!\!\int\!\!\int\!\!\int\!\!\int f(\mathbf{r}, \mathbf{p})\, dxdydzdp_xdp_ydp_z \tag{10.20}$$

We shall only consider cases in which such multiple integrals break up into products of six or fewer one dimensional integrals. It will then only be necessary to find the values of single integrals, and multiply them together to get the result. To evaluate the expectation value of E, we shall take the case in which the kinetic energy of one particle is E = $\frac{1}{2}mv^2$, and there is no potential energy. Then, since p = mv and thus $E = \frac{1}{2}p^2/m$, the expectation value of E is:

$$\langle E\rangle = \frac{NP(0)\,\rho \int\!\!\int\!\!\int\!\!\int\!\!\int\!\!\int (p^2/2m)\exp(-\frac{1}{2}\beta p^2/m)\, dxdydzdp_xdp_ydp_z}{NP(0)\,\rho \int\!\!\int\!\!\int\!\!\int\!\!\int\!\!\int \exp(-\frac{1}{2}\beta p^2/m)\, dxdydzdp_xdp_ydp_z} \tag{10.21}$$

There is no x, y or z dependence in either numerator or denominator, so if V is the volume of the container, the x-y-z integrals give:

$$\int\!\!\int\!\!\int dxdydz = V$$

Substituting this result into the expression for (E) in Equation (10.21), it is easily seen that V cancels out between numerator and denominator. Furthermore, $NP(0)\ \rho$ cancels, since it appears as a factor in both numerator and denominator. This always happens when expectation values of single-particle properties are being calculated; hence, if we are only interested in calculating expectation values, we do not need to know the values of N, P(0) and p.

Thus, after canceling such common factors, (E) reduces to an expression involving only integrals over p_x, p_y and p_z:

$$\langle E\rangle = \frac{\int\!\!\int\!\!\int \frac{1}{2}p^2/m\exp(-\frac{1}{2}\beta p^2/m)\, dp_xdp_ydp_z}{\int\!\!\int\!\!\int \exp(-\frac{1}{2}\beta p^2/m)\, dp_xdp_ydp_z} \tag{10.22}$$

Let us first evaluate the denominator. To separate this denominator into three single integrals, we note that

$$\exp\left(\frac{-\frac{1}{2}\beta p^2}{m}\right) = \exp\left(\frac{-\frac{1}{2}\beta p_x^2}{m}\right)\exp\left(\frac{-\frac{1}{2}\beta p_y^2}{m}\right)\exp\left(\frac{-\frac{1}{2}\beta p_z^2}{m}\right) \tag{10.23}$$

Then the use of integrals given in Table 10.1 leads to the result:

$$\begin{aligned}
\int_{-\infty}^{\infty} \exp\left(\frac{-\frac{1}{2}\beta p^2}{m}\right) dp_x dp_y dp_z
&= \int_{-\infty}^{\infty} \exp\left(\frac{-\frac{1}{2}\beta p_x^2}{m}\right) dp_x \\
&\quad \cdot \int_{-\infty}^{\infty} \exp\left(\frac{-\frac{1}{2}\beta p_y^2}{m}\right) dp_y \int_{-\infty}^{\infty} \exp\left(\frac{-\frac{1}{2}\beta p_z^2}{m}\right) dp_z \\
&= \left[\int_{-\infty}^{\infty} \exp\left(\frac{-\frac{1}{2}\beta u^2}{m}\right) du\right]^3 = \left[\sqrt{\frac{2\pi m}{\beta}}\right]^3
\end{aligned} \qquad (10.24)$$

We shall refer to this result several times later.

TABLE 10.1 Some Definite Integrals

$\int_0^\infty e^{-ax}\,dx = \frac{1}{a}$	$\int_0^\infty e^{-ax^2}\,dx = \frac{1}{2}\sqrt{\frac{\pi}{a}}$
$\int_0^\infty xe^{-ax^2}\,dx = \frac{1}{2a}$	$\int_0^\infty x^2e^{-ax^2}\,dx = \frac{1}{4}\sqrt{\frac{\pi}{a^3}}$
$\int_0^\infty x^3e^{-ax^2}\,dx = \frac{1}{2a^2}$	$\int_0^\infty x^4e^{-ax^2}\,dx = \frac{3}{8}\sqrt{\frac{\pi}{a^5}}$
$\int_0^\infty x^5e^{-ax^2}\,dx = \frac{1}{a^3}$	$\int_0^\infty x^6e^{-ax^2}\,dx = \frac{15}{16}\sqrt{\frac{\pi}{a^7}}$

We next need to evaluate the numerator. The integral we need is:

$$\text{Numerator} = \frac{1}{2m}\iiint \exp\left(\frac{-\frac{1}{2}\beta p^2}{m}\right) p^2\, dp_x dp_y dp_z \qquad (10.25)$$

Again substitute $p^2 = p_x^2 + p_y^2 + p_z^2$ in the two places in this equation.

$$\begin{aligned}
\text{Numerator} &= \frac{1}{2m}\iiint \exp\left[-\frac{1}{2}\beta(p_x^2 + p_y^2 + p_z^2)\right] \\
&\quad \times (p_x^2 + p_y^2 + p_z^2)\, dp_x dp_y dp_z
\end{aligned} \qquad (10.26)$$

Then we have the sum of three integrals to evaluate, with integrands proportional, respectively, to p_x^2, p_y^2 and p_z^2 times the exponential. Since the three integrals are identical except for labeling of axes, they will be equal. Hence, taking the integral with integrand proportional to p_x^2 as representative, we have:

$$\text{Numerator}, = \frac{3}{2m}\int_{-\infty}^{\infty} p_x^2 \exp\left(\frac{-\frac{1}{2}\beta p^2}{m}\right) dp_x dp_y dp_z \qquad (10.27)$$

Upon separation of this threefold integral into the product of three single integrals, the p_y and p_z integrals are the same as the p_y and p_z integrals in the denominator, and may be performed using Table 10.1. The integral then reduces to:

$$\text{Numerator} = \frac{3}{2m}\,\frac{2\pi m}{\beta}\int_{-\infty}^{\infty} p_x^2 \exp\left(\frac{-\tfrac{1}{2}\beta p_x^2}{m}\right) dp_x \qquad (10.28)$$

The remaining integral over p_x, from Table 10.1, gives a factor $\tfrac{1}{2}\sqrt{\pi}(2m/\beta)^{3/2}$ so the numerator is:

$$\text{Numerator} = \frac{3}{2}(2\pi m)^{3/2}\,\beta^{-5/2} \qquad (10.2’3)$$

Taking the ratio of the results for numerator and denominator obtained in Equations (10.24) and (10.29), we find that

$$\langle E\rangle = \frac{3}{2}\beta \qquad (10.30)$$

For the ideal gas, however, $\langle E\rangle$ is given by Equation (10.19) as (E) = $3k_BT/2$, and therefore,

$$\beta = \frac{1}{k_BT} \qquad (10.3’1)$$

Thus, by calculating the average energy per particle using a Maxwell-Boltzmann distribution function, and requiring the result to be the same as for an ideal gas, β is determined. This result is important and should be remembered.

.8 EVALUATION OF $NP(0)\,\rho$

For completeness, we will find $NP(0)\,\rho$, the normalization constant for the ideal gas system. This constant varies from one system to another, and probably should not be memorized for any one system. The constant may be found if the number of particles N in the volume V is known; that is, the integral of $f d\Omega$ over all phase space must equal N. For the Maxwell-Boltzmann distribution function, describing a gas of free particles, the normalization for a system with N particles in a volume V is:

$$N = \int\!\!\int\!\!\int\!\!\int\!\!\int\!\!\int NP(0)\,\rho \exp\left(\frac{-\tfrac{1}{2}\beta p^2}{m}\right) dx\,dy\,dz\,dp_x\,dp_y\,dp_z \qquad (10.341)$$

Equation (10.24) with $\beta = 1/k_BT$ leads to:

$$NP(0)\,\rho = \frac{N}{V}\,(2\pi m k_BT)^{-3/2} \qquad (10.33:)$$

Therefore, at equilibrium for an ideal monatomic gas,

$$\mathbf{f\ (r,\ p)} = \frac{N}{V}\,(2\pi m k_BT)^{-3/2} \exp\left(\frac{-\tfrac{1}{2}p^2}{mk_BT}\right) \qquad (10.34)$$

As mentioned previously, the factor $e^{-\beta E}$ in the distribution function is called the Boltzmann factor. In this factor, $\beta = 1/k_BT$. The most important feature of the function f(r, p) is that it is proportional to $e^{-\beta E}$. The constants $NP(0)\rho$ in front of the exponential are for purposes of normalization, and almost always cancel out in calculating <expectation values.

Thus, in Equation (10.34), we have completely determined the distribution function f (r, p) for an ideal monatomic gas of particles in thermal equilibrium with the container walls. Here each particle is considered to be a system with energy $E = \frac{1}{2}p^2/m$.

10.9 MAXWELL-BOLTZMANN DISTRIBUTION INCLUDING POTENTIAL ENERGY

Now consider a slightly more complicated situation, in which there may be some potential energy present. Suppose, as in Figure 10.8, that the box containing the gas consists of two regions. In the lower region, region I, there is no potential energy, but in the upper region, of equal volume, there is a constant potential energy $V_0 > 0$. There is a tendency for particles to seek the condition of lowest potential energy, so it is natural to ask whether all or most of the particles of the system are in the portion of the box of zero potential energy. If the particles in the box are in thermal equilibrium at temperature T, the value of β is still $\beta = 1/k_BT$. Since f (r, p) $dxdydzdp_xdp_ydp_z$ is the number of particles in the volume element $dxdydzdp_xdp_ydp_z$, the total number of particles in the volume element $dxdydzdp_xdp_ydp_z$ in region I is:

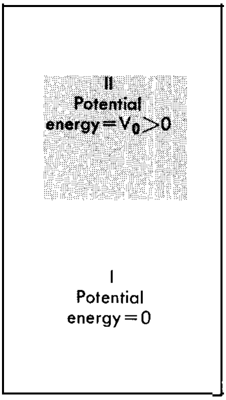


Figure 10.8. Particles in a container which has two distinct regions of different potential energy.

$$N_I = \iiiiiint NP(0)\,\rho\,\exp\left(\frac{-\frac{1}{2}\beta p^2}{m}\right) dxdydzdp_xdp_ydp_z \qquad (10.35)$$

where the integrals over x, y and z go only over region I. The distribution function in region II depends on the energy $E = V_0 + \frac{1}{2}p^2/m$. Therefore, the number of particles in this region is:

$$N_2 = \int\int\int\int\int\int NP(0)\,\rho \exp\left[-\beta\left(\frac{p^2}{2m} + V_0\right)\right] dxdydzdp_xdp_ydp_z \qquad (10.36)$$

where the integrals of dxdydz go **only** over region II.

The ratio N_2/N_1 may be easily evaluated, since V_0 is a constant. The volumes are taken to be equal, and the integrals of exp $(-\frac{1}{2}\beta p^2/m)\ dp_xdp_ydp_z$ are the same for both regions; so these cancel in the ratio N_2/N_1. Therefore,

$$\frac{N_2}{N_1} = e^{-\beta V_0} \qquad (10.37)$$

Thus, the ratio of the numbers N_2/N_1 is just the Boltzmann factor, $e^{-\beta V_0}$, with the energy difference V_0 between the two regions appearing in the exponent.

ple At $T = 300$ K (with $k_B = 1.38 \times 10^{-23}$ joules/K), if $V_0 = 10^{-6}$ joule, what is the ratio of the number of particles in the region of higher potential energy to the number in the region of lower potential energy?

ion $N_2/N_1 = e^{-\beta V_0} = e^{-V_0/k_BT} = e^{-10^{-6}/(1.38\times10^{-23}\times300)} = e^{-2.4\times10^{14}} \cong 10^{-10^{14}}$, an extremely small number. Hence most of the particles will be in the lower potential energy region. If there are on the order of 10^{23} particles, there is negligible probability that even one of them is in the higher potential energy region.

In general, if $\beta V_0 \gg 1$, or $V_0 >> k_BT$, most of the particles would be in the lower part of the box. When k_BT becomes large enough that k_BT and V_0 are comparable, there would be enough thermal energy available so that collisions could knock an appreciable fraction of particles up into region II. This would occur at a temperature given approximately by:

$$k_BT \cong V_0$$

or, if $V_0 = 10^{-6}$ joule, $T = V_0/k_BT \cong 7 \times 10^{16}$ K. Room temperature, about 293 K, corresponds to an energy of k_B J = 4.04 x 10^{-21} j = 0.0252 eV, or about $\frac{1}{40}$ of an electron volt. Energy differences of this order of magnitude occur in some molecular spectra and other atomic systems.

10 GAS IN A GRAVITATIONAL FIELD

Consider next a column of air at temperature 300 K. This is nearly an ideal gas. If the density at sea level is n_0 particles per m^3, what would be the density at height h above sea level? The number of particles in a given volume element of phase space is proportional to the Boltzmann factor times the volume element of phase space. If we are interested only in number of particles in a given volume of ordinary space regardless of momentum, we sum over the momentum part of phase space. Therefore, we take the ratio of $dxdydz\int dp_xdp_ydp_z e^{-\beta E}$ for two equal volumes dxdydz, separated by a height h. The potential energy of a particle of mass m at height h is mgh, and therefore the ratio of number of particles in a unit volume at height h, to the number at sea level, is:

$$\frac{n(h)}{n(0)} = \frac{\int dp_x dp_y dp_z \exp\{-\beta[(\frac{1}{2}p^2/m) + mgh]\}}{\int dp_x dp_y dp_z \exp[-\beta(\frac{1}{2}p^2/m)]} = e^{-\beta mgh} \quad (10.38)$$

example If the mass of a molecule of air, on the average, is $m = 5 \times 10^{-26}$ kg, at what height does the density of the column reduce to half its sea level value for $T = 300$ K throughout the column?

solution $n(h)/n(0) = \frac{1}{2} = e^{-\beta mgh}$. Taking natural logarithms of both sides and solving for h,

$$h = \frac{k_B T}{mg} \ln 2 = \frac{(1.38 \times 10^{-23})(300)}{(5 \times 10^{-26})(9.8)}(0.693)$$

$$= 5.86 \times 10^3 \text{ meters}$$

or 5.86 kilometers.

10.11 DISCRETE ENERGIES

In quantum mechanics it has been shown that in many cases energies are quantized; that is, they take on only discrete values,, rather than continuous values such as the classical kinetic energy $E = \frac{1}{2}mv^2$ does. There are some systems whose particles can, in effect, have only two possible energies; let us denote these energies by E_+ and E_-, with $E_+ > E_-$. An example of such a system is a set of proton spins placed in a magnetic field. The number N_+ of such systems in the energy state E_+ is proportional to the Boltzmann factor. If C is the normalizotion constant, then:

$$N_+ = Ce^{-\beta E_+} \quad (10.39)$$

and the number N_- in the energy state E is:

$$N_- = Ce^{-\beta E_-} \quad (10.40)$$

Thus, $N_+/N_- = e^{-\beta(E_+ - E_-)}$.

If there are a large number of possible discrete energies E,, then the distribution function f (E,) which gives the number of particles in that state is given by the Boltzmann factor:

$$f(E_i) = Ce^{-\beta E_i} \quad (10.41)$$

where C is some proportionality constant. The normalization constant C would be determined by requiring that the system had a (certain given total number of particles and summing over all states i:

$$\sum f(E_i) = C\sum_i e^{-\beta E_i} = N \quad (10.42)$$

when N is the total number of particles. Averages of energy, $\langle E\rangle$, could be computed by the formula:

$$\langle E\rangle = \frac{\sum_i E_i e^{-\beta E_i}}{\sum_i e^{-\beta E_i}} \tag{10.43}$$

2 DISTRIBUTION OF THE MAGNITUDE OF MOMENTUM

In some applications it is necessary to know the number $F(p)$ dp of particles with momenta of magnitude p in the range dp, regardless of position or of the direction of momentum. The number of particles with momenta in the range $dp_x dp_y dp_z$, regardless of position,. may be obtained by integrating f (r, p) . $dp_x dp_y dp_z$ over all positions. We shall denote by f(p) the resulting momentum space distribution function:

$$f(\mathbf{p}) = \iiint dxdydz f(\mathbf{r}, \mathbf{p}) \tag{10.44}$$

Then, since the volume V = $\int$ dxdydz and f (r, p) is independent of r for an ideal gas, we obtain from Equation (10.34):

$$f(\mathbf{p}) = N(2\pi m k_B T)^{-3/2} \exp\left(\frac{-\frac{1}{2}\beta p^2}{m}\right) \tag{10.45}$$

We may now easily rewrite the distribution function in terms of the magnitude of momentum, p = $\sqrt{\mathbf{p}^2}$, because here the distribution function f(p) depends only on p and not on the direction of p. The distribution of particles is therefore spherically symmetric in momentum space.

To obtain the number of particles of momenta in the range of magnitudes dp, we may then consider a thin spherical shell, of radius p and hence of area $4\pi p^2$, in momentum space. If the thickness of the shell is dp, then the volume in momentum space enclosed by the shell is $4\pi p^2 dp$. Alternatively, the volume of a sphere of radius p is $4\pi p^3/3$, and the differential volume contained between two spheres of radii p and p + dp will be just the differential:

$$d\left(\frac{4}{3}\pi p^3\right) = 4\pi p^2 dp \tag{10.46}$$

Thus, using this radial coordinate in momentum space, the volume element becomes:

$$dp_x dp_y dp_z \rightarrow 4\pi p^2 dp \tag{10.47}$$

We then want to look for a function F(p) such that $F(p)$ dp is the total number of particles with momenta of magnitude p in the range dp. Thus, we would set:

$$f(\mathbf{p})\, dp_x dp_y dp_z \rightarrow f(p)\, 4\pi p^2 dp \equiv F(p)\, dp \tag{10.48}$$

This defines a new distribution function as a function only of the variable p. Solving to find F(p) as a function of p, we get:

$$F(p) = 4\pi N(2\pi m k_B T)^{-3/2} p^2 \exp\left(\frac{-\frac{1}{2}\beta p^2}{m}\right) \tag{10.49}$$

The most probable value of p is the value for which $F(p)$ is a maximum. Upon using the condition $dF(p)/dp = 0$ to determine the maximum, we get:

$$0 = \left(2p - \frac{\beta p^3}{m}\right)\exp\left(\frac{-\frac{1}{2}\beta p^2}{m}\right) \qquad (10.50)$$

I.e., the most probable value of p is $\sqrt{2mk_BT} = 1.414\sqrt{mk_BT}$. Since the speed is $v = p/m$, the most probable speed is $\sqrt{2k_BT/m}$.

The average value of p can be computed using F(p) and Table 10.1, noting that $\int_0^\infty F(p)dp = N$. From this we find the average value is:

$$(p) = \frac{1}{N}\int_0^\infty pF(p)\,dp = 4\pi(2\pi mk_BT)^{-3/2}\int_0^\infty p^3 \exp\left(\frac{-\beta p^2}{m}\right)dp$$

$$= \sqrt{\frac{8k_BTm}{\pi}} = 1.595\sqrt{mk_B J} \qquad (10.51)$$

Here the limits range from 0 to ∞, since the magnitude of momentum can never be negative. Comparison of (p) with the most probable value of p is interesting; this is a case in which the most probable value and the expectation value ore almost the same but slightly different, both still being positive, On the other hand, calculation of both the most probable value and the expectation value of one component of momentum such as $p.$, would show that both are zero; this will be discussed below.

Figure 10.9 is a graph of $F(p)$ as a function of p.

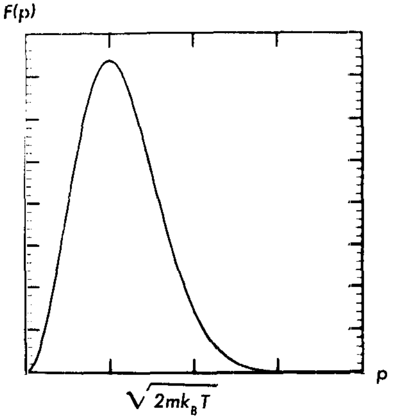


Figure **10.9.** Distribution function $F(p)$ for the magnitude of the momentum.

10.13 EXPERIMENTAL VERIFICATION OF THE MAXWELL DISTRIBUTION

Figure 10.10 shows the results of two runs of an experiment by R. C. Miller and P. Kusch, performed in 1955 to check the validity of the distribution $F(p)$, derived in Equation (10.49). In this experiment, either potassium or thallium was obtained

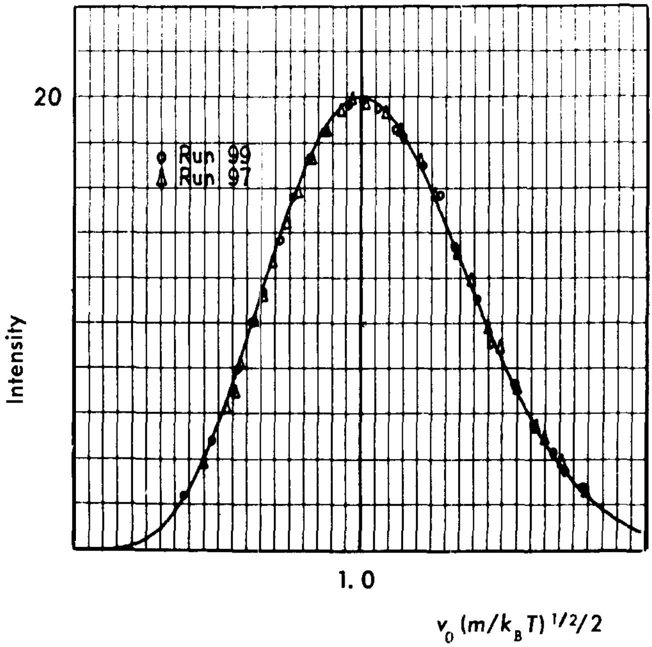


Figure 10.10. Experimental verification of the Maxwell-Boltzmann distribution. The experimental points were for a gas of hot thallium atoms. The dotted line is the theoretical result obtained from the Maxwell-Boltzmann distribution, Equation (10.18). Both curves were multiplied by a factor, so that the maximum is at 20.

in gaseous form by heating the metals to high temperatures in a vacuum oven. A very narrow slit in the oven allowed atoms to escape into an evacuated chamber outside the oven. Presumably, the momenta of the particles in this beam would have the distribution given by F(p). To measure the distribution, it was necessary to be able to select atoms out of the beam having speeds within a very narrow range. To do this, the experimenters inserted a cylinder with its axis parallel to the beam, so that the beam hit the cylinder just inside its rim and was blocked. A straight slot cut in the edge of the cylinder parallel to its axis would then let the beam get through. However, suppose the cylinder were rotating at a constant angular speed. Then, for an atom of a given speed to get through, the slot should not be straight but helical. For a given angular speed and helical slot, only particles in a narrow range of speed could get through. By cutting such a slot in the cylinder and rotating the cylinder at different angular speeds, it was possible to select particles of the desired speed out of the beam. The experimenters then measured the number of particles per second that were transmitted through the slot, versus the speed of the particles.

The particular experimental setup introduced several factors that slightly modified the form of the theoretical distribution which was finally compared with the experimental results. If f is the distribution function for velocities, then the number of particles of speed v hitting an area oriented normal to the direction of v, in one second, is vf. Thus, in this experiment,, the number of particles of speed v hitting the end of the slot nearest the oven, per second, should be proportional to:

$$v^3 \exp\left(\frac{-mv^2}{2k_BT}\right) \tag{10.52}$$

since $p = mv$. Also, if v_0 is the speed that is just right for particles to get through the slot for a given angular speed of the cylinder, then the probability that particles with speeds between v and $v + dv$ will get through will be of the form $A(v/v_0)$, where $A(v/v_0)$ is a probability density depending on the slot width, and is sharply peaked about the value $v = v_0$. Then the number of particles per second that get through the slot is proportional to:

$$\int_0^\infty v^3 \exp\left(\frac{-mv^2}{2k_BT}\right) A\left(\frac{v}{v_0}\right) dv \tag{10.53}$$

Since A is very sharply peaked about $v = v_0$, we can replace v with v_0 everywhere in the integrand, except within A. Then, letting $dv = v_0 d(v/v_0)$, we have an approximate value for the integral:

$$v_0^4 \exp\left(\frac{-mv_0^2}{2k_BT}\right) \int_0^\infty A\left(\frac{v}{v_0}\right) d\left(\frac{v}{v_0}\right) \tag{10.54}$$

The integral is some constant independent of v_0. The experimenters normalized both their experimental results and the theoretical curve, so that the maximum was equal to 20. The theoretical result is then:

$$\text{Intensity at detector} = 36.9 \left(\frac{mv_0^2}{2k_BT}\right)^2 \exp\left(\frac{-mv_0^2}{2k_BT}\right) \tag{10.55}$$

The maximum occurs at $v_0/2\sqrt{k_BT/m} = 1$. In figure 10.10, the theoretical curve is indicated by the solid curve. The experimental results were for thallium vapor. Run 99 was at 870 K and run 97 was at 944 K. The measured peak velocity of the curves agreed with $2\sqrt{k_BT/m}$, within the experimental error of about 1%. Similar results were obtained with potassium vapor at quite different temperatures. One can conclude that to within the experimental error, the Maxwell-Boltzmann distribution agrees with experiment.

10.14 DISTRIBUTION OF ONE COMPONENT OF MOMENTUM

The Maxwell-Boltzmann distribution can be expressed in several other useful ways. For example, let us calculate the total number of particles with x components of momentum in the range dp_x, regardless of their values of p_y and p_z. This means we must integrate over all dp_y and dp_z. The required number of particles is denoted by $f(p_x)\, dp_x$, and is given by

$$dp_x \int_{-\infty}^{\infty} dp_y \int_{-\infty}^{\infty} dp_z f(\mathbf{p}) = f(p_x)\, dp_x \tag{10.56}$$

and so

$$f(p_x) = \int_{-\infty}^{\infty} dp_y \int_{-\infty}^{\infty} dp_z N\left(\frac{1}{2\pi m k_B T}\right)^{3/2} \exp\left[\frac{-(p_x^2 + p_y^2 + p_z^2)}{2mk_BT}\right] \quad (10.57)$$

We may separate the integrals into two single integrals, which are multiplied together. Performing these integrals over p_y and p_z using Table 10.1, we get:

$$f\ (p.) = N(2\pi m k_B\, T)^{-1/2} \exp\left(\frac{-\tfrac{1}{2} p_x^2}{mk_BT}\right) \quad (10.58)$$

In this case, because f (p,) is an even function of p_x, the most probable value of p_x will be zero, as will the expectation value, $\langle p_x \rangle$

If we had performed a similar calculation to obtain f (p,) and f (p_z), we would have found that similarly,

$$\langle p_x \rangle = (P'') = \langle p_z \rangle = 0 \quad (10.59)$$

Also, the most probable values of p_y and p_z would be zero. Thus, although $\langle p_x \rangle = \langle p_y \rangle = \langle p_z \rangle = 0$, $\langle p \rangle > 0$ because p is intrinsically positive.

Previously, we noted that when E is a function only of the magnitude of p, it is useful to use the momentum space volume element in spherical coordinates, $4\pi p^2 dp$. likewise, because the Boltzmann factor, e^{-E/k_BT}, depends only on the energy and temperature, it is often useful to write the differential volume in momentum space, $dp_x dp_y dp_z$, in terms of the corresponding infinitesimal energy change dE. For the free particles we have been discussing,

$$E = \frac{p^2}{2m} \quad (10.60)$$

Since for a free particle E is then a function only of *p,* we can express the volume element in the spherical coordinates of momentum space in terms of energy. Now we noted before that the volume of a sphere of radius p is $4\pi p^3/3$, and thus for the volume of a thin spherical shell:

$$dp_x dp_y dp_z \rightarrow d\left(\frac{4}{3}\pi p^3\right) = 4\pi p^2 dp \quad (10.61)$$

We wish to express $p^2 dp$ in terms of the corresponding energy E, and energy increment dE. From Equation (10.60),

$$p^2 = 2mE \quad \text{or} \quad p = \sqrt{2mE} \quad (10.612)$$

Then differentiation of both sides yields:

$$d\,p = \sqrt{\frac{m}{2E}}\, dE \quad (10.6'3)$$

Thus,

$$dp_x dp_y dp_z \rightarrow 4\pi p^2 dp = 4\pi\sqrt{2m^3E}\, dE \quad (10.64)$$

We may now define an energy distribution function g(E) by equating numbers of particles in the range dE in the two alternative expressions:

$$f(p)\,dp_x dp_y dp_z \rightarrow N(2\pi m k_B T)^{-3/2}\,4\pi\sqrt{2m^3E}\,e^{-\beta E}\,dE \equiv g(E)\,dE \tag{10.65}$$

or for the distribution function in energy,

$$\begin{aligned} g(E) &= \text{const.} \times \sqrt{E}e^{-\beta E} \\ &= [N2\pi(\pi k_B T)^{-3/2}] \times \sqrt{E}e^{-\beta E} \end{aligned} \tag{10.66}$$

A graph of the dependence of g(E) on energy E is given in Figure 10.11. It has a maximum at $\partial g/\partial E = 0$, or at $E = k_B T/2$. Note that the graph is tangent to the vertical axis at small E, whereas $F(p)$ was tangent to the horizontal axis at small p. From equation (10.19), the average energy per particle is $\frac{3}{2} k_B T$, whereas the most probable value of energy, $\frac{1}{2} k_B T$, is considerably different from this.

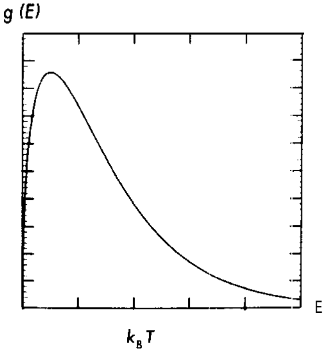


Figure 10.11. Graph of the energy distribution function, g(E) proportional to $\sqrt{E}e^{-\beta E}$.

The total probability that a particle is in the energy range between E and $E + dE$ is $p(E)dE = g(E)dE/N$ or, alternately, $e^{-\beta E}\sqrt{E}\,dE/\int_0^\infty e^{-\beta E}\sqrt{E}\,dE$. It is $p(E)dE = 2\pi(1/\pi k_B T)^{3/2} e^{-\beta E}\sqrt{E}\,dE$.

example What is on expression giving the probability of a particle's having energy between 0 and $1/\beta = k_B T$?

solution

$$\int_0^{k_B T} p(E)\,dE = \int_0^{k_B T} e^{-\beta E}\sqrt{E}\,dE \bigg/ \int_0^\infty e^{-\beta E}\sqrt{E}\,dE$$

The integral in the numerator cannot be written in terms of a closed farm involving simple functions. It may be expressed in terms of error functions which may be found in tables. The numerical result is 0.843.

10.15 SIMPLE HARMONIC OSCILLATORS

The energy dependence of the distribution function in phase space, f = (constant) × $e^{-\beta E}$, was derived for the case of many systems in thermal equilibrium which were weakly interacting with possible heat flow between them. The internal structures of the systems were irrevelant. If we have any set of a large number of identical systems, and the energy of a system takes on the values E, then the number of systems in the set with energy E is proportional to $e^{-\beta E}$. These systems might be macroscopic. Thus, in a cubic mile of air, we might assume the systems to be volumes containing a gallon of air each. Provided the assumption of weak interaction holds, other systems such as liquids can also be treated in the some way.

Suppose we had a box containing a large number of particles, each of which has a mass m and is bound to on equilibrium position by a spring-like farce with spring constant K. At high temperatures, such a picture might be used to represent the behavior of a solid, where atoms oscillate in three dimensions about their equilibrium positions in the crystal lattice. We shall assume the particles to be only very weakly interacting. The energy of a particle is that of a three dimensional harmonic oscillator:

$$E = \frac{1}{2m}(p_x^2 + p_y^2 + pf) + \frac{1}{2}K(x^2 + y^2 + z^2)$$

or

$$E = \frac{1}{2m}\mathbf{p}^2 + \frac{1}{2}K\mathbf{r}^2 \tag{10.67}$$

Here x, y and z are the displacements of the particle in the x, y, z directions from its equilibrium position. The number of particles of this energy is then proportional to

$$\exp\left[-\beta\left(\frac{\mathbf{p}^2}{2m} + \frac{K\mathbf{r}^2}{2}\right)\right] \tag{10.68}$$

The number of particles whose positions x, y and z are in the range dxdydz and whose momenta p_x, p_y, p_z are in the range $dp_x dp_y dp_z$ is then proportional to:

$$\exp\left[-\beta\left(\frac{\mathbf{p}^2}{2m} + \frac{K\mathbf{r}^2}{2}\right)\right] dxdydzdp_x dp_y dp_z \tag{10.69}$$

We shall use this distribution function to calculate the average energy, (E). The formula, written completely out, for this average is

$$\langle E\rangle = \frac{\iiiint\!\!\iint (\tfrac{1}{2}m\mathbf{p}^2 + \tfrac{1}{2}K\mathbf{r}^2)e^{-\beta E}\,dxdydzdp_x dp_y dp_z}{\iiiint\!\!\iint e^{-\beta E}\,dxdydzdp_x dp_y dp_z} \tag{10.70}$$

with all integration limits from $-\infty$ to $+\infty$. There are, altogether, six separate terms in the numerator of this expression. However, there are only two types—integrals involving p_x^2, p_y^2, or p_z^2 and integrals involving x^2, y^2 or z^2 as factors, in the integrand multiplying the exponential. All three of the integrals of a given type are equal, by symmetry. Furthermore, any of the six-fold integrals reduce to a product of six single integrals, so the integrations are straightforward with the use of Table 10.1. Let us calculate this average term by term. First, in the calculation of $\langle p_x^2/2m\rangle$, all factors in numerator and denominator cancel except those involving p_x in the integrands, so

$$\left\langle \frac{\frac{1}{2} p_x^2}{m} \right\rangle = \frac{\int (p_x^2/2m) e^{-\beta p_x^2/2m}\, dp_x}{\int e^{-\beta p_x^2/2m}\, dp_x} = \frac{1}{2} k_B T \tag{10.71}$$

Similarly, by symmetry,

$$\left\langle \frac{\frac{1}{2} p_x^2}{m} \right\rangle = \left\langle \frac{\frac{1}{2} p_y^2}{m} \right\rangle = \left\langle \frac{\frac{1}{2} p_z^2}{m} \right\rangle \tag{10.72}$$

so the average kinetic energy is

$$\left\langle \frac{\frac{1}{2} p^2}{m} \right\rangle = \frac{3}{2} k_B T \tag{10.73}$$

For the average of the potential energy, by symmetry, it is clear that in this case also,

$$\left\langle \frac{1}{2} Kx^2 \right\rangle = \left\langle \frac{1}{2} Ky^2 \right\rangle = \left\langle \frac{1}{2} Kx^2 \right\rangle \tag{10.74}$$

so

$$\left\langle \frac{1}{2} K\mathbf{r}^2 \right\rangle = \frac{3}{2} \langle Kx^2 \rangle \tag{10.75}$$

Now to calculate a typical term such as $\langle Kx^2 \rangle$, using the fact that all factors in numerator and denominator cancel except those involving x, we find that

$$\left\langle \frac{1}{2} Kx^2 \right\rangle = \frac{1}{2} k_B T \tag{10.76}$$

Thus $\langle \frac{1}{2} K\mathbf{r}^2 \rangle = \frac{3}{2} k_B T$, so the total average energy per particle is

$$\langle E \rangle = \frac{6}{2} k_B T \tag{10.77}$$

Note that for every quadratic term in the energy, either of the form $\frac{1}{2} p_x^2/m$ or $\frac{1}{2} Kz^2$, we find a contribution to the average energy per particle of $\frac{1}{2} k_B T$. This result is referred to as the theorem of equipartition of energy. If, for example, the oscillators were restricted to move in only one dimension so that $E = \frac{1}{2} p_x^2/m + \frac{1}{2} Kx^2$, one would immediately expect that

$$\langle E \rangle = \frac{1}{2} k_B T + \frac{1}{2} k_B T = k_B T \tag{10.78}$$

For the three-dimensional oscillator, the average energy per particle is then $\langle E \rangle = 3k_B T$ and the specific heat per particle is $3k_B$. We would expect this specific heat per particle in solids where the particles oscillate about their equilibrium positions. The specific heat per mole, in terms of the gas constant $R = N_0 k_B$ would be equal to $3R = 5.96$ calories/mole-degree K. This behavior is observed in solids at high temperatures where it is called the *Dulong-Petit law.*

At low temperatures, quantum effects come into play which greatly reduce the specific heat. In Table 10.2 the specific heat and molar specific heat at room temperature is given for several common metals. Note that, although the specific heats are quite different, the molar specific heats are close to $3R$.

TABLE 10.2 Molar Specific Heats of Some Metals

Metal	Specific Heat in calories/gram -degree K	Molar Specific Heat in calories/mole degree K 3R = 5.96 cal/mole-degree K
Aluminum	0.21	5.8
Calcium	0.16	6.4
Copper	0.092	5.9
Gold	0.031	6.2
Iron	0.11	6.0
lead	0.031	6.3
Potassium	0.18	7.2
Silver	0.056	6.0
Tin	0.054	6.5
Zinc	0.093	6.1

16 DETAILED BALANCE

When a system of noninteracting particles is in thermal equilibrium, the average density of the cloud of representative points in phase space remains constant in time. Therefore, if we consider some fixed infinitesimal region $d\Omega$ in phase space, there will be just as many points entering this region as there are particles leaving it on the average. It is necessary to keep in mind that these statements refer only to time averages, for at any one instant there may very well be more or fewer points in $d\Omega$ than the average number. However, if a state of the system were to develop in such a way that the number of points in $d\Omega$ was consistently greater or less than the time-averaged or equilibrium number, the system would no longer be in a thermal equilibrium state.

Now suppose we consider any two fixed regions, $d\Omega_1$ and $d\Omega_2$, with volumes of equal magnitudes, $d\Omega_1 = d\Omega_2$, in phase space. If at equilibrium the average rate at which points in $d\Omega_1$ are changing to $d\Omega_2$ is equal to the average rate at which points in $d\Omega_2$ are changing to $d\Omega_1$, and if this equality of rates is maintained for all such pairs of regions in phase space, then the average number of points in each region would remain constant. This would be a sufficient—but not a necessary-condition that thermal equilibrium would be maintained. More detailed calculation of these transition rates using quantum mechanics shows in fact that the rates of transitions between any two such equal regions in phase space are equal.

We shall therefore make the reasonable assumption that this is the case; the assumption may be stated as follows:

The rate of transitions between ***any two equal volume elements in phase*** space are equal at thermal equilibrium.

This statement is called the principle **of detailed balance. It does not mean** that the rate of transition from $d\Omega_i$ to $d\Omega_j$ equals the rate from $d\Omega_j$ to some **other element $d\Omega_k$, but only that the rates from $d\Omega_i$ to $d\Omega_j$, and** back **from** $d\Omega_j$ to $d\Omega_i$, are equal. This is illustrated in Figure 10.12.

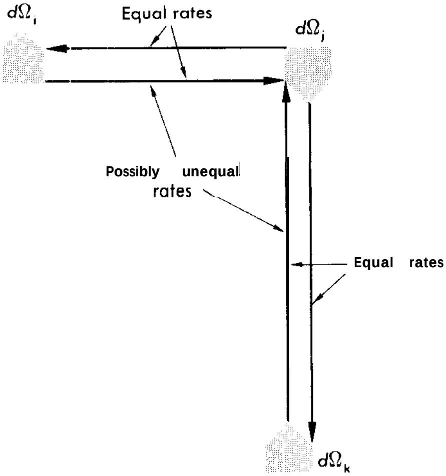


Figure 10.12 The principle of detailed balance asserts that between any pair of regions in phase space with volumes of equal magnitude, the number of particles per unit time making transitions from the first to the second is balanced, on the average, by an equal number making transitions back from the second to the first per unit time.

Now let us consider a classical ideal **gas in which the interactions between** particles may be neglected, but in which the particles may interact with the container walls at temperature T. We define $P_{1\to2}$ to be the probability that one particle in $d\Omega_1$ makes a transition to $d\Omega_2$, per unit time. Similarly, $P_{2\to1}$ is the probability per unit time for a single particle to make a transition from $d\Omega_2$ to $d\Omega_1$. If there are, on the average, $d\bar{n}_1$ particles in $d\Omega_1$, then the number of particles which change to $d\Omega_2$ per unit time is $d\bar{n}_1 p_{1\to2}$. Likewise, if dn_2 **is the average** number of particles in $d\Omega_2$, the average transition rate to $d\Omega_1$ is $d\bar{n}_2 p_{2\to1}$. The equation expressing the principle of detailed balance at **equilibrium may therefore be written:**

$$d\bar{n}_1 p_{1\to2} = d\bar{n}_2 p_{2\to1} \tag{10.79}$$

If the energies of particles in $d\Omega_1$ and $d\Omega_2$ are E_1 and E_2, respectively, for a gas at temperature T, then the ratio $d\bar{n}_1/d\bar{n}_2$ is simply equal to the ratio of the Boltzmann factors. Therefore, because the volumes $d\Omega_1$ and $d\Omega_2$ were taken to be equal in magnitude,

$$\frac{d\bar{n}_1}{d\bar{n}_2} = \frac{e^{-\beta E_1}}{e^{-\beta E_2}} = e^{\beta(E_2-E_1)} = \exp\left[\frac{(E_2 - E_1)}{k_BT}\right] \tag{10.80}$$

Therefore, from Equation (10.79), the ratio of the single-particle transition probabilities is:

$$\frac{p_{2\to 1}}{p_{1\to 2}} = \frac{d\bar{n}_1}{d\bar{n}_2} = \exp\left[\frac{(E_2 - E_1)}{k_B T}\right] \tag{10.81}$$

This important result for the ratio of transition probabilities is generally valid at thermal equilibrium not only for the particles of a classical ideal gas, but also for electrons, photons and other particles having quantum properties. We shall use Equation (10.81) to derive the Fermi-Dirac and Bose-Einstein distribution functions in the following chapter.

.17 TIME REVERSIBILITY

The equations of classical mechanics possess an invariance property known as *time* reversibility. For example, in Newton's equation of motion $\mathbf{F} = m\mathbf{a} = m\, d^2\mathbf{r}/dt^2$, if the sign of the time t is reversed, the equation of motion is unchanged. The velocity, $\mathbf{v} = d\mathbf{r}/dt$, reverses direction when the sign of t is changed. Thus, classically, if t were reversed in sign, all motions would simply reverse exactly, and the particles would retrace their previous paths. Since magnetic forces are proportional to $\mathbf{v} \times \mathbf{B}$, all magnetic fields would have to be reversed in direction under this time reversal in order to have the particles retrace their paths. This would in fact occur, since the currents and spins which are the sources of magnetic fields would all reverse direction.

Another way to state this property of time reversibility is that, for any solution of the equations of motion, another solution exists in which all particles have exactly the opposite velocities, so that they all execute the reverse motions.

Likewise in quantum mechanics, the change of probability density with time would exactly reverse if the sign of the time were reversed, and there exists a motion of the system in which all velocities would correspondingly be reversed. While time cannot be reversed in the laboratory, one can obtain the equivalent result by simply reversing all velocities and hence all magnetic fields. Many experiments have shown that for the usual forces, this principle of time reversibility is valid.

On the other hand, macroscopic systems in general show a type of behavior which is irreversible. For example, a rock dropped into a still pool of water will cause a splash, a succession of circular outgoing waves and turbulence in the water as the rock sinks to the bottom; and after some time a slight increase in the temperature, or heat content, of the water will occur. Although the time-reversed motion-in which a rock at the bottom of a still pool is thrown up into somebody's hand by turbulence and ingoing waves with a resultant cooling of the water-is a possible solution of the equations of motion, it is never observed because of the overwhelmingly small probability of its occurrence. Situations of thermal equilibrium are, however, situations of relatively high probability.

We may illustrate this by considering a container of an ideal gas containing

$N = 10^{23}$ particles. At thermal equilibrium, the particles are randomly distributed in position throughout the box. An example of o nonequilibrium situation might be one in which more particles were in the lefthand half of the box than in the righthand half. We can easily calculate the probability of any distribution of particles between the two halves of the box using the analogy that the probability of finding one particle in, say, the left half is the same os the probability of occurrence of a head in one flip of a fair coin. The probability of finding n particles in the left half of the box is therefore given by the binomial probability distribution, Equation (2.13). and is

$$P_N(n) = \frac{N!}{n!(N-n)!}\frac{1}{2^N}$$

If $N = 10^{23}$, we can certainly use the gaussian approximation for $P_N(n)$ given in Equation (2.53):

$$P_N(n) = \sqrt{\frac{2}{N\pi}}\exp\left[\frac{-(n-N/2)^2}{N/2}\right]$$

Now we can ask, for example, what is the relative probability of finding a macroscopically significant excess of, say, 0.01% of the particles, or $n = 0.5001 \times 10^{23}$ particles, n the left half of the box? The ratio of this probability to that of finding half of the particles on each side is

$$\frac{P_{10^{23}}(0.5001 \times 10^{23})}{P_{10^{23}}(0.5 \times 10^{23})} = \frac{\exp[-(0.0001 \times 10^{23})^2/(N/2)]}{\exp[-(0)^2/(N/2)]}$$

$$= \exp(-2 \times 10^{-8} \times 10^{23}) = \exp(-2 \times 10\text{’:‘})$$

Such an excess would therefore never be observed.

A corollary of this is that if an initial state were artificially created in which there was an excess of particles on one side, such as by injecting particles through a hole in the container wall, then after a short time, due to collisions with the walls, the particles' positions would become randomized, and all positions would become equally probable. The system's apparently irreversible behavior thus consists of an evolution from a nonequilibrium state, of low a priori probability, to a state of thermal equilibrium, which is of much higher a priori probability.

summary

SIX DIMENSIONAL PHASE SPACE

Phase space is a six dimensional space whose coordinates are x, y, z, p_x, p_y, and p_z. The position and momentum of a single particle at a given instant may be represented by a point in phase space. A large number of particles, each represented by a point in phase space, gives rise to a cloud of such points, whose density may be approximated by a continuous distribution function $f(\mathbf{r}, \mathbf{p}, t)$. The number of particles whose representative points are to be found within the volume element $d\Omega = dxdydzdp_xdp_ydp_z$ is equal to $f(\mathbf{r}, \mathbf{p}, t)\, dxdydzdp_xdp_ydp_z$. This results from the assumption that the number of states in $d\Omega$ is proportional to $d\Omega$.

MAXWELL-BOLTZMANN DISTRIBUTION

For a system of weakly interacting particles, or for a number of systems in thermal contact, the distribution function at equilibrium is proportional to $e^{-\beta E}$, where E is the energy of a particular system and $\beta = 1/k_BT$ with k_B the Boltzmann constant and T the absolute temperature. For N particles, each of mass m and energy $E = \frac{1}{2}mv^2$, in a box of volume V, the normalized expression for $f(\mathbf{r}, \mathbf{p})$ is

$$f(\mathbf{r},\mathbf{p}) = f(\mathbf{p}) = \frac{N}{V}\left(\frac{1}{2\pi m k_B T}\right)^{3/2} \exp\left(\frac{-\frac{1}{2}\beta p^2}{m}\right)$$

DISCRETE ENERGIES

If the particles of a system can have only the discrete energies $E_1, E_2, \ldots E_i, \ldots$ then at equilibrium the probability of finding a particle with the energy E_i is proportional to $e^{-\beta E_i}$. The average of any function of energy, $\chi(E)$, is then computed by the formula:

$$\langle \chi \rangle = \frac{\sum_i \chi(E_i)\, e^{-\beta E_i}}{\sum_i e^{-\beta E_i}}$$

MOMENTUM AND ENERGY A!; INDEPENDENT VARIABLES

If the magnitude of the momentum is considered to be an independent variable, then for an ideal gas the number of particles whose momenta are in the range dp is F(p) dp, where F(p) is proportional to $p^2 \exp(-\frac{1}{2}\beta p^2/m)$. If the energy E is considered as independent, then the number of particles whose energies are between E and $E + dE$ is $g(E)\, dE$, where $g(E)$ is proportional to $\sqrt{E}\, e^{-\beta E}$.

EQUIPARTITION OF ENERGY

For a system in equilibrium whose single-particle energies are a sum of M quadratic terms in any of the phase-space coordinates, the average energy per particle is $\frac{1}{2}Mk_BT$. Thus, associated with each quadratic term is an average energy of $\frac{1}{2}k_BT$ per particle.

DETAILED BALANCE

At equilibrium, the number of particles per unit time making transitions from a region $d\Omega_1$ to a region $d\Omega_2$, is equal to the number making transitions from region $d\Omega_2$ to region $d\Omega_1$, provided $d\Omega_1 = d\Omega_2$.

problems

1. Consider the air inside a closed automobile as it travels at a velocity $\mathbf{u}$. The air is at rest relative to the automobile. What is the velocity distribution relative to an observer on the ground? (Neglect gravity.)

   Answer: The Boltzmann factor is exp $\left[\frac{-\frac{1}{2}m(\mathbf{v}-\mathbf{u})^2}{k_BT}\right]$.

2. If the automobile in Problem 1 had an acceleration a, ond the gravitational force $m\mathbf{g}$ acted, what would be the form of the distribution function f (r, p, f)?

   Answer: The Boltzmann factor is

$$\exp\left[\frac{-\frac{1}{2}(\mathbf{p}-m\mathbf{u})^2}{mk_BT}\right]\exp\left[-m(\mathbf{a}-\mathbf{g})\cdot\frac{\mathbf{r}}{k_BT}\right].$$

3. Consider a beach of approximately 1 km^2 area, covered with grains of sand, whose moss is approximately 10^{-4} gm and whose top layer covers the beach at a density of 15 grains/mm^2. Assuming the temperature is 27°C, how many grains of sand on the beach could you expect to see at any one time at a height of 1 mm or more above the level of the beach, assuming the grains are in thermal equilibrium?

   Answer: Approximately exp (-2.4×10^{11}) grains, or effectively none.

4. A particle in a system of weakly interacting particles has energy $E = \frac{1}{2}mv^2 + K(x^4 + y^4 + z^4)$, where K is a positive constant. For what temperature will the average potential energy be $1\frac{1}{2}$ times os great as at 20°C? To solve this you do not need to know explicitly what the integrals equal.

   Answer: 167°C.

5. N smoke particles, each of mass m, are floating in air inside a closed vertical tube of length L and cross sectional area A. Assuming that ot equilibrium the particles at the bottom are far apart compared to their size, find the number of particles per unit volume at height h from the bottom, for gravitational potential energy mgh and temperature T. Find the average height of the particles.

   Answer: $\frac{Nmg}{Ak_BT}\frac{e^{-mgh/k_BT}}{(1-e^{-mgL/k_BT})}$, $\frac{k_BT}{mg} \quad \frac{L}{e^{mgh/k_BT} \quad 1}$

6. N charged smoke particles, each of mass m, are floating in air of temperature T, inside a conducting coaxial cylinder of inner radius a, outer radius b, and length L. The inner cylinder is charged so that the particles have potential energy C ln (r/a), where C is o constant and r is the distance from the cylindrical axis. Assuming that at equilibrium all the particles are far apart compared to their size, find the number of particles per volume at distance r from the axis.

Answer: If $\gamma = C/k_BT$, $n = N\frac{2-\gamma}{2\pi L}\frac{r^{-\gamma}}{b^{-\gamma+2} - a^{-\gamma+2}}$

7. Show that for a Boltzmann distribution,

$$E = \frac{(-d/d\beta \sum_n e^{-\beta E_n})}{\sum_n e^{-\beta E_n}} \quad \text{evaluated at} \quad \beta = \frac{1}{k_BT}$$

or

$$\frac{(-d/d\beta \int e^{-\beta E} f(E)\, dE)}{\int e^{-\beta E} f(E)\, dE} \quad \text{evaluated at } \beta = \frac{1}{k_BT}$$

8. From the result of Problem 7, find the average kinetic energy of a particle in an ideal gas.
Answer: $\frac{3}{2} k_BT$.

9. A "quantum mechanical" one dimensional oscillator has discrete rather than continuous energies, $E_n = (n + \frac{1}{2})\hbar\omega$, where $\omega = \sqrt{K/m}$, $\hbar$ is a constant and $n = 0, 1, 2, .$ From the result of problem 7, show that for a system of weakly interacting oscillators the average energy per oscillator is

$$\langle E\rangle = \hbar\omega\left[\frac{1}{e^{\hbar\omega/k_BT} - 1} + \frac{1}{2}\right]$$

Use the fact that if $a < 1$, $\sum_{n=0}^{\infty} a^n = 1/(1 - a)$ and use $a = e^{\hbar\omega/k_BT}$.

10. From the result of Problem 9, find the heat capacity of a system of N one dimensional harmonic oscillators as a function of T. Plot this versus T up to $T = 4\hbar\omega/k_B$. Also plot the specific heat of a one dimensional classical oscillator on the same graph. (The three dimensional oscillator was discussed in the text.)
Answer: $\frac{d\langle E\rangle}{dT} = (\hbar^2\omega^2 k_BT^2)\frac{\exp(\hbar\omega/k_BT)}{(\exp(\hbar\omega/k_BT) - 1)^2}$

11. In addition to its kinetic energy, a free electron in a magnetic field B has two possible energies, $\pm\mu B$, depending on whether the intrinsic angular momentum, or spin, of the electron is in the same or the opposite direction of B. Here μ is the magnetic moment of the electron, a constant. For an electron weakly interacting with the rest of the system, find what the probability is for an electron spin to be pointing in the direction of the magnetic field. Find the average magnetic interaction energy.
Answer: $e^{\mu B/kT}/(e^{\mu B/kT} + e^{-\mu B/kT})$; $-\mu B(e^{\mu B/kT} - e^{-\mu B/kT})/(e^{\mu B/kT} + e^{-\mu B/kT})$.

12. Suppose a particle in a system had only two possible energies, $E = 0$ and $E = \epsilon > 0$. If the system is in equilibrium at temperature T, what is the average energy per particle?
Answer: $\langle E\rangle = \epsilon e^{-\beta\epsilon}/(1 + e^{-\beta\epsilon})$.

13. Make a sketch of the distribution function $f(p_x)$ for positive p_x for an ideal gas, where $f(p_x)\, dp_x$ is the probability that a particle is between p_x and $p_x + dp_x$.

14. Find the root mean square deviation of the energy of a particle of an ideal gas from the average energy at temperature T. Find the ratio of this root mean square deviation to the average energy of the particle.
Answer: $\sqrt{3/2}\, k_BT$, $\sqrt{2/3} = 0.816$.

15. Find the root mean square deviation of v from its average for a particle of an ideal gas at temperature T if the gas particles have mass m.

Answer: $\sqrt{(3-8/\pi)\,k_BT/m}$.

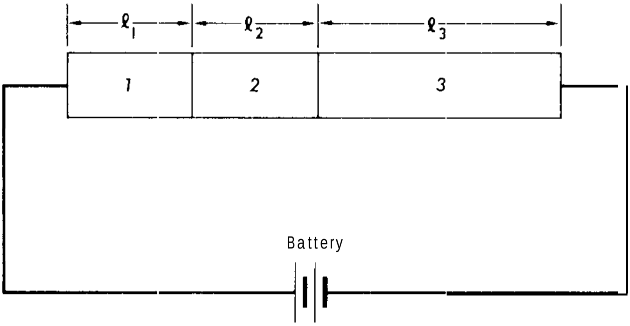
16. At what temperature would the average speed of atoms in an ideal gas be $1\frac{1}{2}$ times as great as at 20°C? At what temperature would the average kinetic energy be 1% times as great as at 20°C?
Answer: 386°C, 166°C.

17. Calculate the average value of $1/v$ in an ideal gas at temperature T.
Answer: $\sqrt{2m/\pi k_BT}$.

18. The molecular weight of O_2 is 16 times that of H_2. In a mixture of H_2 and O_2, what is the ratio of rms speeds of O_2 and H_2?
Answer: ¼.

19. Find the root mean square deviation of v_x from its average for a particle of an ideal gas at temperature T if the gas particles have mass m.
Answer: $\sqrt{k_BT/m}$.

20. In the diagram regions 1, 2 and 3 are three semiconducting solid rods of the same cross sectional area separated by thin insulating films, so that there are changes in electric potential between the two sides of each of the films. Thus, conducting electrons are in regions of three different potential energies in the three semiconductors. If the potential changes at the films are 0.02 volts and 0.01 volts, the potential energies are approximately $V_1 = 0$, $V_2 = 3.2 \times 10^{-21}$ joules, $V_3 = 4.8 \times 10^{-21}$ joules. Assuming the electrons act as an ideal gas, find the ratio of the numbers of conducting electrons in regions 2 and 3 to those in region 1 for $\ell_2 = \ell_1$, $\ell_3 = 2\ell_1$ at 20°C.



Answer: 0.46; 0.63.

21. If the energy as a function of momentum of a particle depended on $ap_z^2 + b(p_x^2 + p_y^2)$, it might be useful to express differential volume in cylindrical coordinates in momentum space, p_z and $p_{xy} = \sqrt{p_x^2 + p_y^2}$. Here p_{xy} is the perpendicular "distance" from the p_z axis. Show that this volume element is $2\pi\, p_{xy}\, dp_{xy}\, dp_z$. An energy depending on momentum this way occurs in some semiconducting solids.

22. We saw that if energy depends on momentum magnitude only, it is useful to use $4\pi p^2 dp$ as the volume element in momentum space, and that nonrelativistically in terms of energy, $E = p^2/2m$, this becomes $2\pi\sqrt{2m^3}\sqrt{E}\,dE$. Using the relativistic relationship between momentum and energy, show that this element of volume in momentum space becomes $4\pi\sqrt{E^2 - m_0^2c^4}\,E\,dE/c^3$. Also show that in terms of kinetic energy, $T = E - m_0c^2$, this is $4\pi\sqrt{T(2m_0c^2 + T)}(m_0c^2 + T)\,dT/c^3$. This becomes $2\pi\sqrt{2m_0^3}\sqrt{T}\,dT$ for $T \ll m_0c^2$.

23. A nucleus can decay, giving off a high energy electron, of rest mass m_0 with energy E and a neutrino of zero rest mass. In many cases, the probability of decay depends only on the magnitudes of the particle momenta so the results of the previous problem can be used. Show that if the sum of the neutrino and electron energies is a constant, E_0, so that the neutrino energy is $E_0 - E$, and if the probability of each particle having a given energy is proportional to volume in phase space, the probability that an electron has an energy between E and $E + dE$ is proportional to $\sqrt{E^2 - m_0^2c^4}\,E(E_0 \quad E)^2\,dE$. The fact that many experimental electron decay distributions follow this equation extremely well leads to proof that the neutrino, which is very difficult to detect, is given off with the electron.

24. Consider a box containing a gas, in which the potential energy of a particle varies from one end of the box to another according to $V = V_0x/L$, where L is the length of the box. What fraction of the particles are in the half of the box for which $\frac{1}{4}L \leq x \leq \frac{1}{2}L$?

Answer: $\dfrac{1}{e^{1/4V_0\beta} + e^{-1/4V_0\beta}}$.

25. For a system of three dimensional classical harmonic oscillators, as discussed in the text, find the root mean square deviation of the energy from the average for one of the oscillators.

Answer: $\sqrt{3}\,k_BT$.

26. Particles of mass 6.2 x 10^{-14} gm are suspended in liquid at 27°C. What should be their rms speed? (Use equipartition)

Answer: 1.4 cm/sec.

27. Colloidal particles in solution are buoyed up by the liquid in which they are suspended by a force equal to the weight of the liquid they displace. Show that the number of particles per unit volume in the liquid varies with height as

$$n = n_0 \exp\left[\frac{-N_0}{RT}V(\rho \quad \rho')gh\right]$$

where N_0 is Avogadro's number, n_0 is the number per unit volume at h = 0, V is the volume of a particle, ρ' is the liquid density, and ρ is the mass per unit volume of the colloidal particles.

11 quantum statistical mechanics

A number of the results obtained in Chapter 10 concerning classical statistical mechanics of a system of particles are still valid when quantum mechanics, rather than classical mechanics, is used to describe the particles. For example, the Boltzmann factor, $e^{-\beta E}$, was found by considering a number of systems in thermal equilibrium, and by assuming that the probability of a system's being in a given state is a function only of the energy of the state and the common temperature. These same assumptions can still be made for large quantum systems. In the classical discussion, β was found to be $1/k_BT$ by evaluating the energy for a classical ideal gas and comparing with the kinetic theory result. This can still be done if it is assumed that the quantum system to be investigated is in equilibrium with at least one classical ideal gas system. Once β is evaluated, it does not matter whether or not the actual system is really in thermal equilibrium with a classical ideal gas. Thus, even for a large quantum system in thermal equilibrium with other systems, the probability that the system is in a state of total energy E is proportional to e^{-E/k_BT}.

How, then, does quantum mechanics change statistical mechanics? There are two main effects of quantum mechanics. First, there are often discrete energy states in quantum mechanics so that, in addition to an integral over phase space for continuous states, there may also be a summation over discrete states in finding average values of quantities. Second, the indistinguishability of particles in quantum mechanics can affect the statistics greatly, especially when we look at the energy distribution of one of the single particles in a system of identical particles. Here the particle itself cannot be treated as an independent system, as was done in the classical case. For a system of identical fermions, this effect can be treated as a consequence of the exclusion principle: no two identical fermions in a system can be described by the same set of quantum numbers. For a system of identical bosons, the effect is quite different; there is, instead, a slight tendency for the particles to collect in states described by the same quantum numbers.

I.1 EFFECTS OF EXCLUSION PRINCIPLE ON STATISTICS OF PARTICLES

In the classical case of a system of identical particles, it was assumed that even identical particles were distinguishable, and that the overall state of a system could be specified by giving the single-particle state of each particle-for example, by specifying the particle's representative point in phase space. However, as has been seen in the discussion of the exclusion principle, for identical particles the wavefunction specifying the overall state is such that each particle appears equally in all the occupied single-particle states. Hence, the state of a system of identical particles may be specified by giving the number of particles in each single-particle state but not which particles are in each state.

This follows because in interchanging particles, the magnitude of the square of the wavefunction does not change; otherwise, the particles would be distinguishable. Then when two bosons, or particles of integral spin, are interchanged, the wavefunction itself remains unchanged. When two fermions, particles of half-odd-integral spin, are interchanged, the wavefunction changes sign. Thus for half-odd-integral spin, there are either no particles or at most one particle in any given single-particle state, while for integral spin particles, any number of particles from zero to infinity may occupy a given single-particle state.

In the case of a system of fermions, since the number of particles in a single-particle state is limited to 0 or 1, the single-particle distribution in energy will differ from the classical Maxwell-Boltzmann distribution.

1 .2 DETAILED BALANCE AND FERMI-DIRAC PARTICLES

We may use the principle of detailed balance to find this distribution. Consider the transitions between states 1 and 2 in a fermion system. In order for thermal equilibrium to be maintained, the average transition rate from 1 to 2 must be the same as the average transition rate from 2 to 1, by the principle of detailed balance. Here the term "transition rate" means the number of particles making transitions per second. The exclusion principle strongly affects these transition rates; for example, if we begin with one particle in state 1 and one particle in state 2, it is impossible for the particle in state 1 to make a transition to state 2: if it were not, there would then be two particles in state 2, which is a violation of the exclusion principle. Transitions between two single-particle states can occur only when, before the transition, the initial state is occupied by one particle and the final state is empty. Actually, the number of particles in a given state may fluctuate considerably in time, because of the large variety of possible transitions between that state and all other states. Hence, there will exist some probability that a state is occupied. Because the maximum number of fermions in a state is unity, like the maximum possible probability, the probability that a state is occupied will be identical to the time-averaged number of particles in the state. Thus, the probability that state 1 is occupied will be the same as $\bar{n}_1$, where the bar denotes the time average of the number of particles n_1 in state 1. The probability that state 2 is occupied will be the same as $\bar{n}_2$, the time average of the number of particles n_2 in state 2. The probability that state 2 is unoccupied will therefore be $1 - \bar{n}_2$.

Let $p_{1\to2}$ be the transition probability per unit time that, given exactly one particle in state 1 and zero particles in state 2, a transition from state 1 to 2 will occur. Similarly, let $p_{2\to1}$ be the transition probability for a transition from 2 to 1 per unit time, given state 2 is occupied and state 1 is unoccupied.

We may now use the rules for combining probabilities given in Equation (2.2) to obtain the transition rate. The probability of occurrence of a transition from state 1 to state 2 must be equal to the product of the probabilities that state 1 is occupied, that state 2 is unoccupied, and that a tronsition occurs; or the transition rate must be

$$\bar{n}_1(1 - \bar{n}_2)p_{1\to2}$$

Similarly, the number of particles per second making transitions from state 2 to state 1 must be

$$\bar{n}_2(1 - \bar{n}_1)p_{2\to1}$$

On the average, for the system to remain in thermal equilibrium, the above two transition rates must be equal, by the principle of detailed balance. The mathematical equality can be expressed as follows:

$$\bar{n}_1(1 - \bar{n}_2)p_{1\to2} = \bar{n}_2(1 - \bar{n}_1)p_{2\to1} \tag{11.1}$$

From Equation (10.81), the ratio of $p_{2\to1}$ to $p_{1\to2}$ in the classical case is

$$\frac{p_{2\to1}}{p_{1\to2}} = e^{(E_2 - E_1)/k_BT} \tag{11.2}$$

where E_1 and E_2 are single-particle energies. The ratio of the transition probabilities $p_{1\to2}$ and $p_{2\to1}$ in the quantum case should be the same as in the classical case, since they are defined for conditions in which only one particle is present in the initial state. Thus the effects of particle exchange are unimportant and Equation (11.2) is still valid. Therefore, combining Equations (11.1) and (11.2) and rearranging, we obtain

$$\frac{\bar{n}_1}{1 - \bar{n}_1}e^{E_1/k_BT} = \frac{\bar{n}_2}{1 - \bar{n}_2}e^{E_2/k_BT} \tag{11.3}$$

On the left side of the above equation is a combination of functions depending only on state 1, and on the right is a combination depending only on state 2. Therefore, both sides of Equation (11.3) must be equal to a constant, independent of the state, and hence independent of the energy of the state:

$$\frac{\bar{n}_1}{1 - \bar{n}_1}e^{E_1/k_BT} = \text{Const.} = \frac{\bar{n}(E)}{1 - \bar{n}(E)}e^{E/k_BT} \tag{11.4}$$

1.3 FERMI ENERGY AND FERMI-DIRAC DISTRIBUTION

It is convenient to write the constant in this equation, which must be a positive number, by introducing a quantity called the *Fermi* energy, E_F. In terms of E_F, the constant in Equation (11.4) is:

$$\text{Const.} \equiv e^{E_F/k_BT} \tag{11.5}$$

This equation constitutes a definition of the constant, E_F, which, in general, is a function of temperature. Substituting the constant into Equation (11.4) and solving for the time-averaged occupation number $\bar{n}(E)$, we find:

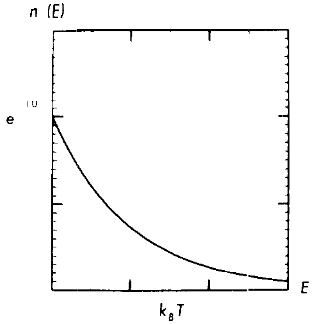
$$\bar{n}(E) = \frac{1}{e^{(E-E_F)/k_BT} + 1} \tag{11.6}$$

This distribution function is called the *Fermi-Dirac* distribution. The additive 1 in the denominator is what distinguishes it from the Maxwell-Boltzmann distribution. The Maxwell-Boltzmann distribution for single particles was valid in the classical case, because with noninteracting particles, each particle could be treated as a single system. For particles where the exclusion principle applies, even though there may be no forces of interaction, the particles affect each other statistically and single particles cannot be treated as single systems. Thus the Maxwell-Boltzmann distribution is not valid for fermion systems.

The form of the Fermi-Dirac distribution depends critically on the magnitude of the exponential function, e^{-E_F/k_BT} appearing in the denominator. This function is independent of the energy of the state and plays the role of a normalization constant. Hence, if the total number of fermions in the system is N, then at a given temperature the Fermi energy will be determined by the condition that

$$N = \sum_i \bar{n}_i = \sum_i \left\{ \exp\left[\frac{(E_i - E_F)}{k_BT}\right] + 1 \right\}^{-1} \tag{11.7}$$

where the summation is taken over all distinct single-particle states labeled by the index i.



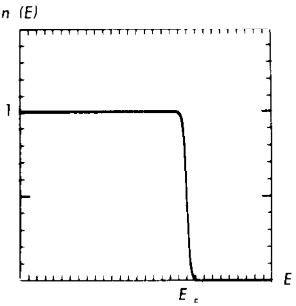


Figure 11.1. **Graph of the Fermi-Dirac distribution function in the nondegenerate case,** E = $-10k_BT$.

Figure 11.2. Graph of the Fermi-Dirac distribution function in the degenerate case, $E = +100k_BT$.

Under some conditions, the Fermi-Dirac distribution closely resembles the Maxwell-Boltzmann distribution. For example, in Figure 11.1 is plotted the average occupation number $\bar{n}(E)$ for the case $E_F = -10k_BT$. The function is substantially just a Maxwell-Boltzmann distribution, since the exponential in the denominator is much greater than unity. On the other hand, if $E_F = +100k_BT$, the function has a completely different character; the Fermi-Dirac distribution for this case is plotted in Figure 11.2. Here all the states are filled up to an energy approximately equal to E_F, and all the states of greater energies are almost empty.

11.4 ONE DIMENSIONAL DENSITY OF STATES FOR PERIODIC BOUNDARY CONDITIONS

In the case graphed in Figure 11.1, with the Fermi energy negative and $E_F \ll -k_BT$, we say that the statistics are nondegenerofe; this case resembles the Maxwell-Boltzmann distribution. In the case of positive Fermi energy with $E_F >> k_BT$, as in Figure 11.2, we say the statistics are degenerate. Which of these cases actually applies in a given system depends on the number of particles, the number of possible states per unit energy interval, and on the temperature. In classical statistical mechanics, the number of possible states could not be calculated; information about the distribution of states was obtained by postulating that the states were uniformly distributed in phase space. Using quantum mechanics, we can calculate from fundamental principles what the distribution of possible states must be.

To derive the number of states per unit energy interval, which is called the density of states, we consider first a problem closely related to the problem of a particle in a one dimensional box. There, the possible wavelengths were limited by the condition that an integral number of half-wavelengths must fit into the box. We consider instead the one dimensional free particle wavefunction, written in the form:

$$\psi = \exp\left[i(kx - \omega t)\right] \tag{11.8}$$

where the wavenumber is related to momentum by $k = p/\hbar$, and the frequency is related to energy by $\omega = E/\hbar$. We then impose the artificial periodic boundary condition that

$$\psi(x + L) = \psi(x) \tag{11.9}$$

where L is some extremely large, but arbitrary length. We will eventually allow L to approach infinity, so that the particular boundary condition imposed is of no importance; that is, for a system of many particles the boundary conditions should affect the system only in the neighborhood of the boundary and should have negligible effect in the interior of the system. The wavefunctions ψ correspond to single-particle states in which the momentum of the particle is completely known and the position is unknown. Thus, if we use free-particle momentum eigenfunctions to describe the single-particle states of the system, it no longer makes sense to talk of phase space in the classical sense, for specification of the particle's momentum and position at the same time would violate the uncertainty principle.

The boundary condition, Equation (11.9), gives us

$$\exp i[k(x+L) - \omega t] = \exp i(kx - \omega t) \qquad (11.10)$$

This condition then means that

$$\exp ikL = 1 \qquad (11.11)$$

In general, $e^{i\theta} = 1$ only if $\theta = 2\pi n$, where n is any integer. Therefore, the boundary condition limits the possible wavenumbers to the set of values:

$$k = \frac{2n\pi}{L} \qquad (11.12)$$

where n = 0, $\pm 1, \pm 2, \pm 3, \ldots$. This is the same as saying that an integral number of wavelengths must fit into the large length L.

Since $p = \hbar k$, the possible values of p are given by:

$$p = \frac{2\pi\hbar}{L} n = \frac{hn}{L} \qquad (11.13)$$

and the corresponding particle positions must be completely undetermined. Therefore, instead of a "phase space" consisting of one axis for x and one for p, we can specify all the possible single-particle states by drawing only one axis, the p axis, and labeling the discrete set of points given by Equation (11.13) with its corresponding set of quantum numbers n, as in Figure 11.3. These states are uniformly distributed in momentum space along the p axis in this case. As the length L approaches infinity, the possible states become more and more densely packed in momentum space, but still form a discrete set.

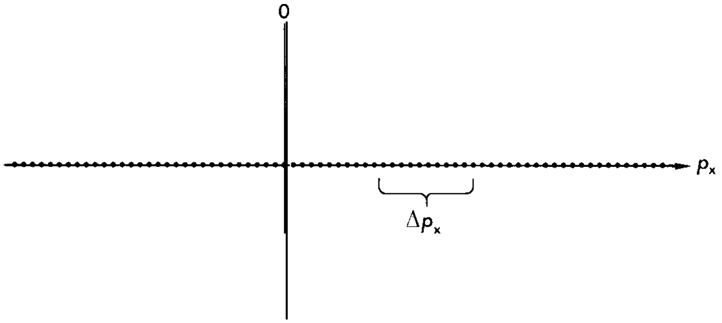


Figure 11.3. Discrete states for a free particle with periodic boundary conditions are uniformly distributed along the momentum axis. Positions along the x axis are undetermined.

Now consider, for some extremely large L, a physical region along this momentum axis of length Δp. In this region as we see from Equation (11.13), there will be a number of momentum states An given by:

$$\Delta p = \frac{h}{L}\Delta n \tag{11.14}$$

The number of states per unit momentum interval is thus $\Delta n/\Delta p$ = L/h. Note that the density of states in momentum space, $\Delta n/\Delta p$, is proportional to L, the length of the periodicity region; this is consistent with the classical idea that states are uniformly distributed in x − p space. We can divide out the factor of L and speak about the number of states per unit momentum interval **per unif** *length,* which will be l/h. In the limit as L approaches infinity, the boundary condition becomes irrelevant, so that this result is completely general.

11.5 DENSITY OF STATES IN THREE DIMENSIONS

We may generalize this result for the one dimensional motion of a particle, to the case of three dimensional motion, by considering the free-particle momentum eigenfunction:

$$\psi(x,y,z,t) = \exp\,[i(k_x\,x + k_y\,y + k_z\,z - \omega t)] \tag{11.15}$$

We assume that periodic boundary conditions are imposed in the x, y and z directions, such that:

$$\psi(x,y,z,t) = \psi(x+L,y,z,t) = \psi(x,y+L,z,t) = \psi(x,y,z+L,t)$$

Then all three components of the wavevector, and hence of the momentum, are quantized similarly. Thus,

$$\begin{aligned} p_x &= \frac{h}{L}n_x \quad n_x = 0, \pm 1, \pm 2, \ldots \\ p_y &= \frac{h}{L}n_y \quad n_y = 0, \pm 1, \pm 2, \ldots \\ p_z &= \frac{h}{L}n_z \quad n_z = 0, \pm 1, \pm 2, \ldots \end{aligned} \tag{11.16}$$

The possible states form a cubical array of points in three dimensional momentum space, (p_x, p_y, p_z). One single-particle state may be specified by giving all three components of the momentum or, equivalently, all three quantum numbers, n_x, n_y, n,. The distance in momentum space, parallel to any one of the axes from one state to the next, is **h/L.** Hence, we can imagine momentum space to be filled up with cubes of side *h/l,* and there will effectively be one possible momentum state per cube, or a volume of $(h/L)^3$ per state.

To put this another way, consider a volume element in momentum space of sides Δp_x, **Ap,,,** and $\Delta p_{:}$. The number of states in this volume element is

$$\Delta n_x\,\Delta n_y\,\Delta n_z = \left(\frac{L}{h}\right)^3 \Delta p_x\,\Delta p_y\,\Delta p_z \tag{11.17}$$

which is the momentum space volume divided by the volume per state. The quantity L^3 in this result could be replaced by V, the volume of the fundamental periodicity region. Since the number of states is proportional to V, then as L approaches infinity and thus V approaches infinity, the number of states in the volume element $\Delta p_x \, \Delta p_y \, \Delta p_z$ will increase without limit. We can then divide out the factor V and speak of the density of states in momentum space per unit volume. This density of states will be $1/h^3$.

ple For a macroscopic system of electrons at room temperature, with dimensions 1 cm on a side, the spacing between energy levels corresponding to a change of 1 in one of the quantum numbers n_x, n_y, n_z is

$$\Delta E = \Delta\left(\frac{p_x^2}{2m}\right) = \left(\frac{h}{L}\right)^2 \frac{[(n_x + 1)^2 - n_x^2]}{2m}$$

$$\simeq \frac{h^2 n_x}{mL^2} \quad \text{if} \quad n_x \gg 1$$

At room temperature, the electrons will, on the average, have at least the energy $k_B T \simeq .02 \text{ eV} \simeq p_x^2/2m = h^2 n_x^2/2mL^2 \sim E$. Then

$$n_x \simeq \frac{L}{h}\sqrt{2mE}$$

$$= \frac{10^{-2}}{6.6 \times 10^{-34}} \sqrt{2 \times 9 \times 10^{-31} \times (0.02 \times 1.6 \times 10^{-19})}$$

$$\simeq 10^6$$

The ratio of the energy spacing to the energy is then $\Delta E/E \sim 1/n_x \sim 10^{-6}$. Thus the energy states are packed so close together that it should be a very good approximation to pass to the limit in which the increments Δp_x, Δp_y, are replaced by differentials and summations over states are replaced by integrations.

Although for a real physical system, periodic boundary conditions may not apply, as long as the volume V of the system is sufficiently large the particular boundary conditions should not appreciably affect the density of states; therefore, to a very good approximation, the number of states in a momentum space volume element $dp_x \, dp_y \, dp_z$ should be given by

$$\Delta n_x \, \Delta n_y \, \Delta n_z = \frac{V}{h^3} \, dp_x \, dp_y \, dp_z \tag{11.18}$$

The density of states in momentum space is V/h^3.

.6 COMPARISON BETWEEN THE CLASSICAL AND QUANTUM DENSITIES OF STATES

In classical statistical mechanics, it is assumed that the number of states in the phase space volume element $d\Omega = dx\,dy\,dz \, dp_x \, dp_y \, dp_z$ is $\rho \, d\Omega$, where ρ is the unknown density of states in phase space. To compare this to the quantum mechanical result, Equation (11.18), we must integrate over all positions:

$$\frac{V}{h^3} dp_x\, dp_y\, dp_z = \left(\iiint \rho dxdydz\right) dp_x\, dp_y\, dp_z = {}^{\prime}V\rho\; dp_x\, dp_y\, dp_z \qquad (11.19)$$

Hence, the density of states in phase space must be

$$\rho = \frac{1}{h^3} \qquad (1.20)$$

It is at once clear why in classical theory the density of states could not be determined; energy quantization was unknown and Plcrnck's constant was effectively zero.

11.7 EFFECT OF SPIN ON THE DENSITY OF STATES

One further point must be mentioned in connection with the state density in Equation (1 1.20), which refers to the density of momentum states only. If, in addition, the particle described by the momentum eigenfunction in Equation (1 1.15) has an intrinsic spin, with a total spin quantum number s, then there will be 2s + 1 spin states for each momentum state. The total number of single-particle states in the momentum space volume dp, dp, dp, will then be

$$(2s+1)\; An,\; An,\; An, = \frac{(2s+1)V}{h^3} dp,\; dp,\; dp, \qquad (11.21)$$

One exception to this rule occurs for particles of zero rest mass. Study of the relativistic quantum theory of such particles shows that no matter what the total angular momentum quantum number is, only two spin "orientations" are possible. The component of angular momentum in the direction of the particle's momentum can be only $\pm s\hbar$, corresponding either to spin parallel to p or spin antiparallel to **p**. An erample of this appears in the case of photons, or light quanta, which are known to be bosons with spin quantum number $s = 1$. Electromagnetic theory shows that light waves are transverse, and have two possible states of circular polarization. A left circularly polarized light wave has a z component of angular momentum $+\hbar$, a right circularly polarized light wave has a z component of angular momentum $-\hbar$. Thus, for particles of zero rest mass, the total number of single-particle states in the momentum space volume element dp, dp, dp, will be

$$2\Delta n_x\; An,\; An, = \frac{2V}{h^3}\, dp,\; dp,\; dp_z \qquad (11.22)$$

11.8 NUMBER OF STATES PER UNIT ENERGY INTERVAL

It is frequently useful to know the number of states in the energy interval dE. When the energy E depends only on the magnitude of momentum, as it does for free particles, this number may be obtained by considering the states in a spherical shell of radius p and thickness dp, in momentum space. This was done in classical statistical mechanics [see Equation (10.64)], where it was shown that the spherical shell corresponds to an increment of energy dE given by

$$dp_x dp_y dp_z \rightarrow 4\pi p^2 dp = 2\pi(2m)^{3/2}\sqrt{E}\,dE \qquad (11.23)$$

The same expression holds in quantum statistical mechanics as well, if the energy momentum relation is $E = p^2/2m$.

The number of states between E and $E + dE$ for free particles of spin quantum numbers in a volume V is then:

$$(2s+1)\Delta n_x \Delta n_y \Delta n_z = (2s+1)2\pi V\left(\frac{2m}{h^2}\right)^{3/2}\sqrt{E}\,dE \qquad (11.24)$$

This is an important result, which will be used a number of times. The quantity multiplying dE, $(2s+1)2\pi V(2m/h^2)^{3/2}\sqrt{E}$, is called the ***density of states in*** energy. It is the number of single-particle states per unit energy interval.

.9 FREE-PARTICLE FERMI ENERGY--NONDEGENERATE CASE

The density of states derived above may now be used to find the Fermi energy E_F for various cases in which the particles can be treated as free particles. As a first example, consider a gas consisting of He^3, the isotope of helium with a nucleus containing two protons and a neutron. This isotope has spin ½, and thus it obeys the exclusion principle. The numerical value of the quantity $2s + 1$ is 2. It is known experimentally that ordinary gases at ordinary temperatures and pressures are described very well by Maxwell-Boltzmann statistics. Let us then assume that He^3 gas is nondegenerate under such conditions, so that E_F/k_BT must be negative, with $e^{-E_F/k_BT} >> 1$, and the Fermi-Dirac distribution function, Equation (11.6), may be approximated by:

$$\bar{n}(E) = \exp\left[\frac{-(E - E_F)}{k_BT}\right] \qquad (11.25)$$

We will check to see if this is a consistent assumption.

To determine the normalization constant, e^{E_F/k_BT}, we will follow a procedure similar to that used in the classical case. The number of states in the range $dp_x\,dp_y\,dp_z$ is $2V\,dp_x\,dp_y\,dp_z/h^3$. For this nondegenerate case, the number of particles N must be

$$N = \iiint_{-\infty}^{\infty} \frac{2V}{h^3}\exp\left[\frac{-(E - E_F)}{k_BT}\right] dp_x\,dp_y\,dp_z \qquad (11.26)$$

In terms of momentum, the energy for a free particle of energy E and mass m is $E = p^2/2m$. After substituting this into Equation (11.26), one may perform the integration by using the definite integral $\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\pi/\alpha}$. The result is

$$N = \frac{2V}{h^3}(2\pi m k_B T)^{3/2} e^{E_F/k_B T} \tag{11.27}$$

Therefore,

$$e^{E_F/k_B T} = \frac{N}{2V}\left(\frac{2\pi m k_B T}{h^2}\right)^{-3/2} \tag{11.28}$$

To check the self-consistency of this result, i.e. to see whether $e^{-E_F/k_B T} \gg 1$ as assumed, we may evaluate the righthand side of Equation (11.28) for He^3 at standard temperature and pressure, using the following values:

$$\begin{aligned} m &= 3 \times (1.67 \times 10^{-27} \text{ kg}) \\ T &= 273\text{K} \\ k_B &= 1.38 \times 10^{-23} \text{ j/K} \\ h &= 6.63 \times 10^{-34} \text{ j-sec} \end{aligned} \tag{11.29}$$

The particle density may be obtained from the fact that at standard temperature and pressure, one mole of a gas has a volume of 0.0224m^3 and contains Avogadro's number $N_0 \doteq 6.023 \times 10^{23}$ molecules. The result is

$$\begin{aligned} e^{E_F/k_B T} &\doteq \frac{6.02 \times 10^{23}}{2 \times .0224} \times \left(\frac{6.28 \times 5.01 \times 10^{-27} \times 1.38 \times 10^{-23} \times 273}{(6.63 \times 10^{-34})^2}\right)^{-3/2} \\ &\doteq 3 \times 10^{-6} \end{aligned} \tag{11.30}$$

This is much less than unity, so that in the Fermi-Dirac distribution,

$$\bar{n} = \left\{\exp\left[\frac{E - E_F}{k_B T}\right] + 1\right\}^{-1} \tag{11.31}$$

the exponential is always much greater than unity, justifying the approximation of nondegeneracy. Other atomic and molecular gases of half-odd-integral spin at standard temperature and *pressure* would give similar results, and thus would obey essentially Maxwell-Boltzmann statistics.

It should be noted that the result in Equation (11.28) is well-defined for a system of a given density, even when the volume V approaches infinity; for N/V is just the density of particles, and then both N and V approach infinity in a constant ratio.

In order for the gas to be degenerate, $e^{E_F/k_B T}$ should be at least comparable to unity. This occurs at such a low temperature that all atomic and molecular gases except helium are solidified, and even helium is liquified. The effect of degenerate Fermi-Dirac statistics of atoms on properties of solids is negligible, so the only substance in which degenerate statistics of atoms can be studied is liquid He^3. We can estimate the temperature at which effects due to degenerate statistics might begin to show up experimentally in He^3, by using the fact that the volume of one mole of liquid He^3 is about $2.5 \times 10^{-5} m^3$. Then, when $e^{E_F/k_BT} \simeq 1$, the temperature should be given by

$$1 \cong \frac{N_0}{2 \times 2.5 \times 10^{-5} m^3}\left(\frac{2\pi m k_B T}{h^2}\right)^{-3/2} \tag{11.32}$$

Taking for e^{E_F/k_BT} the value 3×10^{-6} calculated above at 273° and a molar volume of $0.0224 m^3$, we have

$$3 \times 10^{-6} = \frac{N_0}{2 \times .0224\ m^3}\left(\frac{2\pi m k_B 273}{h^2}\right)^{-3/2} \tag{11.33}$$

Therefore, dividing the first of these equations by the second and solving for T, we get

$$T \simeq 273 \times \left(\frac{.0224 \times 3 \times 10^{-6}}{2.5 \times 10^{-5}}\right)^{2/3} \cong 5.3K \tag{11.34}$$

This can be only an order of magnitude estimate, since a liquid will not act as a degenerate ideal gas because of the important effects of interparticle interactions. Also, expression (11.28), which is obtained assuming $e^{-E_F/k_BT} >> 1$, actually will not be valid at low temperatures, where e^{-E_F/k_BT} is comparable to unity.

10 FREE ELECTRONS IN METALS-DEGENERATE CASE

The most important case where Fermi-Dirac effects are large is that of electrons in metals. Here it is often a good approximation to treat the electrons as free noninteracting particles.

ple Assuming that nondegenerate statistics apply for electrons in a metal, at room temperature $T = 273K$, take $N/V \cong 10^{28}\ m^{-3}$, $m = 9 \times 10^{-31}$ kg, and calculate e^{E_F/k_BT} using Equation (11.28). Check the consistency of the result with the approximation, $e^{E_F/k_BT} << 1$.

ion For this case,

$$e^{E_F/k_BT} = \frac{10^{28}}{2} \times \left(\frac{6.28 \times 9 \times 10^{-31} \times 1.38 \times 10^{-23} \times 273}{6.63 \times 10^{-34}}\right)^{-3/2}$$

$$= 4.6 \times 10^{2}$$

This is much greater than unity, so the assumption that the statistics are nondegenerate must be wrong.

A much better approximation than that used in the above example would be to assume that:

$$\bar{n} = 1, \quad E < E_F$$

$$\bar{n} = 0, \quad E > E_F \tag{11.35}$$

as may be seen from Figure 11.2. In this case, E_F may be evaluated most easily by using the density of states given in Equation (11.24). Then, using the approximations given in Equation (11.35), the number of particles would be given by

$$N = \int_0^{E_F} 4\pi V\left(\frac{2m}{h^2}\right)^{3/2} \sqrt{E}\, dE \tag{11.36}$$

The integral $\int_0^x \sqrt{x}\, dx = \frac{2}{3} x^{3/2}$, leads to the result:

$$N = \frac{8\pi V}{3}\left(\frac{2mE_F}{h^2}\right)^{3/2} \tag{11.37}$$

and the Fermi energy is

$$E_F = \frac{h^2}{2m}\left(\frac{3N}{8\pi V}\right)^{2/3} \tag{11.38}$$

Again using the parameters $N/V = 10^{28}$, $m = 9 \times 10^{-31}$, E_F in electron volts is

$$\begin{aligned} E_F &= \frac{(6.63 \times 10^{-34})^2}{2 \times 9 \times 10^{-31}}\left(\frac{3 \times 10^{28}}{25.1}\right)^{2/3} \times \frac{1}{1.6 \times 10^{-19}\ \mathrm{j/eV}} \\ &= 2.7\ \mathrm{eV} \end{aligned} \tag{11.39}$$

At room temperature, $J = 273$ K, $k_BT = 0.024$ eV, so here $E_F \gg k_BT$; statistics are degenerate, and the approximation in Equation (11.35) should be a good one.

11.11 HEAT CAPACITY OF AN ELECTRON GAS

Because, in the degenerate case, the Fermi energy E_F is much greater than k_BT, and essentially all the states are filled up to the Fermi energy, it is to be expected that the average electron kinetic energy will be much larger than k_BT. Since the number of states in the energy interval dE is proportional to $\sqrt{E}\, dE$, and Equations (11.35) hold approximately, the expectation value of the kinetic energy per particle is

$$\langle E \rangle = \frac{\int_0^{E_F} \bar{n} E \sqrt{E}\, dE}{\int_0^{E_F} \bar{n} \sqrt{E}\, dE} \tag{11.40}$$

with $\bar{n} = 1$ up to E_F. These integrals may be evaluated as follows:

$$\int_0^{E_F} E^{3/2} dE = \frac{2}{5} E_F^{5/2}; \quad \int_0^{E_F} E^{1/2} dE = \frac{2}{3} E_F^{3/2} \tag{11.41}$$

Then

$$\langle E\rangle = \frac{2E_F^{5/2}/5}{2E_F^{3/2}/3} = \frac{3}{5}E_F \qquad (11.42)$$

This is on the order of several electron volts, much greater than k_BT at room temperature. On the other hand, classical statistical mechanics would have given an average kinetic energy of $3k_BT/2$, by the theorem of equipartition of energy.

To calculate the heat capacity of the electron gas, the actual dependence of ii(E) on temperature must be taken carefully into account, so that the average energy per particle can be calculated more accurately. When this is done the average energy per particle is found to be:

$$(E) = \frac{3}{5}E_{F_0}\left[1 + \frac{5\pi^2}{12}\left(\frac{k_BT}{E_{F_0}}\right)^2 + \text{Order of } (k_BT/E_{F_0})^4 + \cdots\right] \qquad (11.43)$$

where E_{F_0} is the Fermi Energy calculated in Equation (11.38), the Fermi energy at zero temperature.

The total energy in a mole of electrons is then $N_0\,(E)$, where N_0 is Avogadro's number. The heat capacity per mole, at constant volume, is just the derivative of N,(E) with respect to temperature and is

$$C_V = \left(\frac{\pi^2 k_BT}{2E_{F_0}}\right)R \qquad (11.44)$$

where we have used the expression for the gas constant, $R = N_0k_B$. On the other hand, the classical heat capacity is $C_V = 3R/2$.

Thus, the heat capacity of an electron gas is reduced by the effect of statistics, by a factor of the order of magnitude $k_BT/E_{F_0} \sim 0.01$ at room temperature. This can be understood qualitatively by noting that for heat to be absorbed by the system, the electrons must make transitions from lower occupied states, to higher empty states. Since the thermal energy available for one electron is about k_BT, only electrons with energies within about k_BT of the Fermi energy can change their states when heat is added to the system. The fraction of the electrons in this region of energy is of order of magnitude k_BT/E_{F_0}. Thus, one would expect a reduction of the heat capacity by about this factor. At ordinary temperatures, the electronic heat capacity is negligible compared to other contributions to the heat capacity in metals, due mainly to lattice vibrations. However, at very low temperatures, the electronic heat capacity, although very small, is larger than the remaining contributions which approach zero as some higher power of the temperature than T. Thus, the electronic heat capacity at low temperatures is the main contribution to heat capacity in metals.

12 WORK FUNCTION

In studying the photoelectric effect, it was found that the incident photons had to be of energies greater than a certain critical energy in order to cause electrons to be ejected from the metal surface. The minimum energy needed to get an electron out of the surface was called the work function, Φ. In terms of the work function, the minimum photon energy required to eject an electron is

$$E_{\min} = h\nu_{\min} = \Phi \tag{11.45}$$

In Figure 11.4, the potential energy of a single electron in or near the surface of a metal slab is sketched. The curved portions outside the surfaces approach

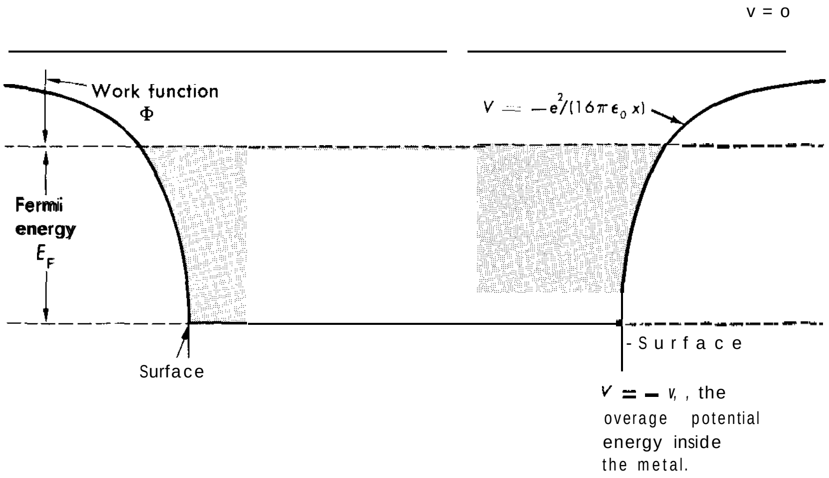


Figure 11.4. Potential energy of a single electron near the surface of a metal.

zero as x approaches infinity according to the equation $-e^2/16\pi\epsilon_0 x$, where x is the distance from the surface. This potential energy results from attraction of the electron by positive charge induced on the surface near the electron. As a result, electrons will be bound to the metal, with an average potential energy $-V_1$ inside the metal, where V_1 is of the order of from 5 to 15 eV for different metals. The electrons then fill the energy levels above $-V_1$ up to $-V_1 + E_F$, which is usually of the order of several eV higher in energy than $-V_1$. The work function is therefore the energy which must be added to the most energetic of the electrons in the metal in order to remove it from the metal, and hence the work function, Fermi energy and minimum potential energy $-V_1$ are related by:

$$\Phi = V_1 - E_F \tag{11.46}$$

The work function is typically several electron volts.

11.13 PHOTON DISTRIBUTION

Calculation of the distribution with energy of the average number $\bar{n}(E)$ of photons of energy E in a cavity is of considerable historical interest, since it was Planck's study of this problem that launched the quantum theory. Photons can be considered as particles of light, described by wavefunctions having the space and time dependence given in Equation (1 1.15). Inside a cubical cavity of side l, the single-particle states are therefore described by giving the momentum quantum numbers n_x, n_y, n_z, just as in Equation (11.16). Photons have spin quantum number $s = 1$, and are therefore bosons. Furthermore, they have zero rest mass, and hence only two spin states—or two polarization states-for each momentum state. The density of states is given in Equation (11.22). Another complication is that, in contrast to a system of massive bosons such as a gas of He”, photons can be emitted and absorbed by the walls of the cavity; thus the number of photons inside the cavity is not fixed, but may fluctuate as energy is exchanged with the cavity walls. Hence, we do not speak of one of the particles making a transition from state 1 to state 2, but rather of a loss of particles from state 1 due to interaction with the walls and a gain of a possibly different number of particles in state 2 from the same cause.

These properties of light waves require that the distribution function for photons be derived by a special method, based on the observation that if the radiation in the cavity is in thermal equilibrium with the walls, then the probability that the radiation has total energy E must be given by the Boltzmann factor, $e^{-\beta E}$. After deriving the photon distribution n(E), we may examine and generalize those special features which are due to the fact that photons obey Bose-Einstein statistics for application to a gas of bosons of nonzero rest mass.

For simplicity of notation we shall let the single index j stand for the combination of integers (n,, n_y, n_z) describing a single particle state. If n_j is the number of photons in one of these states, the total energy of these n, photons is $n_j h\nu_j$, where ν_j is the frequency of the state, given by

$$\nu_j = \frac{c}{\lambda} = \frac{c}{h} p_j = \frac{c}{L}\left(n_{xj}^2 + n_{yj}^2 + n_{zj}^2\right)^{1/2} \qquad (11.47)$$

from Equations (1 1.16). The total energy in the cavity will be a sum over all states j of the energy in each state, $n_j h \nu_j$, so the total energy is

$$E = \sum n_j h \nu_j \qquad (1\ 1.48)$$

The Boltzmann factor is

$$\exp\left[-\beta \sum_j n_j h \nu_j\right] = \exp\left[-(n_1\nu_1 + n_2\nu_2 + \cdots)\frac{h}{k_B T}\right] \qquad (11.49)$$

Different overall states of the system will then differ in the set of occupation numbers n,, $n_2, n_3, \ldots$, that is, they will differ in the numbers of photons in the various single-particle states. To calculate the average number of photons in the particular state i, we therefore have to calculate the following sum:

$$\langle n_i \rangle = \frac{\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\sum_{n_3=0}^{\infty}\cdots n_i \exp\left[-(n_1\nu_1 + n_2\nu_2 + \cdots n_i\nu_i + \cdots)h/k_B T\right]}{\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\sum_{n_3=0}^{\infty}\cdots \exp\left[-(n_1\nu_1 + n_2\nu_2 + \cdots n_i\nu_i + \cdots)h/k_B T\right]}$$

(1 1 SO)

where the sums run over all the possible values of each of the integers; i.e., $n_1 = 0, 1, 2, 3, \ldots, n_2 = 0, 1, 2, 3, \ldots$ corresponding to the fact that in any state j, any number of photons may exist.

The above sum may immediately be simplified because the summations over all of the n_j's, except $j = i$, is exactly the some in numerator and denominator. The constant factor due to these other summations then cancels out. We thus have

$$\langle n_i \rangle = \frac{\sum_{n_i=0}^{\infty} n_i \exp\left(-n_i \nu_i h / k_B T\right)}{\sum_{n_i=0}^{\infty} \exp\left(-n_i \nu_i h / k_B T\right)} \tag{11.51}$$

The sum over n_i may be found by performing the following differentiation:

$$-\frac{d}{dx} \ln\left(\sum_{n_i=0}^{\infty} e^{-n_i x}\right) = \frac{-d/dx \left(\sum_{n_i} e^{-n_i x}\right)}{\sum_{n_i} e^{-n_i x}} = \frac{\sum_{n_i} n_i e^{-n_i x}}{\sum_{n_i} e^{-n_i x}} \tag{11.52}$$

The above result is identical to $\langle n_i \rangle$ if $x = \nu_i h / k_B T$. The remaining sum in the argument of the logarithm in Equation (11.52) is an infinite geometric series, of the form:

$$1 + e^{-x} + e^{-2x} + \cdots$$

In general, if $a < 1$, $\sum_0^{\infty} a^n = (1 - a)^{-1}$. Thus, if x is positive,

$$\sum_{n_i=0}^{\infty} e^{n_i x} = \frac{1}{1 - e^{-x}} \tag{11.53}$$

Combining these results, we obtain the following formula for $\langle n_i \rangle$:

$$\langle n_i \rangle = -\frac{d}{dx} \ln\left(1 - e^{-x}\right)^{-1} \Big|_{x = \nu_i h / k_B T} = \frac{1}{1 - e^{-x}} \left(+e^{-x}\right) \Big|_{x = \nu_i h / k_B T}$$

$$= \frac{1}{e^{h\nu_i / k_B T} - 1} \tag{11.54}$$

or

$$\bar{n}(E) = \left(e^{E/k_B T} \quad 1\right)^{-1} \tag{11.55}$$

where E is a photon energy. This result strikingly resembles the Fermi-Dirac distribution, Equation (11.6), except that -1 appears in the denominator in place of + 1, and there is no constant similar to the Fermi energy. This latter omission is entirely reasonable, as the Fermi energy was determined by a normalization condition, $\sum_i \langle n_i \rangle = N$, the total number of particles. Since the total number of photons is not conserved, no such normalization condition can be written down for photons.

11.14 PLANCK RADIATION FORMULA

To find the infinitesimal number of photons dn in the cavity in the frequency range $d\nu$, we may use the density of states, Equation (11.22). If we use spherical coordinates in momentum space, dp, $dp_y dp_z \rightarrow 4\pi p^2$ dp. For photons, the momentum p and frequency ν are related by $p = h\nu/c$. Hence, the number of states in the frequency range $d\nu$, including polarizations, is

$$\frac{2V}{h^3} 4\pi \left(\frac{h\nu}{c}\right)^2 \left(\frac{hd\nu}{c}\right) = \frac{8\pi V \nu^2 d\nu}{c^3} \tag{11.56}$$

The number of photons in the interval $d\nu$ is therefore

$$\frac{8\pi V}{c^3} \frac{\nu^2 d\nu}{(e^{h\nu/k_BT} - 1)} \tag{11.57}$$

The energy per photon is $h\nu$.

If we then multiply $h\nu$ by the number of photons in the interval du, we obtain the energy $d\bar{E}$, contributed by photons of frequencies in the range $d\nu$, to the total average energy $\bar{E}$ in the cavity. The energy per unit Frequency, per unit volume, is then

$$\frac{1}{V}\frac{d\bar{E}}{du} \quad \frac{8\pi h\nu^3}{c^3(e^{h\nu/k_BT} - 1)} \tag{11.58}$$

This is Planck's radiation formula for the energy density per unit frequency interval, inside a cavity containing only radiation at temperature T. When $h\nu/k_BT << 1$, $e^{h\nu/k_BT} = 1 + h\nu/k_BT + \cdots$, and the Planck formula becomes approximately:

$$\frac{1}{v}\frac{d\bar{E}}{d\nu} = \frac{8\pi\nu^2 k_B J}{c^3} \tag{11.59}$$

which is the Rayleigh-Jeans radiation formula. The Rayleigh-Jeans formula was derived originally by using classical ideas. It is evident that such a derivation is possible because h does not appear in it. The Rayleigh-Jeans formula agreed well with experiment at low frequencies but not at high frequencies. The Planck formula was one of the early triumphs of the idea of quantization of photon energy. Using the same h as found from the photoelectric effect, Planck was able to completely explain the radiation experiments. In Figure 1 1.5 are plotted both the Planck radiation formula and the Rayleigh-Jeans law; the two are seen to agree only at very low frequencies

If the walls of the container were perfectly black, that is, if they absorbed all of the radiation incident upon them, then for thermal equilibrium to be maintained, the frequency distribution of the radiation emiited by the walls would have to have the same form as that of the incident radiation. In other words, since there is equilibrium, if energy is absorbed in a particular frequency range, on the average an equal amount of energy in this frequency range must be emitted by the walls. For ordinary intensities of radiation, it is to be expected that the radiation from the walls should not depend significantly on whether the walls are in equilibrium with the incident radiation. Hence we may conclude that, in general, the radiation from a black body has a frequency distribution the same as that given in Equation (1 1.58) for equilibrium radiation. This is therefore

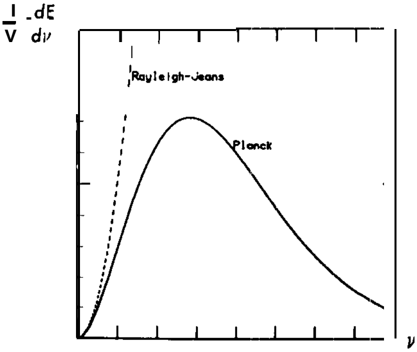


Figure 11.5. Graphs of the classical Rayleigh-Jeans formula for energy density in a cavity and the Planck radiation formula obtained from quantum theory. At high frequencies, the classical energy density per unit frequency interval becomes infinite, whereas Planck's formula agrees with experiment.

called *black body radiation.* Other bodies when heated emit radiation whose frequency distribution closely resembles the radiation from an ideal black body. For instance, in the visible range the light from the sun is very much like that of a black body near 6000K, which would actually be "white hot."

The usual procedure for performing experiments with black body radiation is to form a cavity in any substance so there is equilibrium radiation inside. The radiation is sampled through a very small hole in the cavity wall, so that the radiation is not significantly disturbed by the measurements.

To find the total energy due to radiation in a cavity as a function of temperature, we may simply integrate Equation (11.52) over all frequencies from zero to infinity:

$$\bar{E} = \int_0^\infty \frac{8\pi V h\nu^3}{c^3}\left[\exp\left(\frac{h\nu}{k_B T}\right) - 1\right]^{-1} d\nu \tag{11.60}$$

To simplify the algebra, let-us designate by the variable x the quantity $h\nu/k_B T$ appearing in the exponential. Then

$$\nu = \frac{k_B T}{h}x, \quad d\nu = \frac{k_B T}{h}dx \tag{11.61}$$

We therefore obtain:

$$\bar{E} = \int_0^\infty \frac{8\pi V}{h^3c^3}(k_B T)^4 \frac{x^3 dx}{e^x - 1} \tag{11.62}$$

The required integral is found in definite integral tables, and is

$$\int_0^\infty \frac{x^3 dx}{e^x - 1} = \frac{\pi^4}{15} \tag{11.63}$$

The energy density is therefore

$$u \equiv \frac{\bar{E}}{V} = \frac{8\pi^5 (k_B T)^4}{15h^3c^3} \tag{11.64}$$

The significant feature of this expression is its dependence on the fourth power of the temperature. This fourth power dependence could be calculated from thermodynamics; however, the proportionality constant, because it involves Planck's constant, could not be calculated classically.

The result, Equation (11.64), also implies that the power radiated from a hot black body is proportional to T^4. The radiation from non-black bodies frequently has approximately the same temperature dependence.

1.15 SPONTANEOUS EMISSION

Let us now consider the processes of emission and absorption of radiation in the cavity from the point of view of detailed balance. Suppose, for example, that there is one object inside the cavity which has two energy levels E_1, $E_2 > E_1$, separated in energy by the amount $h\nu_i$, where ν_i is the frequency of a particular one of the single photon states in the cavity. We can assume that the object itself obeys Maxwell-Boltzmann statistics. Thus, an equation such as Equation (11.2) holds:

$$p_{1\to2}e^{-\beta E_1} = p_{2\to1}e^{-\beta E_2} \tag{11.65}$$

This is a way of stating detailed balancing. In Equation (11.65), the Boltzmann factors can be interpreted as the relative probabilities that the object will be found in the upper state E_2 or lower state E_1 at thermal equilibrium.

Suppose that associated with a transition 1 → 2 of the object is the absorption of a photon of frequency ν_i, in the single photon state i. Similarly, associated with a transition 2 → 1 of the object is the emission of a photon of the same frequency.

Now let us analyze the transition probability for absorption of a photon per unit time, $p_{1\to2}$, in more detail. If a beam of light is incident on an absorbing object, such as the surface of a metal, it is well-known, even in classical electromagnetic theory, that a certain fraction of the incident energy is absorbed; this fraction is independent of the intensity of the incident beam. In other words, if n_i photons of the mode i are incident per second on the absorbing object, the rate of absorption by the object should be proportional to n_i. Therefore, $p_{1\to2}$ is proportional to the number of incident photons n_i. We write this as:

$$p_{1\to2} = Cn_i \tag{11.66}$$

where C is some proportionality constant, not dependent on the temperature of the walls because of the way the transition probability $p_{1\to2}$ was defined.

Next consider emission processes. An isolated object tends to spontaneously emit radiation and make transitions downward in energy, until it ends up in the ground state. This process can occur even when there is no radiation initially present. If the emission were due entirely to spontaneous emission, then $p_{2\to1}$ would have to be independent of temperature, and we would write $p_{2\to1} = A$, a constant independent of T. Einstein was the first to notice that thermal equilibrium could not be maintained if the emission were due only to spontaneous emission, for then detailed balance would require that

$$C\bar{n}_\nu e^{-\beta E_1} = Ae^{-\beta E_2} \tag{11.67}$$

or

$$\bar{n}_\nu = \frac{A}{C} e^{-\beta h\nu} \tag{11.68}$$

which is inconsistent with the photon distribution function derived in Equation (11.42). It would be consistent only if the photon distribution were a classical Boltzmann distribution.

11.16 RELATIONSHIP BETWEEN SPONTANEOUS AND STIMULATED EMISSION

Einstein recognized that another process, called *stimulated emission,* contributes to the emission probability. In this process, if the system is initially in the excited State E_2, and some number n_i of photons in a mode frequency ν_i are initially present, then a kind of resonant interaction occurs between the object and the radiation, which increases the probability of emitting another photon in the same mode. In fact, the probability of stimulated emission is proportional to the number of photons n_i initially present. It is this proportionality which leads to the terminology "stimulated emission," because the incident radiation "stimulates" further emission of photons of the same type, the probability of emission being directly proportional to the intensity of the incident radiation.

Thus, the total emission probability must be written:

$$p_{2\to 1} = A + B\bar{n}_i \tag{11.69}$$

where B is another proportionality constant, independent of temperature. At thermal equilibrium we must have, by detailed balance,

$$C\bar{n}_i e^{-\beta E_1} = (A + B\bar{n}_i)e^{-\beta E_2} \tag{11.70}$$

Then, inserting the expression, Equation (11.55), for the photon distribution,

$$Ce^{\beta h\nu_i} - B = A(e^{\beta h\nu_i} - 1) \tag{11.71}$$

In order for this equation to be satisfied at all temperatures, we must have

$$A = B = C \tag{11.72}$$

Thus, from Equation (11.69), the total emission probability is proportional to $A(1 + n_i)$, and hence to $1 + n_i$, which is the number of photons present after emission, or the number of photons present in the final state of the electromagnetic field. In the factor $1 + n_i$, the 1 corresponds to the contribution from spontaneous emission processes, and the n_i corresponds to the contribution from stimulated emission processes.

Stimulated emission is the basis of operation of a celebrated invention--the laser. The name of the device is taken from the initial letters of the words "light amplification by stimulated emission of radiation."

In a laser, a large number of atoms are placed in an excited state by some special means, such as by collisions with other atoms or by shining light of proper frequencies upon them. The atoms are then not in thermal equilibrium, because the number of atoms in the excited state is larger than the number in the ground state-in disagreement with the Boltzmann probability factor, which holds at equilibrium. If one of the atoms should spontaneously radiate a photon of mode n_i, then the subsequent probability of radiation of another photon in the same mode is increased because of the factor $1 + n_i$ in the emission probability --that is, by the effect of stimulated emission. As other atoms then radiate into the same mode, the stimulated emission probability factor for that mode builds up into an enormous factor. A large number of the atoms can thus be made to radiate into the same mode, so that a pulse of radiation containing as many as 10^{19} photons, all going in nearly the same direction and with nearly the same frequency, can result. The buildup of energy in a single mode is enhanced by enclosing the active laser material between partially coated mirrors, so that the light is reflected back and forth many times through the material before getting out, thus contributing further to the stimulated emission. This coherent light is unlike the light emitted by most natural sources, such as hot bodies. Due to its high directionality and the sharpness of the frequency, laser light has many important uses.

1.17 ORIGIN OF THE FACTOR $1 + n_i$ IN BOSON TRANSITIONS

In the preceding section it was seen that the total emission probability for photons in the mode i is proportional to the number of photons in the final state, or proportional to $1 + n_i$ where n_i is the number of photons initially in mode i. This factor, $1 + n_i$, occurs in general for transitions of bosons to a state i, with an initial number n_i of bosons in the state i. By way of contrast, in Equation (11.1), which applies for fermions, there is a factor 1 − A, in the transition rate to state i, where $\bar{n}_i$ is the average occupation number of particles initially in state i. This difference of sign is characteristic of the difference between particles of half-odd-integral spin, which obey Fermi-Dirac statistics, and those of integral spin, which obey Bose-Einstein statistics.

A discussion of the factor $1 + n_i$ for bosons follows. Anyone not interested in this discussion should skip to Section 11.18.

The wavefunction for a system of two or more fermions must be antisymmetric under exchange of any two particles, which requires that when single-particle states are used to describe the system, the wavefunction must be an antisymmetrized combination of single-particle states; this also requires that no two single-particle states in the wavefunction can have the same quantum number. This gives rise to the factor $1 - \bar{n}_i$ in the transition rate.

On the other hand, the wavefunction of a system of two or more bosons must be symmetric, i.e., must not change even in sign, under an exchange of any two particles. For example, the symmetric wavefunction for two particles in different states ψ_1 and ψ_2 would be:

$$\psi(\mathbf{r}_1, \mathbf{s}_1; \mathbf{r}_2, \mathbf{s}_2) = \frac{1}{\sqrt{2}}[\psi_1(\mathbf{r}_1, \mathbf{s}_1)\psi_2(\mathbf{r}_2, \mathbf{s}_2) + \psi_1(\mathbf{r}_2, \mathbf{s}_2)\psi_2(\mathbf{r}_1, \mathbf{s}_1)] \quad (11.73)$$

where the factor $\sqrt{2}$ in the denominator, which is the square root of the number of terms in the symmetrized wavefunction, is for correct normalization. To see that this normalization is correct if ψ_1 and ψ_2 are each normalized, we consider the integral:

$$\begin{aligned} 2\int\psi^*\psi dV_1 dV_2 = & \Big[\Big(\int |\psi_1(\mathbf{r}_1, \mathbf{s}_1)|^2 dV_1\Big)\Big(\int |\psi_2(\mathbf{r}_2, \mathbf{s}_2)|^2 dV_2\Big) \\ & + \Big(\int |\psi_1(\mathbf{r}_2, \mathbf{s}_2)|^2 dV_2\Big)\Big(\int |\psi_2(\mathbf{r}_1, \mathbf{s}_1)|^2 dV_1\Big) \\ & + \Big(\int \psi_2^*(\mathbf{r}_1, \mathbf{s}_1)\psi_1(\mathbf{r}_1, \mathbf{s}_1) dV_1\Big)\Big(\int \psi_1^*(\mathbf{r}_2, \mathbf{s}_2)\psi_2(\mathbf{r}_2, \mathbf{s}_2) dV_2\Big) \\ & + \Big(\int \psi_1^*(\mathbf{r}_1, \mathbf{s}_1)\psi_2(\mathbf{r}_1, \mathbf{s}_1) dV_1\Big)\Big(\int \psi_2^*(\mathbf{r}_2, \mathbf{s}_2)\psi_1(\mathbf{r}_2, \mathbf{s}_2) dV_2\Big)\Big] \end{aligned} \quad (11.74)$$

As shown in Appendix 2, an integral such as $\int \psi_2^*(\mathbf{r}_1, \mathbf{s}_1)\psi_1(\mathbf{r}_1, \mathbf{s}_1) dV_1$ is zero. Also, an integral such as $\int |\psi_1(\mathbf{r}_1, \mathbf{s}_1)|^2 dV_1 = 1$ if ψ_1 and ψ_2 are normalized to unity. Thus $2\int\psi^*\psi dV_1 dV_2 = 2$, and $1/\sqrt{2}$ is the correct normalization. If there are p terms in the symmetrized wavefunction, the normalization is $1/\sqrt{p}$ by the same reasoning. If two particles were in the some state, say ψ_1, the symmetric wavefunction would be

$$\psi(\mathbf{r}_1, \mathbf{s}_1; \mathbf{r}_2, \mathbf{s}_2) = \psi_1(\mathbf{r}_1, \mathbf{s}_1)\psi_1(\mathbf{r}_2, \mathbf{s}_2) \quad (11.75)$$

We may give a brief indication of the origin of the factor $1 + n$ in the transition rate, by considering an initial state of the system with n_2 particles in the final single-particle state 2, and one particle in the initial single-particle state 1. The symmetrized wavefunction of the system would be

$$\begin{aligned} \psi_{\text{initial}} = & \frac{1}{\sqrt{1 + n_2}}[\psi_1(\mathbf{r}_1, \mathbf{s}_1)\psi_2(\mathbf{r}_2, \mathbf{s}_2)\cdots\psi_2(\mathbf{r}_{n_2+1}, \mathbf{s}_{n_2+1}) \\ & + \psi_2(\mathbf{r}_1, \mathbf{s}_1)\psi_1(\mathbf{r}_2, \mathbf{s}_2)\cdots\psi_2(\mathbf{r}_{n_2+1}, \mathbf{s}_{n_2+1}) + \cdots \\ & + \psi_2(\mathbf{r}_1, \mathbf{s}_1)\cdots\psi_1(\mathbf{r}_{n_2+1}, \mathbf{s}_{n_2+1})] \end{aligned} \quad (11.76)$$

Here there are $1 + n_2$ terms in the symmetrized combination, and therefore the normalization constant is ‘I/-\/in,. The wavefunction of the final state, with $1 + n_2$ particles in state 2, is

$$\psi_{\text{final}} = \psi_2(\mathbf{r}_1, \mathbf{s}_1)\psi_2(\mathbf{r}_2, \mathbf{s}_2)\cdots\psi_2(\mathbf{r}_{n_2+1}, \mathbf{s}_{n_2+1}) \quad (11.77)$$

In calculating a transition probability from quantum mechanics, the ***square*** of an integral involving the ***product*** of the above two wavefunctions appears. In the product, ψ_{initial} leads to a factor of $\sqrt{n_2 + 1}$ in the denominator. Also, because there are $n_2 + 1$ terrns in ψ_{initial} and one in ψ_{final}, there are $n_2 + 1$ terms in the product; each contributes equally to the transition probability, so there is a net factor $[(1 + n_2)/\sqrt{1 + n_2}]^2$ in the transition probability. If the initial wavefunction corresponds to n_1 particles in state 1, n_2 in state 2, and the final function corresponds to $n_1 - 1$ in state 1, $1 + n_2$ in state 2, then similar reasoning shows that there is a factor $n_1(1 + n_2)$ in the transition probability.

18 BOSE-EINSTEIN DISTRIBUTION FUNCTION

We may proceed under the assumption that in all boson systems the transition rate for transitions from a single-particle state 1 to a single-particle state 2 is proportional to $1 + n_2$. Let $\bar{n}_1, \bar{n}_2$ be the time-averaged values of the number of particles found in the single-particle states 1 and 2, respectively, of a system of bosons at thermal equilibrium. Then the principle of detailed balance can be written as:

$$\bar{n}_1(1 + \bar{n}_2)p_{1\to 2} = \bar{n}_2(1 + \bar{n}_1)p_{2\to 1} \qquad (11.78)$$

Here, as in the Fermi-Dirac case, we assume that the ratio of transition probabilities per unit time, $p_{1\to 2}/p_{2\to 1}$, is the same as in the classical case. Then, using Equation (11.2), we obtain:

$$\frac{\bar{n}_1}{1 + \bar{n}_1} e^{E_1/k_B T} = \frac{\bar{n}_2}{1 + \bar{n}_2} e^{E_2/k_B T} \qquad (11.79)$$

Since each side of the above equation depends on a different energy, each side must be equal to a constant independent of energy. We shall denote this constant by the symbol Z:

$$\frac{\bar{n}(E)}{1 + A(E)} e^{E/k_B T} = Z \qquad (11.80)$$

Then, solving for $\bar{n}$, we find the Bose-Einstein distribution:

$$\bar{n}(E) = \left[\frac{1}{Z}\exp(E/k_B T) - 1\right]^{-1} \qquad (11.81)$$

Note that for the special case of photons which are not conserved in number, Z = 1. The main difference between the Fermi-Dirac and Bose-Einstein distributions lies in the presence of the sign preceding the 1 in the denominators; this sign arises as a direct consequence of the symmetry, or antisymmetry, of the wavefunction under particle exchange.

The constant Z in the denominator of the Bose-Einstein distribution, for a system of particles of non-zero rest mass, serves substantially as a normalizing constant, just as did the factor $e^{E_F/k_B T}$ in the Fermi-Dirac case. The condition used to determine Z would be

$$\sum_i \bar{n}_i(E_i) = N \qquad (11.82)$$

for a system of N particles. The summation could be written as an integration by using the appropriate density of states, such as in Equation (11.24), for a system of noninteracting bosons with kinetic energy $p^2/2m$.

The most common isotope of helium, He^4, with two protons and two neutrons in the nucleus, has zero spin, and thus these nuclei obey Bose-Einstein statistics. A calculation at room temperature, assuming that the statistics are nondegenerate for He^4 gas (i.e. assuming that $Z << 1$), closely parallels that done for He^3 previously. It shows that Z is indeed much less than 1. The 1 in the denominator of the distribution, Equation (11.81), gives negligible effect in this case, and the gas follows essentially Maxwell-Boltzmann statistics. The order of magnitude of the temperature at which the 1 in the denominator would be important- the case of degenerate statistics-is a few degrees Kelvin; the calculation of this would again be similar to that for He^3. However, in the Bose-Einstein case at low temperature, many particles tend to collect in the state of zero energy rather than filling states up to a Fermi energy. In Figure 11.6, the Bose-Einstein distribution is plotted for $Z = 1 - 0.01 = 0.99$.

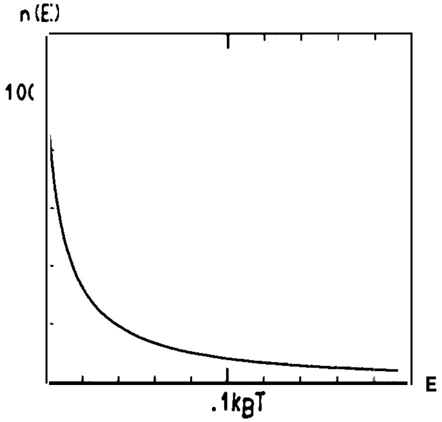


Figure 11.6. Bose-Einstein distribution function for $Z = 1 \quad 0.01 = 0.99$.

Experimentally, it is found that at 2.2K the specific heat of liquid He^4 changes abruptly, and that below this temperature the liquid behaves as if it were composed of two interpenetrating fluids, one of zero viscosity. The fraction of the zero viscosity part increases as temperature decreases. This superfluid exhibits a number of interesting properties connected with the lack of viscosity. The behavior of liquid helium can be explained on the basis of Bose-Einstein statistics, with the zero viscosity component roughly connected with accumulation of helium atoms in the ground state.

summary

NUMBER OF STATES

By consideration of free particle wavefunctions and imposition of periodic boundary conditions at the boundaries of a volume V, it was found that in the limit as V becomes very large, the number of single-particle states in the momentum interval dp,, dp,, dp, is (2s + $1)Vdp_x$ dp, dp_z/h^3, where s is the particle spin.

When the quantities to be integrated depend only on the magnitude of p, it is often useful to write the volume element in momentum space as $4\pi p^2 dp$, so the number of states in dp is $4\pi(2s + 1)Vp^2dp/h^3$. For free particles, the energy is E = $p^2/2m$, and in dE the number of states is $2\pi V(2s + 1)\sqrt{(2m)^3}\,\sqrt{E}\,dE/h^3$.

FERMI-DIRAC DISTRIBUTION

For identical particles of half-integral spin, for which the exclusion principle holds, the average number of particle!; per single particle state of energy E at temperature T is

$$\bar{n} = \frac{1}{e^{(E-E_F)/k_BT} + 1}$$

E_F is a constant called the Fermi energy. If the smallest value of E is taken to be 0, then if $E_F >> kT$, the distribution is much different from the classical Maxwell-Boltzmann statistics, and is said to be degenerate. If $-(E_F) \gg kT$, the distribution is nondegenerate, and is substantially the same as Maxwell-Boltzmann statistics.

For free electrons with degenerate statistics,

$$E_F \cong \left(\frac{3N}{8\pi V}\right)^{2/3} \frac{h^2}{2m}$$

where N is the number of electrons of mass in volume V. Also for this case, the average energy per particle is approximately $^3\!/_5\, E_F$. A more careful calculation results in a correction to the average energy proportional to T^2. This leads to a specific heat on the order of $k_B\, T/E_F$ times the classical specific heat.

BLACK BODY RADIATION

For photons, the Z in the Bose-Einstein distribution is 1. Thus, the average number of photons per state in the equilibrium radiation is $1/(e^{h\nu/k_BT} - 1)$, where $h\nu$ is the photon state energy. In the relation giving the number of states, 2s + 1 should be taken as 2 for a zero rest mass particle. Also, p = $h\nu/c$. Thus, the number of states in $d\nu$ is $8\pi V\nu^2 d\nu/c^3$. Multiplication of this number of states by the average number of photons per state and the energy per photon, *hu,* gives the energy in *du:*

$$dE = \frac{8\pi Vh\nu^3 d\nu}{c^3(e^{h\nu/k_BT} - 1)}$$

The energy radiated by a perfectly black wall, and often approximately by other objects, is proportional to this function. Integration gives a total energy radiated proportional to T^4.

STIMULATED AND SPONTANEOUS EMISSION

The probability of emission of a photon of a particular mode or single-particle photon state, is proportional to 1 + **n**, where n is the number of photons initially present. The term 1 in 1 + n corresponds to the contribution to emission probability from spontaneous emission; the term n arises from stimulated emission. In any system of bosons, the probability for transition to a final state occupied initially by n particles is proportional to 1 + n.

BOSE-EINSTEIN DISTRIBUTION

For identical particles of integral spin, the average number of particles per single particle state of energy E at temperature T is

$$\overline{n} = \frac{1}{(1/Z)e^{E/k_BT} - 1}$$

If Z $\ll$ 1 when the minimum of E is 0, the statistics are nondegenerate, closely like Maxwell-Boltzmann statistics. For Z $\cong$ 1, the degenerate statistics are quite different from Maxwell-Boltzmann statistics. The ground state is much more densely populated for particles obeying Bose-Einstein statistics.

problems

1. Calculate the number of states of electromagnetic radiation using periodic boundary conditions in a cubical region 0.5 meters on a side, between 5000 and 6000 Angstroms in wavelength.
   Answer: 3.53×10^{18}.
2. Suppose a gas of particles of energies **E** =: $p^2/2m$ was confined to move on a flat plane of area A, rather than in three dimensional space. Find the density of states per unit energy interval dE **for** zero spin.
   Answer: $2m\pi A/h^2$.
3. The density of electrons in some regions of interplanetary space is about $10/\text{cm}^3$. Would the statistics be degenerate or nondegenerate? Estimate the Fermi energy in eV for these electrons, assuming they are in thermal equilibrium with the sun. (Temp. of sun $\approx$ 6000K)
   Answer: $E_F = \approx$ --24 eV.
4. The average energy per particle of an electron gas at low temperatures is E = $^3/_5\, E_F + \pi^2 k_B^2 T^2/4E_F$. Calculate the specific heat per particle of the conduction electrons in copper (8.5×10^{22} electrons/cm^3) at a temperature of T = 2.0K. Compare with the classical result, $^3/_2\, k_B$.
   Answer: C_V = 1.66×10^{-27} j/K. Classical result is 12.07×10^{-23} i/K.
5. In aluminum, there are three free electrons per atom. The density of aluminum is

$2.7 g/cm^3$, and the atomic weight of Al is 26.97. Find the Fermi energy at zero temperature.

Answer: 11.7 eV.

6. In a crystal of the compound indium antimonide, the number of "free" electrons can be varied by introduction of impurities. Also, because of the interaction of electrons with the crystal atoms, the electrons behave as free particles with $^1\!/_{80}$ the true electron mass. Show that at concentrations of 10^{14} electrons/cm^3 the statistics are nondegenerate at room temperature. Show that at liquid nitrogen temperature, about 80K, and at a concentration of 10^{18} electrons/cm^3 the statistics are degenerate. Find the Fermi energy.

   Answer:* *0.29 eV.

7. The density of states in energy near $E = E_F$, for the part of a degenerate electron gas with spin parallel to magnetic field, is $2\pi V(2m)^{3/2}\sqrt{E_F}/h^3$. A similar relation holds for the antiparallel spin part. In the magnetic field, in addition to the kinetic energy, the electrons have potential energy $\pm\mu_M B$, where μ_M is the electronic magnetic moment $e\hbar/2m$ and B is the field strength. The plus and minus correspond to the spin parallel and antiparallel cases. If $\mu_M B \ll E_F$, show that the dipole strength of the electron gas at equilibrium is $4\pi V(2m)^{3/2}\mu_M^2 B\sqrt{E_F}/h^3 = 3N\mu_M^2 B/2E_F$. This is on the order of $k_B T/E_F$ smaller than classical statistics would give. (Use the fact that the Fermi energy is the same for the two spin parts, but that the lowest energy of one spin part is $2\mu_M B$ lower than the other, so there are more electrons with the antiparallel spin orientation.)

8. Most metals melt at temperatures below 3000K. Explain why the Fermi energy of a metal is almost independent of temperature.

9. Estimate the decrease in work function of a metal at 1000K, in eV, as compared to 0K.

   Answer: 0.1 eV.

10. In a metal of Fermi energy 7.0 eV, at a very low temperature, what fraction of the electrons have energies between 6.9 and 7.0 eV? In a low density nondegenerate electron plasma at 25,000K, what fraction of the electrons have energies between 6.9 and 7.0 eV?

    Answer: ***0.021; 0.0037.***

11. By the classical equipartition theorem, the average kinetic energy per particle of a Maxwell-Boltzmann gas is $\frac{3}{2}k_B T$. The average thermal wavelength $\lambda_T = h/p$ is defined so that $\frac{3}{2}k_B T = \frac{1}{2}m(h/\lambda_T)^2$. Compute λ_T for a gas of hydrogen atoms at 300K. Show that for a gas of N electrons in a volume V, the statistics will be nondegenerate if $\lambda_T^3 N/V \ll 1$, that is, if the thermal wavelength is small compared to the distance between particles. (Hint: Assume $e^{-E_F/k_BT} \gg 1$, show that $\lambda_T^3 N/V \ll 1$.)

    Answer: $\lambda_T = 1.46 \times 10^{-8}$ cm.

12. If light of energy density ***du*** is hitting a wall at an angle of incidence θ, show that the energy hitting per second per unit area is ***(cdu)*** cos θ. Show that if the ***energy*** density for black body radiation is u, then the contribution to u arising from radiation propagating in the solid angle $d\Omega = 2\pi \sin\theta\, d\theta$ at angle θ from the wall normal is $du \simeq \frac{1}{2}u\sin\theta\, d\theta$. From these results, argue that the total intensity emitted by a black wall is $cu/4$. This quantity, $cu/4 = \sigma T^4$. Evaluate σ.

    Answer: $\sigma \simeq 5.67 \times 10^{-8}$ watt/m^2K^4.

13. Verify that for black body radiation the wavelength for the energy maximum of $1/V \times dE/d\nu$ is at $\lambda_m = hc/2.82k_BT$. If the sun's surface temperature is about 6000K, what is λ_m?

Answer: 8500 Angstroms (the visible region is around 4000 Angstroms to 7000 Angstroms).

14. Show that the energy per unit wavelength per unit volume in black body radiation is $1/V(dE/d\lambda) = 8\pi hc/\lambda^5(e^{hc/\lambda k_B T} - 1)$. Verify that the wavelength for the maximum. of this function is at $\lambda_M = hc/4.97k_BT$. This dependence of λ_M on J is called the Wien displacement law. If J = 6000K for the sun, what is λ_M?

Answer: 4830 Angstroms.

15. If the energy density of black body radiation is u, show that the pressure on the wall at equilibrium due to the radiation is $^1/_3\, u$.

16. A combination of the first and second laws of thermodynamics for a reversible process is $TdS = d(uV) + pdV$, where S is entropy, V is volume, p is pressure, and u is energy density. If the pressure for black body radiation is $^1/_3\, u$ as found in Problem 15, find $(\partial S/\partial u)$ at constant V and $(\partial S/\partial V)$ at constant u. Assuming that u is a function only of T, find $\partial/\partial V(\partial S/\partial u)$ and $\partial/\partial u(\partial S/\partial V)$. Setting these second derivatives equal to each other, show that $4(dT/T) = du/u$, and thus that $u = \text{const.}\,(T)^4$.

17. There exists a kind of excitation in magnetic solids called spin waves, which may be treated as particles like photons but with no spin. The effective particles have an energy $E = v_0 p^2$, where v_0 is a constant and p is the "momentum" associated with a wave. Show that the contribution to the specific heat of the solid, arising from spin waves, is proportional to $T^{3/2}$.

18. There exists in solids a kind of excitation or vibration of atoms called phonons (particles corresponding to sound waves), which may be treated as particles similar to photons but with three kinds of polarization, one longitudinal and two transverse. At low energies, the energy is proportional to the effective phonon momentum, as for light. Show that at low temperatures the specific heat due to phonons is proportional to T^3.

19. The energies of a one dimensional harmonic oscillator of frequency ν are $(n + ½)h\nu$, $n = 0, 1, 2, 3, \ldots$ with one state per n. If $h\nu = 10^{-8}$ eV and there are 3×10^8 particle oscillators, for J = 300K find the approximate n and energy corresponding to the Fermi energy for spin $^3/_2$ particles; find the number of particles approximately in the lowest energy level for spin 1 particles. (Use $\sum_{n=0}^{\infty} 1/(ae^{n\delta} - 1) \cong 1/(a - 1) - 1/\delta \ln(a - e^{-1/2\delta})$ for $\delta \ll 1$. Assume that $a = 1 + \Delta$, where Δ is very small.)

Answer: $n = 75 \times 10^8$; $E_F = 0.75$ eV; 1.8×10^8.

20. An impurity atom in a crystal has one valence electron which has the possibility of either being bound to the atom in either state or being in the continuum with the other crystal electrons. In writing the detailed balance equation, one should include the fact that if there is no electron bound to the atom, continuum electrons of either spin orientation can go to the bound state. However, in the absence of spin-changing interactions, a bound electron with a particular spin state can go to only that some spin orientation in the continuum. Using these ideas, show that if $\bar{n} = 1/[e^{(E - E_F/kT)} + 1]$ for the continuum electrons and E_b is the energy of a bound electron, then $\bar{n} = 1/[½\, e^{(E_b - E_F)/kT} + 1]$ for the average number of bound electrons.

21. In a certain Bose-Einstein liquid at a very low temperature, the value of Z is very close to 1: $Z = 1\ \ 10^{-18}$. If the liquid has 10^{20} particles in a volume 0.2m^3, what is the number of particles in the state of exactly zero energy?

Answer: $1/(1/Z\ \ 1) = 10^{18}$.

22. Show that $0 \le Z \le 1$ for the ideal Bose-Einstein gas.

2 solid state physics

Solid state physics, as the name implies, is the study of physical properties of solids, as distinct from those of liquids and gases. This field has been the subject of intense research activity in the past two decades, which has resulted in many important technological advances. Examples of solid state devices which have recently seen widespread use are transistors, computer memory elements and lasers.

In this chapter we shall discuss some of the most basic properties of solids. In all our discussions, we shall consider only crystalline solids, i.e., solids in which the atoms or molecules are arranged in some simple repetitive pattern. While many solids--such as glass-are not of this type, more progress has been made in understanding crystalline solids because they are simpler to treat mathematically. Some of the consequences of having a crystalline structure will be illustrated in the discussions of crystal lattice vibrations (sound waves) and of electron energy bands in solids.

2.1 CLASSIFICATION OF CRYSTALS

The primary property of crystals which simplifies their discussion is their periodic or repetitive structure, or ***translational*** symmetry. For example, in discussing lattice vibrations, we shall set up an equation of motion for a general atom in a one dimensional crystal; an equation of the same form then describes any other atom. Another way of stating this property is to say that, except at the boundaries, a translation of the crystal by a *lattice* vector leaves the crystal unchanged. A lattice vector is a vector from one atom site in the lattice to a similar site, such as vector **A** in Figure 12.1. Thus we could consider translating the crystal by vectors a, **b** or c in the Figure, and nothing would be changed except at the boundaries. The general lattice vector by which one could translate would be an integer times **a** plus an integer times **b** plus an integer times **c**. Because of the periodicity, it is clear that the crystal can be considered to be composed of small volumes called unit *cells,* which all have the same properties. The three smallest independent lattice vectors **a, b** and c, which can be used to build up the crystal by translations,, are called the ***primitive lattice*** vectors. The unit cell of a crystal can be taken as the parallelepiped formed on **a, b** and c.

Crystals are classified into 14 possible types of *Bravais* ***lattices*** according to other possible symmetries, in addition to translational ones. Figure 12.2 shows

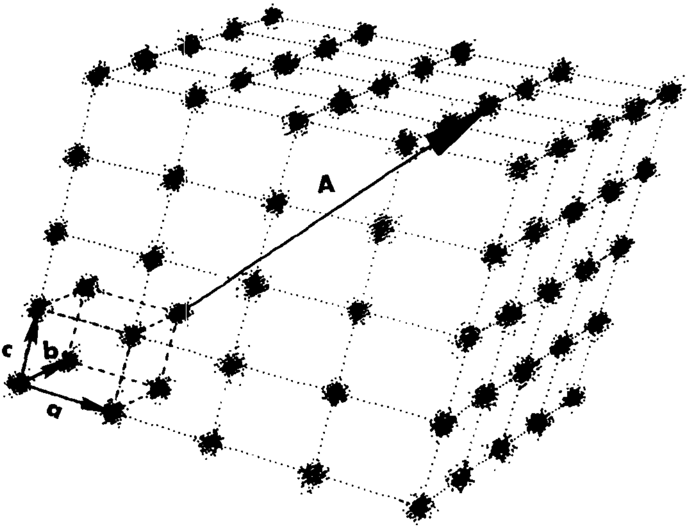
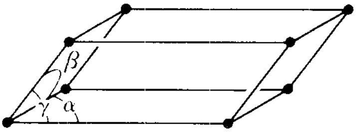


Figure 12.1. Diagram illustrating how a solid crystal may be built up of identical unit cells stacked together.

the basic structures of the 14 types, together with their names and some properties. Each lattice point in these diagrams might represent one atom or a group of atoms. In some crystals there may be several atoms per unit cell represented by the lattice point. The lattice point represents the basic periodic structure, and there is one lattice point per unit cell. Some of the basic structures shown are not unit cells as defined above. That is, the edges shown in Figure 12.2 are not the smallest three independent lattice vectors. For instance, the unit cell of the body-centered cubic is actually a parallelepiped based on the two cube edges and a vector from a corner of the cube to its center. The reason for showing figures other than unit cells is that they allow easier visualization of other types of symmetries.

12.2 REFLECTION AND ROTATION SYMMETRIES

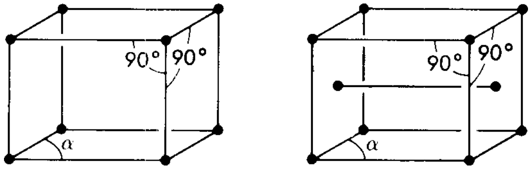
The classifications into these fourteen crystal types are based on symmetries of rotation and reflection. Let us choose an origin of coordinates at the center of each structure in Figure 12.2. All rotation axes and reflection planes we discuss will be assumed to pass through this origin. By "rotation axis" here we mean a line through the origin such that a rotation about the line through some angle would leave the crystal unchanged so far as physical properties are concerned. For example, in Figure 12.3 imagine identical atoms at each of the sites marked A, and imagine a rotation axis normal to the paper at the geometrical center 0. Rotations about 0 by any of the angles a/3, $2\pi/3$, $3\pi/3$, $4\pi/3$, $5\pi/3$, $6\pi/3$, which are multiples of $\pi/3$, would bring the set of atoms back to the sites marked A.



Triclinic

$\alpha \neq \beta, \alpha \neq \gamma, \beta \neq \gamma$

Edges which are not parallel are unequal in length.

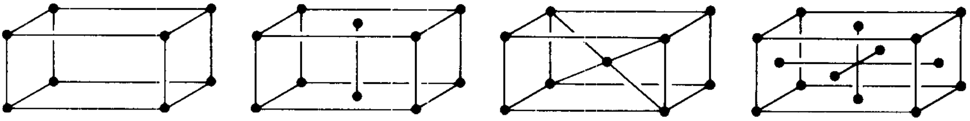


Simple monoclinic

Base centered monoclinic

$\alpha \neq 90°$.

Edges which are not parallel are unequal in length.



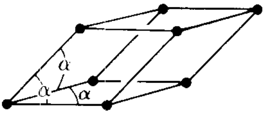
Simple orthorhombic

Base-centered orthorhombic

Body-centered orthorhombic

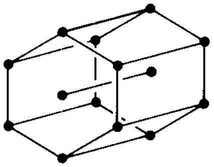
Face-centered orthorhombic

All angles between edges are 90”.
Edges which are not parallel are unequal in length.



Rhombohedral

All angles at one corner are equal but not equal to 90”. All sides are equal.



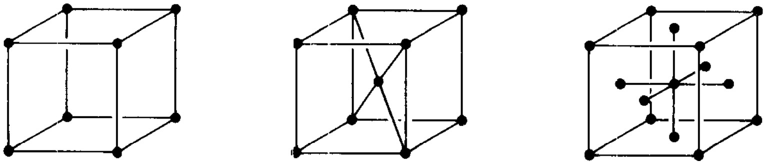
Hexagonal

Two faces are regular hexagons. The edges not in a hexagonal plane are perpendicular to that plane.

Simple tetragonal

Body-centered tetragonal

Two faces are squares. The edges of a different length not in the plane of a square are perpendicular to that plane



Simple cubic

Body centered cubic

Face-centered cubic

All edges meet at right angles and have equal lengths.

Figure 12.2. The fourteen Bravais lattices.

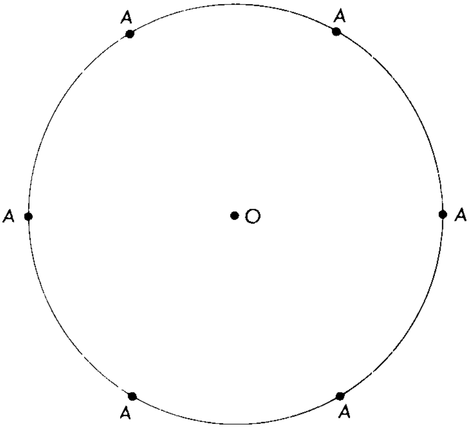


Figure 12.3. A set of positions, marked A, having rotational symmetry. Rotation by any multiple of the angle $\pi/3$ about an axis through zero and normal to the paper takes the set of positions into itself.

Since there are six possible angles of rotation which will leave atoms at the same sites, the axis is called a sixfold rotation axis.

In a similar way, a *reflection plane* is a plane such that a mirror reflection of the crystal relative to the plane leaves the crystal physically unchanged. In Figures 12.4(a, b, c) the plane through M, *M'* is to be imagined normal to the paper. In Figure 12.4(b), the line MM' is a reflection plane, whereas in Figures 12.4(a) and 12.4(c), reflection through MM' would change the positions of some of the atoms; hence in these two figures, *MM'* is not a symmetry reflection plane.

One symmetry that all the structures in Figure 12.2 could have is *inversion* symmetry. Inversion is a change in sign of all coordinates of each atom. As indicated in Figure 12.5, it is equivalent to a rotation by 180" about an axis, (which changes the signs of two coordinates) followed by a reflection of the atom coordinates in a plane perpendicular to the axis (which changes the sign of the third coordinate). The inversion simply interchanges points on opposite sides of the origin, and it may be seen by inspection that it is possible for this operation to leave the crystals unchanged. While there may be some structures in each crystal class which have this symmetry, it is possible that a crystal would not have inversion symmetry if the combination of atoms or ions corresponding to a single cell did not have the proper symmetry. Inversion symmetry' is the only possible symmetry of the triclinic system.

In the monoclinic systern, o reflection in a plane parallel to the face containing the angle α may leave the structure unchanged. Also, a rotation of 180" about an axis perpendicular to the face containing α may leave the structure unchanged. This 180" rotation is called a twofold rotation, because two such rotations would give one complete revolution. Likewise, a threefold rotation axis corresponds to symmetry under 120" rotation, a fourfold axis to 90°, and a sixfold axis to 60" or a/3. Because of the translational crystal symmetry, these four kinds of rotation axes are all that can occur in a crystal.

In the orthorhombic system, there can be symmetry reflection planes each of which is perpendicular to a face and parallel to an edge. Also, there may be a

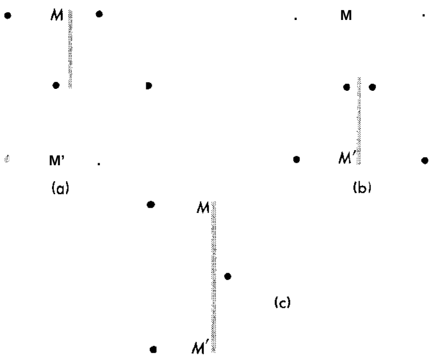


Figure 12.4. Diagrams illustrating symmetry under mirror reflection. Diagrams (a) and (c) do not have reflection symmetry in the MM' plane. In diagram (b), MM' is a mirror reflection symmetry plane.

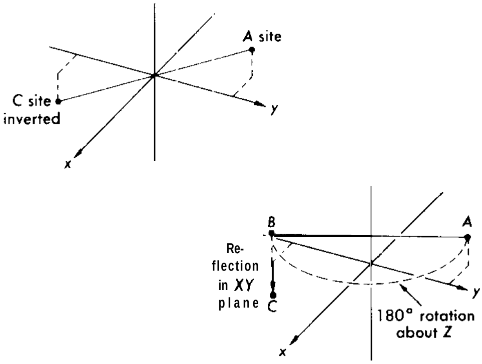


Figure 12.5. Diagrams illustrating symmetry under inversion. Inversion is equivalent to a reflection in one plane, followed by a 180" rotation about an axis normal to the reflection plane.

twofold rotation axis perpendicular to any face. The rhombohedral system, among other possible symmetries, can have a three-fold rotation axis through the diagonal connecting corners, where the angles α meet. Threefold axes may occur in the hexagonal and cubic systems as well. Fourfold rotation axes may occur in the tetragonal and cubic systems, while only hexagonal systems can have six-fold rotation axes.

The reason for being interested in rotation and reflection symmetries is that for a crystal of known symmetry one may derive limitations on the possible values of some physical quantities, i.e. they must be consistent with the symmetries. Such quantities as electrical conductivity, heat conductivity, dielectric constant and permeability can vary with the directions of the corresponding fields. However, for a rotation symmetry axis of order greater than two, it turns out that these quantities have to be independent of direction in the plane perpendicular to the axis. Then, in a hexagonal crystal of a metal such as zinc, the electrical conductivity can vary at most with the angle of the applied field relative ta the axis of the hexagon. Similarly, the conductivity in a cubic crystal is independent of direction since there are three fourfold axes and four threefold axes, oriented at various angles with respect to each other.

12.3 CRYSTAL BINDING FORCES

A different classification of crystals could be made on the basis of the types of forces holding the crystals together. There are four general kinds of binding involved:

(1) Valence crystals are held together by the same kinds of forces that hold organic molecules together. While the electrons of the atoms are bound fairly tightly to the atoms, there is a sharing of electrons between neighboring atoms. For example, Figure 12.6 represents a valence crystal in two dimensions, in which

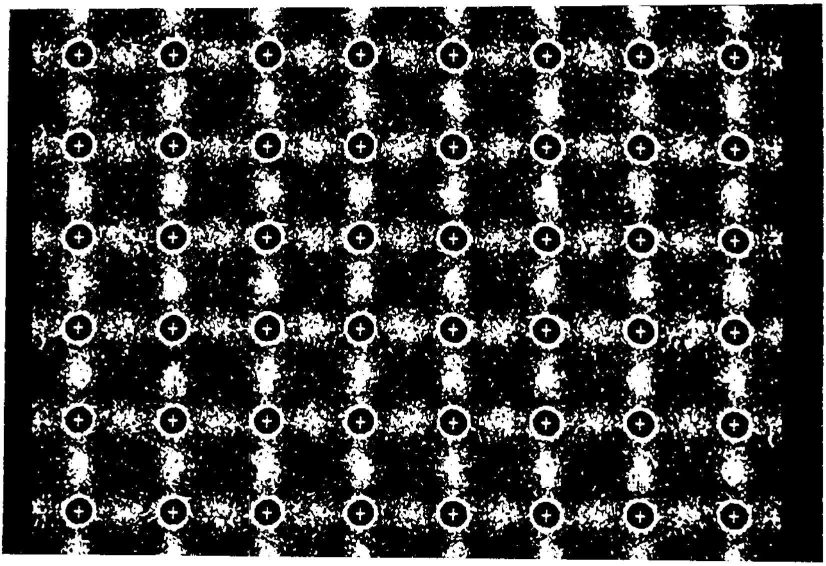


Figure 12.6. In covalent bonding, the crystal is held together by concentrations of negative electronic charge between positively charged cores. The negative and positive charges attract each other, giving a net binding effect to the crystal.

each atom contributes an electron which spends most of its time somewhere in between the atom and its nearest neighbors. Then, on the average, the positively charged atoms which remain will be attracted toward the negative charge clouds, and hence toward the other atoms. The electrons are shared, since one such electron cannot be said to be bound to any particular atom. The attraction caused by this sharing can give rise to a lower energy than if the electrons were all bound to individual atoms; therefore, if the atoms are to be separated, forces must be exerted to give work to make up this change in energy. A typical crystal with this kind of binding is the diamond, made of carbon atoms.

(2) Ionic crystals are held together primarily by Coulomb forces. A typical crystal of this type is sodium chloride-table salt. The outer electron in sodium is

fairly loosely bound, since it is the only electron outside a closed n = 2 shell, whereas the chlorine atom needs one electron in the $n = 3$, $\ell = 2$ orbits in order to form a closed $3p$ subshell. Then, when a sodium atom comes near a chlorine atom, this electron tends to go over to the chlorine atom. The resulting positive and negative ions are then bound by electrical forces. likewise, a crystal made of such dissimilar ions of valences ± 1, or ± 2, is held together by Coulomb forces between ions.

(3) In metals the outer electrons are very loosely bound, and each electron moves through the whole crystal, being shared about equally by all the atoms. As in the case of valence binding, this sharing lowers the energy and causes the atoms to be bound together.

(4) In crystals consisting of neutral atoms or molecules where the electrons are bound so tightly that there is little shuring of electrons, the forces are weaker and are called *van der Waals* forces. These arise primarily from electric dipole interactions. Some molecules have permanent electric dipoles and interact through these. In other cases, such as in solid crystals of argon or neon, there are only fluctuating dipoles to give the binding.

12.4 SOUND WAVES IN A CONTINUOUS MEDIUM

In discussing physical processes which occur in solids, two things are of primary interest: first, the properties of the lattice of atoms; and second, the electronic wavefunctions and energy level structure for the outermost atomic electrons. One of the important lattice properties is that of lattice vibrations. These vibrations are oscillations of atoms in the crystal about their equilibrium positions, and are responsible for such diverse phenomena as sound waves and specific heats at high temperature; they are also important in limiting electrical conduction and heat conduction. The interaction of electrons with lattice vibrations can, under some conditions, cause electrons to be bound together in pairs, and can give rise to the phenomenon of superconductivity at sufficiently low temperatures. Electrons in crystals play an extremely important role in phenomena such as magnetism, propagation and absorption of light in crystals, and conduction of electricity.

In the following two sections we shall discuss the classical and quantum theories of lattice vibrations in crystals and see how they enter into the calculation of the specific heat of a crystal. For purposes of comparison, in the present section we shall consider the classical theory of sound waves in a continuous medium.

To describe wave propagation through an elastic medium in classical mechanics, the medium is treated as a continuous one with a mass density ρ, and a suitably defined elastic constant. The wove equation can then be derived by straightforward application of Newton's laws of motion in an infinitesimal element of the medium.

Consider, for example, compressional waves in a long, thin, elastic, solid rod, as in Figure 12.7. We introduce the variable $\psi(x, t)$ to describe the displacement from equilibrium at time t of a point in the rod whose equilibrium position is x.

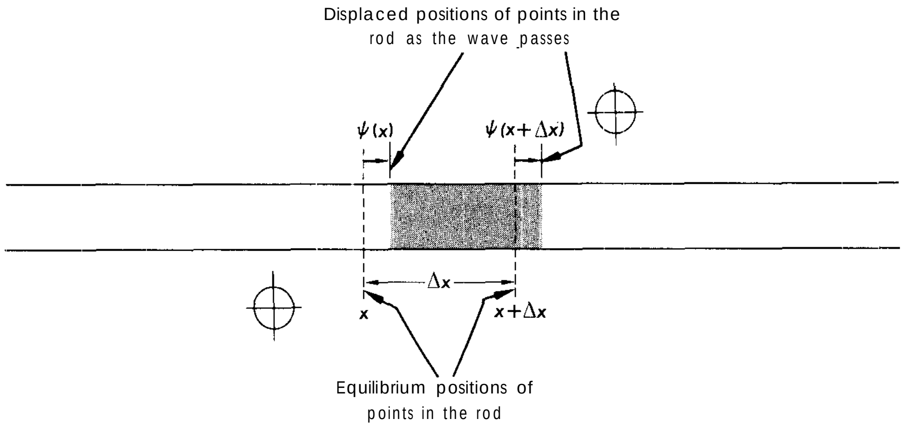


Figure 12.7. The motion of a long, thin rod, as compressional waves propagate through it, is described by a variable ψ(x, f), the displacement at time t of a particle where equilibrium position is x.

Consider an infinitesimal portion of the rod of length Ax, between x and x + Ax at equilibrium. Under the action of the wave as it propagates through the rod, this portion of the rod may be stressed so that its length is changed. The change in length will be

$$\Delta L = \psi(x + \mathrm{Ax},\ \mathrm{f}) \quad \psi(x, t) \tag{12.1}$$

and the fractional change in length will be

$$\frac{\Delta L}{\mathrm{AX}} = \frac{\psi(x + \Delta x, t) - \psi(x, t)}{\mathrm{AX}} - \frac{\partial \psi(x, t)}{\partial x} \tag{12.2}$$

if Ax is sufficiently small. The partial derivative taken here indicates that the change of length is calculated at a particular time.

The fractional change in length, called strain, is related to the elastic constant ***Y-Young's*** modulus-by

$$\frac{\Delta L}{\Delta x} = \frac{T}{AY} \tag{12.3}$$

where T is the tension in the rod at the point x and A is the cross-sectional area of the rod. The quantity T/A is called stress; it is the force per unit area tending to change the length of the rod. Young's modulus is thus the stress divided by the fractional change in length of a piece of material. Combining the above two equations, the equation

$$\frac{\partial}{\partial x}\psi(x, t) = \frac{T(x, t)}{YA} \tag{12.4}$$

expresses the elastic property of the rod.

Next, applying Newton's law of motion to the infinitesimal section Ax of the rod, we find that the net force in the positive x direction is

$$T(x + \Delta x, t) - T(x, t) \cong \frac{\partial T}{\partial x}\Delta x \tag{12.5}$$

This must equal the mass $\rho A \Delta x$, times the acceleration $\partial^2\psi/\partial t^2$:

$$\frac{\partial T}{\partial x}\Delta x = \rho A \Delta x \frac{\partial^2\psi}{\partial t^2} \tag{12.6}$$

Thus, differentiating Equation (12.4) and combining with Equation (12.6), we obtain the ‘wave equation,

$$\frac{\partial^2\psi}{\partial x^2} - \frac{\rho}{Y}\frac{\partial^2\psi}{\partial t^2} = 0 \tag{12.7}$$

It is easily verified that ψ satisfies this equation if it is any function of $x - wt$ or $x + wt$, where $w = \sqrt{Y/\rho}$. Thus, the phase speed of propagation of the waves will be

$$w = \sqrt{Y/\rho} \tag{12.8}$$

For a wave which is of the form $\psi = \psi_0 \cos(kx - \omega t)$, where ψ_0 is a constant, the angular frequency ω and wavenumber k of the wave will be related by $\omega = wk = \sqrt{Y/\rho}\,k$, where w will be essentially independent of k or ω.

12.5 WAVE EQUATION FOR SOUND WAVES IN A DISCRETE MEDIUM

Let us now consider sound waves in a crystalline solid to see the effect of having a medium made up of discrete atoms or molecules, rather than a continuously distributed mass. For simplicity, the discussion will be based on the one dimensional crystal-like system shown in Figure 12.8, in which the forces between neighboring atoms are approximated by massless springs. When all the springs are at their equilibrium length a,. the atoms are said to be in their equilibrium positions. The one dimensional structure pictured is then crystal-like, because it has a simple repetitive, or periodic, structure. If one of the atoms is displaced slightly and then released, it will vibrate about its equilibrium position, and neighboring atoms will start to vibrate because of the elastic forces between

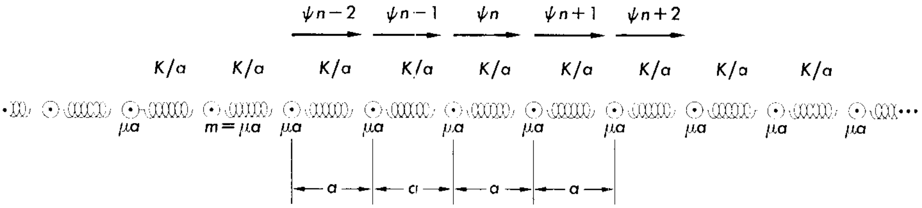


Figure 12.8. A **one** dimensional model of a solid lattice, consisting of atoms of mass μa, connected by springs of spring constant K/a.

atoms. In a real crystal, something very similar occurs, but the vibrations take place in three dimension,;. The basic unit is the mass m $\equiv \mu a$, connected to neighboring masses by the massless springs of spring constant K/a. The equilibrium spacing of the masses is a.

Clearly, μ is the effective mass per unit length, or the linear mass density. If a force tends to compress an object giving a change in length $\Delta \ell$, the same force acting on an object half os long would give a change in length $\Delta \ell/2$; i.e. the spring constant would be twice as big. Thus in our case we have chosen to write the spring constant as K/a, so that the spring constant times the length of an individual spring is a constant, K, which is independent of length. These springs can be thought of as simulating actual forces between atoms in a crystal for small vibrations. The quuntities K and μ for the one dimensional case are analogous to Y and ρ for the three dimensional case.

We shall consider only ongitudinal motion of the atoms, parallel to the length of the system. Then, in analogy to the displacement variable $\psi(x, t)$ used in describing wavemotion in a continuous medium, we define $\psi_n(t)$ as the displacement from equilibrium of the n^{th} atom in the line. In terms of the spring constant K/a, the force on the n^{th} atom is:

$$F = -\frac{K}{a}[(\psi_n - \psi_{n-1}) + (\psi_n - \psi_{n+1})] \tag{12.9}$$

This force gives the mass μa an acceleration $d^2\psi_n/dt^2$. Hence, using Newton's second law for the n^{th} particle,

$$-\frac{K}{a}(2\psi_n - \psi_{n-1} - \psi_{n+1}) = \mu a \frac{d^2\psi_n}{dt^2} \tag{12.10}$$

There is one such equation for each atom in the line of atoms, corresponding to different values of the index n.

The above set of coupled differential equations is closely related to the wave equation, Equation (12.7); in the limit of infinitesimally small spacing a, Equation (12.10) reduces to Equation (12.7). Let us see how this happens. In the limit of small a, the distance na must be replaced by the corresponding distance x of the atom from some reference position. Then,

$$\lim_{a \to 0} \frac{\psi_{n+1}(t) - \psi_n(t)}{a} = \lim_{a \to 0} \frac{\psi(x+a,t) - \psi(x,t)}{a} = \frac{\partial \psi(x,t)}{\partial x} \tag{12.11}$$

Similarly,

$$\lim_{a \to 0} \frac{1}{a^2}[(\psi_n - \psi_{n-1}) + (\psi_n - \psi_{n+1})]$$

$$= \lim_{a \to 0} \frac{1}{a}\left[\frac{\partial \psi(x)}{\partial x} - \frac{\partial \psi(x+a)}{\partial x}\right] = \frac{\partial^2 \psi}{\partial x^2} \tag{12.12}$$

Also, $d^2\psi_n/dt^2$ is the time derivative at a certain particle, so it becomes a derivative at constant x, or the partial derivative $\partial^2\psi_n/\partial t^2$. Hence, Equation (12.10) becomes:

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\mu}{K}\frac{\partial^2\psi}{\partial t^2} \tag{12.13}$$

and the phase speed will be given by $W = \sqrt{K/\mu}$.

In the model for lattice vibrations which we are using here, a is small-of the order of a few Angstroms-but finite. We would expect variations from the continuous wave solutions when the wavelength is comparable to a. We must return to Equation (12.10) and find solutions valid for all n and all t, for finite a.

6 SOLUTIONS OF THE WAVE EQUATION FOR THE DISCRETE MEDIUM

Equation (12.13) has solutions for continuous x and for a definite frequency w, of the form:

$$\psi = A_1 \cos (kx + \omega t + \varphi_1) + A_2 \cos (kx - \omega t + \varphi_2) \tag{12.14}$$

where A_1, A_2, φ_1 and φ_2 are arbitrary constants, and $w = wk = \sqrt{K/\mu}\, k$. Here, the terms in A_1 and A_2 correspond to waves propagating in the negative and positive x directions, respectively. By superposition of such solutions, one can find solutions representing standing waves; for example, one standing wave solution is

$$\psi = A \cos kx \cos (wt + \Phi) \tag{12.15}$$

where Φ is an arbitrary phase constant.

In the discrete case, on the other hand, the variable na corresponds to the position variable x. This leads us to attempt to find solutions for the discrete equation of motion, Equation (12.10), of a form similar to the above but with x replaced by na. Here we shall consider only standing 'wave solutions. let us then try the function

$$\psi_n(t) = A \cos (kna) \cos (wt + \Phi) \tag{12.16}$$

in Equation (12.10), to see if we can obtain a solution. Then on the left side of Equation (12.10), among other terms, the quantity,

$$\begin{aligned} -\psi_{n+1} - \psi_{n-1} = - A \cos(\omega t + \Phi) \\ [\cos (kna + ka) + \cos (kna - ka)] \end{aligned} \tag{12.17}$$

occurs. The trigonometric identity $\cos(\theta + \varphi) + \cos(\theta - \varphi) = 2 \cos \theta \cos \varphi$, with $\theta = kna$ and $\varphi = ka$, then gives us:

$$-\psi_{n+1} - \psi_{n-1} = -2A \cos(\omega t + \Phi)\cos(kna)\cos ka \tag{12.18}$$

Hence, when ψ_n of Equation (12.16) is substituted into Equation (12.10), the factor $A \cos(kna)\cos(\omega t + \Phi)$ occurs in each term. This substitution gives us

$$\begin{aligned} -\frac{K}{a} [A \cos(kna)\cos(\omega t + \Phi)][2 - 2 \cos ka] &= \mu a \frac{d^2\psi_n}{dt^2} \\ &= \mu a[-\omega^2 A \cos(kna) \cos (wt + \Phi)] \end{aligned} \tag{12.19}$$

This equation is satisfied if $\omega^2 = 2K/\mu a^2(1 - \cos ka)$. Since $1 - \cos\theta = 2\sin^2(\frac{1}{2}\theta)$, the relationship between ω and k may be written in the form:

$$\omega^2 = \frac{4K}{\mu a^2}\sin^2\left(\frac{1}{2}ka\right) \tag{12.20}$$

This equation has two solutions for ω which are opposite in sign. Only the positive solution for ω need be considered, so with the choice of the positive square root, this solution for the possible frequencies may be written as:

$$\omega = \sqrt{\frac{K}{\mu}}\left|\frac{\sin(ka/2)}{a/2}\right| \tag{12.21}$$

Thus substitution of the assumed solution, Equation (12.16), into the differential equation gives us a solution if ω and k are related in a certain way given by Equation (12.21). Such a relation between frequency and wave number is called a dispersion *relation.* The same dispersion relation would have resulted it we had worked with any of the other standing wave solutions, such as $B\sin(kna)\cos(\omega t + \Phi)$.

A graph of the dispersion relation, Equation (12.21), is given in Figure 12.9. The corresponding dispersion relation for the continuous medium, $\omega = \sqrt{K/\mu}\,k$,

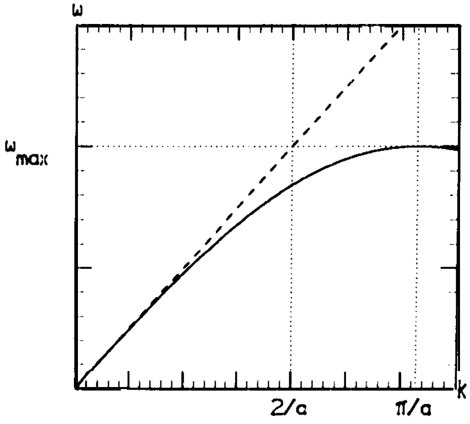


Figure 12.9. Graph of the dispersion relation, Equation (12.21), for waves on a one dimensional linear chain of atoms, connected by springs. Dotted line is the dispersion relation for a continuous medium, Equation (12.7).

is indicated by dashed lines on the same graph. Thus it can be seen that for $k \ll 1/a$ (long wavelengths), the phase speed $w = \omega/k = \sqrt{K/\mu}$ is approximately a constant, and is the same for the continuous and discrete media. For large k in the real solid, the phase speed deviates appreciably from this constant value.

12.7 NUMBER OF SOLUTIONS

To count up the total number of physically different possible standing wave solutions, we note first that from Equation (12.21), it is evident that the frequency ω

is a periodic function of k, with a maximum value of:

$$\omega_{max} = \frac{2}{a}\sqrt{\frac{K}{\mu}}. \qquad (12.22)$$

The frequency ω of Equation (12.21) is unchanged if k is changed to -k *or* if k is changed to $(2\pi/a) - $ k. likewise, $\psi_n = $ A cos (kna) cos (wf + Φ) for a fixed n is the same for these changes in k. Therefore, we can restrict the discussion to values of k in the region 0 to π/a, since we get nothing new by taking a k outside that region. For larger values of k |, the wavelengths $2\pi/k$ would be shorter than the lattice spacing; this would be meaningless, since there are no atoms this close together to vibrate with such wavelengths.

Many solids have wave speeds at low frequencies of around 10^3 m/sec. The spacing, a, between atoms is around 2 x 10^{-10}m. An estimate of the highest possible angular frequency of a wave propagating in such a solid is then:

$$w_{max} \cong \frac{2 \times 10^3}{2 \times 10^{-10}} = 10^{13} \text{ sec}^{-1}$$

The speed of sound differs by only about 1% from its low frequency value at 4 x 10^{11} cps. Thus in the audible range, zero to 20,000 cps, the speed of sound in a solid is essentially independent of frequency.

Up to this point, we have specified neither the size of the one dimensional crystal nor the boundary condition:, on the displacements ψ_n. Once these are specified, even in classical mechanics a discrete set of values of k results. If, as in the discussion of the density of states in Chapter 11, we impose periodic boundary conditions at the ends of a periodicity region of length Na = L, then for $\psi_n = $ A $\cos(kna)$ cos $(\omega t + \Phi)$, we would require that

$$\psi_{n+N} = \psi_n \qquad (12.23)$$

Here N is the number of masses, or crystal cells, in the length L. Equation (12.23) results in:

$$\cos(kna + kNa) = \cos(kna) \qquad (12.24)$$

This means that

$$kNa = kL = 2 m x \qquad (12.25)$$

or

$$k = \frac{2m\pi}{Na}, \quad m = 0, 1, 2, \ldots \qquad (12.26)$$

The other standing wave solutions, $\psi_n' = B$ sin kna cos $(\omega t + \Phi)$, would give these some values for k.

The independent values of k lie in the range 0 to $-a/a, corresponding to m ranging from 0 through ½ N for even N, or 0 through ½ (N − 1) for odd N. The values k = π/a and k = 0 give nothing for the solution $\psi_n' = B$ sin (kna)

$\cos(\omega t + \Phi)$, since:

$$\sin(0) = \sin\left(\frac{\pi}{a} na\right) = 0 \tag{12.27}$$

for any n. Then for even N there are $\frac{1}{2}N - 1$ solutions for the solution ψ'_n and $\frac{1}{2}N + 1$ solutions for the solution $\psi_n = A\cos(kna)\cos(\omega t + \Phi)$. Thus there are N different states. likewise, N states occur for odd N. The number of different oscillation states (or normal modes, as they are called in classical mechanics) is equal to the number of movable atoms in the fundamental periodicity region.

Also, if other types of boundary conditions were used, such as requiring $\psi_{N+1} = \psi_0 = 0$ for fixed endpoints, the number of different modes of oscillation would equal the number of degrees of freedom of the system. In this case, the number of degrees of freedom would equal the number of movable masses or cells, N.

Imposition of the periodic boundary conditions for the one dimensional chain corresponds to taking the long chain of N atoms and bending it into a circle, so that one end fits onto the other. If N is sufficiently large, the slight curvature introduced into the chain has negligible effect on the equations of motion. A wave propagating out past one end, however, must then propagate back in from the other end.

12.8 LINEAR CHAIN WITH TWO MASSES PER UNIT CELL

To see the effects of introducing internal degrees of freedom in the crystal cell, we next consider a slightly more complicated one dimensional crystal with two inequivalent atoms in each repeated unit. The chain is diagramed in Figure 12.10; the alternate masses are denoted by μa and Ma, and the distance between successive masses of similar type is a. The distance between neighboring masses Ma and μa is a/2, and the displacements from equilibrium of the masses μa and Ma are denoted by $\psi_n^{(1)}$, $\psi_n^{(2)}$, respectively. The springs connecting the masses are all assumed to have the same spring constant K/a. The crystal ceil is one complete unit from which the whole crystal can be built by repetition; hence, in this

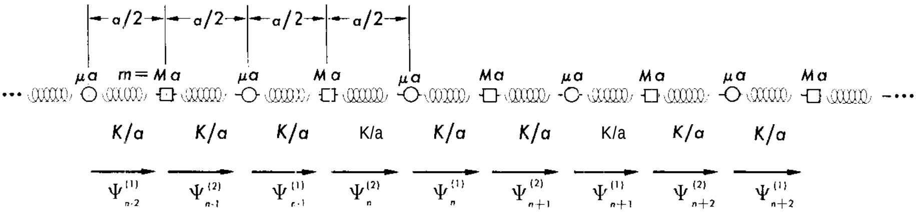


Figure 12.10. linear chain with two dissimilar atoms per unit cell.

case, the cell width or lattice constant is a, and the cell contains two masses: μa, Ma, and two springs.

let us assume that the displacement of the n^{th} mass pa is

$$\psi_n^{(1)} = A_1 \cos(kna)\cos(\omega t + \Phi) \tag{12.28}$$

and the displacement of the n^{th} mass *Ma* is

$$\psi_n^{(2)} = A_2 \cos[k(n + ½)a]\cos(\omega t + \Phi) \tag{12.29}$$

The Newtonian equations of motion are:

$$\begin{aligned} \mu a d^2\psi_n^{(1)}/dt^2 &= -(K/a)(2\psi_n^{(1)} - \psi_n^{(2)} - \psi_{n+1}^{(2)}) \\ M a d^2\psi_n^{(2)}/dt^2 &= -(K/a)(2\psi_n^{(2)} \quad \psi_{n-1}^{(1)} - \psi_n^{(1)}) \end{aligned} \tag{12.30}$$

These equations of motion lead in a straightforward way to:

$$\begin{aligned} A_1\left(\omega^2\mu a \quad \frac{2K}{a}\right) + A_2\left(\frac{2K}{a}\cos\frac{1}{2}ka\right) &= 0 \\ A,\left(\frac{2K}{a}\cos\frac{1}{2}ka\right) + A_2\left(\omega^2 M a \quad \frac{2K}{a}\right) &= 0 \end{aligned} \tag{12.31}$$

For these two equations to be consistent, the determinant of the coefficients of A_1 and A_2 must vanish. The resulting dispersion relation is

$$a^4\mu M\omega^4 - 2Ka^2(\mu + M)\omega^2 + 4K^2\sin^2\frac{1}{2}ka = 0 \tag{12.32}$$

The solutions

$$\begin{aligned} \psi_n^{(1)} &= B_1 \sin(kna)\cos(\omega t + \Phi) \\ \psi_n^{(2)} &= B_2 \sin\left[k\left(n + \frac{1}{2}\right)a\right]\cos(\omega t + \Phi) \end{aligned} \tag{12.33}$$

would lead to this same dispersion relationship. The positive solution!; for ω are:

$$\omega_\pm = \frac{1}{a}\sqrt{K\frac{\mu + M}{\mu M} \pm K\sqrt{\left(\frac{\mu + M}{\mu M}\right)^2 - \frac{4}{\mu M}\sin^2\frac{1}{2}ka}} \tag{12.34}$$

For long wavelengths, ½ ka << 1, the solutions may be approximated by:

$$w + \cong \frac{1}{a}\sqrt{2K\left(\frac{\mu + M}{\mu M} - \frac{1}{4}\,\frac{1}{\mu + M}\cdot k^2a^2\right)} \tag{12.35}$$

and

$$w - \cong \frac{1}{2}\sqrt{\frac{2K}{\mu + M}}\,|k| \tag{12.36}$$

Note that again w is unchanged in changing k to -k, *or* to $2\pi/a - k$.

12.9 ACOUSTIC AND OPTICAL BRANCHES

Sketches of $a\omega_+\sqrt{\mu/K}$ and $a\omega_-\sqrt{\mu/K}$ for the special case M = 2μ are given in Fig. 12.11. There are now two branches to the w versus *k* curve. In general, if there are ℓ masses per cell that differ in mass or geometry, or that have different forces acting upon them, there will be ℓ branches to the curve. In the one dimensional case, only one of these curves will pass through the origin w = 0 at k = 0. This branch is called the acoustic branch because for small k it describes the sound waves to which we are accustomed. The other branches lie at frequencies of the order of 10^{13} cps. Electromagnetic infrared waves also are in this frequency range, and although lattice vibrations are not electromagnetic waves, these branches are called optical branches. The high-frequency branches have been detected experimentally in absorption experiments with infrared light, and also by low energy neutron scattering experiments. Each branch is periodic in k and if periodic boundary conditions are applied, it can be shown, as in the discussion following Equation (10.26), that *each* branch has N modes if N is the number of cells (not necessarily the number of masses).

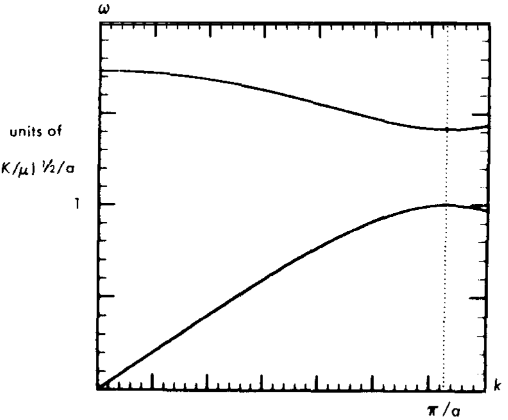


Figure 12.11. The two branches of the dispersion relation for a linear chain of atoms, with two dissimilar atoms per unit cell,

While our discussion has been for one dimensional spring-like forces, a three dimensional discussion with more realistic forces leads to very similar results. Instead of a single k, there is then a vector k with three components. There are still acoustic and optical modes with the number of modes per branch equal to the number of cells in the crystal. The cell now has three characteristic lengths and has a volume. Likewise, the zone giving the independent values of k is a volume in three dimensional “k-space.” The main change is that now, in addition to the longitudinal modes, there are transverse modes in which the actual motion of the atoms is perpendicular to the direction of wave propagation. Consider, for instance, the two dimensional array shown in Figure 12.12. If the n^{th} column of atoms is pulled downward uniformly, it exerts forces on the *n* + 1” column, giving rise to wave propagation to the right with vertical displacement. Of course, the longitudinal modes exist also. In three dimensions, for a given direction of k there can be displacements either parallel to k or displacements in two

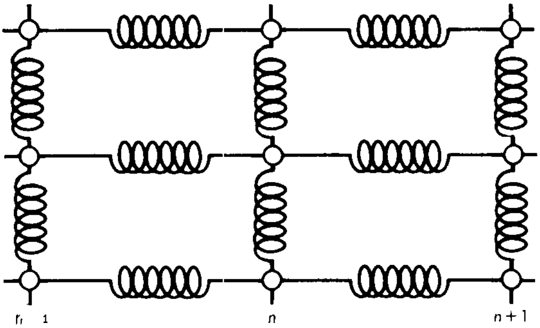


Figure 12.12. Two dimensional solid, consisting of atoms connected by springs. In addition to the longitudinal (compressional) waves supported by a linear chain, this model can support transverse (shear) waves.

directions perpendicular to k. Thus, for each longitudinal branch, there are two transverse branches; a branch may be either acoustic or optical. (Actually, for an anisotropic crystal with different properties in different directions, the various branches or modes of definite frequency are, in general, neither purely longitudinal nor purely transverse, but a mixture of the two.)

0 ENERGY OF LATTICE VIBRATIONS

Now we shall return to the consideration of the simple linear chain, Figure 12.8, in order to discuss the similarity between lattice vibrations and a collection of simple harmonic oscillators.

The solutions to the equation of motion, Equation (12.10), were found to be of the form:

$$\psi_n = A \cos kna \cos(\omega t + \Phi)$$

$$\psi_n' = B \sin kna \cos(\omega t + \Phi) \qquad (12.37)$$

and by superposition of these solutions, one can describe all possible wave motions of the atoms in the crystal lattice. The essential feature of a normal mode solution is that all the atoms vibrate with the *same* frequency. In a standing wave, successive atoms in the line would vibrate with slightly different amplitudes, but the vibrations would be in phase. (In a running wave the amplitudes could all be equal, but the phase could change slightly from one atom to the next.) The changes in vibration amplitude from one atom to the next are described by the factors cos kna or sin kna in the above solutions. The time-dependence for *all* atoms is contained entirely in the factor $A \cos(\omega t + \Phi)$. Thus, the factor $A \cos(\omega t + \Phi)$ describes, in a collective sense, the simultaneous vibrations of all the atoms in the crystal. We can, in fact, introduce a collective displacement "variable" $q_\omega(t)$, and write the solution ψ_n as:

$$\psi_n = \sqrt{2} \cos kna \; q_\omega(t) \qquad (12.38)$$

The factor $\sqrt{2}$ is for convenience. If we had assumed a solution of this form instead of Equation (12.16), in which the time-dependence is given explicitly, then upon substitution into the equations of motion we would have immediately found that $q_\omega(t)$ must satisfy the differential equation of the harmonic oscillator,

$$\frac{d^2 q_\omega}{dt^2} + \omega^2 q_\omega = 0 \tag{12.39}$$

where ω is given by Equation (12.21). Thus $\sqrt{2}\ q_{,,}(t) = A\cos(\omega t + \Phi)$ is the most general real solution of such an equation. Let us think of $q_\omega(t)$ as the displacement variable of a single oscillator.

Since the displacement of each particle in the lattice is proportional to $q_\omega(t)$, each has a kinetic energy proportional to $(dq_\omega/dt)^2$. Therefore, the total kinetic energy T of the lattice is some number C times $(dq_\omega/dt)^2$, or

$$T = \tfrac{1}{2} A^2 C\omega^2 \sin^2(\omega t + \Phi)$$

C is constant in time. Since total energy-kinetic plus potential energy--is conserved, the total energy is a constant in time and the total potential energy must therefore be $\tfrac{1}{2} A^2 C\omega^2 \cos^2(\omega t + \Phi) = C\ \omega^2 q_\omega^2$. The kinetic energy and potential energy of the crystal for this mode are thus the same as for a harmonic oscillator of displacement q_ω, frequency ω, mass $2C$, and spring constant $2C\omega^2$. (Also, q_ω satisfies the harmonic oscillator equation $d^2 q_\omega/dt^2 + \omega^2 q_\omega = 0$). Hence, the whole lattices appears similar to a single harmonic oscillator of mass $2C$. We will show that this mass is $N\mu a$, the total mass of the chain of atoms.

Let us examine the total kinetic energy of the lattice, to find C. The kinetic energy is, from Equation (12.38),

$$T = \sum_{n=0}^{N-1} \frac{1}{2}(\mu a)\left(\frac{\partial \psi_n}{\partial t}\right)^2 = \sum_{n=0}^{N-1} \mu a \cos^2(kna)\left[\frac{dq_\omega(t)}{dt}\right]^2 \tag{12.40}$$

If the phase kna in $\cos^2(kna)$ varies over a large number of values as n goes from 0 to N 1, we would expect that in the summation the square of $\cos^2(kna)$ could be replaced by its average value, ½ . The kinetic energy is therefore simply:

$$T = \frac{1}{2} N\mu a \left(\frac{dq_\omega}{dt}\right)^2 \tag{12.41}$$

In fact, this can easily be proved to be exact by writing $\cos(kna)$ as $\tfrac{1}{2}(e^{ikna} + e^{-ikna})$, using the formula for the sum of a geometric series, and noting that by Equation (12.26), $k = 2m\pi/Na$, where m is an integer. This kinetic energy is exactly the same as that of a single harmonic oscillator of displacement q_ω and mass $N\mu a$, which is the mass of the entire lattice. Hence 2C = Nya. The total energy is thus:

$$E(\omega) = T + V = \frac{1}{2}\mu a N\left[\left(\frac{dq_\omega}{dt}\right)^2 + \omega^2 q_\omega^2\right] \tag{12.42}$$

Both in the equation of motion, and in the expression for the energy, the variable q_ω—which in a sense describes the motion of all the masses in the crystal for this particular mode-is effectively a simple harmonic oscillator displacement variable. Since the Schrödinger equation is obtained from the energy expression, the importance of Equation (12.42) can be partially recognized from the ease with which one may utilize Equation (12.42) to obtain the quantum description of lattice vibrations. This will be discussed in the following section.

I ENERGY FOR A SUPERPOSITION OF MODES

The above expression, Equation (12.42), for lattice vibration energy was derived for a single mode. The question arises as to whether, when several modes are excited simultaneously in the crystal, the total energy will be the sum of individual contributions from each mode. That this is so may be seen from the following argument. Suppose that the displacement were a superposition of the form:

$$\psi_n = \sqrt{2}\, q_{\omega_1} \cos(k_1 na) + \sqrt{2}\, q_{\omega_2} \cos(k_2 na) = \psi_n(\omega_1) + \psi_n(\omega_2) \qquad (12.43)$$

Then the kinetic energy has the form:

$$\begin{aligned} T &= \sum_n \frac{1}{2}\mu a \left(\frac{d\psi_n}{dt}\right)^2 \\ &= \frac{1}{2}\mu a \sum_n \left\{ \left[\frac{d\psi_n(\omega_1)}{dt}\right]^2 + \left[\frac{d\psi_n(\omega_2)}{dt}\right]^2 + 2\frac{d\psi_n(\omega_1)}{dt}\frac{d\psi_n(\omega_2)}{dt} \right\} \\ &= T(\omega_1) + T(\omega_2) + \frac{1}{2}\mu a \cdot 2 \sum_n \frac{d\psi_n(\omega_1)}{dt}\frac{d\psi_n(\omega_2)}{dt} \end{aligned} \qquad (12.44)$$

The cross product summation involves:

$$\sum_n \cos(k_1 na)\cos(k_2 na) = \frac{1}{2}\sum_n \{\cos[(k_1 + k_2)na] + \cos[(k_1 - k_2)na]\} \qquad (12.45)$$

Since $k_1 \neq k_2$, one would expect the cosines to oscillate as n changes and hence to average out to zero. That this sum is exactly zero can be shown by again expressing the cosines as sums of exponentials, and using the equation for the sum of a geometric series. Likewise, even for equal frequencies the cross product of the solutions, proportional to $\cos(kna)$ and sin(kna), sum to zero. Thus the cross product terms never contribute to the kinetic energy. A similar argument holds for the potential energy. Therefore, if a number of modes are excited, the total energy is just the sum of the energies of the individual modes. Thus the normal modes in a sense act like independent particles. Although all the atoms in the lattice participate in a normal vibration mode, the various normal modes do not interfere with each other in any way, even though a great many of them may be present; and the total energy of the system, which is basically a sum of kinetic and potential energies of individual particles, can also be written as a simple sum of energies of the individual normal modes. It is this last fact that makes normal modes so useful.

12.12 QUANTUM THEORY OF HARMONIC OSCILLATORS AND LATTICE VIBRATIONS

All our previous discussion was based on Newtonian mechanics. We wish to see now what modifications arise in quantum mechanics. In quantum mechanics, the Schrödinger equation describing stationary states (states of definite energy) is obtained by expressing the energy E in terms of the coordinates and the momenta, then replacing the momentum component p_x by $-i\hbar\partial/\partial x$, and so forth. The resulting expression is then a differential operator which acts on the wavefunction. In calculating the energy contributed by one normal mode of a lattice vibration, the effective coordinate is q_ω and the mass is $N\mu a$. The effective "momentum" is then $N\mu a\, dq_\omega/dt$. Thus, in treating the quantum theory of lattice vibrations, one would expect that in the energy expression the effective momentum should be replaced by letting

$$N\mu a \frac{dq_\omega}{dt} = -i\hbar \frac{\partial}{\partial q_\omega} \tag{12.46}$$

This can be shown rigorously from the fact that $\mu a\, d\psi_n/dt$, the classical momentum of the i^{th} particle, is replaced by $-i\hbar\partial/\partial\psi_n$, and the fact that in general, ψ_n is a superposition of terms of different frequencies proportional to q_ω. We shall not prove this here, however. The energies of the lattice vibrations in quantum mechanics are, then, found from the quantum mechanical discussion of the one dimensional harmonic oscillator of mass $N\mu a$ and angular frequency ω.

From the study of the simple harmonic oscillator of spring constant k and mass m in Chapter 7, it will be recalled that in Newtonian mechanics the energy of the oscillator is

$$E = \frac{p_x^2}{2m} + \frac{1}{2}kx^2 \tag{12.47}$$

and the natural angular frequency of oscillation is

$$\omega = \sqrt{\frac{k}{m}} \tag{12.48}$$

In solving the Schrödinger equation for this system, it was found that only discrete energies of the system were possible, given by

$$E_n = (n + \tfrac{1}{2})\hbar\omega \tag{12.49}$$

where n is a positive integer or zero. These energy levels are equally spaced; the minimum possible energy is $E_0 = \frac{1}{2}\hbar\omega$, and is called the zero point energy.

In quantum mechanics, whenever a system has energies which can be written in a form corresponding to that of a simple harmonic oscillator, Equation (12.47), the energies will be quantized according to Equation (12.49).

In the case of lattice vibrations, each normal mode then has the possible energies, $(n + \frac{1}{2})\hbar\omega$. The smallest possible vibrational energy of the crystal is $\sum_{N\,\text{modes}} \frac{1}{2}\hbar\omega$. While our discussion was for a one dimensional crystal, except for the fact that k becomes a vector and additional polarizations are possible, all these results still hold for a three dimensional crystal.

'e If the average natural frequency ω of the normal modes in a crystal is about 10^{13}/sec, the number of cells in a crystal of reasonable size is 10^{23}, and A $\simeq 10^{-34}$j-sec, what is the order of magnitude of the zero point energy of the crystal?

n Zero Point Energy $\simeq \frac{1}{2}\hbar\omega N = \frac{1}{2}(10^{-34})(10^{13})(10^{23})$

$= 50$ joules.

e If the binding energy of the crystal is of the order of 1eV per atom, what is the order of magnitude of the ratio of the zero point energy to the binding energy?

n $\dfrac{1\text{eV}}{\frac{1}{2}\hbar\omega} \simeq \dfrac{1.6 \times 10^{-19}}{\frac{1}{2}(10^{-34})(10^{13})} \sim 300$

I PHONONS; AVERAGE ENERGY PER MODE AS A FUNCTION OF TEMPERATURE

Frequently, it is convenient (though not strictly correct) to think of the quantum number n in the energy expression, $(n + \frac{1}{2})\hbar\omega$, as meaning the number of "particles" of sound, called phonons. Thus, if due to an interaction of a lattice vibration mode with an electron, n increases by Δn, we say that Δn phonons were created. Usually, phonons are thought of in association with traveling sound waves rather than standing waves.

The specific heat of a solid due to motions of atoms can be found from a knowledge of the relationship between ω and **k** for the lattice vibrations. The Boltzmann factor of statistical mechanics for one mode is

$$e^{-E_n/k_BT} = e^{(n + 1/2)\hbar\omega/k_BT} \tag{12.50}$$

This factor gives us the relative probability of finding the solid in the state characterized by the eigenvalue E_n of energy.

At high temperatures, when k_BT is large compared with the average of $\hbar\omega$, then the Boltzmann factor $e^{-(n+1/2)\hbar\omega/k_BT}$ is slowly varying for small changes in n, and many states are excited. The quantization of energy should then be of no significance, and one could as well describe the crystal in terms of the classical oscillators. For a simple crystal containing one mole of atoms (N_0 atoms) in N_0 unit cells, there are $3N_0$ modes of oscillation (since there are 1 longitudinal and 2 transverse modes per atom). By the equipartition of energy theorem, each of the quadratic terms proportional to q_ω^2 and $(dq_\omega/dt)^2$ in the energy of one mode, contributes an average energy of $\frac{1}{2}k_BT$ to the total crystal energy. Thus, the total energy is $3N_0k_BT = 3RT$, and the heat capacity per mole is 3R. This is called the Wang-Petit law, and it agrees well with experiment for most solids.

For very low temperatures, only the lowest frequencies can give a Boltzmann factor much different from zero. In calculating a thermal average to find the average total energy, we have to average over all states of the system. This involves an average over all the quantum states with energy $(n + \frac{1}{2})\hbar\omega$ for a given mode, and then a sum over all modes of various frequencies. The average energy for a given mode is

$$\langle E\rangle_{\text{mode}} = \frac{\sum_{n=0}^{\infty} E_n e^{-E_n/k_BT}}{\sum_{n=0}^{\infty} e^{-E_n/k_BT}} \tag{12.51}$$

with $E_n = (n + \frac{1}{2})\hbar\omega$. The summation in the denominator D is

$$D = e^{-1/2\,\hbar\omega/k_BT}\sum_{n=0}^{\infty}\left(e^{-\hbar\omega/k_BT}\right)^n \tag{12.52}$$

and therefore simply involves a geometric series. Thus, the standard formula for the sum of an infinite geometric series, $\sum_{n=0}^{\infty} a^n = 1/(1 - a)$ for $a < 1$, (gives for the denominator: $D = e^{-1/2\,\hbar\omega/k_BT}/(1 - e^{-\hbar\omega/k_BT})$. The reader can easily verify from Equation (12.51) that $\langle E\rangle_{\text{mode}} = (1/D)\,[dD/d(-1/k_BT)]$, so that after carrying out the differentiations, the average energy contributed by one mode—or by phonons of frequency ω—is

$$\langle E\rangle_{\text{mode}} = \hbar\omega\left(\frac{1}{e^{\hbar\omega/k_BT} - 1} + \frac{1}{2}\right) \tag{12.53}$$

12.14 LATTICE SPECIFIC HEAT OF A SOLID

Next, we want to sum over the various modes for a given longitudinal or transverse polarization, to find the average total energy for that given polarization. In discussing statistical mechanics, we found the density of states for particles by considering periodic boundary conditions on a wavefunction of the type $\exp[i(k_xx + k_yy + k_zz)]$; and we found that the number of states in an element of momentum space and volume V of ordinary space was

$$\frac{V\,dk_x\,dk_y\,dk_z}{(2\pi)^3} = \frac{V\,dp_x\,dp_y\,dp_z}{h^3} \tag{12.54}$$

where, in that case, $p = \hbar k$. Here, we could write the spatial dependence of the phonon wavefunctions for running waves as an exponential of this same form, and a similar application of periodic boundary conditions would lead to:

$$\frac{V\,dk_x\,dk_y\,dk_z}{(2\pi)^3} \tag{12.55}$$

for the number of states of each polarization. This can also be seen easily by generalizing Equation (12.26) to the three dimensional case. Since $E_0 = \frac{1}{2}\hbar\omega(\mathbf{k})$

is the minimum possible energy of each mode and does not change when more phonons are created in that mode, it is of more physical interest to calculate the average of the difference $\Delta E_n = E_n - E_0 = n\hbar\omega$ from the zero point or ground state energy. This average is

$$\langle \Delta E \rangle = \frac{V}{(2\pi)^3} \int dk_x\, dk_y\, dk_z \left(\frac{\hbar\omega}{e^{\hbar\omega/k_BT} - 1} \right) \tag{112.56}$$

Since only the lowest frequencies contribute at low temperatures, we can assume that ω is in the acoustic branch, i.e. depends linearly on k . If we are dealing with the longitudinal mode, then we may assume that for small ω,

$$|\mathbf{k}| = \frac{1}{w_\ell}\omega \tag{12.57}$$

where w_ℓ is the speed of propagation of that mode, at low frequencies, which might differ from the speed of propagation of the transverse acoustic modes. Since ω is a function of the magnitude of k, we can choose a spherical shell in ***k*** space of radius k and thickness dk, for the element of volume, and write:

$$dk,\ \mathrm{dk},\ dk,\ \text{--}\ 4\pi k^2 dk \tag{12.58}$$

Since $k = \omega/w_\ell$, this becomes:

$$dk_x\, dk_y\, dk_z \longrightarrow \frac{4\pi}{w_\ell^3}\omega^2 d\omega \tag{12.59}$$

and similarly for the two transverse modes with speed w_t. Thus, $\langle \Delta E \rangle$ has the form of

$$(AE) = \int_0^\infty \omega^3 f(\omega/T)\, d\omega \tag{12.60}$$

where $f(w/J) = \dfrac{V}{2\pi^2}\left(\dfrac{1}{w_\ell^3} + \dfrac{2}{w_t^3}\right)\dfrac{\hbar}{e^{\hbar\omega/k_BT} - }$,

is a function of the ratio ω/T. While the range of ω is actually finite, we have, for simplicity, taken the upper limit to be infinity for temperatures low enough so that $k_BT \ll \hbar\omega_{\max}$. Then the factor $1/(e^{\hbar\omega/k_BT}$ 1) makes the integrand negligible for the large frequencies. Thus at low temperatures,

$$\langle \Delta E \rangle = \text{const.} \times T^4 \int_0^\infty \left(\frac{\omega}{T}\right)^3 f\left(\frac{\omega}{T}\right) d\left(\frac{\omega}{T}\right) = \text{const.} \times T^4 \tag{12.61}$$

The integral involved is the same as was encountered in the discussion of black body radiation in Chapter 11, and has the value $\pi^4/15$. We may then evaluate the constant of proportionality to obtain:

$$\langle \Delta E \rangle = \frac{\pi^2 V}{30}\frac{k_B^4}{\hbar^3}\left(\frac{1}{w_\ell^3} + \frac{2}{w_t^3}\right) T^4 \tag{12.62}$$

If ΔE is proportional to T^4 at low temperatures, then the heat capacity $d\Delta E/dT$ at low temperatures is proportional to T^3. These results agree well with experiments for substances where the phonon energy gives the primary contribution to specific heat at low temperatures. In Figure 12.13 the specific heat C_v is plotted, showing the limiting behavior at low and high temperatures.

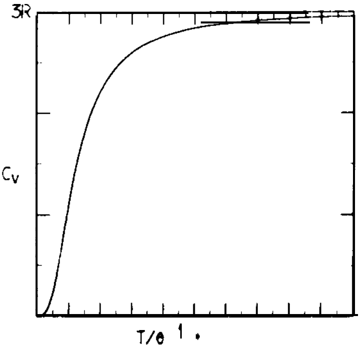


Figure 12.13. Specific heat at constant volume, due to lattice vibrations in a solid.

12.15 ENERGY BANDS OF ELECTRONS IN CRYSTALS

In electric conduction, heat conduction, the photoelectric effect, absorption of light, index of refraction, magnetism, and many other phenomena, the effects are primarily dependent on the behavior of electrons in solids. In this section we shall discuss some of the properties of wavefunctions and of the energies of electrons in crystals.

To get an intuitive idea of the structure of the energy levels of the electrons, let us consider a sodium crystal and begin by imagining the atoms very far apart, so that the wavefunction due to an electron on one atom is negligible at the positions of those atoms closest to it. Also, we will start with the outer electrons (one per atom) on all the atoms in their lowest energy state, except for some one electron which we single out to investigate. This one electron could be in any one of the energy states of its atom, and for each such energy there are two possible orientations of the electron spin. Also, if there are N atoms, there are N possible atoms in which the excited electron can be found. Thus, for any one atomic energy level there are, ir general, at least 2N distinguishable states for this electron.

As the atoms are brought nearer to each other to form the actual crystal, electronic wavefunctions start to overlap, and one can no longer say that an electron is associated with any one atom. Then the 2N energy states, derived from any one single atomic state, will ordinarily develop into 2N states that differ slightly from each other, and have energies that are slightly different. Therefore, a band of energies results containing 2N states. In the final crystal, the electrons will have an energy band structure, the bands being derived from the single atomic energy states and each band containing 2N closely spaced energy states.

.16 BLOCH'S THEOREM

Now, utilizing the translational symmetry of a crystal, we will find some properties of the electron wavefunctions, and we will show more rigorously that energy bands occur with $2N$ states per band. An electron in the crystal sees primarily the Coulomb potential energy of interaction with the atomic nuclei of the crystal, and the Coulomb potential energies of interaction with other electrons. We will assume, as is usually done, that the other electrons can be treated as a continuous charge distribution which, because of the electrons' interactions with atomic nuclei of the lattice, has the spatial periodicity of the lattice. Thus, the overall potential energy has the periodicity of the lattice.

Again for simplicity, let us treat a one dimensional lattice. Then, if V(x) is the periodic potential energy and a is the lattice spacing, $V(x+a) = V(x)$. The one dimensional Schrödinger equation for the wavefunction $\psi(x)$ of the electron is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x) \qquad (12.63)$$

If x is replaced by x + *a* in the above equation, dx → dx, so the kinetic energy operator is unchanged. Also, $V(x + a) = V(x)$, so the potential energy is unchanged. However, all we can say about $\psi(x)$ is that it becomes $\psi(x + a)$; hence the wave equation becomes

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x+a)}{\partial x^2} + V(x)\psi(x+a) = E\psi(x+a) \qquad (12.64)$$

The wavefunction $\psi(x + a)$ therefore satisfies the same equation, with the same energy E, as does $\psi(x)$. Now we can make an argument very similar to that made in discussing the exclusion principle in Chapter 9, to derive information about the possible form of the electron wavefunction. Since the point x, and the point x + a, are physically equivalent, we expect that it is possible for the electron densities at the two points to be the same. Thus, we expect that a wavefunction $\psi(x)$ may be found such that #*(x)$(x) = $\psi^*(x + a)\psi(x + a)$. This can only be true if ψ is of the form

$$\psi(x + a) = e^{ika}\psi(x) \qquad (12.65)$$

where ka is some real constant. That is, if two complex numbers $\psi(x)$ and $\psi(x + a)$ have equal absolute values, they can differ by at most a multiplicative phase factor, which we have written in the form e^{ika}. The phase factor cannot depend on the coordinates, for then both Equations (12.63) and (12.64) could not simultaneously be satisfied. Likewise, then,

$$\begin{aligned}&\psi(x + 2a) = e^{ika}\psi(x + a) = e^{ik(2a)}\psi(x)\\&\psi(x + 3a) = e^{ik(3a)}\psi(x);\ldots;\psi(x + na) = (e^{ikna})\psi(x)\end{aligned} \qquad (12.66)$$

for n an integer. The result is that upon translating by an amount no, the wavefunction is $\psi(x + na) = e^{ik(na)}\psi(x)$ and hence is changed only by a multiplicative factor.

One such function that has this property is

$$\psi(x) = e^{ikx} \tag{12.67}$$

Thus, if in this function x is replaced by x + a, the function becomes $e^{ika} \cdot e^{ikx}$. This function therefore satisfies:

$$\psi(x + a) = e^{ika}\psi(x) \tag{12.68}$$

[but will not satisfy the Schrldinger equation unless V(x) = constant]. Suppose we multiply e^{ikx} by u(x), where u has the property $u(x + a) = u(x)$, i.e. u(x) has the periodicity of the lattice. Thus we set

$$\psi(x) = e^{ikx}u(x) \tag{12.69}$$

Then $e^{ik(x+a)}u(x + a) = e^{ika}e^{ikx}u(x) = e^{ika}\psi(x)$. This is, in fact, the most general function that has the desired periodicity property expressed in Equation (12.65). Thus the wavefunction can be chosen to have the general form,

$$\psi(x) = e^{ikx}u(x) \tag{12.70}$$

where $u(x + a) = u(x)$. In three dimensions, similar reasoning gives us

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u(\mathbf{r}) \tag{12.71}$$

where u(r) has the periodicity of the lattice. This is called the *Bloch* theorem. The fact that the wavefunction takes this simple form allows many calculations to be performed in a relatively simple fashion.

12.17 NUMBERS OF BLOCH FUNCTIONS PER BAND

Once again considering the one dimensional case, Equation (12.65), let us apply boundary conditions to find the number of possible different values of k. The boundary condition we will impose is the periodic boundary ***condition,*** which states that $\psi(x)$ at one side of the crystal is the same as at the opposite side. In our case, this is $\psi(x) = \psi(x + Na)$. While periodic boundary conditions are hardly related to actual physical boundary conditions, they are simple to use and will give the correct number of values of k; this is because, as in the similar problem of lattice vibrations and in the previous discussion of statistical mechanics, the number of values of k is not sensitive to the particular boundary conditions.

Since $u(x + Na) = u(x)$ from the periodicity of u(x), the condition $\psi(x) = \psi(x + Na)$ means that

$$e^{ik(x+Na)} = e^{ikx} \tag{12.72}$$

or that $e^{ikNa} = 1$. But, in general, if $e^{i\Phi} = 1$, Φ must equal $2\pi n$, where n is a positive or negative integer or zero. Thus,

$$k = 2n\pi/Na, \quad n = 0, \pm 1, \pm 2, \ldots \tag{12.73}$$

While these values of k are the only possible ones, not all these values are physically distinct. Suppose, for example, we consider two possible values, k and $k + 2\pi/a$. Then

$$e^{i(k+2\pi/a)x} = e^{ikx}e^{i2\pi x/a} \tag{12.74}$$

Then, when a translation $x \longrightarrow x + a$ is performed, the function $e^{i2\pi x/a} \longrightarrow e^{i2\pi x/a}$, and so is unchanged; i.e. it has the periodicity of the lattice. Thus, $e^{i2\pi x/a}$ could be taken as part of $u(x)$, since it has the lattice periodicity. Hence $k + 2\pi/a$ is equivalent physically to k. We can then restrict k to lie within the Brillouin zone:

$$\frac{-\pi}{a} < k \le \frac{\pi}{a} \tag{12.75}$$

This is very similar to the restriction on k which arose in discussing lattice vibrations. Here it means that allowed wavelengths shorter than twice the lattice spacing are included in the function u(x); the exponential e^{ikx} varies only with wavelengths greater than twice the lattice spacing. The Bloch theorem thus separates the spatial variation of the electron wavefunction into a long-wavelength (slowly varying) part and a short-wavelength (rapidly varying) part: the long-wavelength part, e”“, is completely determined. In many calculations, it is only this long-wavelength part that is needed.

The restriction (12.75) on k, along with the possible values of k from Equation (12.73), means that the total number of independent values of n, and thus of k, is N, the number of unit cells. As n changes by unity, k changes slightly, and we can expect the energy to change slightly. Thus, as k changes over its range, we get a band of energies. The actual values of the energies can be obtained only by solving the Schrödinger Equation (12.63) in a periodic potential. This is ordinarily very difficult. For each k, the spin of the electron can have two orientations. Then the number of states per band is 2N. Likewise, for a three dimensional crystal with N cells there are $2N$ states per band, in agreement with the qualitative reasoning in Section 12.15.

8 TYPES OF BANDS

There will be an infinite number of energy bands in a crystal, but only a relatively small number correspond to bound states which are important in explaining normal crystal properties. The energy E is a function of k and can be complicated. Some possibilities are indicated in Figure 12.14. One simplification is that $E(k) = E(-k)$. This can be shown from the fact that, except for ψ, Equation (12.63) is real. Hence, if $\psi(x) = e^{ikx}u(x)$ is a wavefunction, $\psi^*(x) = e^{-ikx}u^*(x)$ is a solution with the same E. Note the similarity between graphing E versus k here, and graphing ω versus k for lattice vibrations. In some cases there will be an energy gap (or minimum energy difference) between bands, such as E_g between bands 3 and 4 of Figure 12.14, which corresponds to energies not allowed for the electron in the crystal. Such gaps are typically of the order of magnitude of an electron volt. In other cases the bands may overlap, such as in bands 1, 2 and 3, or bands 4 and 5 of the figure.

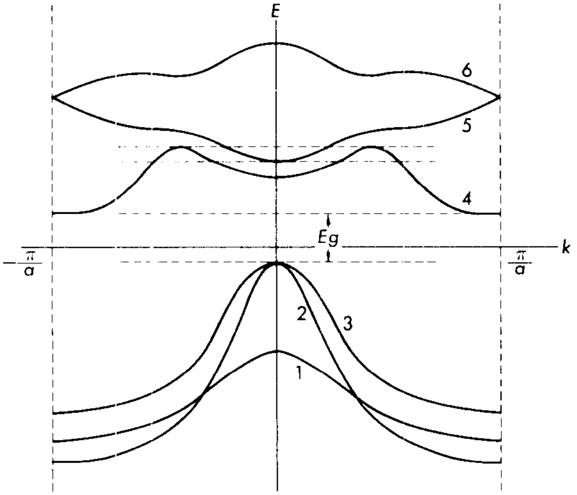


Figure 12.14. Diagram illustrating a number of different possibilities for electron energy bands in crystals.

12.19 EFFECTIVE MASS IN A BAND

For a free particle, $E = \frac{1}{2}p^2/m$, where p is the momentum and m is the mass. The free-particle wavefunction is proportional to e^{ikx} in one dimension, where $k = p/\hbar$. Thus for the free particle, $E = (\frac{1}{2}\hbar^2/m)k^2$. Now if a minimum or maximum occurs at $k = k_0$ for the electron energy $E(k)$ in a crystal band, then when k is near this minimum or maximum, i.e. when $k - k_0$ is small, the energy in the band as a function of $k - k_0$ may be similar to that for the free particle:

$$E(k) \cong E_0 + \alpha(k - k_0)^2 \tag{12.76}$$

where E_0 and α are constants. Let us then rewrite α as $\frac{1}{2}\hbar^2/m^*$, where m^* is a constant. Then, near the maximum or minimum,

$$E(k) \cong E_0 + \left(\frac{\frac{1}{2}\hbar^2}{m^*}\right)(k - k_0)^2 \tag{12.77}$$

Comparison with the energy expression for the free particle leads one to the idea of an "effective" mass,

$$m^* = \frac{\hbar^2}{2\alpha} \tag{12.78}$$

In a sense, the electron can then be treated as a free particle of mass m^*, with no periodic potential energy present. Near a maximum of energy, the effective mass is negative, and near a minimum, the effective mass is the more familiar positive quantity. In three dimensions, where **k** is a vector, α may (and frequently does) vary with direction in **k** space, so that the effective mass is a function of direction. The concept of effective mass is useful in calculating densities of states and in discussing phenomena in applied electric and magnetic fields, for situations in which particles near the minimum or maximum of energy contribute significantly to the effect.

le Suppose that for the one dimensional case,

$$E = \frac{\hbar^2}{ma^2}(1 - \cos ka)$$

For small ka, the expansion, cos $\theta = 1 - \frac{1}{2}\theta^2 + \ldots$, can be used. A similar expansion near ka = π can be used by noting that cos $\theta = -\cos(\pi - \theta)$. Find the effective mass at the energy maximum (k = π/a), and at the minimum (k = 0).

on For $ka < \; < \; 1, E = \frac{\hbar^2}{ma^2}\left[1 - \left\{1 - \frac{k^2a^2}{2}\right\}\right]$

$$\simeq \frac{\hbar^2k^2}{2m}, \quad m^* = m$$

For $\pi \quad ka| << 1$,

$$E = \frac{\hbar^2}{ma^2}[1 + \cos(ka - \pi)]$$

$$\sim \frac{\hbar^2(k^2}{ma^2} \quad \frac{- \quad \pi/a)^2}{2m} \qquad m^* = -m$$

0 CONDUCTORS, INSULATORS, SEMICONDUCTORS

Since the Pauli exclusion principle applies to electrons, in solids it is important to use Fermi-Dirac statistics for the electrons rather than classical statistics. This is, first, because the number of states per band (which equals twice the number of cells) is comparable to the number of outer atomic electrons. Secondly, the energy spread within a band is comparable to electron volts, whereas k_BT at room temperature is about 1/40 eV. Then the electrons will fill up the various different states in a band, and their average energy will be around an electron volt. Thus, the classical equipartition theorem does not hold and the effect of the exclusion principle is important; the <statistics will be degenerate.

Let us first verify that the band width ΔE might be of the order of electron volts. The change in k is about $\Delta k \simeq \pi/a$. If the lattice spacing, a, is 3 x 10^{-10}m, a reasonable value, then

$$\Delta k \simeq 10^{10}\mathrm{m}^{-1}$$

Assuming that $\Delta E \simeq \frac{1}{2}\hbar^2\Delta k^2/m^*$ with m^*, the effective mass, approximately the true electron mass, or about 10^{-30} kg, then ΔE, in electron volts, is $\Delta E \simeq$ 2 eV. If ΔE were a different function of Δk or m were significantly different from the mass of the electron, a different numerical result would be found; but this argument does give the right order of magnitude of the band width for the outer electrons. Inner electron; of the atoms have a very small band width, and the effective mass is very large because of their tight binding to the nucleus.

The average number of electrons per state, using Fermi-Dirac statistics, is

$$n(E) = [\exp(E - E_F)/k_BT + 1]^{-1} \qquad (12.79)$$

and for the degenerate case, $E_F >> k_BT$. Then each state is essentially filled with one electron, up to an energy of about E_F, and there are almost no electrons in states above E_F. The transition region where f(E) drops from ~ 1 to ~ 0 has a width of the order of magnitude of k_BT in energy. In the crystal, therefore, this transition region will ordinarily be a small fraction of the band width. Suppose, then, that the energy bands do not overlap, as indicated for bands 1 and 2 in Figure 12.15, and that tile energy gap E_g is several electron volts. Suppose there

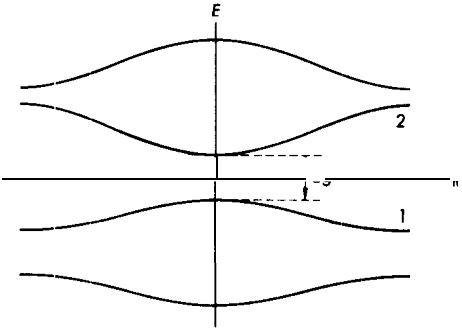


Figure 12.15. The energy difference between the conduction band minimum (band 2) and valence bond maximum is called the energy gap, E_g. In insulators, the valance band is filled, and the energy gap is of the order of several electron volts; the conduction bond is empty.

are enough electrons to fill all the states in band 1 and all of the lower bands, but not enough to fill band 2 completely. If there are N cells, and hence 2N available states per band, then if there are an even number of electrons per cell, there will be almost no electrons in band 2. This is because the even number of electrons will just fill an integral number of bands. The last filled band (band 1), is called the valence band, and the higher unfilled band is called the conduction bond (band 2 in Figure 12.15).

On the other hand, if again the bands do not overlap, but there are an odd number of electrons per cell, there will be only N electrons in the last band, and N unfilled states in that band (the conduction band).

On the basis of the foregoing discussion, one may obtain a simple explanation of the main differences between conductors and insulators. In order for an electric current to flow, there must be more electrons moving in one direction as compared with another. Since $\hbar k$ is somewhat like the electron's momentum, this means the electrons must have wavefunctions with average k different from zero. With no electric field applied, both cases of odd and even numbers of electrons per cell have an average k of zero, since wavefunctions of k and -k correspond to the same energy. When an electric field is applied to a substance having an odd number of electrons per cell, it can easily excite electrons with energies near

E_F into states producing a net current, because there are unfilled available energy states nearby in energy. Thus this crystal will be a conductor. For a substance having an even number of electrons per cell, the unfilled states are several electron volts away in energy, and it would take a very large electric field to produce appreciable current. Such a crystal is then an insulator.

From what has been said so far, all conductors should have obout equal, and large, conductivities. This is because we have assumed a perfectly periodic crystal lattice. One deviation from a perfect crystal lattice that is always present is the lattice vibration, or phonon. Electrons can interact with these phonons and be scattered away from current-carrying states. This is the main effect that limits conductivities in most conductors at room temperature. Other lattice imperfections which reduce conductivities are impurities and atoms missing at lattice sites. Also, in the discussion above it was assumed that the bands do not overlap. Suppose bands 1 and 2 of Figure 12.15 had overlapped. Then there would be more than 2N states having energies below the top of energy band 1, and thus for an even number of electrons per cell, the last 2N electrons could fit in, leaving nearby energy states unfilled. This crystal would then be a conductor. Calcium, with an even number of electrons per cell, is a conductor of this type.

Suppose that a crystal with an even number of electrons per cell had valence and conduction bands which did not overlap, but the energy gap was only a few tenths of an electron volt. Since k_BT at room temperature is about 1/40 eV, then the gap is not enormously greater than k_BT, and there would be a reasonable number of electrons in the conduction band; so the crystal would conduct electricity, but not as well as a normal conductor. A crystal of this type is called a **semiconductor.** Germanium, silicon and various compounds ure of this type. Semiconductors ***are*** used in many devices, especially in transistors.

12.2 1 HOLES

Suppose there is a semiconductor in which the gap E_g between conduction and valence bands is less than an electron volt, as in Figure 12.16. Then at room temperature there will be some electrons in the conduction band, and there will be an absence of electrons in the valence band, primarily at the energy maximum.

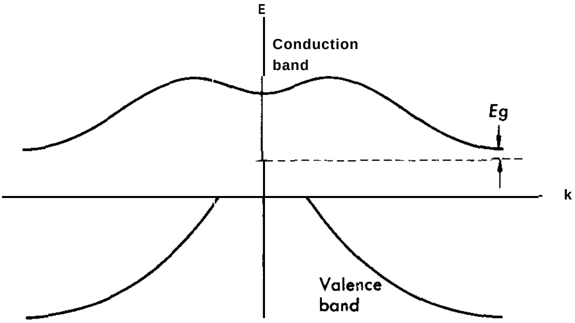


Figure 12.16. Illustration of conduction and valence bands having a very small energy gap.

These unfilled states in the valence band are called hales. The effective mass associated with these unfilled states at the energy maximum is negative.

For simplicity, let us assume that just one state, the j^{th} state, near the energy maximum is unfilled, so there is one hale. If the charge of an electron is $e =$ $e|$ and $\mathbf{v}_j$ is the expectation value of the velocity of the j^{th} state, then the current is proportional ta:

$$\sum_{i\neq j}(-\ e|\mathbf{v}_i) \tag{12.80}$$

Here, the summation is aver all valence band states except the one that is unfilled. This can be written as:

$$\sum_{i\neq j} -\ e\ \mathbf{v}_i = \sum_{\text{all } i}(-\ e\ \mathbf{v}_i) + \ e|\mathbf{v}_j \tag{12.81}$$

If the valence band were completely filled, the electric current would be zero. Thus, $\sum_{\text{all } i}(-|e\ \mathbf{v}_i) = 0$. The net current is then proportional ta $|e|\mathbf{v}_j$. Thus, a hale acts as a particle with a velocity associated with the empty state, and with a positive charge equal in magnitude ta the electronic charge.

The rate of change in time of the current is proportional ta $e\ d\mathbf{v}_j/dt$. Suppose there were an electron of charge $-\ e$ and effective mass m^* in the j^{th} state, and an electric field $\mathbf{E}$ were present. Then, using the expectation value of Newton's second law, we get

$$\frac{e\ d\mathbf{v}_j}{dt} = \frac{-|e|^2\mathbf{E}}{m^*} \tag{12.82}$$

Near a maximum in energy, m^* is negative, $m^* = -|m^*|$, so

$$\frac{e\ d\mathbf{v}_j}{dt} = \frac{+|e|^2\mathbf{E}}{|m^*|} \tag{12.83}$$

The motion is that of positively charged particles with positive mass. Thus, such a hale will contribute ta electric current in the same sense as an electron in the conduction band, which has negative charge and positive effective mass. This discussion shows that in a semiconductor the electric current will consist, in general, of an electron current due ta conduction band electrons, and a hale current due ta valence band hales.

12.22 n-TYPE AND p-TYPE SEMICONDUCTORS

By introducing impurities into a semiconductor, the number of electrons in the conduction band, or the number of hales in the valence band, can be greatly increased. Far example, the germanium atom, like carbon, has a valence of 4 and farms a valence-bound crystal, in which each germanium atom is surrounded by four other germanium atoms. If an arsenic atom impurity with 5 outer electrons is substituted far a germanium atom, 4 of the 5 electrons are bound tightly by the valence bands, but the fifth is loosely bound. To see how loosely, let us treat the impurity as if it were like a hydrogen atom. Thus the arsenic nucleus and all electrons but the fifth outer electron form an effective nucleus of charge e , and the electron of charge $-e$ is bound by the attractive Coulomb-like force between it and the core, and will be described by hydrogen-like energy levels lying below the conduction band minimum. However, the Coulomb force inside a medium with a dielectric constant K is $-e^2/4\pi\epsilon_0 K r^2$, so the effective charge for this hydrogen-like atom is $e/\sqrt{K}$. The dielectric constant in germanium is 16, and all electric fields are hence reduced by a factor $1/16$ in germanium. Also, one should use the effective mass m^* rather than the true electron mass. While the effective mass is dependent on direction, the average effective mass at the minimum of the conduction band is about $m/5$. The binding energy of a true hydrogen atom in free space is 13.6 eV and is proportional to me^4. The binding energy of the fifth electron may then be estimated as:

$$E_b \cong 13.6 \times \frac{1}{K^2} \times \frac{m^*}{m} = \frac{13.6}{(16)^2 \times 5} = .0106\ \text{eV}$$

This result agrees in order of magnitude with the actually measured binding energy. Since the binding energy below the conduction band is about .01 eV and is smaller than $k_B T \sim 1/40$ eV, at room temperature a large fraction of the impurities will be ionized, with the extra electrons going into the conduction band. The Fermi level E_F will lie near the bottom of the conduction band rather than halfway between bands as in a pure material, and so there will be very few holes in the valence band. Almost all conduction electrons will come from the impurities. Because the impurities give electrons to the conduction band, they are called donors. Also, since the current is due to negatively charged particles because there are few holes, this is called an n-type semiconductor.

Likewise, the germanium could be doped with impurities of valence 3 instead of 5. In this case, the impurity would draw an electron out of the valence band, to give itself 4 electrons. The resulting negative ion would then have the resulting hole bound loosely to it. Because this kind of impurity takes electrons out of a band, it is called an ***acceptor.*** Many of the holes are unbound at room temperature and move freely in the valence band. The Fermi energy is near the top of the valence band, and so there are few electrons in the conduction band. Thus the electrical conduction is mainly due to hole motion. Because the hole is effectively a positive particle, we say this is a p-type semiconductor.

A pure semiconductor, where there are equal numbers of electrons and holes, is called an intrinsic semiconductor. When the electrons or holes are due primarily to impurities, it is called an ***extrinsic*** semiconductor.

.23 HALL EFFECT

The fact that both holes and electrons can exist in semiconductors can be observed in the *Hall* effect. Suppose a piece of semiconductor (or any other material) is hooked across a battery as in Figure 12.17. Indicated on the figure by arrows labeled H and E are the average directions of motion of holes and elec-

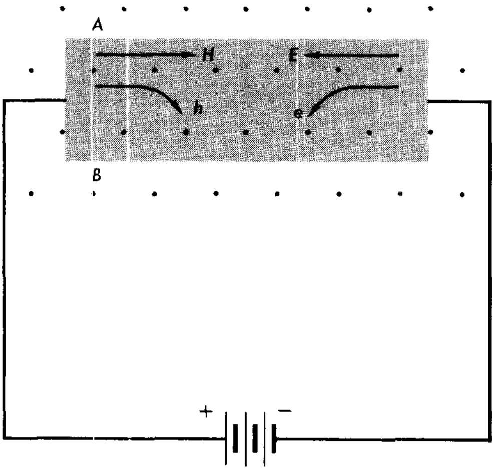


Figure 12.117. Schematic diagram of the experimental setup for observing the Hall effect. The dots indicate a magnetic field out of the paper. Current flowing from right to left in the sample is forced downward by the Lorentz force acting on a moving charge. A resulting potential difference, the Hall voltage, then builds up across the sample.

trons, respectively. If a magnetic field is applied perpendicular to the applied electric field (B out of the paper in the figure), the magnetic forces tend to deflect the charged particles, due to their average velocity. The deflections that a hole and an electron, respectively, would receive, are indicated on the diagram by curved arrows labeled *h* and e. Thus, electrons and holes are deflected in the same direction. If there are more electrons than holes, a negative charge builds up on side B and a positive charge on side A, until the resulting electrostatic forces are equal and opposite to the magnetic forces. If there were more holes, side *B* would be positive and side A would be negative. The electrostatic potential difference resulting between sides A and *B*, proportional to the magnetic field strength, is called the Hall voltage. The fact that experimentally the Hall voltage can be either positive or negative, demonstrates that both holes and electrons can be responsible for electrical conductivity. This is the Hall effect.

summary

CRYSTAL CLASSIFICATION

Crystals are classified into the 14 Bravais lattices of Figure 12.1 according to symmetry axes and reflection planes. The possible symmetry axes consistent with translational symmetry are twofold, threefold, fourfold and sixfold, corresponding to rotations of 180°, 120°, 90° and 60°, respectively. Each lattice point of a Bravais lattice can correspond to several atoms or molecules.

BINDING FORCES

Valence crystals are bound by electrons being shared by neighboring atoms, while metals are bound by each electron's being shared by all the atoms. Ionic crystals are bound by direct Coulomb electrostatic forces. The fourth type of binding is due to permanent or fluctuating electric dipoles.

LATTICE VIBRATIONS

Because a solid is not a continuous medium but consists of discrete atoms, the equation of motion leading to sound vibrations is somewhat different from the wave equation for a continuous medium. Instead of all frequencies being possible, the number of frequency modes is equal to three times the number of atoms (for three dimensions), and there exists a maximum frequency of propagation. There are branches of the ω versus $\mathbf{k}$ curves, with the number of modes in each branch equal to the number of cells. The frequency is a periodic function of $\mathbf{k}$ and thus $\mathbf{k}$ can be restricted to one of these periods. The branches of modes for which $\omega = 0$ when $\mathbf{k} = 0$ are called acoustic branches. There are, in general, one longitudinal and two transverse acoustic branches. If there are several inequivalent atoms per cell, there are other branches which are called optical modes and correspond to $\omega \sim 10^{13}$/sec near $\mathbf{k} = 0$.

ENERGIES OF VIBRATIONS

The total vibration energy of the crystal is the sum of the energies associated with the individual modes. The energy of such a mode can be put in the form of the energy of a harmonic oscillator witn the mass of the crystal and the frequency of the mode.

QUANTIZATION OF LATTICE VIBRATIONS

The quantization of a normal mode is the same as the quantization of a harmonic oscillator. The possible energies are $(n + \frac{1}{2})\hbar\omega$, where $n = 0, 1, 2, \ldots$ and ω is the angular frequency of the mode. For many purposes, it is convenient to think of the vibrations as composed of particles called phonons. Then the integer, n, is considered to be the number of phonons present.

LATTICE SPECIFIC HEAT

At high temperatures, one can treat lattice vibrations as classical harmonic oscillators with $3N$ modes. The equipartition of energy theorem then gives an average energy of k_BT per mode, leading tc a specific heat of 3R per mole. At low temperatures, because the energy is proportional to ω and the density of states is proportional to $k^2 dk \sim \omega^2 d\omega$, the average energy is proportional to T^4 and the specific heat to T^3.

ELECTRON ENERGY BANDS

Due to the periodic potential energy that any one electron sees, the electronic wavefunction can be put in the form of a Bloch function, $\psi(\mathbf{r}) = Ae^{i\mathbf{k}\cdot\mathbf{r}}u(\mathbf{r})$, where $\mathbf{k}$ is a constant vector and $u(\mathbf{r})$ is a function which has the lattice periodicity. Since the energy is a periodic function of $\mathbf{k}$, $\mathbf{k}$ can be restricted to a Brillouin zone. When boundary conditions are imposed, it is found that if N is the number of cells, there are N independent $\mathbf{k}$'s. Then, because of the two possible orientations of electron spin, the resulting electron energy bands contain 2N states each.

EFFECTIVE MASS

If at a maximum or minimum of E versus $\mathbf{k}$ at $\mathbf{k} = \mathbf{k}_0$ the energy varies <quadratically with the components of $\mathbf{k} - \mathbf{k}_0$, by analogy with the free particle energy $E = (\hbar k)^2/2m$, one can find an effective mass for each direction.

CONDUCTORS, INSULATORS, SEMICONDUCTORS

Because of Fermi-Dirac statistics and the fact that there are 2N states per band, if there are large energy gaps between bands, then at normal temperatures a crystal with an even number of electrons per cell has the bands below the Fermi energy completely filled, and those above completely empty. Since the nearest empty states are far away in energy, a reasonable electric field gives little current and the crystal is an insulator. For an odd number of electrons per cell, the Fermi level is in the middle of the last band containing electrons. The band is half-filled, and since unfilled states are nearby in energy, this is a conductor. Likewise, if there is overlap in the last bands containing electrons, there are more than 2N states below the energy gap, and there are unfilled states in these bands, forming a conductor. If there are an even number of electrons per cell, but the energy gap is small, there may be a reasonable number of electrons in the conduction band at room temperature, so there will be some conduction of electricity. The substance is then called a semiconductor.

HOLES

The empty states left in the top of the valence band of a semiconductor when electrons go to the conduction band act as if they were particles of positive charge e and positive effective mass. These particles are called holes. They can conduct electricity just as the electrons in the conduction band.

n AND *p*-TYPE SEMICONDUCTORS

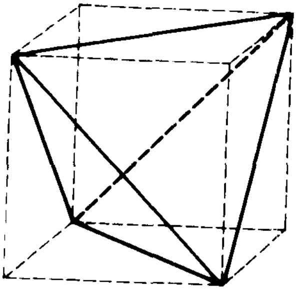
If an impurity is in a semiconductor and has one extra electron, the electron is loosely bound and is easily excited to the conduction band. The impurity is called a *donor.* Conduction is then primarily due to the negative electrons and the material is called n-type. A deficiency of one electron on the impurity causes the impurity to bind an electron tightly from the valence band leaving a hole. The impurity is called an acceptor. The positive hole conduction leads to the term p-type.

HALL EFFECT

When a potential is applied to a substance, current tends to flow parallel to the electric field. If a magnetic field is applied perpendicular to the electric field, the charges are deflected until the new charge distribution produces electric forces equal and opposite to the magnetic forces. The resulting potential difference due to the charge redistribution is the Hall voltage. Because electrons and holes are deflected in the same direction, the Hall voltage has opposite signs for the two kinds of conduction.

problems

1. Sodium has a body-centered cubic structure with two atoms per cubic cell. The density of sodium is 0.952 g/cm^3, and it: atomic weight is 23.0. Calculate the length of the edge of a cubic cell and the smallest distance between atoms.
   Answer: 4.31 Angstroms; 3.73 Angstroms.
2. Copper has a face-centered cubic structure which has on the average four atoms per cubic cell. The density of copper is 8.9 g/cm^3, and its atomic weight is 63.54. What is the length of the edge of a cubic cell, and what is the smallest distance between atoms?
   Answer: 3.62 Angstroms; 2.56 Angstroms
3. Show that a body-centered rhombohedral lattice is equivalent to a different simple rhombohedral lattice.
4. Show that a base-centered tetragonal lattice, where the bases are the square faces, is equivalent to a different simple tetragonal lattice.
5. The diamond structure is a face-ten-tered cubic lattice, but with two carbon atoms per lattice point so that the crystal does not hove the full cubic symmetry. It has the symmetry of the regular tetrahedron instead (equilateral triangle faces). It has four similar threefold axes, three similar twofold axes, and six similar reflection planes. Also, there are three similar axes for which a rotation of 90°, followed by reflection about a plane perpendicular to the axis, returns the tetrahedron to its original configuration. Find all these axes and planer. If the inversion were added and combined with all these operations, one would obtain the complete cubic group of symmetry operations.



6. The rhombohedral lattice has a threefold axis, three similar twofold axes, three similar reflection planes, and the inversion. In addition, there is an axis such that a 60” rotation followed by a reflection about a plane perpendicular to the axis leaves the structure the same. Find these axes and planes.

7. In Equation (12.34) the results for ω versus k were given for the lattice vibrations of a one dimensional crystal of alternate masses μa and Ma. Verify these results.

8. Suppose a one dimensional lattice consists of masses, μa, connected by springs. If alternate springs have spring constants K/a and K'/a, show that there are two branches given by:

$$\omega = \frac{1}{a\sqrt{\mu}} \sqrt{K + K' \pm \sqrt{(K + K')^2 - 4KK' \sin^2 \tfrac{1}{2} ka}}$$

if a is the equilibrium distance between alternate masses, or twice the distance between successive masses. To solve the problem, label masses with springs of constant K/a to the right by displacements ψ_n, and the neighboring masses with a spring of constant K'/a to the right by displacements φ_n Write the two equations of motion, one for each of these types of mass; then assume solutions of the form:

$$\psi_n = A\cos(kna)\cos(\omega t + \Phi)$$

$$\Phi_n = B\cos(kna + \Phi_0)\cos(\omega t + \Phi)$$

where A and B are constants. The phase angle Φ_0 is determined by using identities such as $\cos(kna + \Phi_0) = \cos(kna)\cos\Phi_0 - \sin(kna)\sin\Phi_0$, and setting coefficients of $\sin(kna)$ and $\cos(kna)$ in the equations of motion separately equal to zero.

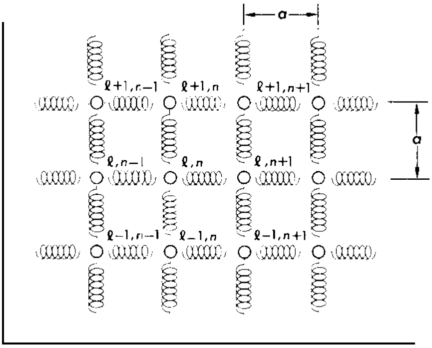
‘9. In the two dimensional lattice shown on the next page, each mass is m, anal the springs all have spring constant K and equilibrium tension T. The horizontal rows are labeled by ℓ and the verticle by n. For small displacements in the plane, the forces on the ℓ, n^{th} mass are (displacements are ξ and η in thex and y directions):

$$F_x = -K(2\xi_{\ell,n} - \xi_{\ell,n+1} - \xi_{\ell,n-1}) - \left(\frac{T}{a}\right)(2\xi_{\ell,n} - \xi_{\ell+1,n} - \xi_{\ell-1,n})$$

$$F_y = -K(2\eta_{\ell,n} - \eta_{\ell+1,n} - \eta_{\ell-1,n}) - \left(\frac{T}{a}\right)(2n_{\ell,n} - \eta_{\ell,n+1} - \eta_{\ell,n-1}).$$

Assume that $\xi_{\ell,n} = \xi_0 \sin(nk, a + \ell k_y a \quad \omega t)$, and find ω as a function of k_x and k,. If $k_y = 0$, a longitudinal wave results, and if $k_x = 0$, it is a transverse wave. Another branch is given by assuming a similar form for $\eta_{\ell,n}$ which just interchanges the roles of k_x and k,.

Answer: $\omega = \dfrac{2}{\sqrt{m}} \sqrt{K \sin^2 \frac{1}{2} k_x a + \left(\frac{T}{a}\right) \sin^2 \frac{1}{2} k_y a.}$



10. If the lattice spacing of a one dimensional lattice of atoms of mass 3.7 x 10^{-27}kg is 3 Angstroms and the effective spring constant is 15 x 10^{-3}nt/meter, what is the maximum angular frequency of waves which can be propagated in the lattice? Of what angular frequency are waves of 0.95 the wavenumber of the maximum frequency waves?

    Answer: 4.03 x $10^{12}\,\text{sec}^{-1}$; 4.02 x $10^{12}\,\text{sec}^{-1}$.

11. The maximum phase speed of an elastic wave in a one dimensional crystal of atoms of mass 6.3 x 10^{-27}kg is 3 x 10^{5}cm/sec. If the atom density is 3.14 x 10^{8} per centimeter, what is the cutoff frequency? Describe the motion of neighboring atoms at this frequency.

    Answer: ν = 3 x 10^{13}cps; 180° out of phase.

12. In a one dimensional crystal with atoms of only one mass, when the wavelength of oscillations is 100 times the interatomic distance, the phase speed is 4 x 10^{5} cm/sec. What is the phase speed and group speed when k is π/a?

    Answer: 2.55 x 10^{5} cm/sec.; 0.

13. In finding the kinetic energy for a mode, it was assumed that

$$\sum_{n=0}^{N-1} \cos^2(kna) = \frac{1}{2}N \quad \text{if} \quad k = \frac{2\pi m}{Na}, \quad m = 0, 1, 2,$$

Prove this by using $\cos(kna) = \frac{1}{2}(e^{ikna} + e^{-ikna})$ and the formula for the sum of a geometric series. Also, in showing that modes do not interfere in energy, it was assumed that

$$\sum_{n=0}^{N-1} \cos(kna)\cos(k'na) = 0$$

if $k \neq k'$. Prove this.

14. If the density of vibrational states between k and k + dk is $kdk/2\pi$ in two dimensions, find what the high temperature lattice specific heat is in two dimensions, and on what power of T it depends at low temperatures.

    Answer: $2R$/mole; T^2.

15. In the chapter on quantum statistical mechanics it was found that the heat capacity per mole of electrons was on the order of $Rk_B T/E_F$, where E_F is the Fermi energy and R is the gas constant. To measure the low temperature dependence of the specific heat of a solid lattice due to phonons, should you use a conductor or an insulator? Why?

16. If the energy in a band is given by $E(k) = E_0 + \beta[3 - \cos(k_x z)\cos(k_y a) - \cos(k_x a)\cos(k_z a) - \cos(k_y a)\cos(k_z a)]$, where E_0 and β are constants, find the effective mass in the x, y and z directions at $k_x = k_y = k_z = 0$, and at $k_x = \pi/a$, $k_y = k_z = 0$.

Answer: $m_x = m_y = m_z = \hbar^2/(2a^2\beta)$; $m_x = -\hbar^2/(2a^2\beta)$, $m_y = m_z = \infty$.

17. If in the conduction band of a conductor, $E = \frac{1}{2}\hbar^2k^2/2m^*$ and the density of states between k and $k + dk$ is k^2dk/π^2, show that the average energy is $\frac{3}{5}$ of the Fermi energy E_F, assuming all states below E_F are filled and all states above E_F are empty.

18. In diamond, the gap width is 7 eV. What frequency of incident electromagnetic radiation would cause an electron to go from the valence to the conduction band?

Answer: 1.689×10^{15} cps.

19. The valence band and conduction band of several crystals are separated by 3.0 eV, 0.3 eV, and 0.00 eV (overlap). Describe the type of electrical conductivity exhibited by each crystal if there are an even number of electrons per cell.

20. The gap width of silicon is 1.21 eV. Arsenic donor atoms in silicon have an energy 0.046 eV below the bottom of the conduction band. Make a sketch of the energy level diagram, roughly to scale, for this situation, and estimate the temperatures at which the donor levels would be filled.

Answer: $T \ll 533$ K

21. In a semiconductor, the effective mass m^* of the holes and electrons are the same, so that the density of states between k and $k + dk$ for each is k^2dk/π^2, and the energy above the bottom of the conduction band or below the top of the valence band (at $\mathbf{k} = 0$) is $(\hbar k)^2/2m^*$. The Fermi energy E_F is halfway between the two bands. Assume that the gap energy E_g is large enough so that $1/[e^{-(E_F-E)/k_BT} + 1] \sim e^{(E_F-E)/k_BT}$ for E in the conduction band, and the distribution function is approximately $1 - e^{-(E_F-E)/k_BT}$ for E in the valence band. If the bands are wide compared to k_BT, find the number of holes per unit volume in the valence band and the number of electrons per-unit volume in the conduction band. For $E_g = 1$ eV and m^* equal to the true electron mass, find this number for $T = 273$ K.

Answer: $2(mkT/2\pi\hbar^2)^{3/2}e^{-E_g/2k_BT}$.

22. When an impurity atom, such as arsenic, in the fifth column of the periodic table, replaces an atom of silicon in a crystal of silicon, there is one extra electron, which effectively sees a charge +e at the position of the arsenic. Assuming the silicon is a medium of dielectric constant $K = 11.9$ and the average effective mass is $0.4m_e$, calculate the binding energy of the electron to the arsenic. atom in electron volts. Also, calculate the radius of the lowest Bohr orbit.

Answer: .038 eV; 15.7 Angstroms.

23. If a small amount of indium is combined with germanium to make a semiconductor, will it be p-type or n-type?

24. In the semiconductor germanium, the energy gap is 0.79 eV in width. What is the wavelength of the photon which, when absorbed by a pure germanium crystal, will create an electron-hole pair? At what temperatures would these pairs be excited thermally in appreciable numbers?

Answer: 15,700 angstroms; $T > 9160$K, far greater than the melting or boiling point of Ge.

25. If silicon is doped with a small amount of aluminum, would you expect it to be a p-type or n-type semiconductor?

3 probing the nucleus

In Chapters 8 and 9 atomic structure was discussed assuming that the nucleus, which actually contains over 99.94% of the mass of the atom, is simply a point mass carrying a charge Ze, where Z is the atomic number. There it was seen how an enormous amount of experimental data can be assembled into a simple conceptual scheme: energy level structure and spectra of the elements, the periodic table, chemical properties of the elements, x-ray spectra, and so on. These phenomena may be understood quantitatively, by largely ignoring any internal structure the nucleus may have. However, it is natural to expect that the nuclei may themselves have an internal structure and exhibit a rich variety of phenomena, particularly if sufficient energy is given to the nuclei so that they can approach one another and react or scatter from each other.

The study of nuclear structure began in 1896 with the discovery of radioactivity by Becquerel, and since then it has been of major concern in physics. In this chapter we shall discuss one of the most important methods used in the study of small particles: scattering. In a scattering experiment, a beam of particles of some type is produced, which may be described by some parameters such as kinetic energy, charge, mass, spin direction, etc. This beam is allowed to strike a selected target, and the angles of deflection, number and type of recoil particles, losses of energy, and other quantities, are observed. This information may then be used in formulating a theory of the forces involved; or, with the aid of a theory or model of the scattering process, information may be obtained about the internal structure of the target particles. For example, Laue spot patterns are observed when x rays are diffracted from crystalline solids. This may be considered as a process involving scattering of the x-ray photons in the incident beam. By observing the spot patterns, one may determine the internal structure and arrangement of the atoms in the crystal.

3.1 A NUCLEAR MODEL

For simplicity, in our first discussions of the nucleus we will consider a model in which the nucleus is assumed to be spherical in shape, and in which the charge, Ze, and the mass are uniformly distributed throughout the sphere. Experiments show that these assumptions are not quite correct in general, but we should nevertheless be able to obtain reasonable estimates of nuclear dimensions using this model.

Let the radius of the sphere in this model be R; this radius is the distance from the nuclear center at which the mass and charge densities fall to zero, and is somewhat of an abstraction because in real nuclei no such sharp outer boundary exists. In order to design a scattering experiment which would reveal some of the internal structure of a nucleus, one would first like to have a rough idea of the radius R for a nucleus of a given charge and mass.

Imagine, for example, a point test charge Q, such as an electron, placed at a distance r from the center of the spherical nuclear charge distribution. The force on this test charge will be a function of both r and R, and hence if this force could be measured, R could be determined. If r is greater than R, so that the test charge is outside the spherical distribution, then by Gauss' law the entire charge Ze of the nucleus may be considered to be concentrated at the center of symmetry. The force between test charge and nucleus would then be equal to $ZeQ/4\pi\epsilon_0 r^2$. However, if r is less than R, so that the test charge is inside the nucleus, then by Gauss' law only the charge at radii less than r effectively acts on the test charge. Since the nuclear charge is assumed to be uniformly distributed, the fraction of nuclear charge acting on the test charge will equal the fraction of nuclear volume at radii less than r. The total nuclear volume is $\frac{4}{3}\pi R^3$. The volume at radii less than r is $\frac{4}{3}\pi r^3$. Therefore, the fraction of nuclear charge acting on the test charge is equal to $(r/R)^3$. The total amount of nuclear charge effectively acting on the test charge at $r < R$ is then equal to Zer^3/R^3, and the force on the test charge is equal to $ZeQr/4\pi\epsilon_0 R^3$. Summarizing, the force is given by:

$$F = \frac{ZeQ}{4\pi\epsilon_0 r^2}, \quad \text{for } r > R$$

$$F = \frac{ZeQr}{4\pi\epsilon_0 R^3}, \quad \text{for } r < R \tag{13.1}$$

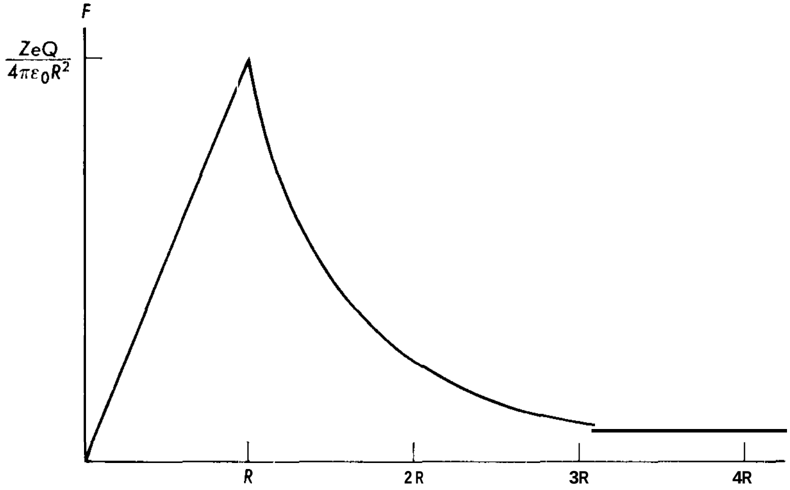


Figure **13.1.** Graph of the force between a test charge Q and a spherically symmetric, uniformly distributed nuclear charge of finite radius R.

In Figure 13.1 the force is plotted as a function of r. Thus, for a distributed charge, at small radii the force does not continue to approach infinity as $1/r^2$ but approaches zero instead. If the edge of the nuclear charge distribution were sharp, there would be a sharp change in the slope of the graph of F(r) at a value of r equal to R, the nuclear radius. Then if we could place a test charge in this region, we could measure R. Actually, we cannot measure forces directly in nuclear physics, but we can measure some of the effects to be expected from different potential energies of interaction.

2 LIMITATIONS ON NUCLEAR SIZE FROM ATOMIC CONSIDERATIONS

From the above considerations, it is seen that for radii $r > R$, the potential will be a Coulomb potential. By (considering deviations between theory and experiment for hydrogen-like atoms with heavy nuclei, we may obtain some idea of the value of R, at which the potential ceases to be Coulombic. Thus, in the theory of the hydrogen atom which was developed in Chapter 8, the calculated electron energies agree with experiment to at least six significant figures. There it was assumed that the nucleus is a point charge, with $R = 0$. In the $1s$ state of hydrogen, the electron spends most of its time in a region of space at radii comparable to the Bohr radius, $a = 4\pi\epsilon_0\hbar^2/me^2 = 0.53$ Angstroms. The fact that the agreement between theory and experiment is so good means that the nuclear radius R must be much smaller than 0.5 Angstroms. To put an upper limit on R, we observe that the order of magnitude of the electron probability density, $|\psi(r)|^2$, does not change significantly for the $1s$ state for radii from $r \cong 0$ to $r \cong a$. Since the volume of a sphere of radius r is $4\pi r^3/3$, the fraction of the time spent by the electron in the neighborhood of the nucleus is of the order of magnitude R^3/a^3, and because the theoretical energy is correct to at least six significant figures, we should have:

$$\frac{R^3}{a^3} < 10^{-6}$$

or R should be less than about 10^{-2} Angstroms.

We can go farther. In a hydrogen-like atom with nuclear charge Z, the radius of the first Bohr orbit is a/Z. In the heavy elements where Z is around 100, this radius can get as small as about 0.005 Angstroms. Moseley's law, which gives x-ray frequencies based on a hydrogen-like model, is in good agreement with experiment. The argument used above in connection with the hydrogen atom, would then indicate that nuclear radii cannot be greater than around 10^{-4} Angstroms.

A μ meson is an elementary particle which has charge $-e$ and a mass m_μ about 200 times that of an electron. It is possible for a μ^- meson to be attracted to a nucleus, and to replace an electron in an atom to form a relatively stable atom with the μ meson in a $1s$ state. The equation for the radius of the Bohr orbit is the same as for the hydrogen atom, but with the mass of the μ meson replacing the mass electron. This radius, $a_\mu = am/m_\mu Z$, is inversely proportional to the mass and is around 0.00025 Angstroms for a Z of 10. The binding energies of μ mesic atoms may be determined by various means, and it is found that the energies begin to differ from that expected for a pure Coulomb potential by 10% or so, for $Z \simeq 10$. This means that the μ meson is spending a significant part of its time at radii r inside the nucleus. Using the argument above,. we find very roughly that $(R/a_\mu)^3 < {}^1/_{10}$, so the nuclear radius is less than around $0.00025/10^{1/3}$ Angstroms, or about 10^{-14} meters. This is probably an over-estimate of the nuclear size, since $|\psi|^2$ is largest near the origin, which was not taken into account.

The point here is that in the 1s state, the wavefunction does not vanish at the nucleus but approaches the constant value $\psi_{100} = \sqrt{4Z^3/a^3}$ as $r \rightarrow 0$. Hence there is some finite probability of finding the electron (or meson) in the region of the nucleus, and hence the internal structure of the nucleus may have some effect on the atomic energy levels. In lead, for example, a 1s μ meson spends most of its time inside the nucleus and the atomic energies are changed by large factors. For lead, Z = 82, and the first Bohr orbit of a μ mesic atom of lead would be $\simeq 4 \times 10^{-5}$ Angstroms.

Historically, nuclear radii were known to be of this general order of magnitude long before mesic atoms were discovered. These radii were found by Rutherford and his co-workers by allowing a beam of heavy charged particles of high speeds to strike a thin foil, and observing that a few of the incident particles were deflected through large angles. To produce a large deflection requires a large force. From Figure 13.1 it can be seen that the maximum possible Coulomb force is inversely proportional to R^2. Hence the smaller R is, the larger is the maximum possible force, and to hove a large force, and hence a large deflection, R must be very small. Quantitative considerations show that if the nuclear charge 'were spread out over the whole atom-i.e. $R \simeq 1$ Angstrom-then the particles in the incident beam should suffer only very slight deflections due to Coulomb forces. The fact that large deflections are observed means that the nucleus must be much smaller than an Angstrom in radius. Of course, it is possible that forces other than Coulomb forces are present. However, as will be discussed later in this chapter, Rutherford's scattering formula, based only on Coulomb forces, completely explained the scattering results down to very small radii.

Because of the rather small lengths that occur in nuclear physics, it is convenient to introduce a unit of length comparable to nuclear radii. A unit called the fermi (named after the nuclear physicist, Enrico Fermi) is frequently used:

$$1 \text{ fermi} \equiv 10^{-15} \text{ meters} = 10^{-5} \text{ Angstroms}$$

Thus nuclear radii, on the basis of our above rough estimates, must be of the order of several fermis.

3 SCATTERING EXPERIMENTS

A great deal of useful information may be obtained by allowing particles to collide with various targets. In investigating the structure of some object by means of a scattering experiment, it is desirable to use a beam of incident particles whose de Broglie wavelengths are either of the same general order of magnitude as, or less than, the size of the structures being investigated. For example, in the scattering of x rays by a crystal, Laue spot patterns are formed when the wavelengths of the incident photons are comparable to the lattice spacings. Similarly, in scattering off of nuclei, interesting phenomena should occur when the wavelengths of the incident particles are of the same order of magnitude as the lengths characterizing nuclear structure, a few fermis. If the incident particles are protons of wavelengths $\lambda \cong 10$ fermis, the protons' momenta would be about $p = h/\lambda = 6.6 \times 10^{-20}$ kg m/sec. The kinetic energy would be $p^2/2m$. Since the proton rest mass $m_0 = 1.67 \times 10^{-27}$ kg, the corresponding kinetic energy is 1.3×10^{-12} joules, or 8.3 MeV. This is roughly the kinetic energy of the incident particles used by Rutherford, Geiger and Marsden in their early experiments. To decrease the proton wavelength to $\lambda \cong 1$ fermi, the required kinetic energy is roughly 600 MeV, in the relativistic range. The speed of the protons would be $c^2p/E = 0.8c$, comparable to the speed of light. To get electrons of wavelengths $\lambda \cong 1$ fermi requires an energy of this same order of magnitude, and hence the electrons would have speeds very close to that of light. The smaller λ is, the larger the kinetic energy of the incident particles must be. Therefore, the smaller the features of nuclear structure are that we wish to detect, the larger the incident kinetic energies must be.

The scattering process will usually depend on the kinetic energies of the incident particles in an important way. Hence, the incident beams should be beams of definite known energies as nearly as possible. If the energy is really very sharply defined, so is the momentum, and so, according to the uncertainty principle, the position of an incoming particle is unknown. The incoming beam would then be described by a wavefunction like that of a plane wave. Consider a beam of particles of known energy traveling in the x direction, as shown in Figure 13.2. Since $p_y = 0$, the uncertainty in p_y is zero, and the y positions of the particles are unknown. The same is true for the z positions. Hence, if this beam falls on some target, the exact positions at which the incident particles will strike the target will be unknown. The target may consist of a solid chunk of material or a vial of liquid; this will be a piece of matter of macroscopic size because in practice, we cannot put one nucleus in a given position and hold it there, unless it is attached rigidly to the laboratory apparatus. In a solid piece of material as big as 1 mm^3, we do not know exactly where the nuclei are. We will only know that the nuclei are distributed in some fashion throughout the target. Hence, we would not know how close a particular incident particle could come to a nucleus even if we knew exactly the position of the incident particle.

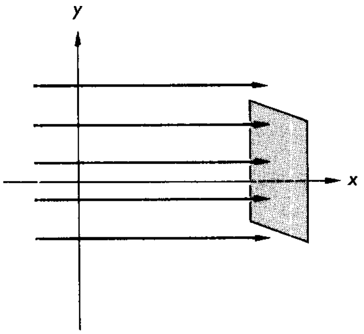


Figure 13.2. A beam of particles traveling in the x direction and striking a target.

Because of these positional uncertainties, it is necessary to describe the scattering process in terms of probabilities. If the beam intensity is uniform across the target, we must assume that an incident particle is just as likely to fall at one position on the target as on any other. In Figure 13.3, a target of area 1 m^2 is represented as it would appear to the incoming beam. It is oriented with its area perpendicular to the beam, and divided up into elements of area A_i. If element A_2 has twice the area of A_1, on the average twice as many particles should fall on A_2 as on A_1. In general, the probability that an incident particle falls on an area A is proportional to A. Suppose that a total of N_i particles per square meter per second are incident on the target. This number N_i is called the *incident flux* density. Then the number of particles incident on the area A per second would be given by:

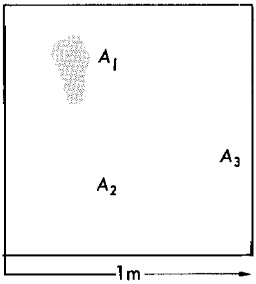


Figure 13.3. The relative probability of an incident particle striking an area A is proportional to the area A.

$$\text{Number incident on A per second} = N_i A \tag{13.2}$$

13.4 CROSS-SECTIONS

Suppose the target consisted of a large number of circular scatterers of equal area σ, as indicated in Figure 13.4, randomly placed throughout the target, and all oriented so that the circles are broadside to the incident beam. If there are η of these scatterers per unit area, and σ is so small that no two circles overlap, the total area covered by the circles in one square meter of target would be just equal to $\eta\sigma$. Then, according to Equation (13.2), the number of particles

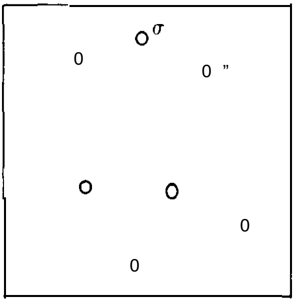


Figure 13.4. Target consisting of randomly placed circular scatterers of area σ.

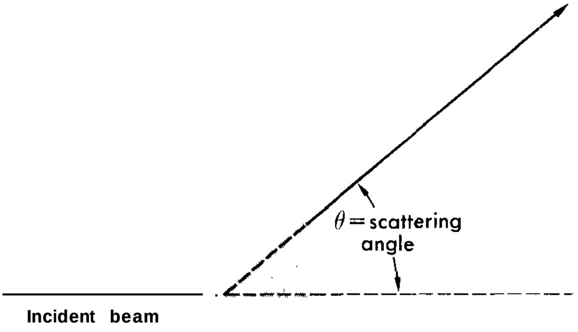
incident on the circles per square meter per second is

$$N_s = N_i \eta \sigma \tag{13.3}$$

The area σ in this expression is called the *fatal scattering cross-section.* We may suppose that, whatever the scattering process actually is, one may represent the probability of the process in terms of an effective cross-sectional area σ, in such a way that the number of particles scattered is given by Equation (13.3). A particle in the incident beam falling inside σ then is scattered, a particle falling outside is not scattered. In actuality, the scattering probability may be a rather complicated function of the distance of the incident particle from the target particle. Equation (13.3) nevertheless serves as a definition of σ. If σ is not known, Equation (13.3) may be used to measure σ experimentally, provided that η is known and N_s and N_i can be measured.

5 DIFFERENTIAL CROSS-SECTION

In practice, when an incident particle is scattered, it may be deflected through any angle θ from zero up to 180”. The scattering angle θ is defined in Figure 13.5. A great deal more information about the scattering forces can be gained by studying the number of scattered particles as a function of angle, than from an experiment in which only σ is found.



We can think of the area σ as being composed of nonoverlapping infinitesimal areas, $d\sigma(\theta)$, with $\sigma = \int da$ da is that part of the total cross-section which corresponds to the scattering of particles into some small range of angles about θ. It is convenient here to consider the number of particles scattered per unit solid angle, into some small range of scattering angles near θ. The solid angle $d\Omega$ subtended by a section of a spherical surface of radius R, between the angles θ and $\theta + d\theta$, is defined, as in Figure 13.6, by $d\Omega = dA/R^2$, where dA is the area cut off on the sphere's surface between the two cones of central angles θ and $\theta + d\theta$. In terms of $d\theta$, the differential solid angle, $d\Omega$ is

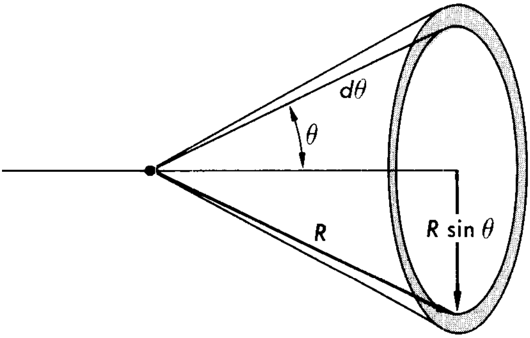


Figure 13.6. Solid angle corresponding to an increment in polar scattering angle θ.

$$d\Omega = \frac{2\pi R \sin\theta \cdot R d\theta}{R^2} = 2\pi \sin\theta \, d\theta \tag{13.4}$$

Thus, $d\sigma(\theta)$ is the cross-section for scattering into $d\Omega$.

The ratio $d\sigma/d\Omega$ is called the differential cross-section. If $dN_s/d\Omega$ is the number of particles scattered per unit solid angle, per unit area of target material, then by analogy with Equation (13.3), the differential cross-section is

$$\frac{d\sigma}{d\Omega} = \frac{dN_s/d\Omega}{N_i \eta} \tag{13.5}$$

or the fraction of particles scattered into angles near 8, per unit solid angle, divided by the number of scatterers per unit area. The total cross-section is then

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^\pi \frac{d\sigma}{d\Omega} (2\pi \sin\theta) \, d\theta \tag{13.6}$$

Suppose, for example, that the scatterers were hard spheres, and that point masses in the incident beam were scattered elastically upon striking the spheres. Then the areas da would be the projections of thin, ring-shaped areas on the surfaces of the spheres, concentric about lines through the center of the spheres, parallel to the incoming beam, as in Figure 13.7. Since the various ring-shaped areas ore inclined at different angles to the beam, they scatter the particles through different angles.

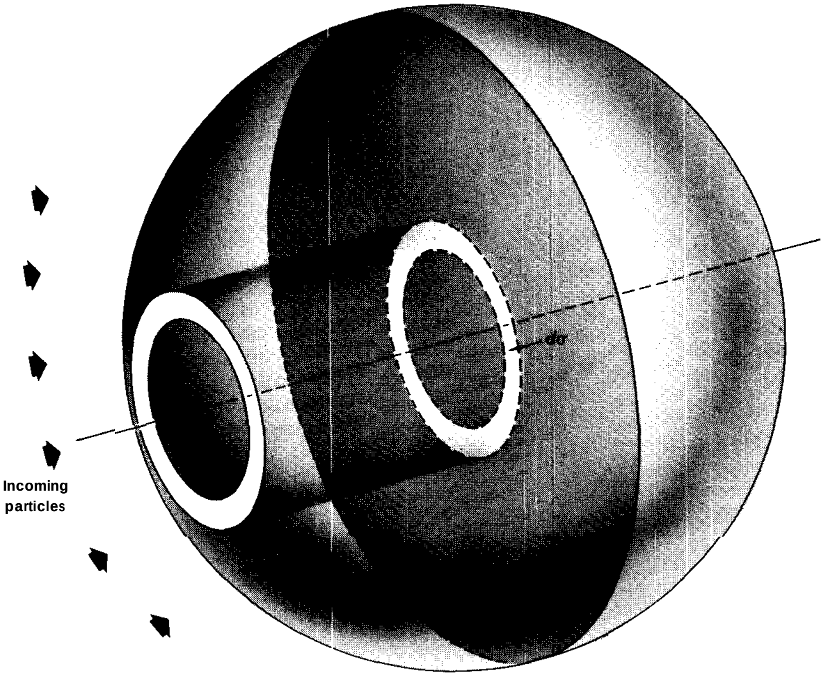


Figure 13.7. Differential scattering area, $d\sigma$, for a hard sphere.

mple If the areal density of scatterers is $\eta = 10^{24}$ per square meter, and the differential cross-section for scattering at 89.5” is $d\sigma/d\Omega = 10^{-31}\,\text{m}^2$, what is the fraction of the particles scattered into angles between 89” and 90°?

ution One degree is about 1/57.3 radians. The solid angle between 89” and 90” is then about $2\pi \sin(89.5^\circ)\Delta\theta \cong 1/10$. Then $\Delta\sigma = d\sigma/d\Omega\, \Delta\Omega \cong 10^{-32}\,\text{m}^2$. The effective scattering area per square meter of target material is then $\eta\Delta\sigma = (10^{24})(10^{-32})$ = 10-s. This is the fraction of particles scattered.

mple Suppose a differential cross-section is given by $d\sigma/d\Omega = a^2 \cos^2\theta$. Find the total cross-section.

ution
$$\sigma = \int_0^\pi \frac{d\sigma}{d\Omega}\,d\Omega = \int_0^\pi a^2\cos^2\theta\,(27r \sin\theta\,d\theta) = \frac{2\pi a^2}{3}\left(-\cos^3\theta\right)\Big|_0^\pi = \frac{4\pi a^2}{3}.$$

13.6 NUMBER OF SCATTERERS PER UNIT AREA

Consider a target made of some solid material which has a known number of scattering centers per unit volume, n. If the target is a thin slab of thickness t, the total number of scattering centers per unit area will be

$$\eta = nt \tag{13.7}$$

Thus, the fraction of particles scattered when the total cross-section is σ, will be

$$\frac{N_s}{N_i} = nt\sigma \tag{13.8}$$

Usually, the number of scatterers per unit volume, n, is not given directly in tables, but the density ρ, in grams per cubic meter, is known. Also, the atomic weight W is given. The number of moles per cubic meter is then p/W. The number of particles in one mole is Avogadro'r. number, $N_0 = 6.022 \times 10^{23}$ per gram-mole. Hence, the number of particles or scatterers per unit volume is

$$n = \frac{N_0\rho}{W} \tag{13.9}$$

example For gold, the atomic weight is W = 197.2 grams per g-mole, and the density is $\rho = 1.93 \times 10'$ g/m^3. Since Avogadro's number is $N_0 = 6.02 \times 10^{23}$, the number of particles per unit volume is

$$n = \frac{N_0\rho}{W}\frac{(6.02 \times 10^{23})(1.93 \times 10^7)}{197.2}$$

$$= 5.89 \times 10^{28}/m^3$$

Suppose the gold is a foil of thickness $t = 6 \times 10^{-5}$ cm. If the cross-section for scattering into angles greater than 1" is $\Delta\sigma = 9.0 \times 10^{-24}$m^2, then the fraction of the incident particles that are scattered into angles greater than 1° is, from Equation (13.8),

$$\frac{\Delta N_s}{N_i} = nt\Delta\sigma = (5.89 \times 10^{28})(6 \times 10^{-7})(9.05 \times 10^{-24})$$

$$= 0.32$$

13.7 BARN AS A UNIT OF CROSS-SECTION

In nuclear scattering problems, many cross-sections are found to be typically on the order of 10^{-32} to 10^{-28} m^2. The quantity 10^{-28} m^2 is a large cross-section, and in nuclear problems it is sometimes taken as a unit of cross-section (area) called the burn.

$$\boxed{1 \text{ barn} \equiv 10^{-28} \text{ m}^2.}$$

Thus a cross-section of 4.2 x 10^{-30} m^2 would be 0.042 barns.

nple If a nucleus is a sphere of 2.5 fermis in radius, then what is the cross-sectional area in barns?

ition The cross-sectional area of a sphere of radius r is πr^2. Here r is 2.5 fermis, or 2.5 x 10^{-15} meters. Then the cross-sectional area is

$$A = a(2.5 \times 10^{-15})^2 = 1.96 \times 10^{-29} \text{ m}^2$$

$$= 0.196 \text{ barns}$$

This cross-sectional area will not necessarily be the same as the scattering cross-section because the forces causing scattering may extend over a larger area.

3.8 α AND β PARTICLES

With the definitions of scattering cross-section given above, we can now study one of the earliest experiments giving direct evidence about the nuclear size. This involved the scattering of alpha particles by thin metal foils. After the discovery of radioactivity by Becquerel, Rutherford and his co-workers studied the radiations given off by uranium and found there were two types: one type which was easily absorbed by thin sheets of material, and another type which was very penetrating. The first type was called alpha radiation and the second was called beta radiation. Both alpha and beta rays were deflected by a magnetic field, but in opposite directions. Also, they both left visible tracks when they passed through a cloud chamber. Hence, one could conclude that both radiations must consist of charged particles. It has since been established that beta rays are high speed electrons, and alpha rays are the nuclei of helium atoms. We are interested here particularly in alpha particles.

In Figure 13.8 is a reproduction of a typical cloud chamber photograph of the α radiation emitted by radioactive nuclei. The α rays leave tracks consisting of tiny droplets of liquid condensing on ions caused by the passage of the particles. By studying the length of a track (called the range), the initial kinetic energy of the α particle may be determined. From a study of the characteristics of the vapor molecules, it has been determined that on the average it takes about 32 eV of energy to form an ion pair. Since a small droplet condenses around each ion, by counting droplets one may measure the total energy lost by the α particle. It has been found that the number of ions formed per unit of track length is nearly constant, except near the end of the path, so the initial kinetic energy of the particle is a well-defined function of the range. If all α particles coming off have the same range, then one could infer that all the particles have

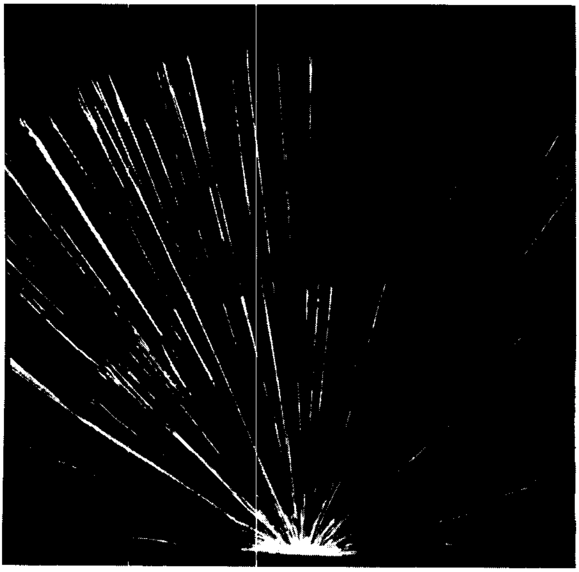


Figure 13.8. Cloud chamber photograph of alpha rays, showing two distinct ranges corresponding to **two different energies of the emitted alpha particles.**

equal kinetic energies. In Figure 13.8 we see that there are α particles of two different initial kinetic energies. In general, the α particles emitted by nuclei all have discrete energies. These kinetic energies have been determined to be of the order of magnitude of a few million electron volts. For example, one a particle emitted by polonium has an average range of 3.84 cm in air at 15°C, and has a kinetic energy of 5.30 MeV.

Let us denote the charge of the α particle by Q and its mass by M. The charge-to-mass ratio, Q/M, may be determined by observing the deflection of the particles in both electric and magnetic fields. The charge Q may be determined in another type of experiment in which a known number of particles, N, are captured in a chamber and the total charge NQ is measured. The results of these experiments are:

$$Q = +3.2 \times 10^{-19} \text{ coulombs}$$

$$Q/M = 4.84 \times 10^{7} \text{ coul/kg}$$

so

$$M = 6.62 \times 10^{-27} \text{ kg}$$

The mass of the proton is $M_p = 1.67 \times 10^{-27}$ kg, so the α particle mass is very closely four times that of the hydrogen nucleus. Also, the charge Q is two times the magnitude of the electronic charge. This suggests that an α particle is a helium nucleus. Rutherford established that this is the case by collecting α particles in a tube, where they attracted electrons to form atoms. Then he observed the emission spectrum of these atoms, and found it identical to that of heliium.

3.9 RUTHERFORD MODEL OF THE ATOM

Until 1911, the structure of the atom and the size of the nucleus were completely unknown. Many physicists felt that the nuclear material occupied most of the region in the interior of the atom, i.e. was spread over a region of approximately one Angstrom in diameter. In 1911, Rutherford proposed that the nucleus occupied only a small region compared to atomic dimensions. In 1913, Geiger and Marsden reported experiments which completely confirmed the predictions of Rutherford's model of the atom. In these experiments, alpha particles were scattered from thin foils of various metals. While quantum mechanics was unknown at that time, we can calculate the wavelength of the α particles used, to see with hindsight that these particles were suitable to use in the experiments. The α particles had an energy of about 8 MeV. Since the rest energy Mc^2 is about 3750 MeV, the rest energy is much larger than the kinetic energy; so a nonrelativistic treatment of the motion may be made. Then $p = \sqrt{2MT}$, where T is the kinetic energy, 8 MeV. Then, numerically, $p = [2(6.6 \times 10^{-27})(8 \times 1.6 \times 10^{-13}\ \mathrm{j/MeV})]^{1/2} = 1.3 \times 10^{-19}$ kg-m/sec. The de Broglie wavelength corresponding to this momentum is $\lambda_\alpha = h/p = 5 \times 10^{-15}\mathrm{m} = 5$ fermis, about the size of a nucleus as we know it today. In the experiment of Geiger and Marsden, a source emitting the 8 MeV α particles was placed behind slits, as shown in Figure 13.9. These slits gave a collimated beam of particles of a single energy, all traveling along essentially parallel paths. Because of the small wavelength of the particles, diffraction by the slits had negligible effect.

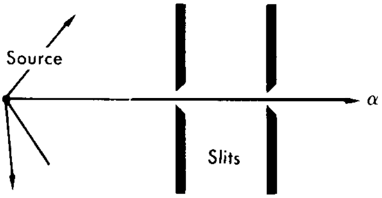


Figure 13.9. Collimation of a beam by a slit-system, to produce a beam going in a well-defined direction.

When α's of kinetic energies of a few MeV collide with an atom having a nuclear charge Ze and Z electrons, the mass of the electrons is around Z/7000 times the mass of the α. Hence the α particle simply smashes right on through the electrons without any appreciable loss of energy, somewhat like an artillery shell passing through a wad of newspapers. Thus the presence of atomic electrons may be neglected when discussing scattering of α particles. We may then calculate the distance of closest approach between a nucleus and an 8 MeV α particle, assuming that the force of interaction all the way in is a purely electrostatic Coulomb force. The Coulomb potential energy for an alpha particle of charge 2e and a nucleus of charge Ze is $2Ze^2/4\pi\epsilon_0 r$, where r is the distance between centers. If all the kinetic energy were converted into potential energy, the two particles would be as close together as they can get. This can occur only if the particles collide headon, and even then only in the frame of reference in which the center of mass is at rest. In any other frame of reference, there is motion of the center of mass and thus some kinetic energy which cannot be converted into potential energy. However, if the nucleus is very heavy, as is the case for gold-which was often used in the early experiments-the nuclear mass is around fifty times that of the alpha particle, and only a few percent error is made using the laboratory rather than the center of mass frame. For gold, Z is 79; also, $1/(4\pi\epsilon_0)$ is 9 x 10^9 numerically. Therefore, if we set the initial α particle kinetic energy equal to the potential energy at closest approach, we have:

$$(8\text{MeV})(1.6 \times 10^{-13}\text{j/MeV}) = 9 \times 10^9(2)(79)(1.6 \times 10^{-19})^2/r$$

or r = 28 fermis. With o target made of silver, the smallest possible distance between particles is 17 fermis. Since these distances are greater than the sizes of the nuclei (as we now know), it is quite reasonable that the Geiger-Marsden experiments confirmed Rutherford's predictions, which were based on the assumption that the nucleus is very small; so the forces are Coulombic down to very small distances. If the nucleus had been greater in size than around 20 fermis, if, in particular, it were around an Angstrom or 10^5 fermis in size, then the scattering experiments would hove given quite different results. Thus the agreement of the experimental results with Rutherford's predictions indicated that the nuclear radii were less than 17 fermis. Actually, we know today that the radii are a little smaller than this. The results of many experiments on measuring nuclear sizes by electron scattering, α scattering, etc., may be summarized in the approximate formula:

$$R =: R_0 W^{1/3} \tag{13.10}$$

where R_0 = 1.1 fermis ond W is the atomic weight of the nucleus. We shall discuss the physical significance of this equation later.

13.10 RU'THERFORD THEORY; EQUATION OF ORBIT

We shall now give an example of a theoretical calculation of a cross-section by discussing the Rutherford Coulomb scattering theory in more detail. In this discussion, we will assume that the scattering nucleus is a point charge, Ze, fixed at the origin. The results obtained will be only approximate in the laboratory system, because the nucleus rebounds to some extent, but will be exact in the center of mass system if the α particle mass is replaced with the reduced mass of the alpha nucleus system.

In Figure 13.10 the dashed line II represents the path that an incoming α particle would follow if it were not deflected by the nucleus at 0, whereas the actual path of the particle along the heavy curved line IS. The angle of scattering, which is the angle between the incident and scattered directions, is labeled in the diagram by the symbol θ. The shortest distance between the line II and the origin 0 is called the ***impact parameter.*** It is labeled b on the diagram. At any point on the trajectory of the α particle, the position may be labeled by the radial distance r and the angle Φ shown in Figure 13.8. As the particle approaches the nucleus and then recedes to infinity, Φ decreases from π to θ, the final scattering angle.

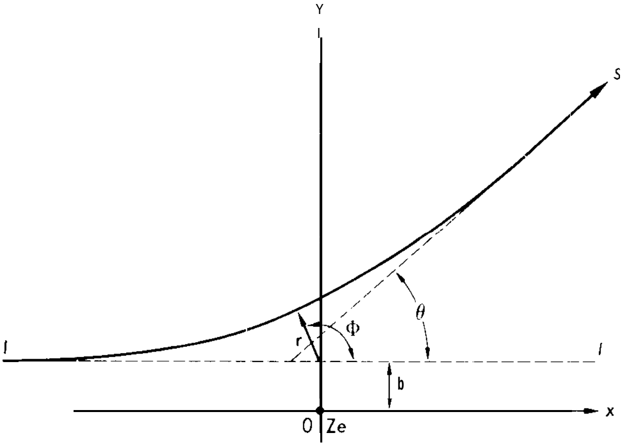


Figure 13.10. Path of an alpha particle scattering from an infinitely **massive nucleus of charge Ze.**

Since the de Broglie wavelength of the alpha particle is smaller than the distance of closest approach, we may use classical mechanics rather than quantum mechanics to analyze the motion. Also, the speeds involved are much less than c, so nonrelativistic mechanics may be used. The equation of the α particle path may be obtained from two conservation equations, conservation of energy and conservation of angular momentum. The latter conservation law holds because the Coulomb force is a central force, so there is no torque about the origin. The resulting expression for the scattering angle in terms of impact parameter and energy is given in Equation (13.23); we shall now derive this equation.

Initially, before the collision, all the energy is kinetic, $T_0 = ½ Mv_0^2$, where v_0 is the initial speed of the alpha particle. Setting the sum of the kinetic energy and potential energy, $V = 2Ze^2/4\pi\epsilon_0 r$, equal to the initial kinetic energy, we find that

$$\frac{1}{2}M\left[\left(\frac{dr}{dt}\right)^2 + \left(r\frac{d\Phi}{dt}\right)^2\right] + \frac{2Ze^2}{4\pi\epsilon_0 r} = \frac{1}{2}Mv_0^2 \qquad (13.11)$$

Here dr/dt and $rd\Phi/dt$ are the radial and tangential components of velocity. The initial angular momentum about the origin is Mv_0b. Then at all times the angular momentum is the same:

$$Mr^2\frac{d\Phi}{dt} = Mv_0b \qquad (13.12)$$

We can solve Equation (13.12) for $d\Phi/dt$, and express dr/dt in the energy equation, Equation (13.11), as $dr/dt = (dr/d\Phi)(d\Phi/dt)$. The result is:

$$\frac{1}{2}M\left[\left(\frac{dr}{d\Phi}\right)^2\frac{(v_0b)^2}{r^4} + \frac{(v_0b)^2}{r^2}\right] + \frac{2Ze^2}{4\pi\epsilon_0 r} = \frac{1}{2}Mv_0^2 \qquad (13.13)$$

We may simplify the notation by defining a constant γ as follows:

$$\frac{1}{2}\gamma = \frac{\frac{1}{2} M v_0^2}{(2Ze^2/4\pi\epsilon_0)}$$

Thus, γ is twice the ratio of initial kinetic energy, to the potential energy the alpha particle would have at a distance b from the nucleus. Then Equation (13.13) can be written:

$$\left(\frac{dr}{d\Phi}\right)^2 \frac{b^2}{r^4} - \frac{b^2}{r^2} + \frac{2b}{\gamma r} = 1 \tag{13.14}$$

Solving for $d\Phi$,

$$d\Phi = -\frac{b\,dr/r^2}{\sqrt{1 - \frac{2b}{\gamma r} - \frac{b^2}{r^2}}} \tag{13.15}$$

The integral of this function of r may be found in most integral tables. The result is:

$$\Phi - \Phi_0 = -\sin^{-1}\left[\frac{(b\gamma/r) + 1}{\sqrt{1 + \gamma^2}}\right] \tag{13.16}$$

The constant of integration Φ_0 may be evaluated by noting that at the initial position, Φ = a and $r = \infty$, so

$$\Phi_0 = \pi + \sin^{-1}\frac{1}{\sqrt{1 + \gamma^2}} \tag{13.17}$$

Hence,

$$\Phi = \pi + \sin^{-1}\frac{1}{\sqrt{1 + \gamma^2}} - \sin^{-1}\left[\frac{(b\gamma/r) + 1}{\sqrt{1 + \gamma^2}}\right] \tag{13.18}$$

Solving for the reciprocal of the radius r, we obtain:

$$\frac{1}{r} = \frac{1}{b\gamma}\sqrt{1 + \gamma^2}\left[\sin\left(\Phi - \sin^{-1}\frac{1}{\sqrt{1 + \gamma^2}}\right) - \frac{1}{\sqrt{1 + \gamma^2}}\right] \tag{13.19}$$

13.11 RUTHERFORD SCATTERING ANGLE

The outgoing particle, long after the collision, is at a distance $r = \infty$, or $1/r = 0$. We see that this will occur in Equation (13.19), when

$$\sin\left(\Phi - \sin^{-1}\frac{1}{\sqrt{1 + \gamma^2}}\right) = \frac{1}{\sqrt{1 + \gamma^2}} \tag{13.20}$$

or

$$\Phi = 2\sin^{-1}\frac{1}{\sqrt{1 + \gamma^2}} \tag{13.21}$$

This value of Φ corresponds to the scattering angle 19. Thus,

$$\sin \frac{1}{2}\theta = \frac{1}{\sqrt{1+\gamma^2}} \tag{13.22}$$

Also.

$$\cot \frac{1}{2}\theta = \frac{\sqrt{1-\sin^2 \tfrac{1}{2}\theta}}{\sin \tfrac{1}{2}\theta} = \gamma = T_0 \frac{4\pi\epsilon_0 b}{Ze^2} \tag{13.23}$$

Equation (13.23) implies that for a given J_0, the smaller b is, the larger is the angle of scattering. If b approaches zero, corresponding to a headon collision, the angle of scattering θ approaches 180"; the alpha particle is scattered straight backwards. If b approaches infinity, θ approaches zero, corresponding to no collision and no deflection.

12 RUTHERFORD DIFFERENTIAL CROSS-SECTION

Now that a relationship between the scattering angle θ and the impact parameter b has been obtained, we may proceed to derive the differential cross-section $d\sigma/d\Omega$. Imagine drawing a circle of radius b around the nucleus, as seen by an incoming α particle. This is depicted in Figure 13.1 1. All α's which hit inside the circle of radius b will be scattered through angles greater than the angle given by Equation (13.23),

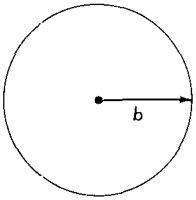


Figure 13.1 1. Circle of radius b; particles striking inside the circle will be deflected through angles greater than that given by Equation (13.23).

$$\cot \frac{1}{2}\theta = T_0 \frac{4\pi\epsilon_0}{Ze^2} b \tag{13.24}$$

Hence, the cross-section for scattering through angles greater than or equal to θ, which will be denoted by $\sigma(\geq \theta)$, will be just the area of the circle. In terms of b, this is

$$\sigma(\geq \theta) = \pi b^2 \tag{13.25}$$

Using Equation (13.23) to express b in terms of θ, we find the cross-section for scattering through angles $\geq\theta$ to be

$$\sigma(\geq\theta) = \pi\left(\frac{Ze^2}{4\pi\epsilon_0}\right)^2 \left[\frac{\cot(\tfrac{1}{2}\theta)}{T_0}\right]^2 \tag{13.26}$$

Consider particles which hit inside the ring bounded by circles of radius b and b + db, shown in Figure 13.12. Such particles will be scattered into angles

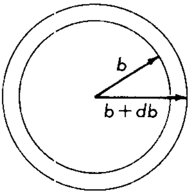


Figure 13.12. Differential area between b and b + db, corresponding to scattering within the range of angles $d\phi$.

between θ and $\theta + d\theta$. The area of this ring is da = $2\pi bdb$. Also, we may differentiate Equation (13.23) to find db in terms of the corresponding range of scattering angles $d\theta$. Since d(cot θ) = $-d\theta/\sin^2\theta$,

$$db = -\frac{1}{2}\left(\frac{Ze^2}{4\pi\epsilon_0 T_0}\right)\frac{d\theta}{\sin^2(\frac{1}{2}\theta)} \tag{13.27}$$

Therefore, with $d\Omega$ = 2n sin $\theta\, d\theta$, in terms of θ and $d\theta$ the differential scattering cross-section is

$$\frac{da}{d\Omega} = \frac{|2\pi bdb|}{d\Omega} = \frac{1}{2}\left(\frac{Ze^2}{4\pi\epsilon_0 T_0}\right)^2\frac{\cos(\frac{1}{2}\theta)}{\sin^3(\frac{1}{2}\theta)\sin\theta} = \frac{1}{4}\left(\frac{Ze'}{4\pi\epsilon_0 T_0}\right)^2\frac{1}{\sin^4(\frac{1}{2}19)} \tag{13.28}$$

since sin θ = 2 sin $(\frac{1}{2}\theta)$ cos $(\frac{1}{2}\theta)$. For large b, cos $\theta/2 \approx 1$ and sin $\theta/2 \approx \theta/2$, so for large impact parameters, the differential cross-section $d\sigma/d\Omega$ approaches infinity. In fact if we tried to integrate da to find the total cross-section σ, we would find that σ is infinite. This reflects the fact that the Coulomb force decreases relatively slowly as distance increases. We say it is a long-range force. In practice, the electrostatic force between nucleus and alpha particle is not really long-range, because if the alpha nuclear distance is greater than a few Angstroms, the nuclear charge is screened out by its bound electrons. Thus, for impact parameters which are too big our assumptions break down, and Equation (13.23) no longer holds; there will be no scattering.

13.13 MEASUREMENT OF THE DIFFERENTIAL CROSS-SECTION

Figure 13.13 shows how the differential cross-section might be measured by a movable detector of fixed area. The scattered α particles are counted by a detector at some fixed distance L from the target, which is arranged so that it may be placed at various angles θ relative to the incident direction. The detector has an area AA. Hence, if θ is small, the detector may detect all of the particles going into $d\theta$, but if θ is large. the detector may detect only a small fraction of the particles going into $d\theta$. This is simply because the detector area is fixed, and the scattering is azimuthally symmetric; that is, it is symmetric about the direction of the incoming beam. The solid angle subtended by a small area A at a distance L from the target is $\Delta A/L^2$. The integral of Equation (13.28) over this solid angle would be proportional to the number of α's counted in the experiment. This

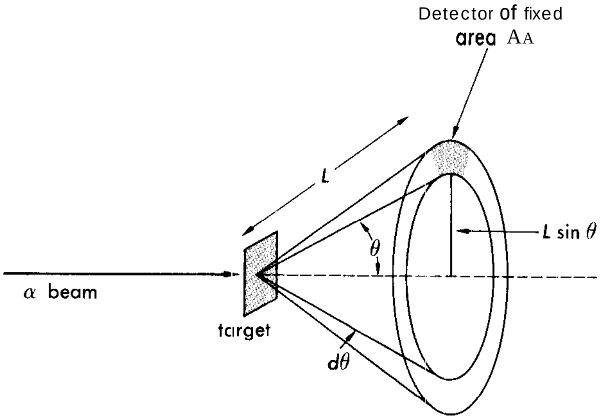


Figure 13.13. A detector of fixed area ΔA subtends an angle of $\Delta A/L^2$.

fractional cross-section times the number of particles incident per unit area per second should give the number of particles hitting the detector per second per target nucleus.

The result, Equation (13.28), is called the Rutherford scattering formula. It says that the effective differential scattering cross-section is proportional to $1/\sin^4 \theta/2$. If this result is combined with the expression, Equation (13.8), relating the scattering cross-section and the numbers of particles scattered, then if the incident flux density is N_i, the number ΔN_s scattered into the detector per second from a target of area 1 square meter, thickness t, and n scatterers per unit volume, will be:

$$\frac{\Delta N_s\,(\text{into detector})}{N_i} = \frac{\Delta A}{L^2}\, nt \cdot \frac{d\sigma}{d\Omega} \tag{13.29}$$

for $\Delta A/L^2$ small, or

$$\frac{\Delta N_s}{N_i} = \frac{\Delta A\, nt}{L^2}\left(\frac{Ze^2}{8\pi\epsilon_0 T_0}\right)^2 \frac{1}{\sin^4(\tfrac{1}{2}\theta)} \tag{13.30}$$

The most important result here is the $\sin^{-4}(\theta/2)$ dependence. The factors $(\Delta A/L^2)nt$ express the choice of detector size, geometrical setup in the lab, choice of scatterer, and thickness of scatterer. The quantity $d\sigma/d\Omega$ depends on the incident α particle energy, and on the nature of the interaction between α and nucleus. Surprisingly, quantum mechanical calculations of $d\sigma/d\Omega$ give the same result for the cross-section as we have obtained here using classical mechanics.

Let us summarize our derivation. We have obtained a specific formula for the number of α particles detected if the force between nucleus and α is a Coulomb force. The problem was treated by using classical mechanics. For an α of incident energy T_0 and impact parameter b, the angle of scattering is given by:

$$\cos\frac{1}{2}\theta = \frac{4\pi\epsilon_0 T_0}{Ze^2}\, b \tag{13.31}$$

All particles falling within a circle of radius b, drawn centered on the nucleus, will be scattered through an angle greater than θ. Particles falling in the area between b and b + db will be scattered into the angles $d\theta$ where $d\theta$ is obtained from db by differentiating the above equation:

$$|db| = \frac{Ze^2}{4\pi\epsilon_0 T_0} \cdot \frac{1/2}{\sin^2\theta/2} |d\theta| \qquad (13.32)$$

The differential cross-section for scattering into $d\theta$ is then

$$\frac{d\sigma}{d\Omega} = \frac{2\pi b \ \mathrm{db}}{d\Omega} = \left(\frac{Ze^2}{8\pi\epsilon_0 T_0}\right) \frac{d\theta}{\sin^4 \theta/2} \qquad (13.33)$$

Since the detector area AA, L meters from the target, is fixed, the detector always subtends a solid angle $\Delta A/L^2$. So the fractional cross-section for scattering into the detector of area AA is

$$\frac{\Delta A}{L^2}\frac{d\sigma}{d\Omega} = \frac{\Delta A}{L^2}\left(\frac{Ze^2}{8\pi\epsilon_0 T_0}\right)^2 \frac{1}{\sin^4 \theta/2} \qquad (13.34)$$

For an incident flux of N, particles per unit area per sec, the number of particles scattered into the detector at θ, from a target of thickness t and n scatterers per m^3, will be given by:

$$\frac{\Delta N_s}{N_i} = \frac{\mathrm{AA}}{L^2} \cdot n\left(\frac{Ze^2}{8\pi\epsilon_0 T_0}\right)^2 \cdot \frac{1}{\sin^4 \theta/2} \qquad (13.35)$$

13.14 EXPERIMENTAL VERIFICATION OF THE RUTHERFORD SCATTERING FORMULA

The above prediction can be used in several ways. The number of a's detected per sec are proportional to:

(1) the reciprocal of $\sin^4 (\theta/2)$;

(2) the reciprocal of kinetic energy squared;

(3) the square of the nuclear charge Z.

There are other dependences, but these are the most important. Let's consider them in order. In Table 13.1 are given some experimental results for scattering from gold foil as a function of scattering angle. According to the theory, the product of ΔN_s and $\sin^4(\theta/2)$ should be constant. The agreement between theory and experiment shown in the last column is reasonably good; that is, AN, is proportional to $1/\sin^4(\theta/2)$.

In another set of experiments, α particles of varying velocity were scattered into a detector held at a fixed angle. According to the scattering formula, AN, is inversely proportional to T_0^2, and $T_0^2 = (\frac{1}{2} Mv_0^2)^2$. So AN, is inversely proportional to v_0^4. In Table 13.2 are given the experimental results in dimensionless form. The results agree well with the formula.

TABLE 13.1 Scattering of Alpha Particles From Gold Foil

Angle of Deflection	Number of Scintillations in Unit Time ΔN_s	$\frac{1}{\sin^4 \theta/2}$	$\Delta N_s \times \sin^4 \theta/2$
150°	33.1	1.15	28.8
135°	43.0	1.38	31.2
120°	51.9	1.79	29.0
105°	69.5	2.53	27.5
75°	211	7.25	29.1
60°	477	16.0	29.8
45°	1435	46.6	30.8
37.5°	3300	93.7	35.3
30°	7800	223	35.0
22.5°	27,300	690	39.6
15°	132,000	3445	38.4

TABLE 13.2 Variation of Scattering with Velocity

Range of Alpha Particles	Relative Values of $1/v_0^4$	Number of Scintillations in Unit Time ΔN_s	$\Delta N_s \times v_0^4$
5.5	1.0	24.7	25
4.76	1.21	29.0	24
4.05	1.50	33.4	22
3.32	1.91	44	23
2.51	2.84	81	28
1.84	4.32	101	23
1.04	9.22	255	28

In another set of experiments, performed by Chadwick in 1920, copper, silver and platinum foils were used with α's of fixed energy and at fixed scattering angles θ, with carefully measured geometrical factors $\Delta A/L^2$, in an attempt to determine the values of Z for these elements. The results are given in Table 13.3.

TABLE 13.3 Nuclear Charges Determined by α-Particle Scattering

Element	Nuclear Charge Ze	Atomic Number Z
Cu	29.3e	29
Ag	46.3e	47
Pt	77.4e	78

These results agree, within the experimental error, with the Rutherford scattering formula, and are additional evidence for the extremely small size of the nucleus.

13.15 PARTICLE ACCELERATORS

The experiments discussed in this chapter employed α particles from naturally occurring radioactive elements. While these were useful for the pioneering scattering experiments in nuclear physics, for a detailed investigation of nuclear forces it is desirable to have a wide range of different types of particles available, with variable energies which go much higher than the 8 MeV available in natural α particles. Therefore, a number of methods have been developed for accelerating particles in the laboratory. The earlier efforts were aimed at obtaining a high difference of potential between two points, and letting charged particles accelerate between the two points. The Van de Graaff generator was the most successful of these accelerators. It utilizes electrostatic induction methods to obtain the high voltages. However, it is limited to energies only slightly higher than the 8 MeV α particles, due to difficulties in insulating between even widely-spaced points, at several million volts potential difference.

An accelerator called the cyclotron, which overcame these difficulties, was developed by E. 0. Lawrence around 1932. In this machine, lower potential differences are used, but the particles move through the potential differences many times, eventually picking up a large energy. This is accomplished by injecting the charged particles into a magnetic field with lines of force oriented perpendicular to the particle velocities. The resulting force causes the particles to move in circular orbits. The particles move as shown by the dashed line in Figure 13.14, inside hollow semicircular conductors called ***dees.*** An alternating voltage is applied between the dees, with a frequency equal to that of the circular motion and synchronized with the passage of the particles across the gap between the dees, in such a way that every time a particle crosses the gap, it is accelerated by the electric field in the gap and gains an energy corresponding to the maximum value of the alternating voltage. One may easily calculate the necessary frequency. If the particle has charge q, speed v and mass m, and moves in a magnetic field B with a radius r and angular frequency w = v/r, then the magnitude of the magnetic force is:

$$F = qvB = qr\omega B \tag{13.36}$$

This equals the mass times the centripetal acceleration, $\omega^2 r$. So

$$m\omega^2 r = qr\omega B \tag{13.37}$$

or

$$\omega = qB/m \tag{13.38}$$

The frequency is then $\nu = \omega/2\pi$. This result is independent of radius if relativistic changes of mass with speed can be neglected. This is very desirable, since as the particles pick up energy, their radius increases until they eventually get to the edge of the dees, where they are extracted to give the particle beam. The limitation on the energy of particles accelerated by a fixed-frequency cyclotron occurs primarily because of the relativistic increase of mass as energy increases. Since the frequency w is inversely proportional to mass, the particles tend to get

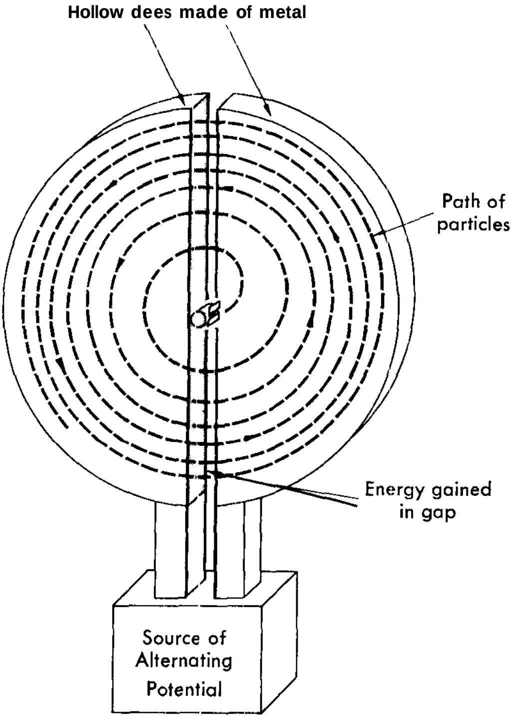


Figure 13.14. Diagram of a cyclotron. The magnetic field is perpendicular to the plane of the figure.

out of phase with the applied alternating potential at higher energy, and cease to be accelerated.

One way to overcome the relativistic effect is to make the magnetic field increase with radius, so that B/m is constant. However, this tends to make the particle motion along the magnetic field lines unstable, so that particles are lost by hitting the dees. This may be cured for energies up to a few hundred MeV, if the particles are nuclei, by making the magnetic field vary periodically around the circular path.

One way of overcoming the relativistic increase of mass effect is to accelerate the particles in bunches, with the frequency of the applied potential decreasing as the bunch of particles gains energy. Such machines are called *synchrocyclotrons.* When one bunch gains maximum energy and leaves the machine, a new bunch is introduced.

In modern high-energy machines in the billion electron volt energy region or higher, the charged particles travel in evacuated circular tubes which may be comparable to a mile in diameter. Carefully designed magnetic fields keep the particles in the proper path.

Electrons are more difficult to accelerate for high energies than more massive particles, because for a given kinetic energy, they tend to lose more energy in the form of radiation when they undergo centripetal acceleration. Therefore, electrons are ordinarily accelerated to very high energies in a linear accelerator.

The electron beam moves down the center of a straight line of cylindrical metal segments. The length of each segment is such that an electron spends the same time inside each segment. Thus, if an alternating potential with period equal to twice that time is applied between segments, the particle can go through the maximum potential change every time it crosses a gap between segments. To obtain electron energies in excess of 10 billion electron volts, the linear accelerator has to be several miles long.

summary

α PARTICLES

Some radioactive heavy elements emit a particles with energies of the order of 4 to 8 MeV. They have a charge $Q = 2e$ and a mass nearly four times the proton mass. They have been identified as helium nuclei.

SCATTERING CROSS-SECTION

An infinitesimal scattering cross-section $d\sigma$ for scattering into a given range of angles $d\Omega$ is the number of particles scattered into $d\Omega$ per scattering particle, divided by the number of particles incident per unit area. Hence do is the effective area of the scatterer for scattering into $d\Omega$. The quantity, $d\sigma/d\Omega$, is called the ***differential cross-section.*** If the scatterer is a thin foil of thickness t containing n scattering centers per unit volume, then the fraction of incident particles scattered into $d\Omega$ is $ntd\sigma$. The totol cross-section is $\int d\sigma$, and is the total number of particles scattered per scattering particle, divided by the number incident per unit area. It is the total effective area of the scatterer. The unit of scattering cross-section is the barn: 1 barn = $10^{-28} \mathrm{m}^2$.

DENSITY OF SCATTERERS

The density of scatterers n per m^3 is given by $n = \rho N_0/W$ where ρ is the density, N_0 is Avogodro's number, 6.02×10^{23} per/gm-mole, and W is the gram molecular weight.

RUTHERFORD SCATTERING

The differential cross-section $d\sigma/d\Omega$ for α particle scattering from nuclei of charge Z is given by:

$$\frac{da}{d\Omega} = \left(\frac{Ze}{8\pi\epsilon_0 T_0}\right)^2 \frac{1}{\sin' \theta/2}$$

NUCLEAR SIZES

Experiments with high-energy electron scattering show that nuclei are roughly spherical, and have radii given by $R = R_0 W^{1/3}$, where R_0 = 1.1 fermis and W is the atomic weight of the element.

problems

1. **The cross-section for interaction of neutrinos** with nuclei is approximately 10^{-18} barns, What thickness of iron could cause 1 % of the neutrinos in a neutrino beam to interact? For iron, $\rho = 7.9$ g/cm^3.
   Answer: 1.2 x 10^{15} meters, or around 10.7 million miles or about 0.1 light years.
2. Using the **value** of the nuclear radius as given in Equation (13.10), calculate the average density of nuclear matter.
   Answer: *3* x 10” kg/m^3.
3. Calculate the rest energy of one cubic Angstrom of pure nuclear matter.
   Answer: *2.7* x 10^4 joules.
4. Scattering of particles with the wavelength h/p by an obstacle is essentially a diffraction effect. If the obstacle is a hard sphere of radius a and p $\gg$ **h/a,** argue that the total cross-section should be greater than πa^2. As $p \rightarrow \infty$ the cross-section approaches $2\pi a^2$. The cross-section increases as p decreases. Explain why this might be. As $p \rightarrow 0$ the cross-section approaches $4\pi a^2$, four times the geometrical cross-section.
5. A beam of electrons with 10^{21} electrons per second per square meter is incident on a gas. The scattering cross-section due to a gas atom is 10^{-19}m^2. How many electrons are scattered per second by a gas atom?
   Answer: 100.
6. A solid has **n** atoms per unit volume. A beam of gamma rays incident on the solid sees a scattering cross-section of σ. In going the infinitesimal length **dx out of** N photons, how many are scattered? What fraction of the gamma rays are unscattered after going the distance x?
   Answer: Nnadx, $e^{-\sigma n x}$.
7. An alpha particle with a speed of 10^6m/sec moves in a circle perpendicular to a magnetic field of 2 weber/m^2. Find the frequency of rotation and the radius of the circle.
   Answer: 1.5 x 10^7 rotations/sec; 1.03 cm.
8. Calculate the distance of closest approach to a silver nucleus (Z = 47) of 12 MeV deutrons with charge e | and mass about twice that of a proton.
   Answer: 5.6 fermis.
9. An alpha particle of speed 1.55 $\times 10^7$ m/sec is scattered through an angle of 25” from a silver nucleus. What was the impact parameter?
   Answer: 61 fermis.
10. What is the distance of closest approach of a 6 MeV α particle to a uranium (Z = 92) nucleus?
    Answer: 44 fermis.
11. A beam of 8.3 MeV α particles is incident on aluminum foil, and significant devi-

otions from the Rutherford scattering formula are observed for scattering angles greater than 60". Assume the α particle has a radius 1.1 x $\sqrt{4}$ fermis, and estimate the radius of the aluminum nucleus.

Answer: 4.6 fermis.

12. Suppose a beam of spherical particles of radius r is incident on a material consisting of fixed spherical particles of radius R. If the scattering is the same as that of elastic collisions of hard spherical particles following classical mechanics, show that the infinitesimal cross-section for scattering angle θ is

$$d\sigma = \pi(r + R)^2 \sin \tfrac{1}{2}\theta \cos \tfrac{1}{2}\theta = \tfrac{1}{2}\pi(r \text{ t } R)^2 \sin\theta \, d\theta$$

What is the differential cross-section? Integrate to show that the total cross-section is $\pi(r + R)^2$.

13. A plane wave e^{ikx} representing a beam of particles with momentum $p = \hbar k$ in the x direction, can be expressed as a sum of wovefunctions, each with definite angular momentum:

$$e^{ikx} = \sum A_\ell \psi_\ell(r, \theta)$$

where A_ℓ is a constant depending on the angular momentum quantum number, ℓ, and θ is the angle relative to the x axis with r the radial distance ($x = r$ cos 0). The scattering can then be found for the individual ψ_ℓ's, and the combination gives the total scattering. If a scattering center gives scattering out to radius R and none for greater radii, argue that there will be negligible scattering for a ψ_ℓ when $\ell \gg kR$. As the momentum goes to zero, argue that we need to consider only ψ_0.

14. Compute the differential scattering cross-section $d\sigma/d\Omega$ for scattering of protons off gold nuclei into the angles near 45°, if the incident proton energy is 4 MeV. Assume Coulomb forces.

Answer: 94 barns/stereradians.

15. A silver foil of thickness 10^{-5} mm and area 4 mm^2 is used as a target in on α particle scattering experiment with α's of 6.5 MeV kinetic energy. The incident flux of particles is 25 per mm^2 per minute. How many α's per minute should be scattered into the detector of area 1 cm^2, placed at 45" relative to the incident beam a distance 5 cm away from the target? For silver, $\rho = 10.5$ g/cm^3.

Answer: 3 x 10^{-6} per minute.

16. For a certain type of scattering process, particles are scattered uniformly in all directions. Then how should do depend on angle?

17. Alpha particles from polonium (Velocity = 1.6 x 10' m/sec) are directed normally against a gold foil of thickness 4 x 10^{-5} cm. The density of gold is 19.32 g/cm^3. What fraction of the alpha particles are scattered through angles greater than 135°?

Answer: 5.9 x 10^{-6}.

18. What fraction of 5.7 MeV α particles incident on copper foil, $\rho = 8.929$ g/cm^3, of thickness 10^{-5} mm, will be scattered through angles greater than 90°?

Answer: 1.4 x 10^{-7}.

19. For the series in Problem 13, take $\psi_0(r, \theta) = (\sin kr)/kr$, and assume that $A_0 \cong 1$ with the other A_ℓ negligible. If a hard sphere of radius R were placed in the path of the plane wave, the wavefunction would then be $\sum B_\ell \psi'_\ell(r, \theta)$ with the constant B_0 the only one of appreciable size. For the $\ell = 0$ case, $\psi'_0 = \dfrac{\sin (kr + 6)}{kr}$.

Show that to satisfy the boundary condition at r = R, $-\delta = kR$. Now sin (kr) =

$\frac{1}{2} i(e^{ikr} - e^{-ikr})$ and $\sin (kr + \delta) = \frac{1}{2} i(e^{ikr+i\delta} \quad e^{-ikr-i\delta})$. Since the time dependence is $e^{-i\omega t}$, the terms in parentheses correspond to outgoing and incoming waves respectively. Thus, for the incoming waves to be the same with and without the sphere, $-e^{-ikr}/2i = -B_0 \frac{1}{2} i e^{-ikr-i\delta}$. Find B_0. If we say that the number of incident particles per unit area per unit time is proportional to $e^{ikx}|^2$, argue that the number scattered per unit area per unit time is proportional to $1/(2kr)^2 \quad e^{2i\delta} - 1 \quad ^2$ for $k \rightarrow 0$, and thus the differential cross-section is $\frac{1}{4k^2}(2 - 2\cos 2kR) = \frac{\sin^2 kR}{k^2} \xrightarrow[k=0]{} R^2$. Show that for $k \rightarrow 0$, the total cross-section is $4\pi R^2$.

14 nuclear structure

The experiments on α particle scattering give direct evidence that the force between a nucleus and an α particle is a Coulomb force, proportional to $1/r^2$, down to distances of the order of several fermis. Hence the size of the nucleus has to be of this order of magnitude (1 fermi = 10^{-15} meters). Later experiments with other types of incident particles from accelerators have established that the matter in the nucleus is distributed throughout the nuclear volume with nearly constant density, and that the radius R of a nucleus of an element of atomic mass W (in amu) may be expressed by: $R = r_0 W^{1/3}$, where $r_0 \cong 1.1$ fermis. Nuclei are thus seen to be extremely small, compared to the size of the atom. In fact, in an ordinary piece of lead, 99.978% of the mass is contained in about 0.000 000 000 000 000 04% of the volume.

It is the aim of nuclear physics to understand the internal structure of these tiny objects-how they are held together, what they are made of, and how they interact with each other. This study is very active at present, and there are a great many unsolved problems. In contrast to atomic physics, where the basic principles of wave mechanics are well understood and where these principles have almost invariably led to o quantitatively precise explanation of atomic phenomena, in nuclear physics the basic principles are only qualitatively understood and accurate numerical calculations are extremely difficult. We shall begin by looking at some of the simplest experimental data. Then we shall discuss the properties of stable nuclei and some models by which we can understand qualitatively the gross features of nuclear structure.

14.1 NUCLEAR MASSES

Over a thousand different kinds of nuclei are now known to exist. Two nuclei are different in kind if their charges or masses are different. The charge Ze on a nucleus can be determined in a number of ways-by particle scattering, by x-ray production, or simply by chemical or spectral identification of the element whose atoms are formed by electrons surrounding the given nucleus. Nuclei with about 100 different values of Z are found in nature. All nuclei having equal values of Z are called isotopes. For example, the element calcium (Z = 20) is found in nature with 6 different nuclear masses which are stable, and others which are not stable. Therefore, calcium has six different stable isotopes.

Some nuclei are stable, while others are unstable and emit radiations in the form of α particles, high-speed electrons or positrons, photons, or other particles. In this chapter we shall be primarily concerned with the stable nuclei, those which do not emit radiations. In Appendix 3 are given the measured values of the atomic masses of the stable nuclei and a few of the more interesting unstable ones. These masses are based on the assignment of exactly 12 units of mass to the most common carbon isotope, which is then used as the standard of mass. (NOTE: These are not nuclear masses, but masses of the entire *electrically* neutral atom.) The reason atomic masses are given, rather than nuclear masses, is that it is atomic masses which are usually measured directly. For example, the mass of 22.4 liters of helium, containing N_0 particles, could be directly measured and the atomic mass, or mass of one atom, could be derived from the measurement. Another way atomic masses are measured is by ionizing an atom (removing one or more electrons) and then accelerating the atom through an electric field, thus giving it a known energy. The charged ion is then allowed to pass through a magnetic field. By measuring the deflection of the ion in the magnetic field, the ion's momentum can be determined. If both momentum and kinetic energy are known, the ion mass and then the atomic mass may be determined. The art of using electric and magnetic fields for determining atomic masses has been developed to a high degree.

If the atomic mass is known, then to find the mass of the nucleus by itself, one should subtract the masses of the electrons in amu from the atomic mass:

$$m_e = 9.108 \times 10^{-31}\ \text{kg} = 0.000549\ \text{amu}$$

Strictly speaking, the mass of an electron bound to a nucleus is effectively slightly less than the electron's rest mass, because the electron has more negative potential energy than it has kinetic energy. However, these binding energies are only a small fraction of the electron's rest energy and can be neglected when using atomic mass tables. A common notation is to denote the value of Z as a subscript to the left of the symbol of the element. Thus, iron (Z = 26) is denoted by $_{26}Fe$. Oxygen, with Z = 8, would be denoted by $_8O$. If $_ZM_{at}$ is the atomic mass of a nucleus having charge Z, and if m_e is the electron's rest mass, then the nuclear mass $_ZM$ is given to sufficient accuracy by:

$$_ZM = {}_ZM_{at} - Zm, \qquad (14.1)$$

From the table of atomic masses, it is seen that the atomic masses are nearly integers, when the masses are measured in atomic mass units (amu). The integer nearest to the atomic mass W is called the mass number and is denoted by A. Thus the mass number of the isotope of zirconium (Z = 40), with an atomic mass W = 91.9046 amu, is A = 92. For a nucleus of a given Z and A, in addition to writing Z as a subscript to the left, the value of A is written as a superscript to the right: $_ZM^A$. Thus the Zirconium nucleus mentioned above would be denoted by $_{40}Zr^{92}$.

ample From the table in Appendix 3, the atomic mass of $_{53}I^{127}$ is 126.90435 amu. The mass of one electron is the mass of a proton, 1.0078 amu, divided by the ratio of proton to electron mass, 1836, or m_e = .000549 amu; so the mass of the electrons in ${}_{53}I^{127}$ is (0.00055)(53) = 0.0292 amu. Therefore, the nuclear mass of ${}_{53}I^{127}$ is 126.9044 − 0.0292 = 126.8752 amu.

14.2 NEUTRONS IN THE NUCLEUS

The fact that the nuclear masses are so nearly integral multiples of a basic unit suggests that a nucleus of mass number A is built out of A smaller particles of equal or nearly equal masses. It is now known that nuclei are basically composed of protons and neutrons. Neutrons are electrically neutral particles having a mass nearly equal to the proton mass. However, for a time it was thought that a nucleus of mass number A might be composed of A protons plus a number of electrons which resided in the nucleus, thus canceling out a part of the protonic charge. We shall consider two of the most important reasons why this cannot be an accurate picture of the nucleus, and shall then discuss the properties of nuclei based on a proton-neutron composition.

A nucleus has a very small size, several fermis in diameter. If an electron exists inside the nucleus, then the magnitude of the uncertainty in position of the electron will be roughly $\Delta x \sim 10^{-15}$ m. For such a small uncertainty in position, the momentum uncertainty will be very large; the average momentum will be of the order of magnitude of the uncertainty in momentum, and from this the average kinetic energy of the electron in the nucleus can be estimated. For an uncertainty Ax, the uncertainty in momentum will be Ap $\cong h/(4\pi\Delta x)$. The average momentum would then be roughly

$$p \sim \frac{6.6 \times 10^{-34}}{(12.6)(10^{-15})} = 5 \times 10^{-20}\ \text{kg-m/sec} = 100\ \frac{\text{MeV}}{c}$$

For an electron with rest energy of about 0.5 MeV, this is an extreme relativistic momentum, so the energy is

$$E = \sqrt{(pc)^2 + (m_0c^2)^2} \cong pc = 100\ \text{MeV}$$

Thus, from the uncertainty principle, if an electron is confined to a region around a fermi in size, it will have a very large kinetic energy. In order for the electron to remain in the nucleus, it must be bound by an even greater negative potential energy. Since the negative potential energy due to Coulomb attraction is at best a few MeV, that would mean that there would have to exist a *very* strong attractive force between proton and electron of some entirely new type. There is no other independent evidence in nature for such a strong force between electron and proton.

Also, the proton-electron model of the nucleus does not give good values for nuclear magnetic moments. An electron has an intrinsic magnetic moment, $e\hbar/2m$ = 1 Bohr magneton. If there were an odd number of electrons inside the nucleus, then the unpaired electron should give rise to a nuclear moment of 1 Bohr magneton. Instead, nuclear moments are more nearly of the order of

$e\hbar/2M_p$, where M_p is the proton mass. In Bohr magnetons, $e\hbar/2M_p$ = 0.00054 $e\hbar/2m$.

When the neutron was discovered by Chadwick in 1932, Heisenberg immediately suggested that nuclei must be composed of neutrons and protons. Chadwick had found that when α particles are incident on nuclei of $_4Be^9$, a very penetrating radiation is given off. Since this radiation leaves no visible tracks in a cloud chamber, it is uncharged. Also, the radiation has the property that when passing through any material containing a large proportion of hydrogen, protons are knocked out with about 5 MeV of kinetic energy. Chadwick showed that these and other similar experiments could be understood by assuming that the radiation consisted of uncharged particles called neutrons, having a mass nearly equal to the mass of the proton. The neutron's mass has been determined to be 1.0086652 amu. The neutron is denoted by the symbol $_0n^1$, which means the mass number of the neutron is one. Neutrons have been found to take part in a number of nuclear reactions.

A nucleus of mass number A can then be considered to be composed of N neutrons and Z protons, with

$$N + Z = A \tag{14.2}$$

The number of neutrons in a nucleus, N, is called the neutron number.

The different kinds of stable nuclei may be characterized by giving them the numbers N, Z and A. Since, from Equation (14.2), there is one equation connecting N, Z and A, it is necessary to give only two (any two) of these three numbers. Knowing the two numbers Z and A corresponds to knowing the charge and mass of the nucleus in question. The N and Z values of all the stable nuclei are given in Figure 14.1. In this table the neutron number is plotted vertically and the proton number horizontally. A dot at a certain point with coordinates (Z, N) represents a stable nucleus, which exists with Z protons and N neutrons. We see from Figure 14.1 that the stable nucleus $_{20}Ca^{46}$ exists, but that the stable nucleus $_{92}U^{238}$ does not exist.

We also see, for example, that there are ten stable isotopes of $_{50}Sn$. Nuclei having equal numbers of neutrons in the nucleus are called *isotones. One* way to remember *which is which:*

isotopes: equal numbers of protons
isotones: equal numbers of neutrons

As an example, Figure 14.1 shows that there are three stable N = 14 isotones. Since nuclei are constituted of protons and neutrons, these fundamental particles are also called nucleons.

.3 PROPERTIES OF THE NEUTRON AND PROTON

In attempting to understand the properties of large nuclei containing up to 240 nucleons, we need to know first what the fundamental properties of the nucleons

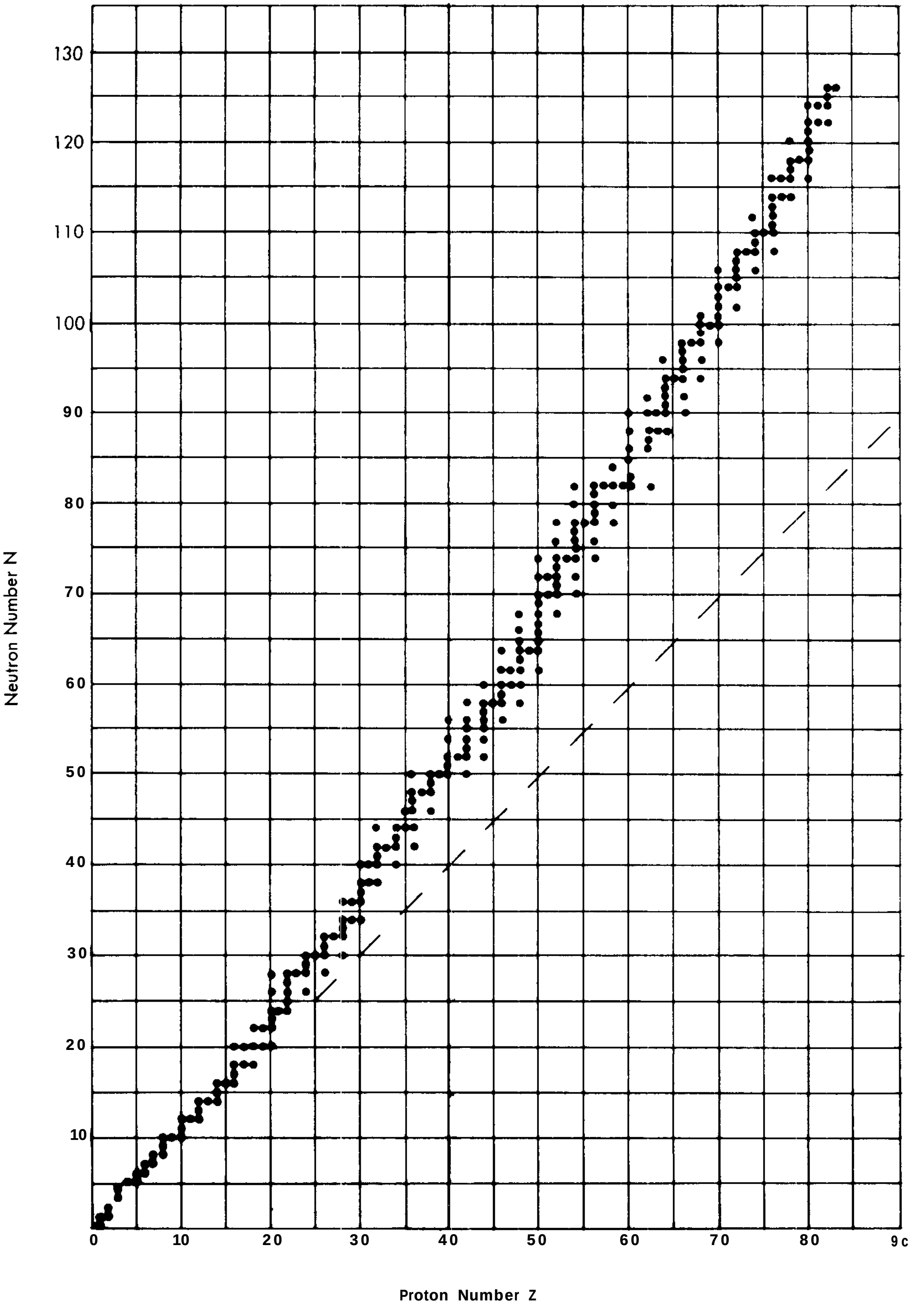


Figure 14.1. Neutron number versus proton number for the stable nuclides.

themselves are. So far, we have discussed charge and mass. In addition, it has been found that neutrons and protons both have intrinsic spin angular momenta characterized by spin quantum numbers of ½ . Nuclear spin quantum numbers are denoted by I, and for both neutron and proton, I = ½ . These spin angular momenta obey the same rules we have discussed several times for electron spin and orbital angular momenta. For example, the eigenvalue of the square of the spin angular momentum of a nucleus would be given, in terms of I, by

$$\mathbf{I}^2 = \hbar^2 I(I+1) \tag{14.3}$$

Since a nucleus may contain several nucleons, I may in general be different from ½ . Specifically for nucleons, however, since I = ½ ,

$$\mathbf{I}^2 = \frac{3}{4}\hbar^2 \tag{14.4}$$

Nuclear spin angular momenta are associated with the presence of magnetic moments. There is a simple relation between magnetic moment $\boldsymbol{\mu}$ and spin I, which is customarily written:

$$\boldsymbol{\mu} = g\frac{e\hbar}{2M_p}\mathbf{I} \tag{14.5}$$

where M_p is the proton mass. The quantity $e\hbar/2M_p$ is a unit called the ***nuclear magneton.*** It is $^1/_{1836}$ of a Bohr magneton. Most nuclear magnetic moments are of the order of a few nuclear magnetons. When writing the magnetic moment as in Equation (14.5), the factor g—simply called the "g factor"-is a pure number of the order of magnitude -5 to +5, which must be determined experimentally. In Equation (14.5), the (convention is adopted that the mass of the proton, rather than the neutron or some other particle, is used in the unit $e\hbar/2M_p$. Then g has some value that cannot be predicted accurately; at present, there is no acceptable theory of nuclear moments.

The relation between $\boldsymbol{\mu}$ and I is such that, if the nuclear spin can have 21 + 1 different z components along some chosen z direction, then the number of different values of μ_z is also $2I + 1$. Thus, if a nuclear spin is placed in a magnetic field, the energy $E = -\boldsymbol{\mu}\cdot\mathbf{B}$, has $2I+1$ different values. Hence, in a magnetic field, isolated protons and neutrons have two different energy states. The g factors of various nuclei can be measured by observing the frequencies of the photons which are absorbed as the nuclei make transitions between different states in a magnetic field. For example, in a magnetic field of 0.5 w/m^2, protons absorb electromagnetic radiation of frequency 2.13 x 10^7 cps in making a transition from the spin-down to the spin-up state. Here, AE = $h\nu = 2\mu B$. With $e\hbar/2M_p = 5.051 \times 10^{-27}$ joule/(weber/m^2) and $I = ½$, the proton's g factor is

$$g_p = \frac{h\nu}{½\,[2(e\hbar/2M_p)\,B]} = \frac{(6.62 \times 10^{-34})(2.13 \times 10^7)}{(5.05 \times 10^{-27})(0.5)} = 5.58$$

In the case of the $_3Li^7$ nucleus, I = $\frac{3}{2}$ and the measured value of g is 2.1688. Therefore, the maximum component in any direction of the nuclear magnetic moment of $_3Li^7$ is $\frac{3}{2}$ (2.1688) = 3.25 nuclear magnetons. Table 14.1 is a brief summary of the numerical values of the constants characterizing nucleons.

TABLE 14.1 Properties of Neutron and Proton

	$_0n^1$	$_1p^1$
Charge	0	$\lvert e \rvert$
Mass (amu)	1.008665	1.007276
Spin	½	½
g factor	-3.8256	+5.5856
Magnetic moment (nuclear magnetons)	-1.9128	+2.7928

14.4 THE DEUTERON ($_1H^2$)

The simplest nucleus which contains more than one particle consists of one proton and one neutron, and is called a deuteron. The Z of a deuteron is one. Since the deuteron has a charge +$\lvert e \rvert$ and a mass number A = 2, it is an isotope of hydrogen. Since the nuclear mass is different from that of ordinary hydrogen, the hydrogen-like atomic energy levels will be shifted slightly away from the values they have in hydrogen. These energy shifts can be used to measure the deuteron's mass M_d in terms of the proton mass M_p. The experimental values of the Rydberg constants in cm-' for $_1H^1$ and $_1H^2$ are:

$$R_H = 109{,}677.581 \text{ cm}^{-1}, \text{ for } {}_1H^1$$

$$R_D = 109{,}707.419 \text{ cm}^{-1}, \text{ for } {}_1H^2$$

The ratio of these two numbers is just the ratio of the reduced masses, so:

$$\frac{R_H}{R_D} = \left(1 + \frac{m_e}{M_d}\right) \Big/ \left(1 + \frac{m_e}{M_p}\right) = \left(1 + \frac{m_e}{M_p} \cdot \frac{M_p}{M_d}\right) \Big/ \left(1 + \frac{m_e}{M_p}\right) \tag{14.6}$$

or

$$\frac{M_d}{M_p} = 1 \Big/ \left(\frac{M_p}{m_e} \frac{R_H - R_D}{R_D} + \frac{R_H}{R_D}\right) \tag{14.7}$$

From this we can calculate the ratio of mass of the deuteron to mass of the proton. With $m_e/M_p = 1/1836$, we obtain:

$$\frac{M_d}{M_p} = 1.9985$$

Then, in amu, the deuteron mass is 2.013. This illustrates how information about nuclei can be obtained by studying the interaction of nuclei with electrons.

More accurate mass values for the deuteron may be obtained by observing the deflections of deuterons in electric and magnetic fields, or by observing the behavior of deuterons in nuclear reactions. The value of the deuteron's mass, from Appendix 3, is:

$$_1M_{at}^2 - m_e = 2.014102 - 0.000549 = 2.013553 \text{ amu}$$

The deuteron's mass is not equal to the sum of the neutron and proton masses, which is:

$$\begin{aligned} M_p &= 1.007276 \text{ amu} \\ + M_N &= \underline{1.008665} \\ &= 2.015941 \text{ amu} \end{aligned}$$

Thus, the total rest mass of the deuteron is less than the sum of the rest masses of its constituent particles. This means that the system is bound. This is due to an attractive force between neutron and proton, and a negative potential energy of interaction. If the system is bound, then it is necessary to add energy to the system to separate it into its component parts. The amount of energy needed to separate the system into its constituents and place them at rest infinitely distant from each other is called the *binding* energy, E_b. The binding energy of a bound system is always positive.

The binding energy of the deuteron may be computed as follows: The rest mass after separating the nucleus into parts = $M_p + M_n = 2.015941$ amu; the rest mass before separating the nucleus into parts = $M_d = 2.013553$ amu; the difference between these masses is due to the addition of energy, in this case an amount equal to the binding energy; therefore, the binding energy will be given by $E_b/c^2 = M_p + M_n - M_d = 0.002388$ amu; since 1 amu is equivalent to 931.48 MeV, we find that the binding energy in MeV is $E_b = 2.224$ MeV. This is extremely large compared to atomic binding energies.

The existence of a large value, 2.224 MeV, for the deuteron's binding energy indicates the presence of a strong, attractive force between neutron and proton. The deuteron can be made to disintegrate by irradiating it with a beam of high energy y-ray photons. If the energy of a photon is greater than the binding energy, the deuteron can absorb the photon and be dissociated into a proton and a neutron with some kinetic energy. This process is called *photodisintegration* and is observed experimentally to occur, provided the incident γ energy is greater than the minimum 2.224 MeV, called the *threshold energy.*

The spin and magnetic moment of the deuteron are also of interest. The nuclear force between nucleons is found to depend very strongly on the relative orientation of the spins; for a neutron and a proton,, the state of lowest energy is one in which the nuclear spins are lined up. The spin quantum numbers of both n and p are ½ If the spins are parallel, then assuming there is no orbital angular momentum, the spin quantum number of the deuteron should be $I_D = 1$. It is found experimentally that this is the spin quantum number of the deuteron. In contrast to the hydrogen atom, which has infinitely many bound states, the deuteron has only this one bound state with spins parallel.

let us next consider the magnetic moment of the deuteron. From Table 14.1, the magnetic moment of the neutron is antiparallel to its spin. The magnetic moment of the proton is, on the other hand, parallel to its spin. So if the spins of n and p are parallel, the two magnetic moments should therefore be in opposite directions, or antiparallel. If this is the case, then we might expect that the magnetic moment of the deuteron would be equal to the difference between the magnetic moments of proton and neutron. This difference is

$$\mu_p - \mu_n = 2.7928 - 1.9128 = 0.8800 \text{ nuclear magnetons}$$

The actually measured value of the moment of the deuteron is +0.8574 nuclear magnetons. This agrees quite well with the above result, but there is a difference of 0.0226 nuclear magnetons, which has not yet been explained.

14.5 NUCLEAR FORCES

In order for a neutron and a proton to form a bound state, it has been said that a strong attractive force must exist between the two particles, and that the force will be spin-dependent. Although from experimental studies of the scattering of nucleons off nucleons, semi-quantitative statements can be made about such strong interactions, the basic force law is not completely known. One way to study the interaction is by scattering neutrons off proton targets. A way to interpret the data is to assume the potential energy of interaction between the particles is a certain mathematical function, then solve the Schrödinger equation to find what the scattering cross-section should be for that potential. If the predictions agree with experiment, this would be evidence that the assumed potential is correct. Thus we do not deal directly with a force, but rather with a potential energy in nuclear physics. In Figure 14.2 is given a potential energy as a function of distance r between neutron and proton, which explains the scattering data for incident neutron energies up to 10 MeV or so. The potential varies somewhat, depending on the relative spins of the two particles. The interaction potential is

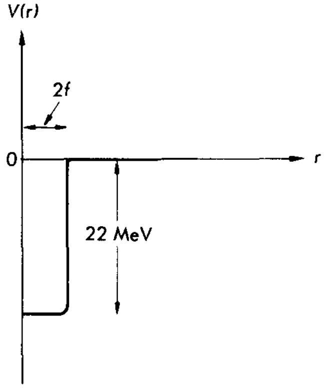


Figure 14.2. Neutron-proton interaction potential.

essentially zero until the particles come to within $\simeq 2$ fermis of each other, and then drops down to a very low value, about -22 MeV. Such a function is called a *potential well*. The exact shape of the well is not too important; in fact, one could draw several other curves which have the same general shape as that in the figure, and which explain the data equally well. They might differ in details, such as in the sharpness of the bend upwards at $r = 2$ fermis, in whether the bottom of the well slants a little, and so forth. One of the most important features of this potential is that it is of very short range and goes to zero at a range of about 2 fermis.

In proton-proton scattering experiments, as contrasted with neutron-proton scattering, it is to be expected that if the distance of closest approach is greater than the proton diameter, the potential energy of interaction should be just a Coulomb potential. It is found that if the incident proton's kinetic energy is large enough for the protons to penetraie the repulsive Coulomb potential and come within a few fermis of each other, then the potential energy of interaction becomes large and negative. This conclusion is reached by interpreting the scattering data in a fashion similar to that used for neutron-proton scattering. The potential of interaction is plotted in Figure 14.3. Apart from the Coulomb repulsion of protons, the interaction between two protons is essentially the same as that between a neutron and proton. That is, the "nuclear" part of the potential is the same in both cases. Experiments on neutron-neutron scattering also indicate that the neutron-neutron potential is the same as the neutron-proton potential. Thus, the nuclear part of the interaction between two nucleons is *charge-independent*; that is, the nuclear potential between two nucleons does not depend appreciably on the charge:; of the nucleons. The internuclear potential between any two nucleons is of the form of a potential well. The range of the potential is approximately 2 fermis, and the well depth is about 22 MeV.

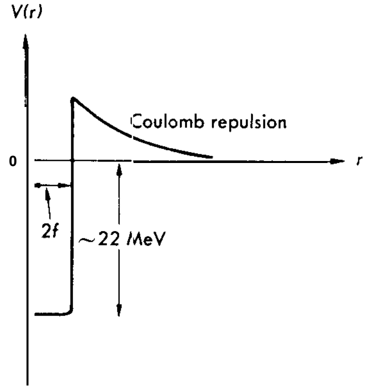


Figure 14.3. Proton-proton interaction potential.

While the description of low-energy interactions of two nucleons may be explained by a simple potential moclel, when many nucleons interact the theory becomes much more difficult. One might expect that with the two-body potential discussed above, each of the nucleons in a nucleus would be attracted by every other nucleon, and all would be within about 2 fermis of each other. This contradicts the fact that the observed radii of nuclei increase as $W^{1/3}$, so that the nuclear density is approximately constant. Thus, the nucleons in a nucleus actually tend to stay a distance apart about equal to the range-2 fermis-of the interaction. If all nucleons in the nucleus stay an average distance from their nearest neighbors which is $\simeq$ 2 fermis, and the range of the force is 2 fermis, a given nucleon can interact with only a few other nucleons at any given instant. This is partially, but not completely,. accounted for by the exclusion principle, which tends to prevent identical spin ½ particles from being at the same position with the same spin. Also, nucleon-nucleon scattering data at higher incident kinetic energies reveals that at even shorter distances, less than $\simeq$ 1 fermi, the nucleon-nucleon potential becomes repulsive rather than attractive; this also tends to keep nucleons in a nucleus from staying too close together.

14.6 YUKAWA FORCES

In 1935, H. Yukawa proposed that the nuclear force was produced by emission and absorption of particles. The following mechanical analogy might make this seem reasonable: Imagine two people standing on carts and throwing bricks at each other, as in Figure 14.4. When one throws a brick, he acquires a net momentum in the backward direction. When the other catches the brick, he also acquires a momentum in the backward direction. If they throw and catch many bricks, there will tend to be a net repulsive force between them. In order for there to be an attractive force, rather than a repulsive one, they must not throw bricks away, but they must pull bricks awoy from each other; in other words, the force between a man on a cart and a brick must be attractive.

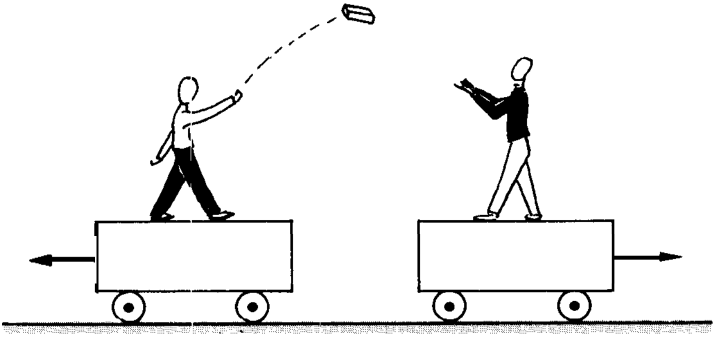


Figure 14.4. A repulsive force between two objects is generated by a mass thrust back and forth.

Similarly, if nucleons interact by exchanging particles, as indicated in Figure 14.5, an attractive force could be produced. We can make some rough order-of-magnitude estimates, based on the uncertainty principle, for the mass of the exchanged particle. Suppose we have two nucleons, about 2 fermis apart, interacting by emitting and absorbing particles. There will be an uncertainty in position of an emitted particle $\Delta x \sim 2f$, so the uncertainty in momentum

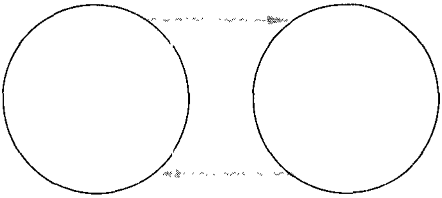


Figure 14.5. Nucleons are attracted by exchange of particles pulled back and forth.

will be given by the uncertainty principle, $\Delta p \Delta x \sim \hbar$. We may assume that the order of magnitude of the momentum is roughly the same as the uncertainty in momentum, so $p \sim \hbar/\Delta x$. We can use this estimate for the momentum to estimate the mass, if we make some reasonable assumption about the speed. The speed can approach ½ c or so without the particle's mass changing much from its rest mass. So assume the particle's momentum is just $p \sim Mc$, where M is the rest mass. Then, combining $p \sim \hbar/\Delta x$ and $p \sim Mc$, we obtain for the mass:

$$M \sim \frac{\hbar}{c\Delta x} \tag{14.8}$$

This estimate should only be good to within a factor of ten or so. Let us calculate the rest mass in terms of the rest mass of the electron:

$$\frac{M}{m_e} \sim \frac{\hbar}{c\Delta x m_e} = \frac{10^{-34}}{(3 \times 10^{8})(2 \times 10^{-15})(10^{-30})} \cong 160$$

By making slightly different assumptions about the speed or about Δx, this estimate can be made to vary by a factor of 2 or so. That is, the theory predicts a rest mass of the order of magnitude $\hbar/c\Delta x$, where Δx is the range of the force. Thus, a new particle is predicted that has a rest mass a few hundred times that of the electron.

A particle of mass about $206m_e$, called a μ meson, was later discovered, and it was thought at first that the μ meson was the particle whose existence was predicted by Yukawa. However, there were difficulties with this interpretation, because the μ was not attracted strongly to nuclei; it could spend a great deal of time inside a nucleus, as in a μ-mesic atom, without being absorbed. It was not until some time later that the particle responsible for the strong nuclear interaction was discovered. In fact, three different types of these so-called π mesons have been found: two charged and one neutral. Some of their properties are listed in Table 14.2.

TABLE 14.2 Some Properties of π Mesons

	π^+	π^0	π^-
charge	$+\lvert e \rvert$	0	$-\lvert e \rvert$
mass	$273.23m_e$	$264.4m_e$	$273.23m_e$
spin	0	0	0
magnetic moment	0	0	0

Figure **14.6.** Successive decay of the π meson, a $\rightarrow \mu \rightarrow$ e. (Courtesy P. H. Fowler.)

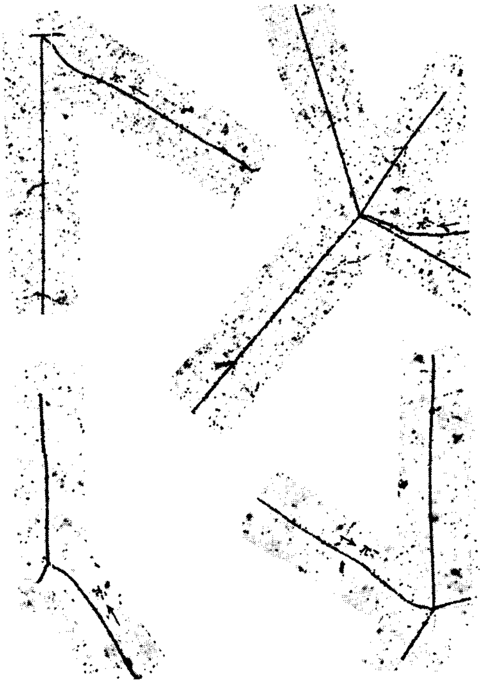


Figure 14.7. Photographs of the disintegration of light elements carbon, nitrogen or oxygen by the nuclear capture of π^- particles. (Courtesy P. H. Fowler.)

The fact that these π mesons have zero spin allows them to be emitted and absorbed readily by nucleons without any difficulties involving conservation of angular momentum. The μ meson on the other hand has spin ½ and could not be emitted alone from a nucleon without causing the nucleon to change its spin to an integral value. However, all nucleons have spin ½.

A π^+ meson tends to be repelled by a nucleus due to its charge, so a free π^+ of low kinetic energy does not come near the nucleus, but decays into a μ meson and a neutrino in around 10^{-8} seconds; the μ, in turn, decays into an electron and two kinds of neutrinos in around 10^{-6} seconds. A typical $\pi \rightarrow \mu \rightarrow e$ decay is shown in Figure 14.6. A π^0 meson ordinarily decays into 2 γ *rays.* If a π^- meson does not enter a nucleus, then it decays into a μ^- and a neutrino. However, a π^- meson is attracted to a nucleus and can be absorbed by it, giving up all its rest energy to the nucleus and causing it to disintegrate. Such an event is shown in Figure 14.7. We shall discuss such decays in more detail later.

The discovery of the new particle predicted by Yukawa was a great triumph of theory. With this theory, Yukawa was also able to write an approximate expression for the internucleon potential energy of the form $-Ce^{-r/a}/r$, where C and a are constants and r is the internuclear distance. This potential can be used to explain the low energy scattering data, just as well as the potential of Figure 14.2. This potential is thus an approximation to the true nuclear potential, and is called a Yukawa *potential.* If the range of the nuclear interaction is about 2 fermis, then one would expect that in the Yukawa potential,

$$a \cong 2 \text{ fermis}$$

7 MODELS OF THE NUCLEUS

Because our present knowledge of the internal structure of the nucleus and of the forces between nucleons is incomplete, many models of the nucleus have been constructed to explain particular nuclear properties. A model is a mathematical construct which supposedly contains all the features essential to explain some physical phenomenon. Each of the models of the nucleus which has been considered is useful in explaining a certain portion of the existing experimental data on nuclei, but no one of them can be used to explain all of the data. In this section we shall consider some of the nuclear models which have been at least partially successful.

Liquid Drop Model

The facts that nuclei have constant densities and moderately well-defined surfaces, and interact with short range forces, suggest that nuclei might be similar in structure to solids or liquids. If one considers a nucleus to be a crystalline aggregate of nucleons, then it turns out that the zero-point vibrations of the nucleons about their equilibrium positions are much too large for the nucleus to remain bound together. So a nucleus cannot resemble a crystalline solid. However, we can think of the nucleus as similar to a drop of liquid in which the particles are able to move about inside the drop, but are prevented from leaving the nucleus by an effective surface tension. This model can be used to explain qualitatively the observed binding energies of the stable nuclei. let us first see how the binding energies are calculated. The binding energy of a bound system is the energy required to break the system into its constituents and place them at rest infinitely distant from each other. For a nucleus of N neutrons and Z protons, of rest masses M_n and M_p respectively, the rest mass of the nucleus after it is broken into its constituent parts will be NM. + ZM,. If the rest mass of the original nucleus is ${}_ZM^A$, then A = N + Z, and the difference in rest mass between the constituents and the nucleus will be proportional to the binding energy E_b. Therefore,

$$\frac{E_b}{c^2} = NM_n + Z M , - {}_ZM^A \tag{14.9}$$

This formula is not very convenient for calculation, because the binding energy is expressed in terms of nuclear masses, whereas tables such as that in Appendix 3 contain atomic masses. To a sufficient approximation, neglecting electronic binding energies, and using m_e for the electron's rest mass,

$${}_ZM^A = {}_ZM^A_{at} - Z m , \tag{14.10}$$

Similarly, in terms of the rest mass of a hydrogen atom,

$$M_p = {}_1M^1_{at} \quad m_e \tag{14.11}$$

and therefore,

$$Z M , = Z\,{}_1M^1_{at} - Z m , \tag{14.12}$$

Substituting for ${}_ZM^A$ and $AM,$ and simplifying, we get

$$\frac{E_b}{c^2} = N M , + Z \,{}_1M^1_{at} - {}_ZM^A_{at} \tag{14.13}$$

Thus, due to the cancellation of all the electron rest masses, the atomic masses of the given element and of hydrogen can be used in calculating the binding energy.

example For iron ${}_{26}\mathrm{Fe}^{56}$, Z = 26, A = 56, N = 30. So we use

$$\begin{aligned} 30M_n &= 30 \times (1.1308665)\ \text{amu} = 30.25995\ \text{amu} \\ 26({}_1M^1_{at}) &= 26 \times (1.007825)\ \text{amu} = \underline{26.20345\ \text{amu}} \\ \text{sum} &= 56.46340\ \text{amu} \\ {}_{26}M^{56}_{at} &= 55.93493\ \text{amu} \end{aligned}$$

Thus, $NM, + Z\,{}_1M^1_{at} -- {}_ZM^A_{at} = 0.52847$ amu. Since 1 amu = 931.48 MeV, the binding energy of the ${}_{26}\mathrm{Fe}^{56}$ nucleus is 492.3 MeV.

The binding energy per particle of a nucleus is the average binding energy of one particle and is just defined as E_b/A. So from the example for $_{26}Fe^{56}$, the binding energy per particle is $492.3/56 = 8.79$ MeV. Likewise the binding energy per particle for $_8O^{16}$ is 7.97 MeV.

The binding energy per particle can be computed in a like manner for all the stable nuclei. The results are shown in Figure 14.8. A fairly smooth curve is found,

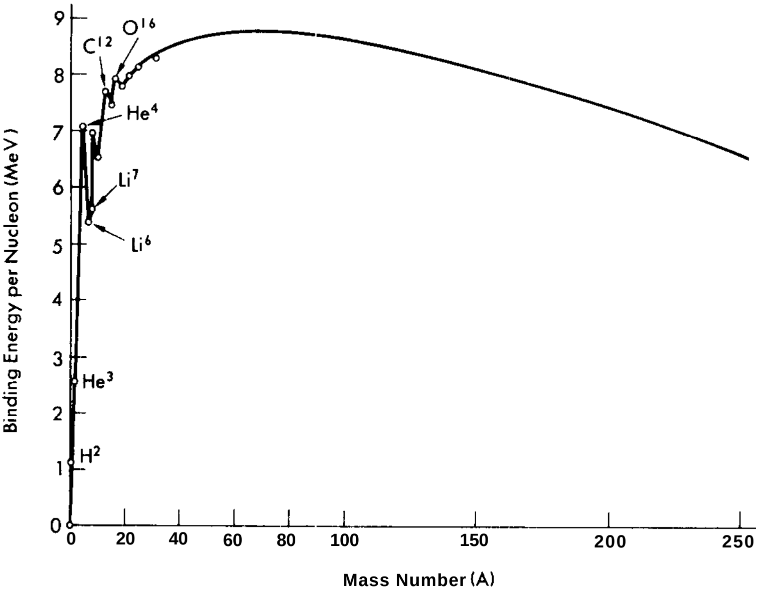


Figure 14.8. The average binding energy per nucleon as a function of mass.

which has a maximum at about the position of iron, but there are a number of peaks at lower values of A. From around A = 20 on up to A = 200, the curve is nearly a constant at a value of E_b/A equal to about 8 MeV per particle. This constancy of the binding energy per particle is very similar to that of a liquid. For example, to boil water requires 80 kilocal/kg, a constant value. However, nuclei do not contain 10^{23} particles, but more like 250 particles at most. Hence there will be important surface effects. If a nucleus held a very large number of particles, then because of the short range of nuclear forces and because of the constant density of nuclei, one nucleon in the interior would interact with only a few others and would have about 8 MeV binding energy. Nucleons near the surface would, however, not interact with so many others and would have less binding energy. The amount by which the binding energy will be less than 8 MeV should be proportional to the number of nucleons "near" the surface. Since nuclear densities are constant, the number of nucleons near the surface should be proportional to the surface area. Because nuclear radii are proportional to $W^{1/3}$ or $(A^{1/3})$, the correction to the total binding energy from the presence of the surface should be proportional to $A^{2/3}$. Then the correction to the binding energy per particle should be proportional to $A^{-1/3}$. The correction to the binding energy will be negative.

For smaller values of A, where the surface-to-volume ratio is larger, this effect should be more important. In fact, as A → ∞, this correction approaches zero, while as A → 0, it becomes very large. This explains why the binding energy per particle becomes small at low A. At large A, the binding energy per particle again gets small, principally due to Coulomb repulsion of protons in the nucleus. Since a nucleus has Z protons, which are on the average distributed uniformly throughout the nucleus, these protons tend to repel each other and make the nucleus fly apart. This is an "unbinding" effect. Thus, there will be a negative correction to the binding energy per particle, which is proportional to the electrostatic self-energy of a spherical charge of magnitude Ze. This energy is $\frac{3}{5}(Ze)^2/R$. Since R is proportional to $A^{1/3}$, the correction to the binding energy per particle will be proportional to $Z^2/A^{4/3}$. This Coulomb repulsion does not occur for neutrons. This means that heavy nuclei can consistently contain more neutrons than protons without the unbinding Coulomb repulsion which tends to make the nucleus unstable. For example, $_{82}Pb^{208}$ has a Z of 82 and an N of 126.

For small nuclei, the Coulomb contribution is small, but for large nuclei, it is large. In fact, as Z → co, this term becomes larger in magnitude than 8 MeV/particle. Hence it is not possible to have bound nuclei for Z too large, because of the Coulomb repulsion between the protons in the nucleus. The binding energy per particle should then be given by the sum of three terms:

$$\frac{E_b}{A} = 8\text{ MeV} - \frac{C_1}{A^{1/3}} - \frac{C_2 Z^2}{A^{4/3}} \qquad (14.14)$$

where C_1 and C_2 are constants. The curve in Figure 14.8 con be fit reasonably well by these three terms. The three separate contributions, and their sum, are shown in Figure 14.9.

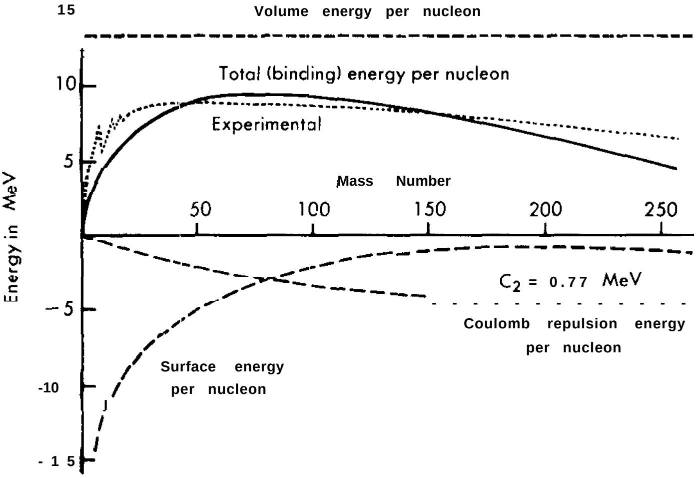


Figure 14.9. Binding energy per nucleon in on atomic nucleus as a function of atomic number.

7.2 Alpha Particle Mode/

Inspection of the binding energy curve, Figure 14.8, shows sharp relative peaks at the positions of $_2He^4$, $_4Be^8$, $_6C^{12}$, $_8O^{16}$, and $_{10}Ne^{20}$. This, and the fact that some heavy nuclei emit α particles, suggests that pairs of neutrons and protons become associated together inside the nucleus, as α particles. The binding energy per particle of $_2He^4$ is about 7 MeV. Thus, if nuclei consisted of α particles, about 87% of the binding energy would be accounted for. Presumably, then, the remaining energy should be due to relatively weak binding between α particles. However, this model has not been very successful. For example, in scattering of α particles off α particles, the data cannot be satisfactorily explained in terms of an interaction between two α particles. Rather, it seems necessary to assume that the two α particles combine into a larger nucleus, and then break up into two new α's. Thus, the α particle model has a very limited range of application.

7.3 She// Model

In describing the electronic structure of atoms, it was seen how a great deal of data could be explained on the basis of a set of electronic shells and subshells. The electrons had spin ½ and obeyed the Paulii exclusion principle, so that into any state such as a 1 S, only two electrons could go with their spins antiparallel. There is considerable evidence that a shell structure exists in nuclei. For example, the numbers 2, 8, 20, 50, 82 and 126 appear to have special significance in nuclear structure. We only mention part of the evidence here. Calcium (Z = 20) has six stable isotopes (see Figure 14.1), an unusually large number. Sn (Z = 50) has ten stable isotopes, more than any other element. The largest group of stable isotones occurs at N = 82. The heaviest stable nuclei are:

$$Pb^{208}\ (Z = 82,\ N = 126)$$

and

$$Bi^{209}\ (N = 126)$$

The numbers 2, 8, 20, 50, 82, 126 are called *magic* numbers, because to earlier investigators their significance was so puzzling.

In the shell model, this and similar data may be understood by assuming that each nucleon moves, nearly independently of other individual nuclei, inside a spherically symmetric potential well which is due to all the other nucleons. Then a nucleon moving in this potential will have states described by a principal quantum number n, orbital angular momentum (S, P, *D*, F,. . .) and total angular momentum j. This is very similar to the situation in atoms. In nuclei the spin-orbit interaction is very large, and when the spin-orbit interaction is included, this leads to the sequence of single-particle states of increasing energy shown in Table 14.3, which are grouped into shells and subshells matching the experimental magic numbers.

TABLE 14.3 An (Ordering of Subshell States Which leads to the Observed Magic Numbers

Spectroscopic Configuration	No. of States in Shell	Total No.
$(1s_{1/2})^2$	2	2
$(2p_{3/2})^4(2p_{1/2})^2$	6	8
$(3d_{5/2})^6(3d_{3/2})^4(2s_{1/2})^2$	12	20
$(4f_{7/2})^8(4f_{5/2})^6(3p_{3/2})^4(3p_{1/2})^2(5g_{9/2})^{10}$	30	50
$(5g_{7/2})^8(4d_{5/2})^6(4d_{3/2})^4(3s_{1/2})^2(6h_{11/2})^{12}$	32	82
$(6h_{9/2})^{10}(5f_{7/2})^8(5f_{5/2})^6(4p_{3/2})^4(4p_{1/2})^2(7i_{13/2})^{14}$ 4	4	126

When using the information in Table 14.3, one should remember that both protons and neutrons have spin ½. Hence they are both fermions and obey the exclusion principle. However, protons are distinguishable from neutrons. Thus, two protons could go into the $1s_{1/2}$ state. Likewise, two neutrons could go into that state. When the $1s_{1/2}$ state contains 2 protons and 2 neutrons, the shell is filled up. This corresponds to an α particle. When the $1s_{1/2}$, $2p_{3/2}$, and $2p_{1/2}$ levels are all filled up with both neutrons and protons, the resulting nucleus is $_8O^{16}$. Notice the peak of the binding energy curve, Figure 14.8, at the positions of $_2He^4$ and $_8O^{16}$.

In applying these ideas to the explanation of the properties of stable nuclei, it would at first appear that, on the average, the number of neutrons in a nucleus should be about equal to the number of protons in a nucleus. However, from Figure 14.1 it is seen that there are more neutrons than protons in heavy nuclei. As mentioned previously, this is because of the Coulomb repulsion between protons: since protons are charged whereas neutrons are not, the potential energy of an extra proton added to a nucleus would be greater than that of an added neutron, other things being equal. Therefore, in the shell model, the potential well used to calculate the neutron energy states will be deeper than that used for the protons. Hence the neutron energy levels will generally lie lower than those of the protons.

The shell model can also be used to explain many features of the **spin** and magnetic moments of stable nuclei. If a nucleus had two protons in a $1s_{1/2}$ state, the total angular momentum should be zero. If a nucleus had any even number of protons, it is not unreasonable to suppose that these would be paired off, two in each state, so that the total spin should be zero. Then the contribution to the total magnetic moment from these paired protons, provided their net orbital angular momentum is zero, should be zero. This is found to be the case. Similarly for a nucleus with even N, the spin and magnetic moment are zero, because the neutrons are paired off with opposite spins in each pair.

A nucleus with even Z and even N is called an ***even-even*** nucleus. In Table 14.4 are given the numbers of stable nuclides (nuclei) as a function of whether Z and N are even or odd.

TABLE 14.4 Effect of Evenness and Oddness of Z and N on Stability of Nuclides

Z	N	Number of Stable Nuclides
even	even	160
even	odd	56
odd	even	52
odd	odd	4

It appears that nuclei have greater stability when bath protons and neutrons are paired, then if there is an unpaired neutron or proton or both. The only examples of stable odd-odd nuclides are the lightest possible odd-odd ones, which are ${}_1H^2$, ${}_3Li^6$, ${}_5B^{10}$ and ${}_7N^{14}$. A nucleus with even Z, odd N or odd Z, even N, has an odd number of nucleons, and therefore should have values of net angular momentum of $\frac{1}{2}\hbar$, $\frac{3}{2}\hbar$, $\frac{5}{2}\hbar$, $\frac{7}{2}\hbar$, ... Usually, only the lower values of the net angular momentum quantum numbers actually occur in nature; this is evidence for the pairing of like nucleons within the nucleus.

The lightest odd Z, even N, nucleus is ${}_1H^3$. One would expect the neutrons to be paired with opposite spins in an s state, and the proton in the s state then gives the nucleus spin $\frac{1}{2}$. The magnetic moment should be about that of the proton, 2.79 nuclear magnetons. Experimentally, it is 2.98 nuclear magnetons. Likewise, an estimate of the magnetic moment of the even Z, odd N, ${}_2He^3$ nucleus would be that of the neutron, $\mu_n = -1.91$ nuclear magnetons. The experimental value is -2.13. An odd-odd nucleus has one unpaired neutron, one unpaired proton. The lightest example of this is the deuteron, where the nuclear forces are such that the spins of the n and p line up, the net spin being 1. In general, for an odd-ocld nucleus the net angular momentum should be integral. The actually observed values of spin quantum numbers for odd-odd nuclei are:

$$ {}_1H^2 \rightarrow 1; \qquad {}_3Li^6 \rightarrow 1; \qquad {}_5B^{10} \rightarrow 3; \qquad {}_7N^{14} \rightarrow 1. $$

We shall not pursue the discussion of nuclear models any further. So far, we have just scratched the surface in discussing the types of experimental data which are observed. Some of this will be discussed in the next chapter. We have not mentioned all the different models which are used to explain different types of data such as scattering and absorption of incident particles, and excited states due to overall rotation of the nucleus.

summary

NUCLEAR MASSES AND BINDING ENERGIES

The nuclear mass of a given nucleus, ${}_ZM^A$, is obtained by subtracting from the atomic mass the rest mass of Z electrons. The nucleus consists of Z protons and

N = A -- Z neutrons. Nuclei having equal Z are called isotopes; those having equal N are called *isotones.* The mass number, A, is the integer nearest to the atomic mass. The binding energy of a nucleus is defined as the energy which must be added to the nucleus in order to separate it into its constituent neutrons and protons, and place them at rest infinitely distant from each other. The binding energy E_b is given by

$$\frac{E_b}{c^2} = NM_n + Z\,{}_1M_{at}^1 - {}_ZM_{at}^A$$

where M_n is the neutron mass, ${}_1M_{at}^1$ is the atomic mass of hydrogen, and ${}_ZM_{at}^A$ is the atomic mass of the nucleus in question.

MAGNETIC MOMENTS

The magnetic moments of nuclei are measured in nuclear magnetons. 1 nuclear magneton = $e\hbar/2M_p = 5.051 \times 10^{-27}$ joule $(\text{weber/m}^2)^{-1}$, where M_p is the proton mass. Nuclear moments are written in the form $\mu = g\, e\hbar/2M_p\, I$, where I is the spin (total angular momentum) of the nucleus. The magnetic moments vary from about -5 to +5 nuclear magnetons, and must be measured experimentally.

NUCLEAR FORCES

The forces between nucleons are short range and strongly attractive. A nucleon in a nucleus interacts with only a few others at a time and stays about 2 fermis away from the other nucleons. For many purposes, the interaction potential between two nucleons may be treated as a potential well of range about *2f* and depth of 22 MeV. Yukawa proposed that nuclear forces were due to the exchange of particles called π mesons, and predicted that the π rest mass should be a few hundred times the electron rest mass.

LIQUID DROP MODEL

The liquid drop model can be used to explain qualitatively the behavior of binding energy as a function of A. Due to nuclear saturation, a nucleon in the interior of a nucleus interacts with only a few others and has a constant binding energy per nucleon, due to the nuclear forces. Nucleons near the surface do not interact with as many other nucleons, and hence there is a surface correction which decreases the binding energy. The resulting binding energy formula is:

$$\frac{E_b}{A} = C_0 - \frac{C_1}{A^{1/3}} - \frac{C_2 Z^2}{A^{4/3}}$$

for the binding energy per particle, where C_0, C_1 and C_2 are constants.

SHELL MODEL

In the shell model the nucleons are treated as through they move in a spherically symmetric potential well, which is deeper for neutrons than for protons. This gives rise to a set of energy levels described by quantum numbers n, ℓ, and the total angular momentum j. Neutrons and protons are both fermions, and satisfy the exclusion principle; hence only two neutrons and two protons can go into each orbital state. Filled levels are more stable configurations and this leads to exceptional preference in nature for nuclei with N or Z equal to 2, 8, 20, 50, 82, 126. Nuclei with even Z have their protons paired off with opposite spins, and there is no net contribution to spin or magnetic moment from these particles. Similarly for nuclei with even N. There are more stable even-even nuclei in nature than any other type. Nuclei with both odd N and odd Z are rare, and have spins 1 or 3. Even-odd and odd-even nuclei have at least one unpaired particle and have spins $1/2$, $3/2$, $5/2$, $7/2$, . . .

problems

In nuclear magnetic resonance experiments, nuclear magnetic moments in a strong magnetic field, with energy $-\mu \cdot \mathbf{B}$, are caused to go from a state with one spin orientation to a state with a different spin orientation and energy, by absorption of radio frequency photons. The following three problems are based on this.

1. In a field of 0.2 webers/m^2, what photon frequency will cause a proton to go from a state with spin component ½ in the direction of the field to one of spin component ½?
   Answer: 8.51 x 10^6 cycles/sec.
2. If hydrogen fluoride has an 18-megacycle electromagnetic field applied to it, by how much must the strong applied static magnetic field be changed to go from absorption of photons by fluorine to the absorption by hydrogen? Use Appendix 3.
   Answer: 0.0266 webers/m^2.
3. In a field of 0.35 webers/m^2, at what frequency is there photon absorption by the $_5B^{11}$ nucleus, corresponding to the $s_z = 3/2$ to $1/2$ transition? Use Appendix 3 and note that the maximum magnetic moment listed corresponds to $s_z = 3/2$
   Answer: 4.78 x 10^6 cycles/sec.
4. What is the g factor of the $_{35}Br^{79}$ nucleus? Use Appendix 3.
   Answer: 1.4039.
5. Find the nuclear mass of $_{27}Co^{59}$ from Appendix 3.
   Answer: 58.9184 amu.
6. Treat the deuteron as if it were a particle in a cubic box of side ℓ and mass equal to the reduced mass $M_nM_p/(M_n + M_p)$. According to the data in this chapter, how far is the deuteron energy above the potential energy of interaction? Let this be equal to the ground state energy of the particle in the three dimensional box to get ℓ, and thus a rough estimate of the nuclear diameter.

7. A A" meson decays into two gamma rays. If the π° is at rest, what is the energy of each gamma ray?
Answer: 67.5 MeV.
8. If the mass of the μ^+ meson is m_μ and that of a π^+ is m,, find the kinetic energy of the μ^+, and the neutrina energy for a π^+ decaying at rest. The neutrina has zero rest mass.
Answer: $(m, - m_\mu)^2 c^2/2m_\pi$; $(m_\pi^2 - m_\mu^2) c^2/2m_\pi$.
9. Find the binding energy per nucleon of chlorine 35 from Appendix 3.
Answer: 8.5 MeV.
10. Find the binding energies per nucleon for F^{18}, F^{19} and F^{20} from Appendix 3. Which is likely to be the more stable?
Answer: 7.63 MeV; 7.78 MeV; 7.71 MeV.
11. From the data in Appendix 3, decide which of the following should be the more stable: $_7N^{17}$; $_8O^{17}$; $_9F^{17}$.
Answer: $_8O^{17}$.
12. From Appendix 3, calculate the energy necessary to remove one proton from $_7N^{14}$. Compare this with the energy to remove one neutron and also with the average binding energy per nucleon. Why are these different?
Answer: 7.54 MeV; 10.55 MeV; 7.47 MeV.
13. Find the energy necessary to remove the least tightly bound nucleon from the following stoble nuclei: $_{10}Ne^{20}$; $_9F^{19}$; $_8O^{18}$; $_8O^{17}$; $_8O^{16}$; $_7N^{15}$. Compare this energy for even A with that for neighboring nuclei of odd A, and explain in terms of filling proton and neutron levels.
Answer: 6.9 MeV; 8.0 MeV; 8.1 MeV; 4.1 MeV; 12.1 MeV; 10.2 MeV.
14. By considering bringing in infinitesimal spherical shells of charge from infinity to build up a total sphere of charge e and radius R, show that the work necessary is $\frac{3}{5} e^2/4\pi\epsilon_0 R$. Thus, show that to bring into superposition Z uniformly charged spheres of radius R, the work is'/, $Z(Z - 1)\ e^2/4\pi\epsilon_0 R$. Use the relationship between the nuclear radius and A to show that this energy is 0.79 $Z(Z - 1)\ A^{1/3}$ MeV. Compare this 0.79 with the constant C_2 in the discussion of the liquid drop model.
15. In terms of the alpha-particle model, explain why there are no stable nuclei of A = 5 or A = 8.
16. On the basis of the shell model levels in Table 14.3, explain why $_6C^{12}$ and $_8O^{16}$ should both have spin zero.
17. On the basis of the shell model levels in Table 14.3, explain why it is reasonable that $_7N^{14}$ should have a nuclear spin of 1.
18. On the basis of the shell model, explain why you might expect $_3Li^7$ to have a nuclear spin of $\frac{3}{2}$ and a nuclear magnetic moment near 3 nuclear magnetons.

5 transformation of the nucleus

Of the approximately 1200 different nuclides known to exist, only about 270 are stable; the remainder decay sportaneously into lighter fragments. Further, some nuclei may be induced to undergo such decomposition by irradiating them with beams of particles of various types. Under certain conditions, two or more nuclei may combine to form a heavier nucleus. The study of such processes is of great importance in attempting to understand the structure of nuclei and of the elementary particles, and has led to a wide variety of applications in other scientific fields.

We shall study here only some of the more important features of these processes and their applications.

5.1 LAW OF RADIOACTIVE DECAY

The spontaneous decay of a nucleus into lighter particles is called natural radioactivity. An example of this process is the emission of alpha particles by the uranium nucleus, ${}_{92}U^{238}$. A given (unstable nucleus may decay in more than one way; for example, ${}_{83}Bi^{212}$ may emit either an alpha particle or an electron; this latter process is called beta ***decay.*** Nuclei may also emit gamma rays (photons) of discrete energies. All of these processes are fundamentally statistical in nature. That is, it is impossible to predict when any one given nucleus will decay, and the process must be described in terms of a probability of decay per unit time, or a transition rate.

Consider a sample of N nuclei of a given type, where N is sufficiently large that statistical variations in the decay rate will average out. Suppose we count the number of decays in a small time interval dt, starting with N nuclei, and study the number of decays as dt and N are varied. Let us describe the number of decays in terms of the change in the number of nuclei during dt. If dN is the increase in N in the time dt, then the number of decays is $-dN$. The number dN is negative because N is decreasing due to the decays. When $-dN$ is observed experimentally, then over short time intervals the sample is observed to decay at a constant rate. That is, if in dt a certain number of decays are observed, then, on the average, in 2dt twice as many decays will be observed, and so we may conclude that -dN is proportional to dt.

Another observed fact is that nuclei in atoms decay independently of each other; the proximity of one atom to another does not affect the nuclear decay rate. Thus, if starting with N nuclei, -dN decays were observed in df, then with 5N nuclei, the number of decays in dt should be increased by a factor of five. Thus, on the average, -dN is proportional to both dt and to N. These facts may be expressed in the equation,

$$-dN = \lambda N dt \tag{15.1}$$

where λ is a proportionality constant, called the *decay* constant or disintegration constant. The quantiy λ is independent of t and N, and depends only on the particular type of decay.

example If, in a sample of 2.52×10^{18} atoms, of ${}_{92}U^{238}$ (one milligram), 740 α particles are produced per minute, what is the decay constant in $\sec^{-1}$?

solution $\lambda = -\Delta N/N\Delta t = 740/(2.52 \times 10^{18})(60 \text{ sec})$

$= 4.9 \times 10^{-18} \text{ sec}^{-1}$

Equation (15.1) is a differential equation which expresses the rate of change of N with time. We can solve the differential equation to find N as a function of time as follows: divide by N to obtain

$$\frac{dN}{N} = -\lambda dt \tag{15.2}$$

In this form, we can integrate each side separately and equate the results. Apart from a constant of integration,

$$\int \frac{dN}{N} = \ln N \tag{15.3}$$

Also,

$$\int -\lambda dt = -\lambda t + C' \tag{15.4}$$

where C' is some constant of integration. Therefore,

$$\ln N = -\lambda t + C' \tag{15.5}$$

We take exponentials of both sides of this equation to obtain the number of particles:

$$N = Ce^{-\lambda t} \tag{15.6}$$

where $C = e^{C'}$ is a constant. Lastly, we may express the constant C in terms of the number of nuclei N_0 which are present at the initial instant $t = 0$. If $N = N_0$ at $t = 0$, then $N_0 = Ce^0$ or $C = N_0$. Hence, in terms of N_0 and λt, the number of particles remaining undecayed at time t will be given by:

$$N = N_0 e^{-\lambda t} \tag{15.7}$$

This is the fundamental equation describing the average way in which samples of radioactive nuclei decay.

5.2 HALF-LIFE

Decay rates are usually given in terms of the decay constant λ, or else in terms of a closely related number called the half-life and denoted by $T_{1/2}$ The half-life is defined as the time it takes for half the nuclei in a sample to decay. Thus, if we set t = J,,, in Equation (15.7), this would correspond to setting N = ½ N_0. We then find a relation between half-life and decay constant:

$$\tfrac{1}{2} N_0 = N_0\, e^{-\lambda T_{1/2}} \quad \text{or} \quad e^{\lambda T_{1/2}} = 2 \tag{15.8}$$

We can solve Equation (15.8) for $\bar{T}_{1/2}$ in terms of λ by taking logarithms of both sides of the equation. Using the identities

$$\text{In } 2 = 3.693, \qquad \text{In } e^x = x$$

we get

$$7_{1/2} = \frac{0.693}{\lambda} \tag{15.9}$$

nple If $\lambda = 4.90 \times 10^{-18}\ \text{sec}^{-1}$, as in the previous example, and if 1 year = 3.15×10^7 sec., then measured in years,

$$J_{1/2} = \frac{0.693}{\lambda} \quad \frac{0.693}{[(4.9 \times 10^{-18})(3.15 \times 10^7\ \text{sec/yr})]}$$

$$= 4.49 \times 10^9 \text{ years}$$

This is the number of years it would take until only half the original nuclei were left. The decay of the remainder of the nuclei is still described by the same statistical law. Hence, it takes an additional half-life, or a total of 8.98×10^9 years, to reduce the number of nuclei to ¼ the original number.

5.3 LAW OF DECAY FOR UNSTABLE DAUGHTER NUCLEI

When a nucleus such as ${}_{92}U^{238}$ emits an α particle, a resultant nucleus of thorium is left, ${}_{90}\text{Th}^{234}$. In this case, the uranium is called the parent nucleus and the thorium is called the daughter. For every U nucleus which decays, one daughter is formed. So if at time t, $N = N_0 e^{-\lambda t}$ uranium nuclei remain, $N_0 - N$ uranium nuclei have decayed, and so $N_0 - N$ new daughter nuclei have formed. In terms of the time, from Equation (15.7) the number N_d of new daughters is

$$N_d = N_0(1 - e^{-\lambda t}) \tag{15.10}$$

Figure 15.1 shows a graph of number of remaining parents as a function of time, and Figure 15.2 is a similar graph of the total number of daughters formed as a function of time.

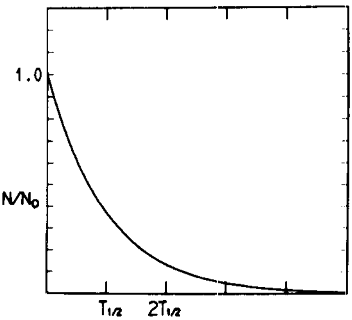


Figure **15.1.** Radioactive decoy low; decoy of the parent nucleus.

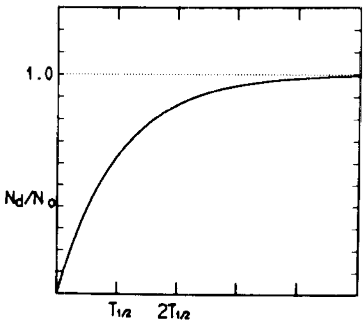


Figure **15.2.** Radioactive decoy low; growth of a stable daughter.

If the daughter is stable, then the actual number of daughter nuclei is equal to the number formed by the parent's decay. However, if the daughter is itself unstable, the actual number of daughter nuclei will be less than that given by Equation (15.10). In this case, we have to reconsider the rate of change of the number N_d of daughter nuclei. Suppose the daughter is unstable and has a decay constant λ_d. Then f N_d is the number of daughter nuclei at a particular time, in a time dt the number which decay will be $\lambda_d N_d$ dt. This will contribute to the rate of decrease of N_d. But daughters are continually being formed by decay of the parent; the number formed in time dt is $\lambda_p N_p$ dt. Therefore, the total increase in number dN_d of daughter atoms will be

$$dN_d = \lambda_p N_p\, dt \qquad \lambda_d N_d\, dt \tag{15.11}$$

The number of parent atoms is $N_p = N_0 e^{-\lambda_p t}$, so we obtain the following differential equation for the rate of change of daughter atoms:

$$dN_d = \quad (-N_d \lambda_d + \quad \lambda_p N_0 e^{-\lambda_p t})dt \tag{15.12}$$

This differential equation can be solved after some manipulation. It is easily verified that the solution is:

$$N_d = \lambda_p N_0 \frac{(e^{-\lambda_d t} - e^{-\lambda_p t})}{\lambda_p - \lambda_d} \tag{15.13}$$

To give some feeling for the behavior of this solution, the ratio N_d/N_0 is plotted in Figure 15.3 for the particular choices, $\lambda_p = 2.0$ sec^{-1}, $\lambda_d = 1.0$ sec^{-1}. From the plot, it may be seen that after a long time has elapsed, N_d approaches zero. This is because all of the parent will have decayed, and all the previously formed daughter nuclei will also decay.

The form of the above result depends on both λ_d and λ_p. One interesting case, which occurs often in nature, is that in which the parent decays much more slowly than the daughter. Then λ_p is much smaller than λ_d, and $\lambda_p - \lambda_d$ is approximately equal to $-\lambda_d$. Also, $e^{-\lambda_p t}$ is much larger than $e^{-\lambda_d}$ for large t. Thus, under these assumptions, Equation (15.13) simplifies to:

$$N_d = N_0 \frac{\lambda_p}{\lambda_d} e^{-\lambda_p t}$$

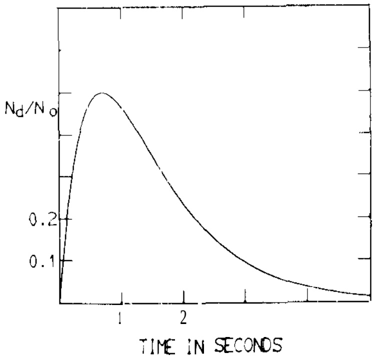


Figure 15.3. Radioactive decay law, growth and decay of an unstable daughter, for decay constants given by $\lambda_p = 2.0\ \text{sec}^{-1}$, $\lambda_d = 1.0\ \text{sec}^{-1}$.

Since the number of parent nuclei is $N_0 e^{-\lambda_p t}$ = N,, the equation states that after a long time,

$$\lambda_d N_d = \lambda_p N_p \tag{15.14}$$

Physically, this means that the rate of production of daughter nuclei is equal to their rate of decay. Hence, the net increase dN_d will be zero. Thus, if the decay constant of the daughter nuclei is much larger than the decay constant of the parent nuclei, at first the number of daughter nuclei will increase, because initially no daughter nuclei are present; the formation process dominates. After a long time has elapsed, the number of daughter nuclei will have increased to the point where they decay as fast as they are formed. The result could also have been obtained from Equation (15.11) by setting $dN_d = 0$. When this situation applies, the daughter is said to be in equilibrium with its parent.

One application of this result is to the determination of extremely long half-lives. Equation (15.14) can also be written in terms of half-lives:

$$\frac{N_d}{(T_{1/2})_d} = \frac{N_p}{(T_{1/2})_p} \tag{15.15}$$

Thus the relative numbers of atoms of the two types will be directly proportional to their respective half-lives.

ple A nucleus of ${}_{92}U^{238}$ decays into ${}_{90}Th^{234}$ by emitting an alpha particle, and ${}_{90}Th^{234}$ is also unstable, emitting an electron with a half-life of 24.1 days. If ${}_{90}Th^{234}$ is found in rocks containing uranium, with the number of thorium atoms equal to only 1.47 x $10^{-9}\%$ of the number of uranium atoms, what is the half-life of ${}_{92}U^{238}$ in years?

ion $(T_{1/2})_U = (T_{1/2})_{Th}\dfrac{N_U}{N_{Th}}$

$$= \left(\frac{24.1}{365\ \text{days/year}}\right)\left(\frac{1}{1.47 \times 10^{-11}}\right)$$

$$= 4.47 \times 10^{9}\ \text{years.}$$

15.4 RADIOACTIVE SERIES

The naturally occurring radioactive elements with $Z > 82$ have been found to fall into three series. Within a given series, the nuclides decay into each other and eventually end as some isotope of lead. There is a fourth series, which has been produced in the laboratory. In all of these series, the decay particles are either alphas (helium nuclei) or betas (electrons). On emission of an alpha,

$$\begin{aligned} Z &\text{ decreases by } 2 \\ N &\text{ decreases by } 2 \\ A &\text{ decreases by } 4 \end{aligned}$$

By conservation of charge, the change in Z of a nucleus on emission of an electron in beta decay by the nucleus, is $+1$. The change in A is zero. Thus, in all decays within a single series, A either decreases by 4 or else does not change. Hence, if n is some integer, all members of a series have mass numbers given by:

$$A = 4n, 4n + 1, 4n + 2, \text{ or } 4n + 3$$

These series are named, respectively, the thorium series, neptunium series, uranium series and actinium series. The properties of the series are given in Tables 15.1, 15.2, 15.3 and 15.4.

Consider first the $4n + 2$, or uranium series. ${}_{92}U^{238}$ decays by α emission to ${}_{90}Th^{234}$, called uranium X_1. The Th nucleus decays, in turn, by beta decay into either uranium X_2 or uranium Z; each of these has the same Z and A, and is a nucleus of the element ${}_{91}Pa^{234}$. Uranium Z may be formed when uranium X_2 emits a gamma ray. Hence, uranium Z and uranium X_2 are two different states of the same nucleus, called isomers. From the last column of Table 15.3 one may predict the energy of the gamma ray emitted. It is

$$E = 2.31 - 0.5 = 1.81 \text{ MeV} \qquad (15.16)$$

If the earth was formed in some process which took place a long time ago, and if the naturally radioactive elements were formed at the same time, then the fact that not all of these elements have decayed yet should give some indication of the age of the earth. The neptunium series, for example, is not found in nature. Since the longest half-life of any member of the neptunium series is 2.2×10^6 years, this means the earth must be many times as old as 2.2×10^6 years. On the other hand, the other three series are found in nature. The longest half-lives found in these other series are between about 10^9 and 10^{10} years roughly. This indicates roughly that the age of the earth may be a few billion years. In addition to these series, there are a few other naturally occurring radioactive nuclides which have been found, with $Z < 82$. There are possibly others whose decay rates are so small that they have not yet been detected. Table 15.5 gives a list of these known unstable elements. Decay by electron capture from an atomic level by the nucleus is indicated by **EC.**

TABLE 15.1 Thorium (4n) Series

Nuclide	Common Name	Particle Emitted	$T_{1/2}$	E^* (MeV)
$_{90}Th^{232}$	Thorium	α	1.39 x 10^{10} yr.	3.99, 3.93
	↓			
$_{88}Ra^{228}$	Mesothorium,	β	6.7 yr.	< 0.02
	↓			
$_{89}Ac^{228}$	Mesothorium$_2$	β	6.13 hr.	1.11, 0.45 – 2.18
	↓			
$_{90}Th^{228}$	Radiothorium	α	1.90 yr.	5.42, 5.34
	1			
$_{88}Ra^{224}$	Thorium X	α	3.64 days	5.68, 5.44
	↓			
$_{86}Em_{220}$	Thoron	α	54.5 sec	6.28, 5.75
	↓			
$_{84}Po^{216}$	Thorium A	α, β	0.16 sec	a6.77
	99.987% 0.013%			
$_{82}Pb^{212}$	Thorium B	β	10.64 hr.	0.34, 0.58
$_{85}At^{216}$	Astatine	α	0.3 × 10^{-3} sec	7.79
	↓			
$_{83}Bi^{212}$	Thorium C	α, β	60.5 min	β2.25; α6.05, 6.09
	33.7% 66.3%			
$_{84}Po^{212}$	Thorium C′	α	3 × 10^{-7} sec	8.78
$_{81}Tl^{208}$	Thorium C″	β	3.1 min	1.79, 1.28
	↓			
$_{82}Pb^{208}$	Thorium D	Stable		

*The energies given ore those of the most important alpha-particle groups, or those of the most energetic beta particles.

TABLE 15.2 Neptunium (4*n* + 1) Series

Nuclide	Common Name	Particle Emitted	$T_{1/2}$	E^* (MeV)
$_{93}Np^{237}$	none	α	2.2×10^6 yr.	4.79, 4.52 – 4.87
$_{91}Pa^{233}$		β	27.4 days	0.26, 0.14, 0.57
$_{92}U^{233}$		α	1.62×10^5 yr.	4.82, 4.78, 4.73
$_{90}Th^{229}$		α	7300 yr.	4.85, 4.94, 5.02
$_{88}Ra^{225}$		β	i 4.8 days	0.32
$_{89}Ac^{225}$		α	10 days	5.80
$_{87}Fr^{221}$		α	4.8 min.	6.30, 6.07
$_{85}At^{217}$		α	1.8×10^{-2} sec	7.02
$_{83}Bi^{213}$		α, β	47 min.	81.39; a5.90
2 %				
$_{81}Tl^{209}$	98 %	β	2.2 min.	1.8, 2.3
$_{84}Po^{213}$		α	4.0×10^{-6} sec.	8.34
↓				
$_{82}Pb^{209}$		β	3.3 hr.	0.62
$_{83}Bi^{209}$		Stable		

*The energies given ore those of the most important alpha-particle groups or those of the most energetic beta particles.

Nuclide	Common Name	Particle Emitted	$T_{1/2}$	E^* (MeV)
${}_{92}U^{238}$	Uranium I	α	4.51 x 10^{9} yr.	4.18
${}_{90}Th^{234}$	Uranium X_1	β	24.1 days	**0.19, 0.10**
${}_{91}Pa^{234}$	Uranium X_2	β	1.18 min.	2.31
	↓ 0.15% 99.85%			
${}_{91}Pa^{234}$	Uranium **Z**	β	6.66 hr.	0.5
	↓			
${}_{92}U^{234}$	Uranium II	α	2.50 x 10^{5} yr.	4.76
${}_{90}Th^{230}$	**Ionium**	α	8.0 x 10^{4} yr.	4.68, 4.61
${}_{88}Ra^{226}$	Radium	α	1620 yr.	**4.78, 4.59**
${}_{86}Em^{222}$	Radon	α	3.825 days	5.48
${}_{84}Po^{218}$	Radium A	α, β	3.05 min.	α**6.00**
	↓ 99.97% 0.03%			
${}_{82}Pb^{214}$	Radium **B**	β	26.8 min.	0.7
${}_{85}At^{218}$	Astatine	α	1.3 sec.	6.63
${}_{83}Bi^{214}$	Radium C	α, β	19.7 min.	α**5.5–10.5**
	0.04% ↓ 99.96%			pl.6, 3.17
${}_{84}Po^{214}$	Radium **C′**	α	1.6 x 10^{4} sec.	7.68
${}_{81}Tl^{210}$	Radium C″	β	1.32 min.	1.9
${}_{82}Pb^{210}$	Radium D	β	20 yr.	0.02
${}_{83}Bi^{210}$	Radium E	α, β	5.0 days	β**1.17**; cu4.94
	↓ 5 x 10^{-5}%			
${}_{81}Tl^{206}$	**Radium E″**	β	4.2 min	1.51
${}_{84}Po^{210}$	**Polonium**	α	138 days	5.30
	↓			
${}_{82}Pb^{206}$	Radium **G**	Stable		

*The energies given are those of the most important alpha-particle groups or those of the most energetic **beta** particles.

TABLE 15.4 Actinium (4n + 3) Series

Nuclide	Common Name		Particle Emitted	$T_{1/2}$	E^* (MeV)
$_{92}U_{235}$	Actinouranium		α	7.1 x 10^8 yr.	4.40, 4.58
$_{90}Th^{231}$	Uranium Y		β	25.6 hr.	0.09, 0.30, 0.22
$_{91}Pa$ 231	Protoactinium		α	3.4 x 10^4 yr.	5.0, 4.64-5.05
$_{89}Ac^{227}$	Actinium		α, β	22 yr.	0.046
	↓ 1.2 %	98.8%			
$_{87}Fr^{223}$	Actinium K		β	22 min.	1.0, 1.3
$_{90}Th^{227}$	Radioactinium		α	1 a.2 days	5.97, 5.65-6.03
	↓				
$_{88}Ra$ 223	'Actinium X		α	11.6 days	5.70-5.68
$_{86}Em_{219}$	Actinon		α	3.97 sec.	6.82, 6.56
$_{84}Po^{215}$	Actinium A		α, β	1.8 x 10^{-3} sec.	7.36
	↓	5 x 10^{-4}%			
$_{82}Pb^{211}$	/Actinium B		β	36.1 min.	1.4, 0.5
$_{85}At^{215}$	Astatine		α	1 x 10^{-4} sec.	a.00
	↓				
$_{83}Bi_{211}$	Actinium C		α, β	2.15 min.	po.35; α6.62, 6.27
	99.68%	0.32%			
$_{81}Tl^{207}$	Actinium C''		β	4.78 min.	1.45
$_{84}Po^{211}$	Actinium C'		a	0.52 sec.	7.43
	↓				
$_{82}Pb^{207}$	Actinium D		Stable		

*The energies given ore those of the most important alpha-particle groups or those of the most energetic beta particles.

TABLE 15.5 Naturally Occurring Unstable Nuclides Not Found in Series

Element	Abundance %	Type of Activity	Half-life Years
$_{19}\mathrm{K}_{40}$	0.0119	β^-, EC	1.2 x 10”
$_{23}\mathrm{V}_{50}$	0.25	EC	4 x 10^{14}
$_{37}\mathrm{Rb}_{a7}$	27.85	β^-	6.2 x 10^{10}
$_{49}\mathrm{In}_{115}$	95.77	β^-, EC	6 x 10^{14}
$_{57}\mathrm{La}_{138}$	0.089		1.0 x 10^{11}
$_{58}\mathrm{Ce}_{142}$	11.07	a	5 x 10^{15}
$_{60}\mathrm{Nd}^{144}$	23.87	a	3 x 10^{15}
$_{62}\mathrm{Sm}_{147}$	15.07	α	1.2 x 10^{11}
$_{71}\mathrm{Lu}_{176}$	2.60	β^-	4 x 10^{10}
$_{75}\mathrm{Re}^{187}$	62.93	β^-	4 x 10^{12}
$_{78}\mathrm{Pt}_{192}$	0.78	α	~ 10^{15}

There are, in addition, a few radioactive elements continually being formed near the earth's surface due to cosmic ray bombardment. These will be discussed later.

5.5 ALPHA-PARTICLE DECAY

In order for a nucleus to decay spontaneously, the process must be energetically feasible. Since the decay products come off with kinetic energy, the necessary energy must be supplied at the expense of energy of some other form. This can be described quantitatively in terms of a net loss of rest mass of the resulting particles. If the parent nucleus is initially at rest, when the alpha is emitted the remaining daughter nucleus will have to carry off some kinetic energy in order to conserve momentum. So to account for all energy, we must consider the motion of both alpha and daughter. Let us call ${}_{Z}M_p^A$ the rest mass of the parent, ${}_{Z-2}M_d^{A-4}$ the mass of the daughter, and ${}_{2}M_{\mathrm{He}}^4$ the rest mass of the alpha. The net decrease in rest energy in the process, which is also the total kinetic energy of the α particle and the daughter nucleus, is called the Q of the decay, and will be given by

$$\frac{Q}{c^2} = {}_{Z}M_p^A - {}_{Z-2}M_d^{A-4} - {}_{2}M_{\mathrm{He}}^4 \qquad (15.17)$$

Suppose we wish to compute Z using a table of atomic masses. In terms of the atomic **mass** ${}_{A}M^A_{p(at)}$, **we have**

$$ {}_{Z}M_p^A = {}_{Z}M^A_{p(at)} - Zm_e \qquad (15.18)$$

and similarly for the masses of the alpha and the daughter. However, since $-Zm_e + (Z\quad 2)m_e + 2m_e$ **is zero**, the Q of the decay may be written in terms of atomic masses:

$$Q/c^2 = {}_{Z}M^A_{p(at)} - {}_{Z-2}M^{A-4}_{d(at)} - {}_{2}M^4_{\mathrm{He}(at)} \qquad (15.19)$$

Using the table in Appendix 3, we shall compute Q for the case where the parent nucleus is ${}_{92}U^{238}$ and the daughter is ${}_{90}Th^{234}$. From the table,

$$\begin{aligned} {}_{Z-2}M^{A-4}_{d(at)} &= 234.043583 \\ {}_{2}M^{4}_{He(at)} &= \underline{4.002603} \\ \text{sum} &= 238.046186 \\ {}_{Z}M^{A}_{p(at)} &= 238.050770 \\ \text{Sum of final rest masses} &= \underline{238.046186} \\ Q/c^2 = \text{difference} &= 0.00458 \text{ amu} \\ 1 \text{ amu} &= 931.48 \text{ MeV} \end{aligned}$$

so

$$Q = 4.27 \text{ MeV} \tag{15.20}$$

This Q is greater than the observed alpha-particle energy of 4.18 MeV, because the daughter also carries off some kinetic energy. The final kinetic energy of the decay products are in the nonrelativistic region, so Newtonian mechanics may be used to calculate the fraction of energy carried off by the alpha. Let v_α be the final speed of the alpha, and v_d be the final speed of the daughter. We assume that the parent nucleus is initially at rest, and take the masses of the α particle and residual nucleus to be proportional to their rest masses, approximately 4 and $A - 4$ amu respectively. Then, from conservation of momentum, $4v_\alpha = (A-4)v_d$, or

$$\frac{v_\alpha}{v_d} = \frac{(A-4)}{4} \tag{15.21}$$

Then the ratio of the kinetic energies of the alpha and the daughter nucleus is

$$\frac{T_\alpha}{T_d} = \frac{[\frac{1}{2}(4)(v_\alpha^2)]}{[\frac{1}{2}(A-4)(v_d^2)]} = \frac{(A-4)}{4} \tag{15.22}$$

Then

$$Q = T_\alpha + T_d = T_\alpha + \frac{4T_\alpha}{A-4} = \frac{A}{A-4}T_\alpha \tag{15.23}$$

For the ${}_{92}U^{238} \rightarrow {}_{90}Th^{234}$ decay, we saw that $Q = 4.27$ MeV. Then $T_\alpha = [(A-4)/A]Q = (234)(4.28)/238 = 4.19$ MeV. This agrees well with the observed α-particle energy, 4.18 MeV.

example The nucleus of Io (or ${}_{90}Th^{230}$) emits an α particle of kinetic energy 4.73 MeV. What is Q?

solution $Q = AT_\alpha/(A-4) = 230(4.73)/226 = 4.81$ MeV.

ple $_{90}Th^{232}$ emits an α particle of 4.05 MeV. What is the Q of the decay?

ion $Q = 232(4.05)/228 = 4.12$ MeV.

i.6 THEORY OF ALPHA DECAY

The potential energy of interaction of the alpha particle and the daughter nucleus, of charge $(Z-2)e$ and mass number $A-4$, is frequently approximated by a constant nuclear interaction potential energy out to the nuclear radius r_0, and by a coulomb potential energy for radii greater than r_0. The expression for this coulomb potential energy in terms of r and $Z-2$ is

$$V = \frac{2(Z-2)e^2}{4\pi\epsilon_0 r} \tag{15.24}$$

This potential energy is shown in Figure 15.4. The actual energy, Q, is indicated by a dashed horizontal line on the diagram. If the alpha particle is initially at a position inside the well, then it is seen that in classical mechanics the alpha particle could not escape with this model for the potential. However, in quantum mechanics it may escape by tunneling. In MeV, the potential coulomb energy may be expressed as $2.88(Z-2)/r$, with r in fermis. It has been found that a good choice for r_0 for α emission is $1.4(A-4)^{1/3}$ fermis (as compared with $1.1A^{1/3}$ mentioned in Chapter 13). Then, in terms of A and Z, the coulomb energy in MeV at $r = r_0$ is

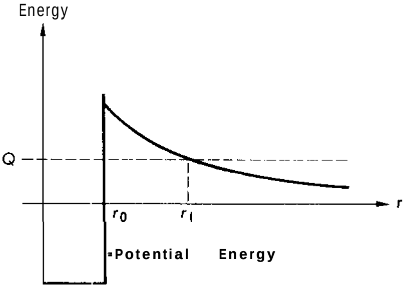


Figure 15.4. Potential energy curve for an alpha particle emitted by an unstable nucleus; alphas initially inside the well, at radii $r < r_0$, have a finite probability of tunneling out of the well and escaping.

$$V_0 = 2.06(Z-2)(A-4)^{-1/3}\ \text{MeV} \tag{15.25}$$

For $A = 230$ and $Z = 90$ ($_{90}Th^{230}$) this peak coulomb energy is 29.8 MeV. Note that this is large compared to Q, which is usually several MeV.

Because Q is less than the maximum of the potential barrier, classically the alpha particle could not get out. However, the quantum mechanical wave function is not quite zero outside the barrier, so there is a small probability of finding the alpha particle outside. To find the relative sizes of the wavefunctions on the two sides of the potential barrier, we will deviate from our main discussion to develop an approximate method of solving a one dimensional Schrödinger equation. The approximate result is given in Equation (15.31). The reader may skip directly there if he is not interested in the mathematical details.

We shall suppose that the alpha particles are emitted symmetrically in all directions; this corresponds to assuming that the wavefunction is a function only of the radial distance r, and that there is no angular dependence. Then the Schrödinger equation for the alpha-daughter system is:

$$\frac{1}{2\mu} p_r^2 \psi(r) + V(r)\psi(r) = Q\psi(r) \tag{15.26}$$

Here, if the parent nucleus is initially at rest, the total energy of the system is Q, the reaction energy, and p_r is the radial component of momentum. μ is the reduced mass, given approximately by

$$\mu = \frac{m_\alpha M_d}{m_\alpha + M_d} \cong \frac{m_\alpha(A-4)}{A} \tag{15.27}$$

The operator corresponding to p_r was discussed in Chapter 8, and it was seen there that the free particle eigenfunctions of p_r, corresponding to outgoing waves, were of the form $(1/r)e^{ikr}$. Hence, if the potential varies sufficiently slowly with r, we would expect to find solutions of this form with $k = \sqrt{2\mu(Q-V)/\hbar^2}$ when $Q > V$, and $k = i\sqrt{2\mu(V-Q)/\hbar^2}$ when $Q < V$. In this problem, however, V cannot be treated as a constant.

If V changes very slowly as r changes, then the change in the phase of the wavefunction, as r varies from r to $r + \Delta r$, should be just $k(r)\Delta r = \sqrt{2\mu[Q - V(r)]/\hbar^2}\,\Delta r$. A further change in r to $r + 2\Delta r$ should result in an additional change of phase $k(r+\Delta r)\Delta r = \sqrt{2\mu[Q - V(r+\Delta r)]/\hbar^2}\,\Delta r$. Hence, by adding a large number of such contributions in passing over a finite distance up to r_1, we might expect the phase of the wavefunction to change by a finite amount given by

$$\Delta\text{phase} = \lim_{\Delta r_i \to 0} \sum_i k(r_i)\Delta r_i = \int dr\, k(r) = \int dr \sqrt{2\mu[Q - V(r)]}/\hbar \tag{15.28}$$

This would, of course, be exact if V were constant. Thus we expect an approximate solution of the form:

$$\psi(r) = \frac{1}{r}\Phi(r) = \frac{\text{const}}{r} \exp\left\{ i \int^r dr \frac{\sqrt{2\mu[Q - V(r)]}}{\hbar} \right\} \tag{15.29}$$

That this is an approximate solution may be checked by substituting Equation (15.29) into (15.26). Then evaluating the first term, we have

$$\frac{1}{2\mu} p_r^2 \left\{ \frac{\text{const}}{r} \exp\left[i \int^r dr \frac{\sqrt{2\mu[Q - V(r)]}}{\hbar} \right] \right\}$$

$$= \frac{1}{2\mu} p_r \left\{ \frac{\text{const}}{r} \sqrt{2\mu[Q - V(r)]} \exp\left[i \int^r dr \frac{\sqrt{2\mu[Q - V(r)]}}{\hbar} \right] \right\}$$

If V(r) is sufficiently slowly-varying that radial derivatives of $\sqrt{Q \quad V}$ can be neglected, this becomes approximately:

$$\sim \frac{1}{2\mu} \sqrt{2\mu[Q - V(r)]}\, p_r \left\{ \frac{\text{const}}{r} \exp\left[i \int^r dr \frac{\sqrt{2\mu[Q - V(r)]}}{\hbar} \right] \right\}$$

$$= \frac{1}{2\mu} \{2\mu[Q - V(r)]\} \frac{\text{const}}{r} \exp\left[i \int^r dr \frac{\sqrt{2\mu[Q - V(r)]}}{\hbar} \right]$$

Equation (15.26) is then obviously satisfied. Hence (15.29) is an approximate solution if $d\sqrt{Q - V}/dr$ is negligible in comparison to $\sqrt{Q - V}/r$.

To apply this to the present problem, in the region between r_0 and r_1, V > Q, so

$$i \int^r dr \frac{\sqrt{2\mu(Q - V)}}{\hbar} = \int^r dr \frac{\sqrt{2\mu(V \quad Q)}}{\hbar} \qquad (15.30)$$

The wavefunction $\psi(r)$ is then of the form:

$$\psi(r) = \frac{\text{const}}{r} \exp\left[- \int_{r_0}^{r} dr \frac{\sqrt{2\mu(V - Q)}}{\hbar} \right] \qquad (15.31)$$

The factor of r^{-1} in Equation (15.31) gives rise to a probability density ψ^{2}, which is proportional to $1/r^2$, corresponding to the inverse squared radial dependence of intensity from a small radiating source.

We can now use this wavefunction to estimate the number of alpha particles which penetrate the Coulomb barrier and are emitted. The speed of the alphas hitting the inside of the barrier is not too different from the speed of the alphas escaping from the other side of the barrier. Therefore, the fraction of particles escaping will be approximately equal to the ratio of probabilities of finding α's in equal volumes at the points r_0 and r_1 in Figure 15.4. The total number of alpha particles in a range of radii *dr* is proportional to $\psi(r)^{2} \cdot 4\pi r^2 dr$, because the volume element corresponding to dr is a spherical shell of area $4\pi r^2$ and thickness *dr.* Hence in terms of $\Phi(r) = r\psi(r)$, the number of particles in dr is proportional to $4\pi \Phi(r)^{2} dr$. The ratio of the number of particles in dr at r_1, to the number of particles in an equal *dr* at r_0, should be just that fraction of alpha particles hitting the inside of the barrier which get out. Hence, from Equation (15.34), the fraction of particles which get out should be

$$\frac{4\pi \Phi(r_1)^{2} dr}{4\pi \Phi(r_0)^{2} dr} = \exp\left[-2 \int_{r_0}^{r_1} \frac{\sqrt{2\mu(V - Q)}dr}{\hbar} \right] \qquad (15.32)$$

Let us call this ratio e^{-I} with

$$I \equiv 2 \int_{r_0}^{r_1} \frac{\sqrt{2\mu(V - Q)}dr}{\hbar} \qquad (15.33)$$

Since the potential between r_0 and r_1 in Figure 15.4 is given by Equation (15.21), the integral which has to be done is

$$I = \frac{2}{\hbar}\int_{r_0}^{r_1}\sqrt{2\mu\left[\frac{2(Z-2)e^2}{4\pi\epsilon_0 r} - Q\right]}\,dr$$

This is a standard integral that can be found in most integral tables. Let $\gamma = Q/[2(Z-2)e^2/4\pi\epsilon_0 r_0]$, the ratio of reaction energy to barrier peak energy. The result is then

$$I = 2.53\sqrt{\frac{A-4}{A}}\,\frac{Z-2}{\sqrt{Q}}\left\{\frac{\pi}{2} - \tan^{-1}\left[\sqrt{\frac{\gamma}{(1-\gamma)}}\right] - \sqrt{\gamma(1-\gamma)}\right\} \qquad (15.34)$$

with Q in MeV. The factor 2.53 arises from the factors $4e^2\sqrt{2m_\alpha}/(4\pi\epsilon_0\hbar)$, with m_α the mass of the α particle, and from the conversion of Q to MeV. The factor $\sqrt{(A-4)/A}$ comes from use of the reduced mass, given in Equation (15.27).

Let us summarize what has been done. By solving the Schrödinger equation approximately, an expression has been derived for the fraction of alpha particles which actually penetrate and escape if they hit the barrier. This fraction is approximately e^{-I} where I depends on the available energy Q, on the mass number A, and on the nuclear charge Ze. Because of the exponential dependence, e^{-I} is an extremely sensitive function of Q and Z.

example It was found in a previous example that Q for the alpha decay of $_{90}Th^{230}$ is 4.82 MeV. Also, the peak of the potential barrier was found to be 29.8 MeV. Thus, $\gamma = 4.82/29.8 = 0.1617$, and from Equation (15.33),

$$I = 2.53\sqrt{\frac{226}{230}}\,\frac{88}{\sqrt{4.82}}\left\{\frac{\pi}{2} - \tan^{-1}\left(\sqrt{0.1617/0.8383}\right) - \sqrt{(0.1617)(0.8383)}\right\}$$

$$= 100.6\left(\frac{\pi}{2} \quad 0.414 - 0.368\right)$$

$$= 79.4$$

Similarly, we found that for the alpha decay of $_{90}Th^{232}$, $Q = 4.12$ MeV. Also, from the peak potential expression of Equation (15.25), the peak of the barrier is at 29.7 MeV. Then $\gamma = 0.1387$ and I = 91.6.

These results can be used to predict quantitatively some half-lives. The exponential e^{-I} is the ratio of the number of particles getting out per unit time to the number inside hitting the barrier per unit time. If we think of the α particle as bouncing back and forth inside the nucleus, the number of times it hits the barrier per unit time is comparable to the α particle's speed divided by the nuclear radius. If we estimate its speed at about $c/10$ (the exact speed does not matter much), and the radius, r_0, as $1.4 \times 10^{-15}(A-4)^{1/3} \cong 8 \times 10^{-15}$ for A around 230, the number of times the alpha particle hits the barrier per second is comparable to 10^{22} per second. Then the fraction of particles coming out per second is comparable to $10^{22}e^{-I} = 10^{22-0.434I}$. This would be the decay constant. The half-life in seconds is then comparable to $10^{0.434I-22}$.

nple In the last example we found that $I = 79.4$ for ${}_{90}\mathrm{Th}^{230}$. The predicted half-life is then about

$$T_{1/2} \approx \frac{\{10^{[(0.434)(79.4)-22]}\}}{3.15 \times 10^{7}\ \text{sec/year}}$$

$$= 1 \times 10^{5}\ \text{years}$$

Likewise for ${}_{90}\mathrm{Th}^{232}$, with $I = 91.6$, the predicted half-life is about 2×10^{10} years. The experimental values are 80,000 years and 1.4×10^{10} years, respectively.

The agreement in this example is somewhat fortuitous, since we dropped various factors multiplying e^{-I} which were comparable to unity. Also, one should take into account the fraction of the time the alpha particle exists in the nucleus, the width of the energy levels, a more accurate solution for the wavefunction, and so forth. This theory was originally given by G. Gamow and E. U. Condon, and was considered a great triumph for quantum mechanics, since it was the first quantitative prediction for nuclear theory. Note that because I appears in the exponent, the small changes in A and Q between the elements ${}_{90}\mathrm{Th}^{230}$ and ${}_{90}\mathrm{Th}^{232}$ gave an enormous half-life ratio.

The most important part of the dependence of this estimated decay constant is on $1/\sqrt{Q}$ in the exponent, I. Thus, if we computed $\log \lambda = -\log(T_{1/2}/0.693)$, we would find that as far as the energy is concerned,

$$\log \lambda = A - \frac{B(Z-2)}{\sqrt{Q}} \qquad (15.35)$$

where A and B are slowly varying functions of A, Z and Q. This law, called the *Geiger-Nuttall law*, is well verified experimentally in its dependence on energy for a given radioactive series.

i.7 BETA DECAY

Unstable nuclei which have an excess of neutrons—that is, whose positions lie generally above the "stability line" on a plot of N versus Z—tend to decay by emitting an electron and another particle called an *antineutrino*, which is extremely hard to detect. The simplest such process is the beta decay of the neutron: When a neutron is not inside some nucleus, it is unstable and decays with a half-life of 12.8 min, according to the process:

$$\text{(a)}\quad {}_{0}n^{1} \rightarrow {}_{1}p^{1} + e^{-} + \overline{\nu}$$

The symbol $\overline{\nu}$ represents the antineutrino, which has zero charge. The symbol e^{-} represents the electron, which has a charge $-e$. Similarly, nuclei lying well below the stability line may decoy by emitting a positron (or, in other words, a β^+) and a neutrino. An example of this is the β^+ decay of the $_7N^{12}$ nucleus:

$$(b) \quad {}_7N^{12} \rightarrow {}_6C^{12} + e^+ + \nu$$

The positron, designated by e^+, has the same rest mass and spin as the electron but a charge of $+e$. On the N -- Z diagram in Figure 15.5 the positions of

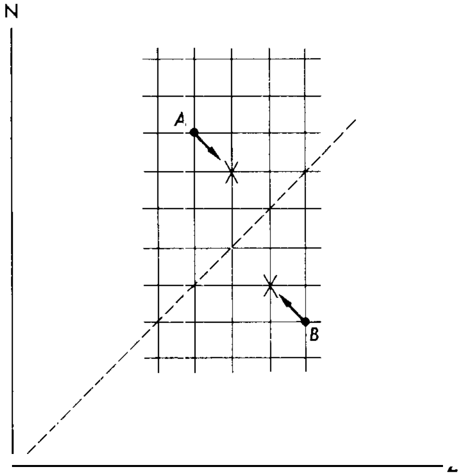


Figure **15.5. N-Z diagram, showing that under beta decay, nuclei lying generally above the stability line tend to decay by β^- emission (A); nuclei lying below the stability line tend to decay by β^+ emission (*B*).**

two unstable nuclei are shown at the points A, *B*. A undergoes β^- decay, *B* undergoes β^+ decay. The crosses indicate the final positions of the nuclei.

In these processes, all the conservation laws we have discussed up to now are satisfied, as well as some new ones. For example, angular momentum and mass-energy are conserved. Conservation of charge is expressed by equolity of the sum of subscripts, together with electron or positron charges on both sides of reactions like (a) and (b). In reaction (a), the total charge to start with is Z = 0, because the neutron is uncharged. The charge finally is that of a proton plus that of an electron, or again zero. In reaction (b), the total charge finally is $6e + 1e = 7e$, agreeing with the initial charge. The antineutrino and neutrino both have charge zero. In beta decay, the mass number of the nucleus does not change; this is expressed by equality of the sum of superscripts on both sides of (a) and (b). This means physically that during a beta decay, the number of neutrons plus the number of protons, or N + Z, does not change. Thus in beta decay there is a new conservation **law: The total number of *nucleons*** is conserved.

Now let us consider mass-energy conservation in β decay. Any mass decrease, due to both the change of nuclear mass and the creation of a β particle, goes into kinetic energy of the final particles. Because of the small masses of the electron and neutrino compared to nuclear masses, most of this kinetic energy goes to them and little goes to the daughter nucleus. As in alpha decay discussed above, we shall designate the energy corresponding to loss of rest mass by Q. We shall call the electron rest mass m_e, the initial or parent atomic mass M_p, and the final or daughter atomic mass M_d. We assume for the present that the neutrino rest mass is zero. We shall see evidence for the validity of this assumption later. Recall that atomic, not nuclear, masses are given in the tables; thus, if the parent atom has Z electrons, the nuclear mass is close to $M_p - Zm_e$. Likewise, if an electron is emitted, the daughter nucleus has one more proton, so its mass is $M_d - (Z + 1)m_e$. Then mass energy conservation is expressed by:

$$(M_p - Zm_e) = M_d - (Z + 1)m_e + m_e + \frac{Q}{c^2} \tag{15.36}$$

The electron masses cancel, so the equation is

$$M_p = M_d + \frac{Q}{c^2} \tag{15.37}$$

In order for β decay to be possible with an electron given off, Q must be positive, so the parent nucleus must have greater mass than the daughter nucleus. It is found that whenever this condition is satisfied, β^- decay does occur, although in some cases the half-life is so large that other decay processes are more important.

ple For the decay ${}_7N^{16} \rightarrow {}_8O^{16} + e^- + \bar{\nu}$, from Appendix 3 the rest mass of ${}_7N^{16}$ is 16.006103 amu, and that of ${}_8O^{16}$ is less at 15.994915 amu. Thus Q is positive. The change in mass is 0.01118 amu, so Q (1 amu = 931 MeV) is 10.4 MeV.

Two other conservation laws that should be satisfied in β^- decay are conservation of momentum and conservation of angular momentum. These two laws lead to the necessity for a neutrino or antineutrino to be present among the β decay products, even though for many years it was impossible to detect these particles directly. For example, consider conservation of angular momentum in connection with the reaction:

$${}_0n^1 \rightarrow {}_1p^1 + e^- + \bar{\nu}$$

The neutron and proton each have spin ½ The electron also has spin ½ . Therefore, if there were no neutrino, angular momentum could not be conserved, because the spin of the end product; would be integral, and could not equal the initial spin of ½ . Thus, if angular momentum is to be conserved, there must be at least one more unobserved particle. If there is only one particle, it must have half-integral spin. Experiments show that the neutrino indeed has spin ½

Now let us consider the effects of momentum conservation along with energy-mass conservation. If there were just two end product particles, , p^1 and e^-, in the center of mass system the two particles would have to have momenta of the same magnitude but opposite in direction, because in the center of mass system the initial momentum is zero. Also, the sum of the kinetic energies equals Q. This gives sufficient information to determine the individual particle energies. Then the electron energies observed should be discrete, just as alpha decay results in discrete alpha-particle energies. However, experimentally it is found that the electrons have a continuous energy distribution from 0 to Q. This indicates that there must be at least one more particle, in addition to the proton and neutron, given off in the decay.

15.8 PHASE SPACE AND THE THEORY OF BETA DECAY

Experimentally observed values of the number of electrons, per unit energy interval, versus electron kinetic energy for the β decay of $_{49}\mathrm{In}^{114}$ are shown in Figure 15.6. Similar results are found in other beta decays. Let us see if we can make some simple arguments to explain the shape of the curve formed by these points. We shall assume first that one particle, an antineutrino of zero rest mass, is given off in addition to the daughter nucleus and the electron. Then the relationship between the energy E_ν and the momentum p_ν of the antineutrino is:

$$p_\nu = \frac{E_\nu}{c} \tag{15.38}$$

just as for a photon. Likewise, if the kinetic energy, momentum and rest mass of the electron are T_e, p_e and m_e, respectively, the relativistic equation relating these three quantities is

$$p_e = \frac{\sqrt{T_e^2 + 2T_e m_e c^2}}{c} \tag{15.39}$$

Now we make a probability argument. As in statistical mechanics, we assume that the probability of finding the particles in a given range of momenta in the final state, is determined only by the availability of final states. Hence we assume their probability is proportional to the corresponding volume in momentum space. Since two particles come off, momentum space here consists of three coordinates for each particle. Therefore, the probability will be proportional to:

$$d\Gamma \equiv (dp_x\, dp_y\, dp_z)_\nu\, (dp_x\, dp_y\, dp_z)_e \tag{15.40}$$

Thirdly, we make the assumption that there is no correlation in direction between the electron and antineutrino. This allows us to use spherical coordinates in momentum space, and to ignore the angular dependence of the distribution of decay products. Then the volume in momentum space becomes

$$d\Gamma = (4\pi p_\nu^2 dp_\nu)(4\pi p_e^2 dp_e) \tag{15.41}$$

From Equations (15.38) and (15.39). in terms of energies E_ν, dE_ν, T_e and dT_e, the volume in momentum space is

$$d\Gamma = (4\pi)^2 \left(\frac{E_\nu^2 dE_\nu}{c^3}\right) \left\{\sqrt{T_e^2 + 2\,T_e\, m_e\, c^2}\,\frac{(T_e + m_e c^2)dT_e}{c^3}\right\}. \tag{15.42}$$

The antineutrino energy E_ν cannot be measured directly, so we would like to sum this expression over all allowed values for E_ν for a given T_e, to find the probability of emitting an electron with kinetic energy T_e. The conservation of energy and momentum equations lead to an approximate relationship between

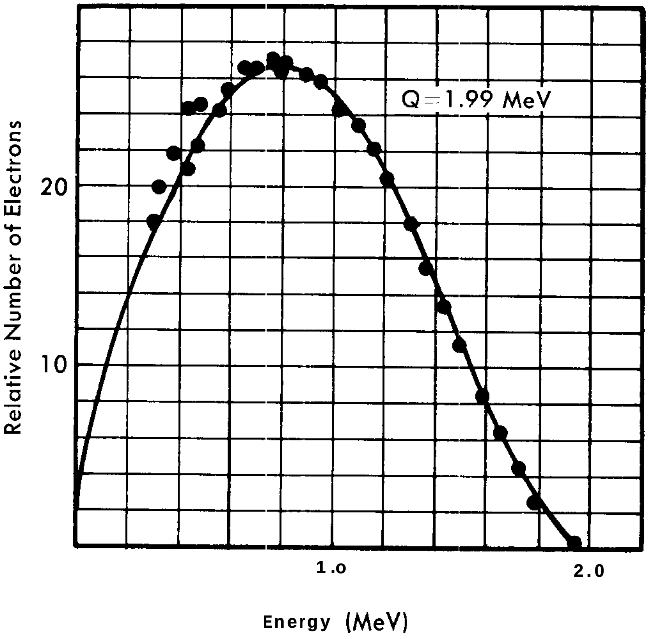


Figure 15.6. Beta decay spectrum far $_{49}\mathrm{In}^{114}$, showing fit obtained by phase space probability argument.

E_ν and T_e. In order to conserve momentum, the nucleus, in general, recoils with a momentum comparable in magnitude to that of the electron and antineutrino. But then, because the nuclear mass is large compared to those of the other particles, it will have negligible kinetic energy. Thus the electron and antineutrino kinetic energies must add to approximately Q. Hence by conservation of energy,

$$E_\nu = Q - T_e \tag{15.43}$$

For a given infinitesimal range of electron kinetic energies near T_e, the antineutrino energies are closely grouped about the value given by Equation (15.43). The factor dE_ν may then be absorbed into a proportionality constant multiplying the factors in $d\Gamma$ which depend on T_e. The number of electrons emitted per unit energy interval, n,, is proportional to the probability divided by dT_e. Then, gathering together the results of Equation (15.42) and (15.43), we see that dropping multiplicative constants, we have:

$$n_e \alpha (Q - T_e)^2 \sqrt{T_e^2 + 2T_e m_e c^2}\,(T_e + m_e c^2) \tag{15.44}$$

For the β decay of ${}_{49}\mathrm{In}^{114}$, $Q = 1.09$ MeV. The expression in Equation (15.44) is plotted as the solid curve in Figure 15.6, using this value of Q and multiplying by the proper constant to make the peak of the curve match the experimental peak. The excellence of the fit indicates strongly that only one additional particle, the antineutrino, is emitted. The dependence on $(Q - T_e)^2$ arose from the assumption that the antineutrino rest mass is zero. The good fit near $T_e = Q$ indicates that this assumption is correct. Thus we conclude that the additional particle emitted in β decay (antineutrino or neutrino) has zero charge, zero rest mass, and a spin of ½ . It also has no magnetic moment. Because of these properties, it interacts very little with matter and is very difficult to detect. It was first detected directly by Reines and Cowan in 1953. They used a large antineutrino flux from a reactor and a very large liquid detector. The reaction used was $\bar{\nu} + {}_1p^1 \to {}_0n^1 + e^+$, and the resulting positron was detected.

While a good fit was obtained to the data of Figure 15.6, many β decays give a curve of different slope. This has been explained in detail by the presence of correlations in the momenta of electron and antineutrino; in the above derivation we assumed no such correlations existed.

15.9 ENERGY IN β^+ DECAY

Let us now consider the condition on parent and daughter atomic masses imposed by energy-mass conservation for β^+ decay, where a positron is emitted. Again let the masses of parent and daughter atoms be M_p and M_d, with m_e the rest mass of the positron (the same as that of the electron). If the charge number of the parent nucleus is Z, that of the daughter nucleus is Z 1. Then if the kinetic energy of the decay products is Q, energy-mass balance is given by the equation:

$$(M_p - Zm_e) = [M_d - (Z - 1)m_e] + m_e + \frac{Q}{c^2} \tag{15.45}$$

Cancellation of *Zm,* on both sides leads to:

$$M_p = M_d + 2m_e + \frac{Q}{c^2} \qquad (15.46)$$

ple Which of the following nuclei could disintegrate by β^+ decay? Find the Q of each decay:

$$_{19}K^{40},\ _4Be^7,\ _{57}La^{138}$$

tion From Appendix 3,

$$\begin{aligned} \text{Mass of } {}_{19}K^{40} &= 39.964000 \text{ amu} \\ \text{Mass of } {}_{18}A^{40} &= \underline{39.962384 \text{ amu}} \\ \text{Difference} &= 0.001616 \text{ amu} \\ 2m_e &= \underline{0.001098 \text{ amu}} \\ \text{Difference} &= 0.000518 \text{ amu} > 0 \end{aligned}$$

Thus the reaction may take place.

$$C? = (931)(0.000516) = 0.48 \text{ MeV}$$

For $_4Be^7 \rightarrow {}_3Li^7 + e^+ + \nu$, the mass difference is -0.000173 amu, which is less than zero, and so the reaction does not take place. For $_{57}La^{138} \rightarrow {}_{56}Ba^{138} + e^+ + \nu$, the mass difference is 0.00081 amu, so the reaction takes place.

$$Q = (931)(0.00081) = 0.75 \text{ MeV}$$

The positron given off in β^+ decay eventually annihilates with an electron, giving off two gamma rays. For a short time before the annihilation, the electron and positron may be bound together to form a system called positronium, somewhat similar to a hydrogen atom. Since the reduced mass, $m_e m_e/(m_e + m_e)$, is $\frac{1}{2} m_e$, the binding energies are one-half the hydrogen energies.

The neutrino given off in β^+ decay has the same properties as the antineutrino except in one respect: the spin of the antineutrino always points in the direction of its motion, and that of the neutrino is always opposite to the direction of the motion. This, together with conservation of angular momentum, leads to the fact that the spins of the electrons or positrons emitted can be lined up, which can be detected experimentally.

10 ELECTRON CAPTURE

A reaction somewhat similar to β decay is that in which an atomic orbital electron is absorbed by the nucleus, with a neutrino being given off. Since the electrons in the K shell spend more time near the nucleus than the other electrons, it is generally a K electron that is captured. The general reaction can be written:

$$e^- + {}_ZP^A \rightarrow {}_{Z-1}D^A + \nu$$

The energy-mass balance equation here is:

$$m_e + [M_p - Zm,] = [M_d - (Z - 1)m_e] + \frac{Q}{c^2} \qquad (15.47)$$

or

$$M_p = M_d + \frac{Q}{c^2} \qquad (15.48)$$

In this case, there are only two particles coming out of the reaction, so their energies should be discrete. Careful measurements, of the recoil energy of the daughter nucleus show that this is the case and that the energy is of the correct mugnitude.

15.11 GAMMA DECAY AND INTERNAL CONVERSION

If a nucleus is bombarded by particles, it may be excited to higher energy levels, just as electrons in atoms can be excited by collisions with particles. Also, if α or β decay takes place, the daughter nucleus may be left in an excited state rather than in the ground state. Ther the nucleus can emit a photon to return to the ground state. These excited state: are typically on the order of an MeV above the ground state. The wavelength of a 1 MeV photon emitted is $\lambda = hc/E = (6.63 \times 10^{-34})(3 \times 10^8)/(1.6 \times 10^{-13}\text{ joules}) = 12 \times 10^{-13}$ m, or about a hundredth of an Angstrom. Such high-energy photons are called gamma rays.

The interaction that leads to γ-ray emission is electromagnetic in origin. Thus, since the interaction potential energies are known, quantum mechanical transition probability theory may be used to estimate the half-life for the transition. The result is that if there are no selection rules preventing the transition, it should occur in about 10^{-14} seconds. If there are selection rules preventing a ready transition, the half-life may be quite large, possibly on the order of days. When there is a long half-life, say greater than 10^{-6} seconds, the various energy states of the nucleus are called isomers. An alternate reaction that may take place to reduce the nucleus to its ground state is interaction with external electrons. Again the K-shell electrons are most important because they spend the most time near the nucleus. In this process of internal *conversion,* the external orbital electron interacts with the nucleus and flies out of the atom, carrying an amount of kinetic energy corresponding to the energy difference between nuclear levels, minus the electron's original binding 'energy.

Measurement of γ-ray energies and conversion electron energies, along with the half-lives, gives information about the spacing and symmetries of nuclear energy levels.

15.12 LOW-ENERGY NUCLEAR REACTIONS

Since there are well over 1200 different known nuclides, or types of nuclei, there are many different ways in which these particles can combine and react. We shall consider here only the simplest type of nuclear reaction, involving two incoming and two outgoing particles of low kinetic energies. By low energy here we mean that the kinetic energies are smaller than about 50 MeV. The lightest nuclear particle (the proton) has a rest energy of about 938 MeV. Therefore, the kinetic energy is small compared to the rest energy, $v/c \ll 1$, and so we can use nonrelativistic mechanics in describing the motion of such a particle. A typical two-particle reaction is as follows:

$$ {}_2He^4 + {}_7N^{14} \rightarrow ({}_9F^{18}) \rightarrow {}_1H^1 + {}_8O^{17} $$

In this reaction, a beam of alpha particles might be allowed to fall on a nitrogen target at rest in the lab. An α particle may combine temporarily with a nitrogen nucleus to form a compound nucleus, in this case a nucleus of fluorine, which is highly unstable and which decays into two new particles. From a study of such reactions, much information can be obtained about the energy levels of the compound nucleus and about nuclear interactions. The Q of a nuclear reaction is defined as the negative of the change in rest energy, that is, Q is the initial particles' rest energy minus the final particles' rest energy. Let us express Q for a two-particle reaction in terms of atomic masses of the incoming and outgoing particles. Assume there are two particles initially of nuclear masses m, M, with M at rest. Let m be incident with velocity v or kinetic energy $T = \frac{1}{2}mv^2$. The initial rest energy is $(m + M)c^2$. If the final particles have masses m', M', the final rest energy is $(m' + M')c^2$. Therefore the Q of the reaction is given by

$$ Q = (m + M - m' - M')c^2 \tag{15.49} $$

These are nuclear masses. However, atomic masses from the tables may be used in this formula, because the electron masses cancel out. Since total energy is conserved in the reaction, if $T_{m'}$ and $T_{M'}$ are the final kinetic energies of the outcoming masses, we have:

$$ T + (m + M)c^2 = (m' + M')c^2 + T_{m'} + T_{M'} \tag{15.50} $$

Therefore, in terms of kinetic energies,

$$ Q = T_{m'} + T_{M'} - T \tag{15.51} $$

This gives another way to define Q: Q equals the increase in kinetic energy of the particles during the reaction.

ample Calculate in MeV, the Q of the reaction, ${}_2He^4 + {}_7N^{14} \rightarrow ({}_9F^{18}) \rightarrow {}_1H^1 + {}_8O^{17}$, using the atomic mass table of Appendix 3.

lution

Mass of ${}_2He^4$ = 4.00260131 amu
Mass of ${}_7N^{14}$ = 14.0030744 amu
Sum = 18.0056775 amu

Mass of ${}_1H^1$ = 1.007825 amu
Mass of ${}_8O^{17}$ = 16.999133 amu
Sum = 18.006958 amu
18.005677 amu
Difference = 0.001281 amu

$$ Q = (931)(-0.001281) = -1.19\ \text{MeV} $$

The fact that Q is negative in the above example means that excess rest mass is created in the reaction, and that some kinetic energy disappears. Such reactions are called endothermic. Reactions in which $Q > 0$, or in which excess kinetic energy is produced, are called exothermic.

example Calculate the Q of the reaction, ${}_3\text{Li}^7 + {}_1\text{H}^1 \rightarrow ({}_4\text{Be}^8) \rightarrow {}_2\text{He}^4 + {}_2\text{He}^4$

solution

Mass of ${}_3\text{Li}^7$ = 7.016004 amu
Mass of ${}_1\text{H}^1$ = 1.007825 amu
Sum = 8.023829 amu
Mass of two ${}_2\text{He}^4$ = 8.005206 amu
Difference = 0.018623 amu

This is an exothermic reaction with

$$Q = (931)(0.018623) = 17.3\ \text{MeV}.$$

15.13 THRESHOLD ENERGY

In an endothermic reaction, excess kinetic energy must be supplied in order for the process to be allowed by energy conservation; if the kinetic energy T of the incident particle falls below Q, the reaction cannot take place. For the reaction to take place, not only must the initial kinetic energy be greater than Q, but enough additional kinetic energy must be supplied to conserve momentum because the final particles are not created at rest. In classical mechanics, it is shown that the total kinetic energy of a system of particles may be written as a sum of two positive contributions: kinetic energy of the center-of-mass motion, plus kinetic energy of the motion relative to the center of mass. The contribution from the center of mass motion is $\frac{1}{2}(m' + M')V^2$, where V is the speed of the center of mass. This speed V is not zero, because for momentum to be conserved,

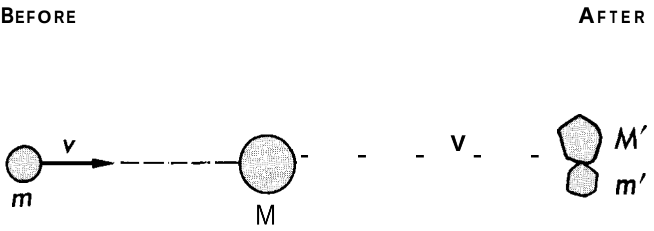


Figure **15.7.** Threshold conditions for an endothermic nuclear reaction.

$$mv = (m' + M')V \tag{15.52}$$

Therefore, the kinetic energy due to the center-of-mass motion is

$$T_{\text{c.m.}} = \left[\frac{m}{(m' + M')}\right]T \tag{15.53}$$

The reaction will not take place unless the incident kinetic energy T supplies $|Q| + T_{\text{c.m.}}$, at the very minimum. If $T = Q + T_{\text{c.m.}}$, there can be no motion of the final particles relative to the center of mass, and the final particles travel along together with speed V. The equation for an endothermic reaction,

$$T = |Q| + T_{c.m} = -Q + \frac{m}{m' + M'} T \tag{15.54}$$

can be solved for T. The solution is:

$$T = T_{th} = -\frac{m' + M'}{m' + M' - m} Q \tag{15.55}$$

Since this is the minimum possible incident kinetic energy which allows the reaction to take place, it is called the threshold energy. Hence the subscript, th, is placed on T.

mple Calculate the threshold energy for the reaction ${}_2He^4 + {}_7N^{14} \rightarrow ({}_9F^{18}) \rightarrow {}_1H^1 + {}_8O^{17}$.

ution The masses and Q are given in the next to last example, $Q = 1.19$ MeV. $m' + M' \simeq 18$ amu; $m' + M'\ m \simeq 14$ amu, assuming that the target ${}_7N^{14}$ nucleus is initially at rest. Then $T_{th} = (18/14)(1.19) \simeq 1.53$ MeV.

The threshold energies we have been discussing are for endothermic reactions. There is, of course, no threshold energy necessary for an exothermic reaction.

15.14 NUCLEAR FISSION AND FUSION

Another very important type of nuclear reaction occurs when a heavy nucleus, far out on the binding energy curve, divides into two lighter nuclei which themselves have larger binding energies per particle. A typical example of this is:

$${}_0n^1 + {}_{92}U^{235} \rightarrow ({}_{92}U^{236}) \rightarrow {}_{56}Ba^{141} + {}_{36}Kr^{92} + 3{}_0n^1 \tag{15.56}$$

This is called fission. Since the overall binding energy per particle increases, kinetic energy is liberated in this process. The Q of the U^{235} fission reaction is about 200 MeV. Atomic bombs utilize this energy release when uranium or plutonium isotopes undergo fission. Again looking at the binding energy curve, Figure 14.8, it may be seen that if a reaction could be made to occur starting with very light particles and ending with heavier particles near Fe^{56}, the binding energy per particle would increase and therefore kinetic energy would be liberated. Such reactions are called *fusion* reactions, and are used in devices such as the hydrogen bomb. Such reactions are also responsible for the energy output of the sun. A typical sequence of fusion reactions which occur in the sun, is the ***proton-proton*** cycle: Starting with pure hydrogen,

$$\begin{aligned} H^1 + H^1 &\rightarrow H^2 + \beta^+ + \nu \\ H^1 + H^2 &\rightarrow He^3 + \gamma \\ He^3 + He^3 &\rightarrow He^4 + 2H^1 \end{aligned} \tag{15.57}$$

Thus, the net result is that 4 protons are "burned" to produce He^4, with β^+ and neutrino particles also appearing. About 25 MeV of energy is released. Such cycles of nuclear fusion reactions can be used to explain the genesis of heavier elements from hydrogen and the large energy output from the sun. Reactions such as these burn up about 1% of the sun's rest mass every 10^9 years. They also give rise to a large flux of neutrinos. From the sun, this flux is about 10^{11} neutrinos/cm^2 sec measured at the earth's surface.

15.15 RADIOACTIVE CARBON DATING

Some radioactive materials are continually being produced by collisions of high-energy, cosmic ray particles, with nuclei of the earth's atmospheric constituents. An important example of this is the production of radioactive $_6C^{14}$, by collisions of cosmic ray neutrons with nitrogen, in the reaction:

$$_0n^1 + {}_7N^{14} \rightarrow {}_6C^{14} + {}_1p^1 \tag{15.58}$$

The carbon nuclei formed in this reaction decay by β emission with a half-life of 5568 years, according to the reaction:

$$_6C^{14} \rightarrow {}_7N^{14} + \beta^- + \bar{\nu} \tag{15.59}$$

In a relatively short time, this radioactive carbon becomes thoroughly mixed with the ordinary $_6C^{12}$ atoms in the atmosphere and near the earth's crust, and is ingested by living organisms. Thus a certain fraction of the carbon in the structure of a living organism consists of radioactive $_6C^{14}$; the amount corresponds to an activity of about 15 disintegrations per minute per gram of fresh carbon. After the death of the organism, the exchange of carbon with the environment ceases and the radioactive carbon atoms decay-the fraction of $_6C^{14}$ atoms decreasing by half in one half-life of 5568 years. By measurement of the carbon activity of an ancient archeological object such as wood or bone, the fraction of the remaining $_6C^{14}$, and hence the age of the object, can be determined. This method of dating organic remains works well if the age of the object is no more than five or six half-lives, or roughly 30,000 years. Beyond that, the fraction of $_6C^{14}$ atoms has decayed to an undetectable level. This method of dating is called radiocarbon dating, and was invented by W. F. Libby in 1952.

summary

LAW OF RADIOACTIVE DECAY

In general, the decay rate for nuclei with decay constant λ is given by $dN/dt = -\lambda N$. Of a sample of N,, nuclei at time $t = 0$ which undergoes spontaneous radioactive decay, at time t there will remain $N = N_0e^{-\lambda t}$ nuclei. The half-life $T_{1/2}$ is the time it takes for half the nuclei in a sample to decay, and is given by

$$T_{1/2} = 0.693/\lambda$$

If there are N_p parent nuclei having a decay constant λ_p, in radioactive equilibrium with N_d daughter nuclei of decay constant λ_d, then the rate at which parent atoms decay is equal to the rate at which daughter atoms decay, and

$$\lambda_d N_d = \lambda_p N_p$$

RADIOACTIVE SERIES

Radioactive elements with $Z > 82$ fall into four series; within each series the nucleon numbers A differ by 4. These series are named the Thorium ($A = 4n$), Neptunium ($A = 4n + 1$), Uranium ($A = 4n + 2$) and Actinium ($A = 4n + 3$) series. The nuclei in these series decay by α or β emission, and ultimately end as stable isotopes of lead or bismuth.

ALPHA-PARTICLE DECAY

Alpha-particle decay is a two-particle decay, in which the atomic number of the parent nucleus decreases by 2 and the nucleon number decreases by 4. An alpha particle is given off with discrete energy. The Q of the decay is the net decrease in rest energy of the particles, and is given in terms of atomic masses by

$$Q/c^2 = {}_ZM_p^A - {}^{A-4}_{Z-2}M_d^A - {}_2M_{He}^4$$

The discrete kinetic energy of the outcoming alpha particle in terms of the nucleon number A of the parent is approximately:

$$T_\alpha = \frac{A-4}{A}Q$$

A relation between the half-life, Q and Z can be obtained approximately on the basis of an alpha-particle model of the nucleus, assuming the alpha particle is bound by a potential energy $V(r)$ which is the positive repulsive Coulomb potential energy for $r > r_0$, but regative for $r < r_0$, where $r_0 = 1.4(A-4)^{1/3}$ fermis. The alpha-particle wavefunction outside the potential barrier is given approximately by

$$\psi \sim \frac{1}{r}\exp\left[-\int_{r_0}^{r} dr\,\frac{\sqrt{2m(V(r)-Q)}}{\hbar}\right]$$

The potential energy for $r > r_0$ is $V = 2(Z-2)e^2/4\pi\epsilon_0 r$. This leads to a half-life:

$$T_{1/2} \simeq 10^{0.434I-22}$$

where

$$I = 2.53\sqrt{\frac{A-4}{A}}\,\frac{Z-2}{\sqrt{Q}}\left[\frac{\pi}{2} - \tan^{-1}\left(\sqrt{\frac{\gamma}{1-\gamma}}\right) - \sqrt{\gamma(1-\gamma)}\right]$$

with γ the ratio of Q to the barrier peak energy,

$$\gamma = \frac{Q}{[2(Z - 2)e^2/4\pi\epsilon_0 r_0]}$$

This result may also be expressed in the form (the Geiger-Nuttall law):

$$\log \lambda = \frac{A - B(Z - 2)}{\sqrt{Q}}$$

where A and B are slowly varying functions of A, Z and Q.

BETA DECAY

In beta decay, electrons are given of: with a continuous range of energies, indicating that in order to conserve energy, momentum and angular momentum, a third particle must also be given off. This third particle has zero rest mass, zero charge, and spin quantum number ½ ; it is called an *antineutrino.* The Q of a beta decay is given in terms of atomic masses by

$$\frac{Q}{c^2} = M_p \quad M_d$$

The number of electrons per unit energy interval which come off in a beta decay process is approximately proportional to:

$$(Q - T_e)^2 \sqrt{\left(\frac{T_e + m_e c^2}{c}\right)^2} - m_e^2 c^2 (T_e + m_e c^2)$$

where T_e is the electron's kinetic energy.

In β^+ decay, a positron and a neutrino are given off, the Q of the reaction being:

$$\frac{Q}{c^2} = M_p - M_d - 2m_e$$

This occurs for nuclei lying generally below the stability line on an N -- Z diagram.

In electron capture, an atomic orbital electron is captured and a neutrino is emitted with a discrete energy.

GAMMA DECAY

Transitions between excited states of a nucleus may occur with the emission or absorption of an energetic photon, called a gamma ray. Typical half-lives for such processes are $\sim 10^{-14}$ sec. Nuclear states with half-lives longer than $\simeq 10^{-6}$ sec are called isomers.

TWO-PARTICLE NUCLEAR REACTIONS

The Q of a nuclear reaction is defined as the negative of the change in rest energy. In terms of the initial masses m, M and final masses m', M': $Q = (m + M \quad m' \quad M')c^2$. Q is also the increase in kinetic energy of the particles. In an endothermic reaction, $Q < 0$; for an exothermic reaction, $Q > 0$. If $Q < 0$ the reaction will not take place unless the incident particle has a minimum kinetic energy:

$$T_{th} = -\frac{m' + M'}{m' + M' - m} Q$$

In a fission reaction, heavy nuclei increase their binding energy by dividing into lighter nuclei which lie closer to the peak of the binding energy curve. In a fusion reaction, light particles are "burned" to produce heavier particles nearer the peak of the binding energy curve.

problems

1. In the actinium series, the parent nucleus U^{235} has a half-life of 8.8 x 10^8 years, much longer than the half-lives in any of the succeeding generations. If 1 gram of U^{235} is in radioactive equilibrium with its decay products (14 generations), what would be the total number of decay particles per second (a's and p's) of the sample?
   Answer: 8.96 x 10^5/sec.
2. A parent nucleus decays into a daughter with decay constant λ_1; the daughter decays into a stable granddaughter with decay constant λ_2. Find the numbers N_1 N_2 and N_3 of parent, daughter and granddaughter nuclei if $N_1 = N_0$, $N_2 = N_3 = 0$ initially. Show that if $\lambda_2 \gg \lambda_1$, $N_1\lambda_1 = N_2\lambda_2$ after a long time has elapsed.
   Answer: $N_1 = N_0 e^{-\lambda_1 t}, N_2 = \lambda_1 \dfrac{N_0(e^{-\lambda_1 t} - e^{-\lambda_2 t})}{(\lambda_2 - \lambda_1)}$,
   $$N_3 = N_0\left[1 - \frac{\lambda_2 e^{-\lambda_1 t} - \lambda_1 e^{-\lambda_2 t}}{\lambda_2 - \lambda_1}\right]$$
3. Calculate the average lifetime of a radioactive substance in terms of its half-life $T_{1/2}$.
   Answer: $1.44\, T_{1/2}$.
4. One curie is defined as an activity of 3.7 x 10^{10} disintegrations per second. Calculate the activity in curies of 1 gram of radium, which has a half-life of $T_{1/2}$ = 1622 years.
   Answer: 0.98 curies.
5. U^{233} has a half-life of 1.62 x 10^5 years. How long will it take for 98% of the original U^{233} atoms to decay?
   Answer: 9.1 x 10^5 years.

6. Calculate the kinetic energy of the α particle arising from α decay of ${}_{92}U^{234}$ using atomic mass tables.

Answer: 4.76 MeV.

7. Calculate the power generated solely by α decay of 1 kg of radium of half-life 1622 years.

Answer: 0.028 watts.

8. From Table 15.3, calculate the Q for α decay of ${}_{85}At^{218}$.

Answer: 6.81 MeV.

9. Which of the following could decay by α decay? Use the atomic mass table. ${}_{4}Be^{8}$, ${}_{22}Ti^{48}$, ${}_{92}U^{235}$.

10. Substitute the WKB approximation, $\psi(x) \simeq (\mathrm{const}/\sqrt{K})\exp\left(\int_0^x K\,dx\right)$ with $K = \sqrt{2m(V - E)}/\hbar$, into the Schrödinger equation, $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{\hbar^2}{2m}K^2(x)\psi = 0$, to see what the error is in this approximation. Show that this error is small if $(dK/dx)/K^2$ and $(d^2K/dx^2)/K^3$ are small compared to one. Near $K = 0$ this is not a good approximation.

11. A particle is in a one dimensional box between $x = 0$ and $x = \ell$. Inside the box, its potential energy is $V = V_0 x/\ell$, where V_0 is small compared to the lowest energy of the particle. Thus $K = \pm\sqrt{2m(V - E)}/\hbar$ is purely imaginary. Use a linear combination of the WKB approximations for positive and negative K to find the energy levels, E, to second order in V_0 (See Problem 10)

Answer: $\frac{n^2\pi^2\hbar^2}{2m\ell^2} + \frac{1}{2}V_0 + \frac{1}{24}\frac{m\ell^2}{n^2\pi^2\hbar^2}V_0^2; \quad n = 1, 2, 3, \ldots.$

12. From Table 15.1, Po^{212} decays with the emission of an α particle, of energy 8.78 MeV. Estimate its half-life using Equation (15.13), and compare with the 3×10^{-7} sec value given in the table.

Answer: 4×10^{-7} sec.

13. From Table 15.3, the half-life of ${}_{92}U^{234}$ is 2.5×10^5 years. By trial and error using Equation (15.13), estimate the a-particle energy that gives this half-life. Compare with 4.76 MeV, as given in the table.

Answer: 4.72 MeV.

14. Find the Q for β^- decay of ${}_{47}Ag^{108}$, of atomic mass 107.9059 amu.

Answer: 1.64 MeV.

15. Suppose the antineutrino had a small rest mass m_ν. Assuming no directional correlation between electron and antineutrino momenta, show that the β^- spectrum should be proportional to:

$$\sqrt{(Q - T_e)(Q - T_e + 2m_\nu c^2)}\,\sqrt{T_e(T_e + 2m_e c^2)}(Q - T_e + m_\nu c^2)(T_e + m_e c^2)$$

where Q is the maximum electron kinetic energy. Sketch this spectrum for T_e near Q, when $m_\nu c^2$ is small.

16. The cross-section for the interaction between nuclei and neutrinos is approximately 10^{-18} barns. Assume that atoms are a few Angstroms apart in the earth, so that there *are* about 10^{28} atoms per cubic meter. What fraction of the neutrinos from the sun, hitting perpendicular to the surface of the earth, are absorbed by the earth?

Answer: 1.3×10^{-11}

17. Find the Q for β^+ decay of ${}_{47}Ag^{108}$, of atomic mass 107.9059 amu.

Answer: 0.90 MeV.

18. Find the Q for K capture in $_{19}K^{40}$.

    Answer: 1.51 MeV.

19. $_{43}Tc^{98}$ has on atomic mass of 97.9071 amu. Can it undergo a β^- decay; a β^+ decay; a K capture?

    Answer: All are possible.

20. $_{15}P^{29}$ has an atomic moss of 28.9818. Can it undergo a K capture; a β^+ decay?

    Answer: Both are possible.

21. Show that for the reaction $\bar{\nu} + {}_ZP^A \rightarrow {}_{Z-1}D^A + e^+$, $M_p = M_d + 2m_e + Q/c^2$. Is it possible to have this reaction if Q is negative?

22. $_6C^{14}$, the radioactive isotope of carbon, has a half-life of 5568 years, decaying by β^- emission. The ratio of $_6C^{14}$ to $_6C^{12}$ in the earth's atmosphere is nearly a constant in time, as $_6C^{14}$ is produced at a constant rate by cosmic rays. If the fraction of $_6C^{14}$ in a sample of wood from an archeological excavation only has 0.30 of the normal fraction of radioactive carbon, what is the age of the sample?

    Answer: 9,700 years.

23. $_{83}Bi^{212}$ decays by n-particle emission, with α particles of kinetic energies 5.60, 5.62, 5.76, 6.07, and 6.11 MeV. Some γ rays observed following the decay have energies of 0.164, 0.452, 0.492, 0.144, 0.432, 0.472, 0.288, 0.328, 0.040 MeV. Construct an energy level diagram showing the various α and γ transitions, and calculate the difference in mass between the $_{83}Bi^{212}$ nucleus and the $_{81}Tl^{208}$ nucleus.

    Answer: 4.0081 amu.

24. Calculate the energy of the γ ray produced by using thermal neutrons, of negligible kinetic energy, in the $n \rightarrow \gamma$ reactions:

$$_0n^1 + {}_1H^1 \rightarrow {}_1H^2 + h\nu; \quad {}_{29}Cu^{65} + {}_0n^1 \rightarrow {}_{29}Cu^{66} + h\nu.$$

    Answer: 2.23 MeV; 7.06 MeV.

25. Calculate the γ energy of the electron capture reaction:

$$_4Be^7 + e^- \rightarrow ({}_3Li^7) \rightarrow {}_3Li^7 + h\nu.$$

    Answer: 0.870 MeV.

26. 5 MeV a particles are absorbed in several centimeters of air; 5 MeV β particles are absorbed in several meters of air. The absorption coefficient of 5 MeV γ rays in air is 0.35×10^{-4}/cm. In what distance would 90% of these γ rays be absorbed?

    Answer: 658 meters.

27. In an internal conversion process, electrons of energies 30.95 keV and 46.10 keV are ejected, followed by x rays of energies 16.3 keV and 1.0 keV, respectively. The nucleus also can emit a γ ray as an alternate way of going from its excited to its ground state. What is the energy of the γ?

    Answer: 47.2 keV.

28. Calculate the Q of the U^{234} fission reaction in which a neutron is absorbed, and $_{56}Ba^{138}$ and $_{36}Kr^{84}$ plus some neutrons are produced.

    Answer: 1050 MeV.

29. Calculate the energy given off during a proton-proton cycle in which four protons are burned to form helium.

    Answer: 25.7 MeV.

16 elementary particles

When the kinetic energies of two colliding particles are made sufficiently high, a variety of particles having new and interesting properties can be created out of the available kinetic energy. An enormous amount of effort has, in the past few decades, been poured into construction of high-energy particle accelerator facilities for the production and study of these so-called elementary particles, and into attempts to classify them and understand their properties. We shall in this chapter present the results of some of these investigations: The successful particle classification schemes, newly discovered conservation laws and quantum numbers will be discussed. The broadest classification schemes are the groupings of particles into different classes, such as the baryons and lepfons. Quantum numbers are assigned to the baryons in such a way that the total number of baryons involved in any reaction among elementary particles remains constant in tirne. Similar conservation laws hold for leptons.

16.1 LEPTONS

Let us first consider the class of particles called leptons. This class includes the electron, positron, neutrinos, antineutrinos and the μ mesons, or muons. All of the leptons have spin ½. In general, for each particle of a given rest mass, charge, and spin within this group there also exists a particle of equal rest mass, opposite charge and the same spin, called an antiparticle. This terminology arises because of the annihilation process which can occur when a particle and its antiparticle combine and disappear in a burst of energy-usually this energy comes out in the form of gamma ray photons. The positron is the antiparticle of the electron. Some neutral particles may be their own antiparticles, as is the case for the π^0 meson to be discussed in Section 16.2. However, in the case of the neutral leptons, such as the neutrino, the antiparticles are different from the particles.

It has been found that there are two distinct types of neutrinos; one type is associated with the appearance or disappearance of electrons in weak decays, while the other type is associated with the appearance or disappearance of muons. The latter type is called a mu neutrino and is denoted by ν_μ. The antiparticle is frequently indicated by putting a bar over the symbol for the particle. The bar changes the sign of the charge; for example, K^+ and K^- are the same. Also, ν_μ, $\bar{\nu}_\mu$ refer to the mu neutrino and the mu antineutrino, respectively.

Examples of the decay of π mesons into muons have been discussed in Chapter 14. A typical decay reaction is:

$$\pi^+ \rightarrow \mu^+ + \nu_\mu \tag{16.1}$$

Here ν_μ is the mu neutrino associated with the appearance of the muon. The μ^+ is the antiparticle of the μ^-. The masses of μ^+ and μ^- correspond to a rest energy of 105.66 MeV, as compared to 0.51 10 MeV for the electron and positron. The ratio of muon mass to electron mass is 206.8.

It has been found experimentally that when leptons are involved in interactions, both the ***electronic lepton number*** and the ***muonic lepton number are*** conserved. By electronic lepton number here we mean that the electron and neutrino are each counted as plus one electronic lepton, and the corresponding antiparticles-the positron and the antineutrino-are counted as minus one electronic lepton each. Likewise, the μ^- and mu neutrino each count as one muonic lepton, and the μ^+ and the mu antineutrino each count as minus one muonic lepton. The total lepton numbers are then found by adding algebraically the lepton numbers of the individual particles appearing on one side of a reaction equation. For example, in the decay reaction (16.1), the muonic lepton number on the lefthand side of the reaction is zero, because no leptons are present. On the righthand side, the total muonic lepton number is -1 for the μ^+ and $+1$ for the mu neutrino; the total is $-1 + (+1) = 0$, the same value as on the left side.

Thus, if in a reaction an electron is created, either another electronic lepton must have been destroyed or an electronic antileptan must have been created at the same time. Using this conservation law and conservation of charge, one may deduce the reaction for the beta decay of the μ^- meson:

$$\mu^- \rightarrow e^- + \nu_\mu + \bar{\nu} \tag{16.2}$$

The muonic lepton number on each side is + 1 and the total electronic lepton number on each side is zero. The mean life for this decay is 2.20×10^{-6} sec. A similar decay involving the antiparticles occurs with the same mean life:

$$\mu^+ \rightarrow e+ + \bar{\nu}_\mu + \nu \tag{16.3}$$

The mu neutrino and the neutrino are distinctly (different particles. In difficult experiments with mu neutrinos from a meson decay, it has been shown that mu neutrinos do not interact with nuclei to form electrons, whereas the creation of electrons from similar nuclear interactions with neutrinos does occur. Charged leptons interact with nuclei primarily through electromagnetic forces, i.e. Coulomb interactions. They do not interact through shortrange strong nuclear forces. The uncharged, zero rest mass leptons cannot interact by means of electromagnetic potentials. Their interaction with the charged leptons is through forces which are very small and are called, appropriately, ***weak interactions.*** Because of the smallness of such interactions, neutrinos go through matter almost as freely as through a vacuum.

16.2 MESONS

As was discussed in Chapter 14, the existence of the π meson was predicted by Yukowa to explain nuclear forces in terms of particle exchange. By an uncertainty principle argument, the π mass was predicted to be several hundred electron masses. Two charged π mesons exist, 'denoted by π^+ and π^-, with rest energies of 139.58 MeV. Also, there is a neutral π meson, π^0, which has a rest energy of 134.98 MeV. The corresponding masses are around 270 times the electron rest mass. The π^0 is its own antiparticle. The antiparticle for the π^+ is the π^-. The π mesons have spin zero and, thus, obey Bose-Einstein statistics. They and the other mesons to be discussed are therefore often called ***bosons.***

If two nucleons collide with sufficient initial kinetic energy, they can create a π meson. Thus, if two protons collide, some possible reactions are:

$$\begin{aligned} {}_1p^1 + {}_1p^1 &\rightarrow {}_1p^1 + {}_1p^1 + \pi^0 \\ {}_1p^1 + {}_1p^1 &\rightarrow {}_1p^1 + {}_0n^1 + \pi^+ \end{aligned} \tag{16.4}$$

Since the rest energy of the π^+ is 139.58 MeV, this is the minimum initial kinetic energy in the center of momentum system needed to create a π^+ meson. Some reactions that might occur for a proton, neutron collision are:

$$\begin{aligned} {}_1p^1 + {}_0n^1 &\rightarrow {}_1p^1 + {}_0n^1 + \pi^0 \\ {}_1p^1 + {}_0n^1 &\rightarrow {}_0n^1 + {}_0n^1 + \pi^+ \\ {}_1p^1 + {}_0n^1 &\rightarrow {}_1p^1 + {}_1p^1 + \pi^- \end{aligned} \tag{16.5}$$

The occurrence of processes such as (16.4) and (16.5) shows that there is no conservation law for meson number.

One decay mode of a charged π meson is the reaction given in (16.1). The mean life for such a decay is 2.55 x 10^{-8} sec. Another decay mode which occurs only in a very small fraction of the decays is

$$\pi^+ \rightarrow e^+ + \nu \tag{16.6}$$

These involve neutral leptons and thus weak interactions. Note that both of these decays have lepton numbers of zero on each side of the equation. Since electromagnetic interactions are much stronger than weak interactions, the most likely decay mode of the π^0 meson is

$$\pi^0 \rightarrow \gamma + \gamma \tag{116.7}$$

-two gamma rays. The mean life here is about 2 x 10^{-16} sec. No leptons are necessary in the decay of the π^0, since no charged particles are needed to conserve charge. Also, the π^0 cannot decay into only one photon because then momentum could not be conserved. In fact, in all these decays at least two particles must result in order to conserve momentum.

The meson exchange theory of nuclear forces is thought to be essentially correct. However, many other mesons have been found which could affect nuclear forces. These mesons all have integral spin and are thus bosons. For instance, the K^+ and K^0 mesons have spin zero and decay in around 10^{-8} sec. Their antiparticles are designated K^-, or $\overline{K^+}$, and K^0. [When discussing the class of particles called mesons, the muon (μ meson) is not included. The muon is a lepton and has spin ½ .] Table 16.1 summarizes the kinds of mesons that fit into the patterns which will be discussed later, along with their rest energies and spins. All of these particles are unstable and decay. For instance, a K^+ meson can decay into $\mu^+ + \nu_\mu$, or into two or three π mesons, etc. It cannot, however, decay into 4 π mesons, because it does not have enough rest energy to form four π's.

TABLE 16.1 Rest Masses and Spin Quantum Numbers of Some of the Mesons

Meson	**Rest Energy (MeV)**	**Spin**
$\pi^\pm$	**139.58**	**0**
π^0	**134.97**	**0**
$K^\pm$	**493.8**	**0**
K^0, K^0	**497.8**	**0**
η	**548.8**	**0**
η'	**958.3**	**0**
$\rho^\pm, \rho^0$	**~ 765**	1
ω	**783**	1
$K^{\pm *}$	**891**	1
$K^{0*}, \overline{K^0}*$	**~ 897**	1
ϕ	**1019**	1
$A_2^\pm, A_2^0$	**-1315**	**2**
$K^{\pm**}$, ^{0**}, K^{0**}	**~ 1405**	**2**
f	**1264**	**2**
f'	**1515**	**2**

.3 BARYONS

There is another class of particles whose number is conserved, called baryons, which includes the proton and neutron, and their antiparticles. These particles all have half-odd-integral spin, and all except the proton—the baryon with the least mass-are unstable. The baryons interact by electromagnetic and short-range nuclear forces, as do mesons. The combined set of mesons and baryons that can interact with nuclear forces is called *hadrons.* The only thing that prevented early discovery of the longer-lived baryons was the lack of particle beams with energy sufficient to produce them. Soon after the bevatron, with enough energy to produce antiprotons, was completed, the antiproton and anti-neutron were detected by several teams of experimenters. The short-lived baryons are more difficult to detect.

Table 16.2 lists some of the baryons that fit into the classification patterns to be discussed later, along with their rest energies and spins. The bars aver symbols indicate antiparticles. The antiparticle always has the opposite sign of

TABLE 16.2 Rest Energies and Spins of Some of the Baryons

Baryon	Rest Energy (MeV)	Spin
$p, \overline{p}$	938.26	1/2
$n, \overline{n}$	939.55	1/2
$\Lambda, \overline{\Lambda}$	1115.6	1/2
$\Sigma^+, \overline{\Sigma^+}$	1189.4	1/2
$\Sigma^0, \overline{\Sigma^0}$	1192.5	1/2
$\Sigma^-, \overline{\Sigma^-}$	1197.3	1/2
$\Xi^0, \overline{\Xi^0}$	1315	1/2
$\Xi^-, \overline{\Xi^-}$	1321	1/2
N^{++*}, N^{++*}	~ 1236	3/2
N^{+*}, [illegible]		3/2
$N^{0*}, \overline{N^{0*}}$		3/2
$N^{-*}, \overline{N^{-*}}$		3/2
Y_1^{+*}, Y_1^{+*}	1382	3/2
$Y_1^{0*}, \overline{Y_1^{0*}}$	-1385	3/2
$Y_1^{-*}, \overline{Y_1^{-*}}$	1388	3/2
$\Xi^{0*}, \overline{\Xi^{0*}}$	1529	3/2
$\Xi^{-*}, \overline{\Xi^{-*}}$	1534	3/2
$\Omega^-, \overline{\Omega^-}$	1672	3/2

charge from the particle. The two plusses on the N^{++*} indicate a charge of 2e.

In any reaction involving baryons, the total baryon number is always conserved. In calculating $\mathcal{B}$, the total baryon number, the antiparticles are assigned -1 and the particles are assigned $+1$. Then the algebraic sum of the numbers of the baryons or antibaryons appearing on one side of a reaction equation must be the same as the number appearing on the other side. Thus in the reaction $\Sigma^0 \to \Lambda + \gamma$, the initial and final baryon numbers are $\mathcal{B} = +1$. In the reaction $n \to \bar{p} + e^+ + \nu$, the initial and final baryon numbers are $\mathcal{B} = -1$. In the reaction $n + n \to 2\gamma$, the initial and final baryon numbers are $\mathcal{B} = 0$.

16.4 CONSERVATION LAWS

In discussing various quantities that are conserved in a particle interaction, it is useful to note what kinds of forces are predominant in causing the reaction. For example, β decay processes go by weak interactions and the numbers of electronic leptons and muonic leptons are conserved. It has been found that there exist quantities that are conserved in nuclear interactions, in which mesons are produced, which might not be conserved for other forces. The four kinds of forces that are known are nuclear or strong, electromagnetic, weak, and gravitational. For particles with nucleon masses, on the order of one fermi apart, the relative sizes of these forces are approximately:

$$\text{Strong: Electromagnetic: Weak: Gravitational:} = 1 : 10^{-2} : 10^{-7} : 10^{-39} \qquad (16.8)$$

Clearly, in reactions where only a few particles are involved, gravitational effects can be ignored. Also, weak forces, where leptons are involved, are important only when a reaction by nuclear or electromagnetic interactions is ***very*** unlikely. A conservation law that holds for all these interactions is conservation of baryon number B.

I. 1 *Isotopic* Spin

Another quantity, which is conserved in strong or nuclear interactions but which is not conserved in electromagnetic or weak interactions, is ***isotopic spin.*** This new quantum number is closely analogous to ordinary spin. It arises from considering that the neutron and the proton are practically identical particles. Nuclear forces are charge independent; the neutron and the proton exhibit the same nuclear forces. They also have nearly the same mass. The only essential difference is that the proton has a charge. As a first approximation, then, one can think of the proton and neutron as different states of the same particle, distinguished only by an internal property (charge), which is described by assigning appropriate internal ***quantum numbers*** to the neutron and proton. Since there are two particles in this case, an internal quantum number having two possible values is needed. If the value $T_3 = \frac{1}{2}$ is assigned to the proton and $T_3 = -\frac{1}{2}$ is assigned to the neutron, these numbers are very closely analogous to the z components of spin of a particle of spin quantum number $T = \frac{1}{2}$, which would have $2T + 1 = 2$ possible states. There are found among the elementary particles numerous exomples of such groups of particles, which can be described as ***isotopic spin multiplets,*** different states described by $2J + 1$ different values of T_3 for the isotopic spin quantum number J. In the case of the proton and neutron, the similarity to ordinary spin $\frac{1}{2}$ is clear; thus the name, isotopic spin. In general, T_3 is analogous to the azimuthal quantum number m,, or the z component of spin, and J is analogous to the total spin quantum number j.

The general utility of the concept of isotopic spin rests on the fact that when several particles are present, the isotopic spin of the system may be obtained by adding isotopic spins just like #ordinary spins, leading to the same possible values for the total T and T_3, as for the analogous j and m. The number of states is $2J + 1$, similar to $2j + 1$ for ordinary spin. The highest T_3 is assigned to the most positive particle in a group of the same J.

For example, from Table 16.2 there are 3 Σ particles. If this number, 3, is $2J + 1$, then

$$J = 1 \tag{16.9}$$

Also, T_3 for each of the three particles is

$$\Sigma^+,\ T_3 = 1;\ \Sigma^0,\ T_3 = 0;\ \Sigma^-,\ T_3 = -1 \tag{16.10}$$

For the "cascade" particles Ξ,

$$T = \frac{1}{2} \tag{16.1 1}$$

and the values of T_3 are:

$$T_3 \text{ for } \Xi = -\frac{1}{2}; \quad T_3 \text{ for } \Xi^0 = +\frac{1}{2} \tag{16.12}$$

For Λ, which has zero charge,

$$T = 0; \quad T_3 = 0 \tag{16.13}$$

In all cases, the antiparticles would have the same T and opposite signs for T_3. The three π mesons have T = 1 and the K mesons have T = ½, with K^+, K^0 having $T_3 = +\frac{1}{2}, -\frac{1}{2}$ respectively.

Let us consider which of the following reactions do not violate any conservation laws discussed so far:

(a) $\Sigma^0 \rightarrow \Lambda + \gamma$
(b) $K^- + p \rightarrow \Xi^0$
(c) $K^0 + n \rightarrow \Lambda + \pi^0$
(d) $\Lambda \rightarrow p + \pi^-$ by strong interaction
(e) $\Lambda \rightarrow p + \pi^-$ by weak interaction.

In all reactions, the charge conservation law is satisfied. Also in all reactions, total spin ½ may occur on each side, so there is no difficulty with angular momentum conservation. Also, the baryon number is + 1 on each side of the equations. No leptons occur in the reactions, so conservation of leptons is irrelevant. In (a), γ indicates an electromagnetic interaction where T need not be conserved; so this reaction appears possible. In reaction (b), the total T_3 is 0 on the left but ½ on the right, so conservation of isotopic spin is violated. In (c), $T_3 = 0$ on both sides; so this appears possible. Likewise in (d), $T_3 = 0$ on the left and $-\frac{1}{2}$ on the right. Thus, this reaction cannot occur by strong interaction. Equation (e) is possible since T, T_3 are not conserved in weak interactions.

76.4.2 Hypercharge

Another quantity that is conserved in strong and electromagnetic interactions, but not necessarily in weak interactions, is strangeness, S. This number was originally introduced to explain *associated* production. For example, in the reaction,

$$p + \pi^+ \rightarrow K^+ + \Sigma^+ \tag{16.14}$$

the K^+ and Σ^+ occur together, or are associated. It was found that a reaction such as

$$n + \pi^+ \rightarrow \Sigma^+$$

in which the Σ^+ would occur not associated with a K^+, and which does not violate previously known conservation laws, does not occur in nature. Later it seemed more useful to introduce a number Y, called hypercharge, in place of S, with

$$Y \equiv S + B \tag{16.15}$$

The law of conservation of strangeness is a combination of conservation of hypercharge and conservation of baryon number. We will use hypercharge, Y, in the rest of this chapter, rather than S. One of the reasons for introducing hypercharge is to explain why two of the Σ's, the Ξ's and the Λ decay in a time characteristic of weak interactions, -- 10^{-10} sec, rather than in a time characteristic of strong interactions, $\sim 10^{-23}$ sec. (The decay time is, roughly, inversely proportional to the square of the strength of the interaction.) We may then say that the reaction

$$\Sigma^+ \rightarrow p + \pi^0 \qquad (16.16)$$

does not occur by strong interactions, because the value of Y or hypercharge of the Σ^+ is different from that of p plus that of π^0. The ***values*** of Y for all of the elementary particles may be determined from considerations similar to those we shall now discuss.

The zero for Y and the spacing between Y numbers may be chosen arbitrarily. The reaction,

$$\Sigma^0 \rightarrow A + \gamma \qquad (16.17)$$

takes place in less than 10^{-14} seconds, and is an electromagnetic interaction because a γ ray is produced. Since γ rays occur in a wide variety of reactions where hypercharge does not enter, and Y is conserved in electromagnetic interactions, we should take $Y = 0$ for photons. Then we see that Y for the Σ^0 particle is equal to that of A. Therefore, we may take $Y = 0$ for the A and Σ^0. Also, since the value of T_3 is the quantum number that differentiates between different Σ particles, Y is the same for the different Σ's. Then $Y = 0$ for $\Sigma^\pm$ also. To define the spacing of Y numbers, the hypercharge of the proton is taken to be $Y = 1$.

The reaction,

$$p + p \rightarrow p + p + \pi^0 \qquad (16.18)$$

takes place by strong interactions. Therefore, Y for the π^0 meson is zero. The reaction,

$$K^- + p \rightarrow \Lambda + \pi^0 \qquad (16.19)$$

takes place through strong interactions. Thus we can say that the Y for K^- and Y for the proton have the same magnitude but opposite signs; or for the K^-, $Y = -1$. The Y for an antiparticle is negative to that of the particle. Therefore we conclude that the hypercharge of the K^+ is + 1, as for the proton. The reaction,

$$K^- + p \rightarrow K^+ + \Xi^- \qquad (16.20)$$

takes place by strong interactions. The total hypercharge on the left is zero, while on the right the hypercharge of the K^+ is + 1. Therefore, the Ξ particle must have a hypercharge of -1. Table 16.3 lists the Y and isotopic spin T for some of the particles in Tables 16.1 and 16.2.

TABLE **16.3** Hypercharge and Isotopic Spins of Some Hadrons

Particles	Y	T
$\pi^{\pm}, \pi^{0}$	0	1
K^{+}, K^{0}	1	1/2
$K^{-}, \overline{K}^{0}$	-1	1/2
p, n	1	1/2
$\overline{p}, \overline{n}$	-1	1/2
$\Lambda^{0}, \overline{\Lambda}^{0}$	0	0
$\Sigma^{\pm}, \Sigma^{0}, \overline{\Sigma}^{\pm}, \overline{\Sigma}^{0}$	0	1
Ξ^{0}, Ξ^{-}	-1	1/2
$\overline{\Xi}^{0}, \overline{\Xi}^{-}$	1	1/2
$N^{-*}, N^{0*}, N^{+*}, N^{++*}$	1	3/2
Y^{-*}, Y^{0*}, Y^{+*}	0	1
Ξ^{-*}, Ξ^{0*}	-1	1/2
Ω^{-}	-2	0

The Ω^{-} particle has $Y =$ 2 and $T = 0$. It does not decay by strong interactions. In the reaction,

$$\Omega^{-} \rightarrow K^{-} + \Xi^{0} \tag{16.21}$$

all quantities are conserved satisfactorily, but the mass of the Ω^{-} is not great enough to produce a K and a Ξ. This reaction is therefore impossible.

A relationship between the charge Q of a hadron in units of $|e|$, its hypercharge Y, and its isotopic spin number T_3, is

$$Q = T_3 + \frac{1}{2} Y \tag{16.22}$$

Thus, for the proton, $Q = 1$, $T_3 = \frac{1}{2}$ and $Y = 1$. Hence, the equation is satisfied.

There are other conservation properties associated with strong and electromagnetic interactions, related to time inversion, space inversion (parity) and charge conjugation (change of particles into antiparticles mathematically). We shall not discuss these in detail.

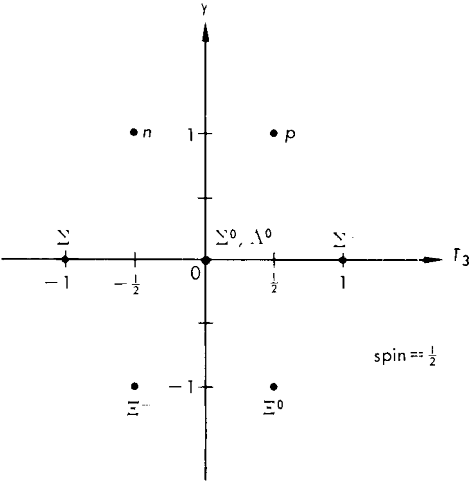
16.5 DETECTION OF PARTICLES

Thus, we have the following particles which are stable under strong and electromagnetic interactions: p, n, Λ, $\Sigma^{\pm}$, Ξ^{-}, Ξ^{0}, Ω^{-}, K^{+}, K^{0}, π^{+} and their corresponding antiparticles. These particles last long enough so that their path length is of reasonable size in a bubble chamber, and they can be detected by this means. The π^{0}, Σ^{0} and η decay rapidly by electromagnetic interaction. All the other particles listed in Tables 16.1 and 16.2 decay by strong interactions in a time comparable to 10^{-23} seconds. In this time, the maximum distance a particle could move is about $10^{-23} c \approx 3 \times 10^{-15}$ m = 3 fermi, about the size of nuclei.

This distance is not detectable on photographic plates. Thus, these particles must be detected indirectly. In the discussion of β decay, we used a phase space argument to find the energy distribution of the electrons. The result was a smooth curve of number of electrons versus energy. Any sharp peak on the curve would indicate the presence of other particles. Similarly, in nuclear scattering experiments one can look for peaks in phase space plots to find these short-lived particles. This is the primary method used to discover them. Statistical analyses of this kind necessitate detailed study of hundreds of thousands of photographs of decay products.

16.6 HYPERCHARGE-ISOTOPIC SPIN PLOTS

Suppose we plot points on a graph of Y versus T_3, for hadrons of the ***same spin.*** Then some interesting symmetries become apparent. Two such plots for the



igure **16.1.** Hypercharge-isotopic spin plot of the aryon octet.

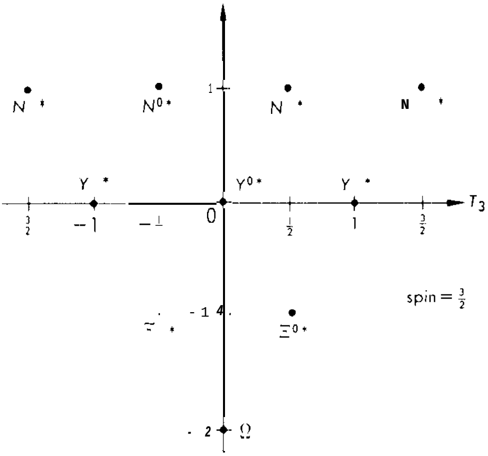


Figure 16.2. The baryon decuplet on a hypercharge-isotopic spin plot.

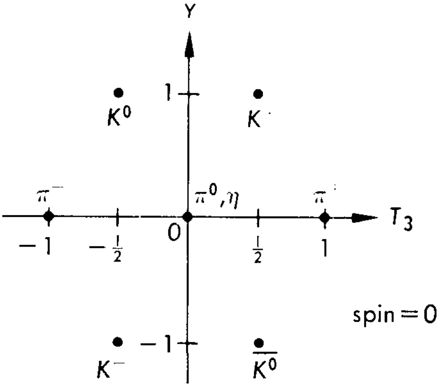


Figure **16.3.** Hypercharge-isotopic spin plot of meson octet for spin zero.

baryons of Table 16.2 are shown in Figures 16.1 and 16.2. Figure 16.3 shows a similar plot of mesons in Table 16.1. The η' particle, which has $Y = 0$, $T_3 = 0$, for reasons of symmetry which will not be discussed here, should be in a diagram by itself. The spin 1 mesons form a similar set of diagrams, with $K^{*\prime}$s replacing K's, ρ's replacing π's, Φ replacing η, and ω replacing η'. Likewise for spin 2, $K \rightarrow K^{**}$, $\pi \rightarrow A_2$, $\eta \rightarrow f$, $\eta' \rightarrow f'$.

These various symmetrical combinations of quantum numbers can be shown to occur naturally in certain "groups" in group theory. Group theory is a branch of mathematics which is useful for systematically finding the physical consequences of symmetries. An alternate simple way of getting these same combinations of quantum numbers is by means of the following model. In atomic physics, the regularities in the periodic table are connected with the fact that combinations of electrons lead to chemical properties. In nuclei, the various regularities in isotopes, isotones, etc. are due to the fact that nuclei are composed of neutrons and protons. This suggests by analogy that the hadrons might be composed of still more fundamental particles. Also, high-energy electron scattering experiments show that there is internal structure-shells of charge-within the proton and neutron, giving further evidence that they might be composed of other particles. While the charge density is positive in the proton, it varies irregularly with radius. The neutron appears to have a positive charge density at the center and negative density further out.

16.7 QUARKS

All of the diagrams of Figures 16.1, 16.2 and 16.3 have at least threefold symmetry about the origin. This suggests that we should consider that each of the hadrons is composed of possibly three fundamental particles. Let us denote these three particles by n', p', Λ'. They have been called *quarks.* Consider the least symmetric of the diagrams exhibiting threefold rather than sixfold symmetry -the one involving the spin $^3/_2$ $N^{*\prime}$s, in Figure 16.2. This contains the $N^{*\prime}$s, $Y^{*\prime}$s, $\Xi^{*\prime}$s, and Ω. Further, to find the values of Y and T_3 to be associated with the quarks, we assume that N^{-*} is made of three n' quarks, N^{++*} of three p' quarks, and Ω^- of three Λ' quarks. Then, for the N^{-*}, $3Y_{n'} = 1$ or $Y_{n'} = ⅓$. For the n' quark, $3T_3 = -^3/_2$ or $T_3 = -½$. Similar arguments for N^{++*} and Ω^- give us:

$$Y_{p'} = \frac{1}{3}$$

$$T_{3p'} = \frac{1}{2}$$

$$Y_{\Lambda'} = -\frac{2}{3}$$

$$J_{3\Lambda'} = 0$$

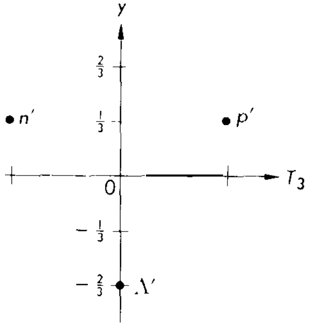


Figure 16.4. Y-T_3 plot for the three quarks.

These three quarks are shown on a $Y - T_3$ plot in Figure 16.4. Again, there is threefold symmetry about the origin. If $Q = T_3 + \frac{1}{2}Y$, for the quarks, as in Equation (16.22), the charges of n′, p', Λ' in units of $|e|$ are $-\frac{1}{3}, \frac{2}{3}, -\frac{1}{3}$, respectively.

Since three quarks can give rise to an ordinary intrinsic spin quantum number of $\frac{3}{2}$, the spin of each quark should be $\frac{1}{2}$. Also, since combinations of three quarks should always give a baryon number of 1, we take $B = \frac{1}{3}$ for each quark. A careful search has been made for particles of fractional charge $-\frac{1}{3}|e|$, $\frac{2}{3}|e|$, but none have yet been definitely identified. The reason could be that quark masses are so large that present machines cannot produce them. (Another possibility is that quarks do not really exist.)

Now let us see if the other baryons can be explained as combinations of three quarks. Consider a baryon made up of two n′ quarks, and a p'. The resulting particle has $Q = 0$, $Y = 1$, $T_3 = -\frac{1}{2}$. These agree with the numbers for n and N^{0*}. The three baryons consisting of an n′, a p′ and a Λ' are the Λ, Σ^0 and Y^{0*}. Similarly, it can be verified that all possible combinations of quarks taken three at a time correspond to baryons.

This quark scheme was worked out before the Ω^- particle had been observed. The theory predicted the charge, isotopic spin and hypercharge of the Ω^-, along with an estimate of its mass, and showed that because of the associated conservation laws, the Ω should decay by weak interactions. Hence it would leave an observable track in a bubble (chamber. An experimental search yielded the first observation of the Ω^-, shown in Figure 16.5.

TABLE 16.4 Quantum Numbers for then′, p′ and Λ' Quarks

	Charge	**B**	**Spin**	**T**	**T_3**	**Y**
n'	$-e/3$	1/3	1/2	1/2	$-1/2$	1/3
p'	$+2e/3$	1/3	1/2	1/2	$+1/2$	1/3
Λ'	$-e/3$	1/3	1/2	0	0	$-2/3$

It is possible that more than one baryon can correspond to a given combination of quarks. We might, for example, take the wavefunction of N^{-*} to

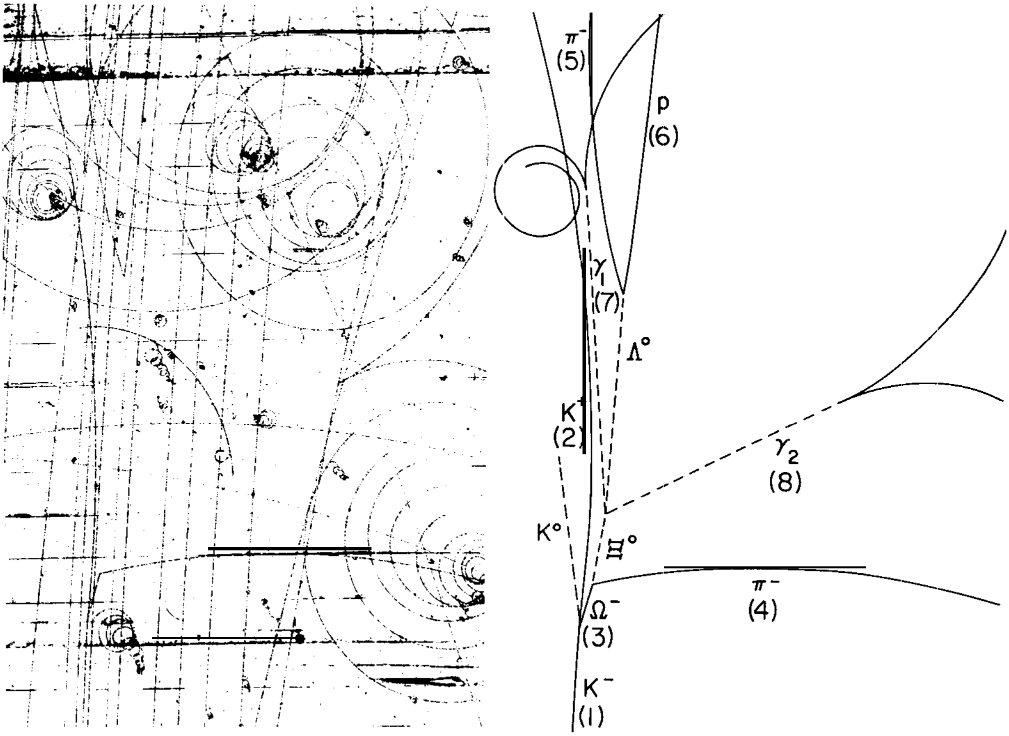


Figure 16.5. Discovery of the Ω^- particle. Measurements on track 4 indicate that it must be a π^-. The decay of the Ξ^0 was previously well-established; analysis of the track and decay of particle 3 indicates that it must be the Ω^- particle, predicted by the theory leading to Figure 16.2. (Courtesy Brookhaven National Laboratories.)

be a product of three quark wavefunctions (labeled 1, 2, 3), as follows:

$$\Psi_{N^*} = \Psi_{n}(1)\,\Psi_{n'}(2)\,\Psi_{n'}(3) \qquad (16.23)$$

Likewise, we might take for the wavefunction of Y^{-*} the combination:

$$\Psi_{Y^*} = \frac{1}{\sqrt{3}}[\Psi_{n'}(1)\,\Psi_{n'}(2)\,\Psi_{\Lambda'}(3) + \Psi_{n'}(1)\,\Psi_{\Lambda'}(2)\,\Psi_{n'}(3) + \Psi_{\Lambda'}(1)\,\Psi_{n'}(2)\,\Psi_{n'}(3)] \qquad (16.24)$$

Both of these wavefunctions are symmetric under exchange of any two quarks. $\Psi_{Y^{0*}}$ would be a symmetric combination of the six products under interchange of 1, 2, 3 in the products of the form:

$$\Psi_{n'}(1)\,\Psi_{p'}(2)\,\Psi_{\Lambda'}(3)$$

Since there are three independent product functions making up Ψ_{Y^*}, there are two other independent linear combinations which could represent $Y = 0$, $T_3 = -1$ baryons. One of these is the Σ^-. The other belongs to another group of eight particles-an octet similar to that containing the n, p and Σ^-. Also, there are six linear combinations that give $Y = 0$, $T_3 = 0$ particles. Three of these are the Y^{0*}, A and Σ^0. Two belong to the second octet of particles just mentioned. The sixth forms a singlet, a group containing only one particle. Particles have been found experimentally which fit into all these various sets. Some of the properties of the particles in the second octet are still not known experimentally. The total number of these baryons is a group of 10 (containing N^{-*}, Ω^-, etc.), one group of eight (containing p, n, etc.) and another group of eight plus one of 1 = 27 baryons. This corresponds to three quarks making up each particle, with three possibilities for each quark. The total number of possibilities is then 3 x 3 x 3 = 27. All these baryons have antibaryons, presumably made of antiquarks.

.8 MESONS IN TERMS OF QUARKS

To form mesons with integral spin from spin ½ quarks, it is necessary to use an even number of quarks. We shall assume that combinations of two quarks form the mesons. Since the baryon number of a meson is zero, we need one quark and one antiquark for each meson. The values of Y, T_3 and Q for all the combinations of a quark with an antiquark are given in Table 16.5.

TABLE 16.5 Formation of Mesons From Quarks

	$n'\bar{n}'$	$n'\bar{p}'$	$n'\bar{\Lambda}'$	$p'\bar{n}'$	$p'\bar{p}'$	$p'\bar{\Lambda}'$	$\Lambda'\bar{n}'$	$\Lambda'\bar{p}'$	$\Lambda'\bar{\Lambda}'$
Y	0	0	1	0	0	1	-1	-1	0
T_3	0	-1	$-1/2$	1	0	$1/2$	$1/2$	$-1/2$	0
Q	0	-1	0	1	0	1	0	-1	0

For the spin zero mesons, combinations of $n'\bar{n}'$, p'p', $\Lambda'\bar{\Lambda}'$ form π^0, η, η', respectively. Also, $n'\bar{p}'$ forms π^-, $n'\bar{\Lambda}'$ forms K^0, $p'\bar{\Lambda}'$ forms K', etc. Higher-spin mesons can be considered to consist of similar combinations of quarks in excited states, with some additional (orbital) angular momentum. Since one quark and an antiquark are needed to create a meson, whereas an odd number of quarks are required to create a boryon, one can understand both baryon conservation and non-conservation of mesons in terms of conservation of quark baryon numbers.

One can believe either that the quarks correspond to actual particles or are simply a convenient way of seeing regularities in hadrons. In the former way of looking at the elementary particles, the only thing special about the proton and neutron is that they have the lowest masses of all the baryons, so that nuclei composed of other types of baryons would eventually decay into nuclei composed of protons and neutrons.

summary

LEPTONS

The leptons are the electron, positron, neutrino, antineutrino, positive and negative μ mesons, and the μ meson neutrino and antineutrino. If the electronic lepton number for the electron and neutrino is taken as + 1, and that for the other electronic leptons is 1, in reactions the sum of the electronic lepton numbers is conserved. A similar conservation law holds for the muonic lepton number. All the leptons have spin ½ . The neutrinos have zero rest mass. The μ meson has a mass of about 207 times the electron mass, and decays in 2.2 x 10^{-6} sec. The neutral leptons, the neutrinos, can interact only through weak interactions.

MESONS

The mesons (not including the μ) have integral spin, and can interact through strong or nuclear interactions. The most easily observed mesons are the π^+, π , π^0, with mass 270 times that of the electron, and the $K^+, K^-, K^0, \overline{K^0}$. The mesons typically decay in $10^{-8} - 10^{-10}$ sec to other mesons or leptons, by weak interactions, or in a shorter time to γ rays by electromagnetic interactions. Some decay in a much shorter time by strong interactions. Exchange of mesons by nuclei is thought to be the source of the interaction forces between the nuclei.

BARYONS

Particles of proton mass and above, with half-integral spin, and with electromagnetic, nuclear and weak interactions, are called baryons. If a baryon number of $+1$ is assigned to the particles and -1 to antiparticles, it is found that the sum of baryon numbers is conserved in interactions. Thus baryons decay to other baryons with various combinations of mesons and leptons. The proton and neutron are the most easily observed of these baryons.

CONSERVATION LAWS

Conservation of lepton and baryon numbers have already been mentioned. Also always conserved in particle interactions in which external forces are negligible, are mass energy, momentum, angular momentum and charge. A number used to distinguish different particles with the same nuclear interactions is isotopic ***spin.*** This is conserved for strong particle interactions. Isotopic spins add like ordinary spins. Another quantum number which was necessary to distinguish different groups of baryons and mesons is hypercharge. This is conserved in strong and electromagnetic interactions. Another related quantum number sometimes used is ***strangeness.*** Strangeness is hypertharge minus baryon number.

QUARKS

It is found that by postulating that three kinds of basic particles, called ***quarks,*** exist, with the proper charges, spins, isotopic spins, hypercharges and baryon numbers, the various baryons and mesons can be considered to be composites of three or two quarks, respectively.

problems

1. μ^- mesons con become bound with atomic nuclei, displacing the inner electrons, to form μ-mesic atoms. Calculate the radius of the first Bohr orbit for a μ-mesic atom of tin; compare with the nuclear radius. What would the binding energy of the μ meson be if the nucleus were of zero radius?
   Answer: 4.46 fermis; nuclear radius = 6.5 fermis; 8.08 MeV.
2. In what region of the spectrum—x-ray, infrared, etc.-would the photons be, arising from transitions due to a μ meson dropping down into lower and lower states in a μ-mesic iron atom?
3. If the π^+ is initially at rest, in the reaction $\pi^+ \rightarrow \mu^+ + \nu_\mu$, what is the kinetic energy of the μ^+?
   Answer: 4.12 MeV.
4. In the reaction $p + p \rightarrow p + p + p + \bar{p}$, a proton-antiproton pair is created. What is the threshold kinetic ard total energy of each of the original protons in the center of momentum system far this reaction to occur? The total energy E_{cm} in the c.m. system is given in terms of the-total energy E_ℓ in the lab system

as $E_c = \sqrt{2E_\ell m_0c^2}$, when one of the two identical initial particles of rest mass m_0 is at rest in the lab. Find the threshold kinetic and total energies in the lab system.

Answer: 5630 MeV lab kinetic energy.

5. If the Σ^0 is at rest, what is the gamma ray energy in the reaction $\Sigma^0 \rightarrow \Lambda + \gamma$, by an electromagnetic interaction?

Answer: 75 MeV.

6. For a A at rest, what is the kinetic energy of the π^- meson given off in the weak decay, $\Lambda \rightarrow p + \pi^-$?

***Answer:* 32** MeV.

7. The K^+ meson has a *mean* life in its rest system of 1.2 x 10^{-8} sec. About how for could a beam of 1 billion eV K^+ particles go before half the particles decayed?

***Answer:* 6.77** m.

8. One unlikely decay mode of the π^+ results in a gamma ray in addition to the μ^+. Write the reaction. An even more unlikely mode produces a π^0 and a positron. Write the reaction.

9. In inelastic proton-alpha particle collisions, either n^0 and π^+, or p^+ and π^0, can come off along with the alpha. The spin and isotopic spin of the alpha particle are both zero. Discuss the possible values of spin and isotopic spin of the outcoming particles which are consistent with the spin and isotopic spin of the incoming particles. What are the total T and T_3 of the combination of outgoing particles?

Answer: $S = ½$, $T_3 = ½$.

10. What are the isotopic spins, T and T_3, of $_2He^4$, $_2He^3$ and , H^3, assuming these quantum numbers are as small as possible? For the reactions, $p + He^3 \rightarrow He^4 + \pi^+$ and $p + H^3 \rightarrow He^4 + \pi^0$, show that the initial and final total T_3's are the same. What must the total initial T's be?

Answer: 0, 0; ½, ½; ½, −½, 1.

11. A Λ^0 decays in flight into a π^- and a proton; it has a kinetic energy of 150 MeV. Calculate the angle at which the proton is projected, if the π^- goes off at 90" with respect to the incident direction of the Λ^0.

Answer: 5.4" from direction of incident A.

12. What is the threshold γ energy such that a π^+ meson can be created when a γ collides with a proton? What is the other particle produced?

Answer: 151 MeV.

13. Which of the following reactions are impossible?

(a) $K^+ \rightarrow \pi^+ + \pi^- + \pi^+$

(b) $K+ \rightarrow \pi^0 + \pi^0 + \pi^+$

(c) $K^+ \rightarrow n^0 + \pi^0 -- \pi^+$

(d) $K^+ \rightarrow \Lambda^0 + \pi^0 + \pi^+$

14. A selection rule that appears to hold for weak interactions is that the magnitude of the change in hyperchorge is unity, $\Delta Y = 1$. Which of the following two sequences is possible?

(a) $\Xi^- \rightarrow n^0 + \pi^-$

(b) $\Xi^- \rightarrow \Lambda^0 + \pi^- \rightarrow n^0 + \pi^0 +$ *a- --* $n^0 +$ *2-y* $+ \pi^-$

15. A π^0 meson decays in flight into 2γ's, which make equal angles of θ with respect to the incident π^0 direction. Derive an expression for the total energy of the π^0.

Answer: $E = m_\pi c^2/\sin\theta$.

16. What conservation laws prevent $\Lambda^0 \rightarrow \pi^+ + \pi^-$?

17. Why doesn't the decay $n \to p + \pi^0$ occur by strong interaction? It doesn't occur by weak interaction either. Why?

18. As pointed out in this chapter, $\Sigma^0 \to \Lambda + \gamma$ goes by electromagnetic interaction. Give two reasons why Σ^0 does not decay by a strong interaction such as $\Sigma^0 \to \Lambda + \pi^0$.

19. One of these reactions can occur by strong interaction but the other cannot. Explain why.

(a) $\pi + n \to K^- + \Lambda$

(b) $\pi^+ + n \to K^+ + \Lambda$

20. The decay $\Sigma^0 \to \Lambda + \gamma$ occurs very rapidly, in far less than 10^{14} sec. The decay $\Sigma \to p + \gamma$ occurs in about 10^{6} sec. Why is there this large difference in decay probability?

21. What conservation laws prevent the reaction, $\pi^+ + p \to p + \Lambda + K^+$?

22. The reaction $\Sigma^+ \to p + \gamma$ is about 10^{-4} times as likely as the reaction $\Sigma^+ \to p + \pi^0$. Why do you think this is so? Both are weak interactions.

23. What conservation laws prevent the decay, $\Sigma^- \to \Sigma^+ + \gamma$?

24. Why doesn't the reaction $\Xi^0 \to \Lambda + \pi^0$ go by strong interaction?

25. To what baryons listed in Table 16.2 does the combination of two λ' quarks and one p' quark correspond?

26. To what baryons listed in Table 16.2 does the combination of two p' quarks and one n' quark correspond?

27. To what mesons in Table 16.1 does the combination of a p' quark and an $\bar{n}'$ quark correspond?

appendix 1

In this appendix the detailed proofs of results quoted in Chapter 8, for the kinetic energy and angular momentum operators in spherical polar coordinates, will be given. The kinetic energy operator, $p^2/2m$, in rectangular coordinates is

$$\frac{1}{2m}p_{\mathrm{op}}^2 = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \qquad \text{(A1.1)}$$

We wish to express this operator in spherical polar coordinates r, θ and φ, defined by the coordinate transformations:

$$\begin{aligned} x &= r\sin\theta\cos\varphi & \qquad & & r &= (x^2+y^2+z^2)^{1/2} \\ y &= r\sin\theta\sin\varphi & & \text{or} & \tan\theta &= \frac{(x^2+y^2)^{1/2}}{z} \\ z &= r\cos\theta & & & \tan\varphi &= \frac{y}{x} \end{aligned} \qquad \text{(A1.2)}$$

Since the operator in Equation (A1.1) is a second-order differential operator, after making the transformation to spherical polar coordinates, no derivatives of order higher than the second can appear. The most general form of such an operator is:

$$A_1\frac{\partial^2}{\partial r^2} + A_2\frac{\partial}{\partial r} + B_1\frac{\partial^2}{\partial\theta^2} + B_2\frac{\partial}{\partial\theta} + C_1\frac{\partial^2}{\partial\varphi^2} + C_2\frac{\partial}{\partial\varphi}$$
$$+ D_1\frac{\partial^2}{\partial r\partial\theta} + D_2\frac{\partial^2}{\partial r\partial\varphi} + D_3\frac{\partial^2}{\partial\theta\partial\varphi}$$

where the coefficients $A_1, A_2, \ldots D_3$ are some functions of the coordinates r, θ and φ.

This expression may be simplified somewhat by noting that apart from the factor $-\hbar^2/2m$ appearing in Equation (A1.1), every term has the physical dimensions of $(\text{length})^{-2}$. In spherical polar coordinates, the only variable with physical dimensions of length is the radius r; hence, the coefficients $A_1, A_2, \ldots D_3$ must each contain the factor $-\hbar^2/2m$ and enough factors of $1/r$ to give each term the same physical dimensions as in Equation (A1.1). Thus we must have:

$$T_{op} = \frac{1}{2m} p^2_{op}$$

$$= -\frac{\hbar^2}{2m}\left(a_1 \frac{\partial^2}{\partial r^2} + a_2 \frac{1}{r}\frac{\partial}{\partial r} + b_1 \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} + b_2 \frac{1}{r^2}\frac{\partial}{\partial \theta} + c_1 \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}\right.$$

$$\left. + c_2 \frac{1}{r^2}\frac{\partial}{\partial \varphi} + d_1 \frac{1}{r}\frac{\partial^2}{\partial r \partial \theta} + d_2 \frac{1}{r}\frac{\partial^2}{\partial r \partial \varphi} + d_3 \frac{1}{r^2}\frac{\partial^2}{\partial \theta \partial \varphi}\right) \qquad \text{(AI .3)}$$

wliere now, at most, $a_1, a_2, \ldots d_3$ can be dimensionless real functions of θ and φ.

These functions may be identified by the following argument. In Cartesian coordinates, the vector momentum operator is

$$\mathbf{p}_{op} = \hat{\imath}\frac{\partial}{\partial x} + \hat{\jmath}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z} \qquad \text{(AI .4)}$$

where $\hat{\imath}, \hat{\jmath}$ and $\hat{k}$ are unit vectors along the x, y and z directions, respectively. The operator p^2_{op} appearing in Equation (AI .l) is the square of $\mathbf{p}_{op}$,

$$p^2_{op} = \mathbf{p}_{op} \cdot \mathbf{p}_{op} \qquad \text{(A1.5)}$$

which reduces immediately to the sum of second derivatives in Equation (A1 .l), because of the orthogonality and constancy of the three unit vectors, $\hat{\imath}, \hat{\jmath}$ and $\hat{k}$. If we can derive an expression for the vector momentum operator in spherical polar coordinates, analogous to Equation (A1.4), then Equation (AI.5) can be used to calculate the kinetic energy.

To derive the vector momentum operator in these coordinates, we introduce unit vectors as follows:

(1) $\hat{r}$ is parallel to r;

(2) $\hat{\theta}$ is in the φ = constant plane, pointing in the direction a particle would move if only its coordinate θ were increased;

(3) $\hat{\varphi}$ normal to $\hat{r}$ and $\hat{\theta}$, such that $\hat{r} \times \hat{\theta} = \hat{\varphi}$. $\hat{\varphi}$ is parallel to the x-y plane and is in the direction a particle would move if only its coordinate φ were increased.

These vectors, each of unit length, are indicated at the point (r, θ, φ) in Figure AI .1. They are mutually perpendicu ar at each point, and change direction when the angles φ and 19 change. These changes in direction must be accounted for when taking the scalar product, as in Equation (A1.5), to calculate the kinetic energy; for then $\mathbf{p}_{op} \cdot \hat{r}$, $\mathbf{p}_{op} \cdot \hat{\theta}$, and $\mathbf{p}_{op} \cdot \hat{\varphi}$ are not zero.

The momentum operator p may be written in terms of its components in the $\hat{r}$, $\hat{\theta}$ and $\hat{\varphi}$ directions by noting that if θ and φ are held constant, and r is changed, the differential increment of distance is

$$ds_r = dr \qquad \text{(Pil.6)}$$

If r and φ are held constant while θ is changed,, the differential increment of distance is

$$ds_\theta = r d\theta \qquad \text{(AI .7)}$$

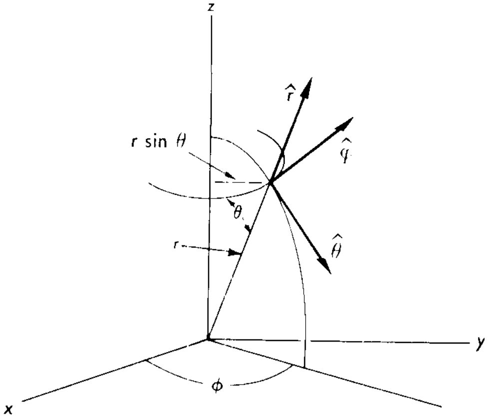


Figure A1.1 Directions of unit vectors r, θ, and φ in spherical polar coordinates.

and changing φ while keeping r and θ constant gives the differential element of distance:

$$ds_\varphi = r \sin\theta \, d\varphi \qquad \text{(A1.8)}$$

In general, the component of the vector momentum operator in the direction corresponding to an increase of linear distance ***ds*** is

$$p_s = \frac{\hbar}{i}\frac{\partial}{\partial s}$$

So, using Equations (A1.6) through (A1.9), in spherical polar coordinates the momentum operator must be:

$$\mathbf{p}_{\text{op}} = \frac{\hbar}{i}\left(\hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\varphi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\right) \qquad \text{(A1.9)}$$

We need to calculate $\mathbf{p}_{\text{op}} \cdot \mathbf{p}_{\text{op}}$, or

$$p_{\text{op}}^2 = -\hbar^2\left(\hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\varphi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\right) \cdot \left(\hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\varphi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\right) \qquad \text{(A1.10)}$$

Consider first only the terms arising from the scalar product in Equation (A1.10), which involve derivatives of second order. Since $\hat{r}$, $\hat{\theta}$ and $\hat{\varphi}$ form an orthogonal set of unit vectors, the only second derivative terms which survive are

$$\hat{r}\cdot\hat{r}\frac{\partial^2}{\partial r^2} + \hat{\theta}\cdot\hat{\theta}\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \hat{\varphi}\cdot\hat{\varphi}\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}$$

$$= \frac{\partial^2}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} \qquad \text{(A1.11)}$$

There can, for example, be no term involving $\partial^2/\partial r\partial\theta$, because this would have to arise from a term such as $\hat{r}\cdot\hat{\theta}\, 1/r\, \partial^2/\partial r\partial\theta$, which vanishes because $\hat{r}\cdot\hat{\theta} = 0$. Other cross-terms vanish for similar reasons.

Hence, from Equation (A1.11), the coefficients a_1, b_1, c_1, d_1, d_2 and d_3 of the second-derivative terms in Equation (A1.3) may immediately be determined. These are:

$$a_1 = 1, \quad b_1 = 1, \quad c_1 = \sin^{-2}\theta, \quad d_1 = d_2 = d_3 = 0 \qquad \text{(A1.12)}$$

Only the coefficients a_2, b_2 and c_2 of the derivatives of first order in Equation (A1.3) remain to be determined. These coefficients may be identified by comparing the effect of the two alternate expressions, (A1.1) and (A1.3), when differentiating arbitrarily chosen functions of r, θ and φ. One sequence of choices of functions which allows the unique determination of the three remaining coefficients is: r^2, z and x.

(A) Let (A1.3) act on r^2. For brevity, we put $C = -\hbar^2/2m$. The result is:

$$T_{op}r^2 = C(2a_1 + 2a_2) = C(2 + 2a_2) \qquad \text{(A1.13)}$$

Let (A1.1) act on $r^2 = x^2 + y^2 + z^2$. A typical term is calculated as follows:

$$\frac{\partial r^2}{\partial x} = 2x \qquad \frac{\partial^2 r^2}{\partial x^2} = 2$$

Similarly, $\partial^2 r^2/\partial y^2 = \partial^2 r^2/\partial z^2 = 2$. Hence,

$$T_{op}r^2 = 6C \qquad \text{(A1.14)}$$

Equating (A1.13) and (A1.14), we must have

$$2 + 2a_2 = 6$$

or

$$\boxed{a_2 = 2} \qquad \text{(A1.15)}$$

The results are unique, since letting Equations (A1.13) and (A1.14) act on r^ℓ, for any $\ell > 2$, gives results for a_2 identical to the above.

(B) Let (A1.3) act on $z = r\cos\theta$. The result, after utilizing (A1.12) and (A1.15), is:

$$T_{op}(r\cos\theta) = C\left(\frac{2}{r}\cos\theta - \frac{1}{r}\cos\theta - \frac{b_2}{r}\sin\theta\right) \qquad \text{(A1.16)}$$

Letting (A1.1) act on z, the result is obviously zero. Hence, from (A1.16),

$$0 = C\left(\frac{2}{r}\cos\theta - \frac{1}{r}\cos\theta - \frac{b_2}{r}\sin\theta\right) \qquad \text{(A1.17)}$$

and therefore,

$$b_2 = \frac{\cos\theta}{\sin\theta} \qquad \text{(A1.18)}$$

(C) Let (A1.3) act on $x = r \sin\theta \cos\varphi$. The result is:

$$T_{op}(r \sin\theta \cos\varphi) = \left(\frac{2}{r} \sin\theta \cos\varphi - \frac{1}{r} \sin\theta \cos\varphi + \frac{1}{r}\frac{\cos^2\theta}{\sin\theta} \cos\varphi - \frac{1}{r} \sin\theta \cos\varphi - \frac{c_2}{r} \sin\theta \cos\varphi\right) \qquad \text{(A1.19)}$$

But letting the alternate expression, (A1.1), act on x, the result is zero. Hence,

$$\begin{aligned} 0 &= \frac{2}{r} \sin\theta \cos\varphi - \frac{1}{r} \sin\theta \cos\varphi + \frac{1}{r}\frac{\cos^2\theta}{\sin\theta} \cos\varphi \\ &\qquad \frac{1}{r}\frac{\sin\theta}{\sin^2\theta} \cos\varphi - \frac{c_2}{r} \sin\theta \cos\varphi \\ &= \frac{\cos\varphi}{r \sin\theta}\left(\frac{\sin^2\theta + \cos^2\theta - 1 - c_2 \sin^2\theta \sin\varphi}{\cos\varphi}\right) \\ &= \frac{-c_2 \sin\theta \sin\varphi}{r} \end{aligned} \qquad \text{(A1.20)}$$

Therefore,

$$c_2 = 0 \qquad \text{(A1.21)}$$

Collecting our results, we find:

$$T_{op} = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial^2}{\partial \theta^2} + \frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)\right] \qquad \text{(A1.22)}$$

which was to be proved.

One method of obtaining components of the angular momentum operator was given in Chapter 8. Here, to obtain the expression for the angular momentum operator, we use instead a straightforward transformation of variables based on the chain rule, from calculus. The same method could have been used in finding p^2_{op} above. This rule states that the net change in a function of several variables such as $\psi(r, \theta, \varphi)$, is the sum of contributions due to changes in the variables separately:

$$d\psi = dr\frac{\partial\psi}{\partial r} + d\theta\frac{\partial\psi}{\partial\theta} + d\varphi\frac{\partial\psi}{\partial\varphi}$$

If the changes in r, θ and φ are due to a change in x, then upon dividing by dx, we have

$$\frac{\partial\psi}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial\psi}{\partial r} + \frac{\partial\theta}{\partial x}\frac{\partial\psi}{\partial\theta} + \frac{\partial\varphi}{\partial x}\frac{\partial\psi}{\partial\varphi}$$

Using the transformations (A1.2), we have:

$$\frac{\partial r}{\partial x} = \frac{x}{r} = \sin\theta\cos\varphi, \quad \frac{\partial\theta}{\partial x} = \frac{1}{r}\cos\theta\cos\varphi, \quad \frac{\partial\varphi}{\partial x} = -\frac{1}{r}\frac{\sin\varphi}{\sin\theta}$$

Thus,

$$\frac{\partial\psi}{\partial x} = \cos\varphi\left(\sin\theta\frac{\partial\psi}{\partial r} + \frac{\cos\theta}{r}\frac{\partial\psi}{\partial\theta}\right) - \frac{\sin\varphi}{r\sin\theta}\frac{\partial\psi}{\partial\varphi} \tag{A1.23}$$

Similarly, for $\partial\psi/\partial y$ we need:

$$\frac{\partial r}{\partial y} = \frac{y}{r} = \sin\theta\sin\varphi, \quad \frac{\partial\theta}{\partial y} = \frac{1}{r}\cos\theta\sin\varphi, \quad \frac{\partial\varphi}{\partial y} = +\frac{1}{r}\frac{\cos\varphi}{\sin\theta}$$

Thus,

$$\begin{aligned}\frac{\partial\psi}{\partial y} &= \frac{\partial r}{\partial y}\frac{\partial\psi}{\partial r} + \frac{\partial\theta}{\partial y}\frac{\partial\psi}{\partial\theta} + \frac{\partial\varphi}{\partial y}\frac{\partial\psi}{\partial\varphi}\\ &= \sin\varphi\left(\sin\theta\frac{\partial\psi}{\partial r} + \frac{\cos}{r}\frac{\partial\psi}{\partial\theta}\right) + \frac{\cos\varphi}{r\sin\theta}\frac{\partial\psi}{\partial\varphi}\end{aligned} \tag{A1.24}$$

For the calculation of $\partial\psi/\partial z$,

$$\frac{\partial r}{\partial z} = \frac{z}{r} = \cos\theta, \quad \frac{\partial\theta}{\partial z} = -\frac{\sin\theta}{r}, \quad \frac{\partial\varphi}{\partial z} = 0$$

Then, using the chain rule, we find:

$$\frac{\partial\psi}{\partial z} = \cos\theta\frac{\partial\psi}{\partial r} - \frac{\sin\theta}{r}\frac{\partial\psi}{\partial\theta} \tag{A1.25}$$

We may combine Equations (A1.23), (A1.24) and (A1.25) to obtain expressions for the angular momentum operators. For example, for L_z we have:

$$\begin{aligned}L_z &= \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\\ &= \frac{\hbar}{i}\left[r\sin\theta\cos\varphi\left(\sin\varphi\sin\theta\frac{\partial}{\partial r} + \frac{\sin\varphi\cos\theta}{r}\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}\right)\right.\\ &\quad\left. - r\sin\theta\sin\varphi\left(\cos\varphi\sin\theta\frac{\partial}{\partial r} + \frac{\cos\varphi\cos\theta}{r}\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}\right)\right]\\ &= \frac{\hbar}{i}(\cos^2\varphi + \sin^2\varphi)\frac{\partial}{\partial\varphi} = -i\hbar\frac{\partial}{\partial\varphi}\end{aligned} \tag{A1.26}$$

This is the same as the result derived in Equation (8.50). To obtain L_x in spherical polar coordinates, we use:

$$L_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$= -i\hbar\left[\sin\theta\sin\varphi\left(\cos\theta\frac{\partial}{\partial r} \quad \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}\right)\right.$$

$$\left. -r\cos\theta\left(\sin\varphi\sin\theta\frac{\partial}{\partial r} + \frac{\sin\varphi\cos\theta}{r}\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}\right)\right]$$

$$= -i\hbar\left(-\sin\varphi\frac{\partial}{\partial\theta} \quad \frac{\cos\theta\cos\varphi}{\sin\theta}\frac{\partial}{\partial\varphi}\right) \tag{A1.27}$$

Similarly,

$$L_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$= -i\hbar\left[r\cos\theta\left(\cos\varphi\sin\theta\frac{\partial}{\partial r} + \frac{\cos\varphi\cos\theta}{r}\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}\right)\right.$$

$$\left. -r\sin\theta\cos\varphi\left(\cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}\right)\right]$$

$$= -i\hbar\left(\cos\varphi\frac{\partial}{\partial\theta} \quad \frac{\cos\theta\sin\varphi}{\sin\theta}\frac{\partial}{\partial\varphi}\right) \tag{A1.28}$$

The square of the angular momentum, L^2, is given by

$$L^2 = L_x^2 + L_y^2 + L_z^2 \tag{A1.29}$$

Calculating these squares term by term, we have (using $d\cot\theta = -\sin^{-2}\theta d\theta$),

$$L_x^2\psi = -\hbar^2\left(-\sin\varphi\frac{\partial}{\partial\theta} + \frac{\cos\theta\cos\varphi}{\sin\theta}\frac{\partial}{\partial\varphi}\right)\left(\sin\varphi\frac{\partial\psi}{\partial\theta} + \frac{\cos\theta\cos\varphi}{\sin\theta}\frac{\partial\psi}{\partial\varphi}\right)$$

$$= -\hbar^2\left(\sin^2\varphi\frac{\partial^2\psi}{\partial\theta^2} - \frac{\sin\varphi\cos\varphi}{\sin^2\theta}\frac{\partial\psi}{\partial\varphi} \quad \frac{\cos\theta\sin\varphi\cos\varphi}{\sin\theta}\frac{\partial^2\psi}{\partial\varphi\partial\theta}\right.$$

$$+\frac{\cos\theta\cos^2\varphi}{\sin\theta}\frac{\partial\psi}{\partial\theta} + \frac{\cos\theta\cos\varphi\sin\varphi}{\sin\theta}\frac{\partial^2\psi}{\partial\varphi\partial\theta}$$

$$\left. - \frac{\cos^2\theta\sin\varphi\cos\varphi}{\sin^2\theta}\frac{\partial\psi}{\partial\varphi} + \frac{\cos^2\theta\cos^2\varphi}{\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}\right) \tag{A1.30}$$

Similarly,

$$L_y^2\psi = -\hbar^2\left(\cos\varphi\,\frac{\partial\psi}{\partial\theta} - \frac{\cos\theta\sin\varphi}{\sin\theta}\,\frac{\partial\psi}{\partial\varphi}\right)\left(\cos\varphi\,\frac{\partial\psi}{\partial\theta} - \frac{\cos\theta\sin\varphi}{\sin\theta}\,\frac{\partial\psi}{\partial\varphi}\right)$$

$$= -\hbar^2\left(\cos^2\varphi\,\frac{\partial^2\psi}{\partial\theta^2} + \frac{\cos\varphi\,\sin\varphi}{\sin^2\theta}\,\frac{\partial\psi}{\partial\varphi} - \frac{\cos\theta\cos\varphi\sin\varphi}{\sin\theta}\,\frac{\partial^2\psi}{\partial\varphi\partial\theta}\right.$$

$$+ \frac{\cos\theta\sin^2\varphi}{\sin\theta}\,\frac{\partial\psi}{\partial\theta} - \frac{\cos\theta\sin\varphi\cos\varphi}{\sin\theta}\,\frac{\partial\psi}{\partial\varphi\partial\theta}$$

$$\left. + \frac{\cos^2\theta\sin\varphi\cos\varphi}{\sin^2\theta}\,\frac{\partial\psi}{\partial\varphi} + \frac{\cos^2\theta\sin^2\varphi}{\sin^2\theta}\,\frac{\partial^2\psi}{\partial\varphi^2}\right) \qquad \text{(A1.31)}$$

Adding these two results, we obtain:

$$L_x^2 + L_y^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{\cos\theta}{\sin\theta}\,\frac{\partial}{\partial\theta} + \frac{\cos^2\theta}{\sin^2\theta}\,\frac{\partial^2}{\partial\varphi^2}\right) \qquad \text{(A1.32)}$$

Then, since $L_z^2 = -\hbar^2(\partial^2/\partial\varphi^2)$, we get

$$L^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{\cos\theta}{\sin\theta}\,\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\,\frac{\partial^2}{\partial\varphi^2}\right) \qquad \text{(A1.33)}$$

which is the expression given in Equation (8.52) for the angular momentum squared.

The tedium of the above calculations can be greatly reduced by using more powerful calculational methods derived from vector and tensor analysis.

appendix 2

ORTHOGONALITY OF WAVEFUNCTIONS

The eigenfunctions of operators which have only real eigenvalues satisfy *orthogonality* relations. For example, for two eigenfunctions ψ_n, ψ_m which have ***different*** energy eigenvalues E_n, E_m respectively, the orthogonality relation is

$$\int \psi_m^* \psi_n \, dV = 0, \quad m \neq n \tag{A2.1}$$

where the integral goes over all the space in which the wavefunctions are defined. More generally, the orthogonality relations state that the integral over space, of the product of one eigenfunction of an operator, times the complex conjugate of another eigenfunction of the operator, vanishes when the eigenfunctions correspond to different eigenvalues.

As an important first example, we will consider the operator,

$$\frac{p_{\mathrm{op}}^2}{2M} + V \tag{A2.2}$$

-the total nonrelativistic energy operator-kinetic, plus potential. Suppose that ψ_n and ψ_m are eigenfunctions of this operator with eigenvalues E_n and E_m, respectively. Then,

$$-\frac{\hbar^2}{2M}\left(\frac{\partial^2\psi_n}{\partial x^2} + \frac{\partial^2\psi_n}{\partial y^2} + \frac{\partial^2\psi_n}{\partial z^2}\right) + V\psi_n = E_n\psi_n \tag{A2.3}$$

and

$$\frac{\hbar^2}{2M}\left(\frac{\partial^2\psi_m}{\partial x^2} + \frac{\partial^2\psi_m}{\partial y^2} + \frac{\partial^2\psi_m}{\partial z^2}\right) + V\psi_m = E_m\psi_m \tag{A2.4}$$

Taking the complex conjugate of the equation for ψ_m, we have:

$$-\frac{\hbar^2}{2M}\left(\frac{\partial^2\psi_m^*}{\partial x^2} + \frac{\partial^2\psi_m^*}{\partial y^2} + \frac{\partial^2\psi_m^*}{\partial z^2}\right) + V\psi_m^* = E_m\psi_m^* \tag{A2.5}$$

because the potential energy and energy eigenvalues are real numbers. Let us multiply Equation (A2.3) by ψ_m^* and Equation (A2.5) by ψ_n. The difference of the resulting two equations is

$$-\frac{\hbar^2}{2M}\left[\left(\psi_n\frac{\partial^2\psi_m^*}{\partial x^2}-\psi_m^*\frac{\partial^2\psi_n}{\partial x^2}\right)+\left(\psi_n\frac{\partial^2\psi_m^*}{\partial y^2}-\psi_m^*\frac{\partial^2\psi_n}{\partial y^2}\right)+\left(\psi_n\frac{\partial^2\psi_m^*}{\partial z^2}-\psi_m^*\frac{\partial^2\psi_n}{\partial z^2}\right)\right] + (V\psi_n\psi_m^* - V\psi_m^*\psi_n) = (E_m - E_n)\psi_m^*\psi_n \qquad (A2.6)$$

or by adding and subtracting terms of the form $(\partial\psi_n/\partial x)(\partial\psi_m^*/\partial x)$, the difference can be written as:

$$-\frac{\hbar^2}{2M}\left[\frac{\partial}{\partial x}\left(\psi_n\frac{\partial\psi_m^*}{\partial x}-\psi_m^*\frac{\partial\psi_n}{\partial x}\right)+\frac{\partial}{\partial y}\left(\psi_n\frac{\partial\psi_m^*}{\partial y}-\psi_m^*\frac{\partial\psi_n}{\partial y}\right)+\frac{\partial}{\partial z}\left(\psi_n\frac{\partial\psi_m^*}{\partial z}-\psi_m^*\frac{\partial\psi_n}{\partial z}\right)\right] = (E_m - E_n)\psi_m^*\psi_n \qquad (A2.7)$$

The terms in the potential, V, cancel out. Integration over a volume ($dV = dxdydz$) gives

$$-\frac{\hbar^2}{2M}\left[\iint\left(\psi_n\frac{\partial\psi_m^*}{\partial x}-\psi_m^*\frac{\partial\psi_n}{\partial x}\right)_{x_1}^{x_2}dy\,dz+\iint\left(\psi_n\frac{\partial\psi_m^*}{\partial y}-\psi_m^*\frac{\partial\psi_n}{\partial y}\right)_{y_1}^{y_2}dx\,dz+\iint\left(\psi_n\frac{\partial\psi_m^*}{\partial z}-\psi_m^*\frac{\partial\psi_n}{\partial z}\right)_{z_1}^{z_2}dx\,dy\right] = (E_m - E_n)\int\psi_m^*\psi_n\,dV \qquad (A2.8)$$

Here x_1 and x_2, the values of x at the boundary of the volume, could be functions of y and z, depending on the shape of the boundary of the volume. If $(\psi_n(\partial\psi_m^*/\partial x) - \psi_m^*(\partial\psi_n/\partial x))$ is the same when evaluated at x_1 and at x_2, and similarly for the terms involving derivatives with respect to y and z, then the left side of Equation (A2.8) is zero. This would occur,. for example, for periodic boundary conditions. Also, for a localized particle, where the wavefunction approaches zero as the coordinates go to infinity, the quantities in parentheses would all be zero as the volume of integration approaches the volume of all space. If the wavefunctions or the derivatives of the wavefunctions are zero at the boundaries, as is the case for a particle in a box, then again all terms on the left side of Equation (A2.13) vanish. We then have:

$$(E_m - E_n)\int_V \psi_m^*\psi_n\,dV = 0 \qquad (A2.9)$$

For $E_m \neq E_n$, this equation can be satisfied only if

$$\int_V \psi_m^*\psi_n\,dV = 0 \qquad (A2.10)$$

This is the orthogonality relation. The eigenfunctions are said to be orthogonal. If there is degeneracy, it is possible that $E_m = E_n$, in which case $\int_V \psi_m^*\psi_n\,dV$ might not be zero. However, it is still always possible to find linear combinations of different eigenfunctions ψ_m and ψ_n, such that for the new combinations, relations like Equation (A2.10) hold.

Clearly, a similar proof could have been made for the one dimensional Schrodinger equation. In particular, let us consider the one dimensional case when V(x) = 0, and $p^2 = p_x^2$. The energy eigenfunctions may then also be eigenfunctions of p_x. If two energy eigenvalues are different, and $E = p^2/2m$, then the momentum eigenvalues are different. Hence, for periodic boundary conditions, the momentum eigenfunctions are orthogonal. Likewise, the Bloch functions in solid state physics, discussed in Chapter 12, are orthogonal, since they satisfy periodic boundary conditions.

Let us investigate the orthogonality relations for the hydrogen atom wavefunctions. The previous discussion shows that the wavefunctions $\psi_{n\ell m}$ and $\psi_{n'\ell'm'}$ are orthogonal for different energies, i.e. if the principal quantum numbers n and n' are different. However, we may show that the individual product functions are also orthogonal if n $\neq$ *n'*, $\ell \neq \ell'$, *or* $m \neq m'$. The hydrogen wavefunctions discussed in Chapter 8 are of the form:

$$\psi_{n\ell m} = R_{n,\ell}(r)\Theta_{\ell,m}(\theta)e^{im\varphi} \qquad \text{(A2.11)}$$

with n, ℓ and m integers. The orthogonality of the functions $e^{im\varphi}$ may be demonstrated directly. Thus,

$$\int_0^{2\pi} e^{-im'\varphi}e^{im\varphi}\,d\varphi = \frac{e^{i(m-m')\varphi}}{i(m-m')}\Bigg|_0^{2\pi} = 0 \quad \text{if} \quad m' \neq m \qquad \text{(A2.12)}$$

If $m = m'$, the integral is not zero but 2π. Hence, the eigenfunctions $e^{im\varphi}$, of the z component of the angular momentum, L_z, are orthogonal.

The functions $R_{n,\ell}$ and $\Theta_{\ell,m}$ satisfy the equations:

$$-\frac{\hbar^2}{2M}\left[\frac{d^2R_{n,\ell}}{dr^2} + \frac{2}{r}\frac{d^2R_{n,\ell}}{dr} - \frac{\ell(\ell+1)}{r^2}R_{n,\ell}\right] - \frac{e^2}{4\pi\epsilon_0 r}R_{n,\ell}$$

$$= E_nR_{n,\ell}, \quad \text{with} \quad E_n = -\frac{me^4}{2(4\pi\epsilon_0\hbar)^2n^2} \qquad \text{(A2.13)}$$

$$\frac{d^2\Theta_{\ell,m}}{d\theta^2} + \frac{1}{\tan\theta}\frac{d\Theta_{\ell,m}}{d\theta} - \frac{m^2}{\sin^2\theta}\Theta_{\ell,m} = -\ell(\ell+1)\Theta_{\ell,m} \qquad \text{(A2.14)}$$

The orthogonality of the functions $R_{n,\ell}$ for different n's and the same ℓ, and of $\Theta_{\ell,m}$ for different ℓ and the same m, may be demonstrated in a fashion similar to that used above for the solutions of the Schrödinger equation. The infinitesimal volume in spherical coordinates is $r^2dr\sin\theta\,d\theta\,d\varphi$. The $d\varphi$ was used above for the proof of the orthogonality of the eigenfunctions of L_z. The one dimensional volume elements needed in discussing the orthogonality of the $R_{n,\ell}$ and of the $\Theta_{\ell,m}$ may therefore be taken to be r^2dr and $\sin\theta\,d\theta$, respectively.

For the radial wavefunctions, $R_{n,\ell}$, orthogonality will be shown for functions of the same ℓ. Hence let us, for simplicity, drop the ℓ subscript. Then, multiplying Equation (A2.13) by $R_{n'}^*$,

$$-\frac{\hbar^2}{2M}\left[R_{n'}^*\frac{d^2R_n}{dr^2} + \frac{2}{r}R_{n'}^*\frac{dR_n}{dr} - \frac{\ell(\ell+1)}{r^2}R_{n'}^*R_n\right] - \frac{e^2}{4\pi\epsilon_0 r}R_{n'}^*R_n = E_n R_{n'}^*R_n \qquad \text{(A2.15)}$$

A similar equation is obtained by taking the complex conjugate of Equation (A2.15) and interchanging n and n'. The difference of the two equations leads to:

$$-\frac{\hbar^2}{2M}\frac{1}{r^2}\frac{d}{dr}\left[r^2\left(R_{n'}^*\frac{dR_n}{dr} - R_n\frac{dR_{n'}^*}{dr}\right)\right] = (E_n - E_{n'})R_{n'}^*R_n$$

The integral over r^2dr for r running from zero to infinity is

$$-\frac{\hbar^2}{2M}\left[r^2\left(R_{n'}^*\frac{dR_n}{dr} - R_n\frac{dR_{n'}^*}{dr}\right)\right]_0^\infty = (E_n - E_{n'})\int_0^\infty R_{n'}^*R_n r^2 dr \qquad \text{(A2.16)}$$

Since both R and dR/dr approach zero exponentially as $r \to \infty$ and are finite at $r = 0$, the left side of Equation (A2.16) is zero. Thus, for different energies, which is the same as for different n's,

$$\int_0^\infty R_{n',\ell}^* R_{n,\ell}\, r^2 dr = 0 \qquad \text{(A2.17)}$$

This could also have been deduced from the general orthogonality relation, Equation (A2.10), for the eigenfunciions in the time independent Schrödinger equation, since for two functions with the same ℓ and m but different n, there is no energy degeneracy and the angular integrals over θ and φ cannot give zero. Therefore, the radial part of the function must satisfy an orthogonality relation. Since R may be chosen real, the complex conjugate used here was not really necessary.

For the angular functions $\Theta_{\ell,m}$, orthogonality will be demonstrated for functions of the same m. Therefore, for simplicity the m subscript will be dropped. Then, from Equation (A2.14),

$$\Theta_{\ell'}^*\frac{d^2\Theta_\ell}{d\theta^2} + \frac{1}{\tan\theta}\Theta_{\ell'}^*\frac{d\Theta_\ell}{d\theta} - \frac{m^2}{\sin^2\theta}\Theta_{\ell'}^*\Theta_\ell = -\ell(\ell+1)\Theta_{\ell'}^*\Theta_\ell \qquad \text{(A2.18)}$$

and a similar complex conjugate equation, with interchange of ℓ and ℓ', is valid. The difference between these two equations leads to:

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left[\sin\theta\left(\Theta_{\ell'}^*\frac{d\Theta_\ell}{d\theta} - \Theta_\ell\frac{d\Theta_{\ell'}^*}{d\theta}\right)\right] = [-\ell(\ell+1) + \ell'(\ell+1)]\Theta_{\ell'}^*\Theta_\ell \qquad \text{(A2.19)}$$

The integral over $\sin\theta\, d\theta$ for θ running from 0 to π is

$$\left[\sin\theta\left(\Theta^*_{\ell'}\frac{d\Theta_\ell}{d\theta}-\Theta_\ell\frac{d\Theta^*_{\ell'}}{d\theta}\right)\right]_0^\pi$$

$$= [-\ell(\ell+1)+\ell'(\ell'+1)]\int_0^\pi \Theta^*_{\ell'}\Theta_\ell \sin\theta\, d\theta \qquad \text{(A2.20)}$$

The left side of Equation (A2.20) is zero. Thus, for $\ell' \neq \ell$,

$$\int_0^\pi \Theta^*_{\ell',m}\Theta_{\ell,m} \sin\theta\, d\theta = 0 \qquad \text{(A2.21)}$$

Since $\Theta_{\ell,m}e^{im\varphi}$ is an eigenfunction of the square of the angular momentum operator, L^2, Equations (A2.12) and (A2.21), show that the angular momentum wavefunctions are orthogonal either for different total angular momenta, specified by different ℓ's, or for different z components of angular momenta, specified by different m's.

Similar orthogonality relations for eigenfunctions with different eigenvalues can be proved for all operators with real eigenvalues.

appendix 3

ATOMIC MASSES, NUCLEAR SPINS AND MAGNETIC MOMENTS OF THE STABLE NUCLIDES

Given here are the masses of the neutral atoms of all stable nuclides and a few unstable ones. The unstable nuclides are indicated by an asterisk following the mass number A. Nuclear spins and magnetic moments are also given. Errors in listed values are in the last significant figure only. The C^{12} atom is the standard at 12.000000 amu.[1]

[1] 1 amu on the C^{12} scale = 931.48 MeV

Z	Element	A	N	Atomic Mass	Spin I	μ (nuclear magnetons)
0	n	1	1	1.0086652	1/2	-1.91314
1	H	1	0	1.00782519	1/2	+2.79277
		2	1	2.0141022	1	+0.857406
		3*	2	3.0160497	1/2	+2.97885
2	He	3	1	3.0160297	1/2	-2.12755
		4	2	4.0026031	0	0
		5*	3	5.012297		
		6*	4	6.018893		
3	Li	5*	2	5.012538		
		6	3	6.015125	1	+0.822010
		7	4	7.016004	3/2	+3.25628
		a*	5	8.022487		
4	Be	7*	3	7.016929		
		8*	4	8.005308		
		9	5	9.012186	3/2	-1.17744
		10*	6	10.013534		
5	B	8*	3	8.024609		
		9*	4	9.013332		
		10	5	10.012939	3	+1.80063
		11	6	11.0093053	3/2	+2.68857
		12*	7	12.0143537		
6	C	10*	4	10.016810		
		11*	5	11.011432		
		12	6	12.000000000	0	0

‘References: J. H. E. Mattauch, W. Thiele, A. H. Wapstra, **Nuclear Physics** 67, 1, (1965). C. M. Lederer, J. M. Hollander, I. Perlman, Table **of Isotopes,** 6th ed., John Wiley & Sons, New York, (1967).

Z	Element	A	N	Atomic Mass	Spin *I*	μ (nuclear magnetons)
		13	7	13.003354	1/2	+0.702381
		14*	8	14.003242	0	0
		15*	9	15.010600		
7	N	12*	5	12.018641		
		13*	6	13.005738		
		14	7	14.0030744	1	+0.40361
		15	8	15.000108	1/2	-0.28309
		16*	9	16.006103		
		17*	10	17.00845		
8	O	14*	6	14.0085971		
		15*	7	15.003070		
		16	8	15.9949150	0	0
		17	9	16.999133	5/2	-1.89370
		18	10	17.9991600	0	
		19*	11	19.003578		
9	F	17*	8	17.002095		
		18*	9	18.000937		
		19	10	18.9984046	1/2	+2.6287
		20*	11	19.999987		
10	Ne	18*	8	18.005711		
		19*	9	19.001881		
		20	10	19.992440		
		21	11	20.993849	3/2	-0.66176
		22	12	21.991385		
		23*	13	22.994473		
11	Na	23	12	22.989771	3/2	+2.21751
12	Mg	24	12	23.985042		
		25	13	24.985839	5/2	-0.85512
		26	14	25.982593		
13	Al	27	14	26.981539	5/2	+3.64140
14	Si	28	14	27.976929		
		29	15	28.976496	1/2	-0.55525
		30	16	29.973763		
15	P	29	14	28.981808		
		31	16	30.973765	1/2	+1.13166
16	S	32	16	31.972074	ID	
		33	17	32.97146	3/2	+0.64327
		34	18	33.967865	0	
		36	20	35.96709		
17	Cl	35	18	34.968851	3/2	+0.82183
		37	20	36.965897	3/2	+0.68409
18	Ar	36	18	35.967544		
		38	20	37.962728		
		40	22	39.962384		
19	K	39	20	38.963710	3/2	+0.39140
		40*	21	139.964000	4	-1.2981
		41	22	40.961832	3/2	+0.21483
20	Ca	40	20	39.962589		
		42	22	41.958625		
		43	23	42.958780	7/2	1.3172
		44	24	43.955490		

Z	Element	A	N	Atomic Mass	Spin I	μ (nuclear magnetons)
		46	26	45.95369		
		48	28	47.95253		
21	SC	45	24	44.955919	7/2	+4.75626
22	Ti	46	24	45.952632		
		47	25	46.95’1768	5/2	-0.7881
		48	26	47.947950		
		49	27	48.947870	7/2	-1.1036
		50	28	49.944786		
23	V	50*	27	49.947164	6	+3.347
		51	28	50.943961	7/2	+5.148
24	Cr	50	26	49.946054		
		52	28	51.940513		
		53	29	52.940653	3/2	-0.47434
		54	30	53.9313881		
25	Mn	55	30	54.938050	5/2	+3.4678
26	Fe	54	28	53.939617		
		56	30	55.934936		
		57	31	56.9315398	1/2	+0.0902
		58	32	57.933273		
27	co	59	32	58.933189	7/2	+4.6583
28	Ni	58	30	57.935342		
		60	32	59.930787		
		61	33	60.931056		
		62	34	61.928342		
		64	36	63.927958		
29	cu	63	34	62.929592	3/2	+2.2261
		65	36	64.927786	3/2	+2.3849
		66	37	65.928871		
30	Zn	64	34	63.929115		
		66	36	65.926052		
		67	37	66.927145	5/2	+0.87552
		68	38	67.924857		
		70	40	69.925334		
31	Ga	69	38	68.925574	3/2	+2.01602
		71	40	70.924706	3/2	+2.56161
32	Ge	70	38	69.924251		
		72	40	71.922082		
		73	41	72.923462	9/2	-0.8788
		74	42	73.921181		
		76	44	75.92’1405		
33	AS	75	42	74.921596	3/2	+1.4390
34	Se	74	40	73.922476	0	0
		76	42	75.919207		
		77	43	76.919911	1/2	+0.5344
		78	44	77.917314	0	0
35	Br	79	44	78.9113329	3/2	+2.1056
		81	46	80.916292	3/2	+2.2696
36	Kr	78	42	77.920403		
		80	44	79.9116380		
		82	46	81.91.3482		
		83	47	82.914131	9/2	-0.97017
		84	48	83.911503		

Z	Element	A	N	Atomic Mass	Spin I	μ (nuclear magnetons)
36	Kr	86	50	85.910616		
37	Rb	85	48	84.911800	5/2	+1.35267
		87*	50	86.909 186	3/2	+2.7505
38	Sr	84	46	83.913430		
		86	48	85.909285		
		87	49	86.908892	9/2	--1.0930
		88	50	87.90564 1		
39	Y	89	50	88.905872	1/2	-0.137316
40	Zr	90	50	89.904700		
		91	51	90.905642	5/2	- 1.30285
		92	52	91.90503 1		
		94	54	93.906313		
		96	56	9.5.908286		
41	Nb	93	52	9’2.906382	9/2	+6.1671
42	Mo	92	50	91.906810		
		94	52	93.905090		
		95	53	94.905839	5/2	-0.9133
		96	54	95.904674		
		97	55	96.90602	5/2	-0.9325
		98	56	97.905409		
		100	58	99.907475		
43	TC	98	55	97.90711		
44	Ru	96	52	915.907598		
		98	54	97.905289		
		99	55	98.905935	5/2	-0.62
		100	56	99.9042 18		
		101	57	100.905577	5/2	-0.7
		102	58	101.904348		
		104	60	103.905430		
45	Rh	103	58	102.90551 1	1/2	-0.0883
46	Pd	102	56	101.905609		
		104	58	103.904011		
		105	59	104.905064	5/2	-0.615
		106	60	1051.903479		
		108	62	107.903891		
		110	64	109.905164		
47	Ag	107	60	106.905094	1/2	-0.113548
		108	61	107.905949		
		109	62	1088.904756	1/2	-0.130538
48	Cd	106	58	105.906463		
		108	60	107.904187		
		110	62	109.903012		
		111	63	110.904188	1/2	-0.59501
		112	64	111.902762		
		113	65	112.904408	1/2	- 0.62243
		114	66	113.903360		
		116	68	115.904762		
49	In	113	64	112.904089	9/2	+5.5233
		115*	66	114.901745	9/2	+5.5351
50	Sn	112	62	111.904835		
		114	64	113.902773		
		115	65	114.903346	1/2	-0.91781

Z	Element	A	N	Atomic Mass	Spin I	μ (nuclear magnetons)
		116	66	115.901745		
		117	67	116.002958		-0.99983
		118	68	117.901606		
		119	69	118.903313	1/2	-1.04621
		120	70	119.902198		
		122	72	121.903441		
		124	74	123.905272		
51	Sb	121	70	120.903816	5/2	+3.3590
		123	72	122.904213	7/2	+2.547
52	Te	120	68	119.904023		
		122	70	121.903066		
		123	71	122.904277	1/2	-0.73585
		124	72	123.902842		
		125	73	124.904418	1/2	-0.88715
		126	74	125.903322		
		128	76	127.904426		
		130	78	129.906238		
53	I	127	74	126.904470	5/2	+2.8091
54	Xe	124	70	123.90612		
		126	72	125.90429		
		128	74	127.90354		
		129	75	128.90478	1/2	-0.77686
		130	76	129.90351		
		131	77	130.90509	3/2	+0.69066
		132	78	131.90416		
		134	80	13390540		
		136	82	135.90722		
55	cs	133	78	132.90536	7/2	+2.5789
56	Ba	130	74	129.90625		
		132	76	131.90512		
		134	78	133.90461		
		135	79	134.90555	3/2	+0.83718
		136	80	135.90430		
		137	81	136.90550	3/2	+0.93654
		138	82	137.90500		
57	La	138*	81	137.90691	5	+3.7071
		139	82	138.90614	7/2	+2.7781
58	Ce	136	78	135.90710		
		138	80	137.90583		
		140	82	139.90539		
		142	84	141.90914		
59	Pr	141	82	140.90760	5/2	+4.3
60	Nd	142	82	141.90766		
		143	83	142.90978	7/2	-1.064
		144*	84	143.91004		
		145	85	144.91254	7/2	-0.653
		146	86	145.91309		
		148	88	147.91687		
		150	90	149.92092		
61	Pm	147	86	14t5.91511		

Z	Element	A	N	Atomic Mass	Spin I	μ (nuclear magnetons)
62	Sm	144	82	143.91199		
		147*	85	146.91487	7/2	-0.8
		148	86	147.91479		
		149	87	148.91718	7/2	--0.65
		150	88	149.91728		
		152	90	151.91976		
		154	92	lS3.92228		
63	Eu	151	88	150.91984	5/2	+3.465
		153	90	152.92124	5/2	+1.52
64	Gd	152	88	1511.91979		
		154	90	1513.92093		
		155	91	15~4.92266		
		156	92	155.92218		
		157	93	156.92403		
		158	94	157.92418		
		160	96	159.92712		
65	Tb	159	94	158.92539	3/2	
66	Dy	156	90	155.92392		
		158	92	157.92445		
		160	94	159.92520		
		161	95	160.92695		
		162	96	161.92680		
		163	97	162.92876		
		164	98	163.92920		
67	HO	165	98	164.93042	7/2	
68	Er	162	94	161.92874		
		164	96	16.3.92929		
		166	98	16.5.93031		
		167	99	166.93206	7/2	
		168	100	1617.93238		
		170	102	169.93556		
69	Tm	169	100	1613.93425	1/2	
70	Yb	168	98	167.9342		
		170	100	169.93502		
		171	101	170.93643	1/2	+0.4930
		172	102	17'1.93636		
		173	103	172.93806	5/2	-0.678
		174	104	173.93874		
		176	106	175.94268		
71	Lu	175	104	174.94064	7/2	+2.23
		176*	105	17S.94266		
72	Hf	174	102	173.94036		
		176	104	17S.94157		
		177	105	176.94340	7/2	+0.61
		178	106	177.94388		
		179	107	178.94603	9/2	-0.47
		180	108	179.94682		
73	Ta	181	108	180.94801	7/2	+2.35
74	W	180	106	179.94700		
		182	108	181.94830		

Z	Element	A	N	Atomic Mass	Spin I	μ (nuclear magnetons)
		183	109	182.95032	1/2	+0.117224
		184	110	183.95103		
		186	112	185.9.5444		
75	Re	185	110	184.95306	5/2	+3.1718
		187*	112	186.95583	5/2	+3.2043
74	OS	184	108	183.95275		
		186	110	185.95387		
		187	111	186.95583		
		188	112	187.95608		
		189	113	188.95830		
		190	114	189.95863		
		192	116	191.96145		
77	Ir	191	114	190.96064	3/2	+0.16
		193	116	192.96301	3/2	+0.17
78	Pt	190*	112	189.95995		
		192	114	191.96115		
		194	116	193.96272		
		195	117	194.96481	1/2	+0.60602
		196	118	195.96497		
		198	120	197.96790		
79	Au	197	118	196.96654	3/2	+0.74485
80	Hg	196	116	195.96582		
		198	118	197.96676		
		199	119	198.96828	1/2	+0.502702
		200	120	199.96833		
		201	121	200.97031	3/2	-0.556701
		202	122	201.9'7064		
		204	124	203.97349		
81	Tl	203	122	202.972353	1/2	+1.61169
		205	124	204.974442	1/2	+1.62254
		206*	125	205.976104		
		207*	126	206.977450		
		208*	127	207.982813		
		209*	128	208.985296		
		210*	129	209.990054		
82	Pb	204	122	203.973044		
		206	124	205.974468		
		207	125	206.975903	1/2	+0.5895
		208	126	207.976650		
		209	127	208.981082		
		210*	128	209.984187		
		211*	129	210.988742		
		212*	130	211.991905		
		214*	132	213.99977		
83	Bi	209	126	208.980394	9/2	+4.0802
		210*	127	209.984121		
		211*	128	210.987300		
		212*	129	211.991279		
		213*	130	212.994317		
		214*	131	213.998686		

Z	Element	A	N	Atomic Mass	Spin *I*	μ (nuclear magnetons)
84	PO	209*	125	208.982426	1/2	
		210*	126	209.982876		
		211*	127	210.986657		
		212*	128	211.988866		
		213*	129	212.992825		
		214'	130	213.995201		
		215*	131	214.999423		
		216*	132	216.001922		
		218*	134	218.008930		
85	At	215*	130	214.998663		
		216*	131	216.002411		
		217*	132	217.004648		
		218*	133	218.008607		
86	Rn	219*	133	219.009481		
		220*	134	220.011401		
		222*	136	222.017531		
87	Fr	221'	134	221.014183		
		223*	136	223.019736		
88	Ra	223*	135	223.018501		
		224*	136	2'24.02021		
		225*	137	2'25.02352		
		226*	138	2'26.02536		
		228*	140	2'28.03114		
89	Ac	225*	136	2'25.02315		
		227'	138	227.02775		
		228*	139	228.03108		
90	Th	227*	137	227.02771		
		228*	138	228.02875		
		229*	139	229.03165		
		230*	140	230.03309		
		231*	141	231.03629		
		232*	142	232.03812		
91	Pa	231*	140	231.03588		
		233*	142	233.04013		
		234*	143	234.04330		
92	U	233'	141	233.03952		
		234*	142	234.04090		
		235*	143	235.04392		
		238*	146	238.05377	7/2	
93	Np	237*	144	237.04806		
94	Pu	240*	146	240.05388		
95	A m	241'	146	241.05671	5/2	l-l.4

appendix 4

SOME PHYSICAL CONSTANTS AND CONVERSIONS[1]

Table of physical constants

Speed of light, $c = 2.998 \times 10^{8}$ m/sec.

Planck's constant, $h = 6.626 \times 10^{-34}$ joule-sec.

$\hbar = h/2\pi = 1.0545 \times 10^{-34}$ joule-sec.

Reciprocal of fine structure constant, $1/\alpha = 1/(e^2/4\pi\epsilon_0\hbar c) = 137.04$.

Gravitational constant, $G = 6.67 \times 10^{-11}$ nt-m^2/kg^2.

Boltzmann constant, $k_B = 1.381 \times 10^{-23}$ joule/K.

Avogadro's number, $N_0 = 6.022 \times 10^{23}$/mole.

Gas constant, $R = N_0 k_B = 8.31$ joule/K-mole $= 1.99$ calories/K-mole.

Electron:

Charge, $e = 1.602 \times 10^{-19}$ coulombs;

Mass, $m_e = 9.109 \times 10^{-31}$ kg $= 0.5110$ MeV;

Magnetic moment (Bohr magneton), $\mu_B = e\hbar/2m_e$
$= 9.273 \times 10^{-24}$ joule/(weber/m^2);

Compton wavelength, $\lambda_c = h/m_e c = 2.426 \times 10^{-12}$ m;

Bohr radius, $a = 4\pi\epsilon_0\hbar/m_e e^2 = 5.2917 \times 10^{-11}$ m;

Rydberg constant, $R_\infty = \frac{1}{2} m_e e^4/\hbar c(4\pi\epsilon_0\hbar)^2 = 1.0973731 \times 10^{7}$/m.

Proton:

Mass, $m_p = 1.673 \times 10^{-27}$ kg $= 938.2$ MeV $= 1836.1\, m_e$;

Nuclear magneton, $\mu_N = e\hbar/2m_p = 5.051 \times 10^{-27}$ joule/(weber/m^2).

Constant in Coulomb's law, $1/(4\pi\epsilon_0) = 8.987 \times 10^{9}$ nt-m^2/coul^2.

Stefan-Boltzmann constant in black body radiation,

$\sigma = 2\pi^5 k_B^4/15c^3h^3 = 5.67 \times 10^{-8}$ watts/m^2-K^4.

Table of conversions

1 radian = 57.3 degrees; 1 degree = 0.01745 radians

1 amu = 1.660×10^{-27} kg = 931.48 MeV

1 eV = 1.602×10^{-19} j; 1 j = 6.242×10^{18} eV

1 MeV = 1.602×10^{-13} j

1 fermi = 10^{-15} m

1 Angstrom = 10^{-10} m

1 foot = 0.3048 m; 1 m = 3.281 ft.

1 mile = 1.609 km; 1 km = 0.621 mi

1 burn = 10^{-28} m^2

1 day = 86400 sec

1 year = 3.156×10^{7} sec

1 curie = 3.7×10^{10} disintegrations/sec.

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