LECTURE NOTES

ON QUANTUM MECHANICS

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Contents

0.1 General Information

- **Aim/Following-up**: The course provides an introduction to advanced techniques in quantum mechanics and their application to several selected topics in condensed matter physics.
- **Contents**: Dirac notation and formalism, time evolution of quantum systems, angular momentum theory, creation and annihilation operators (the second quantization representation), symmetries and conservation laws, permutation symmetry and identical particles, quantum statistics, non-degenerate and degenerate perturbation theory, time-dependent perturbation theory, the variational method
- **Prerequisites**: PHYS2321, PHYS2322, PHYS2323, and PHYS2325
- **Co-requisite**: Nil
- **Teaching**: 36 hours of lectures and tutorial classes
- **Duration**: One semester (1st semester)
- **Assessment**: One-three hour examination (70%) and course assessment (30%)
- **Textbook**: J. J. Sakurai, Modern Quantum Mechanics (Addison-Wesley, 1994)
- **Web page:** http://bohr.physics.hku.hk/~phys3332/ All lectures notes in pdf files can be download from the site.

- **References**: L. Schiff, Quantum Mechanics (McGraw-Hill, 1968, 3nd ed.); Richard Feynman, Robert B. Leighton, and Matthew L. Sands, Feynman Lectures on Physics Vol. III, (Addison-Wesley Publishing Co., 1965); L. D. Landau and E. M. Lifshitz, Quantum Mechanics

Time and Venue: Year 2004 (Weeks 2 – 14)

11:40 -12:30: Monday/S802

11:40 -12:30: Wednesday/S802

11:40 -12:30: Friday/S802

Numerical values of some physical quantities

$$\begin{aligned}
\hbar &= 1.054 \times 10^{-27}\text{erg-sec (Planck's constant divided by } 2\pi \\
e &= 4.80 \times 10^{-10}\text{ esu (magnitude of electron charge)} \\
m &= 0.911 \times 10^{-27}\text{g (electron mass)} \\
M &= 1.672 \times 10^{-24}\text{g (proton mass)} \\
a_0 &= \hbar^2/me^2 = 5.29 \times 10^{-9}\text{ cm (Bohr radius)} \\
e^2/a_0 &= 27.2\text{eV (twice binding energy of hydrogen)} \\
c &= 3.00 \times 10^{10}\text{cm/sec (speed of light)} \\
\hbar c/e^2 &= 137\text{ (reciprocal fine structure constant)} \\
e\hbar/2mc &= 0.927 \times 10^{-20}\text{erg/oersted (Bohr magneton)} \\
mc^2 &= 5.11 \times 10^{5}\text{eV (electron rest energy)} \\
Mc^2 &= 938\text{MeV (proton rest energy)} \\
1\text{eV} &= 1.602 \times 10^{-12}\text{erg} \\
1\text{ eV/c} &= 12,400\text{Å} \\
1\text{eV} &= 11,600\text{K}
\end{aligned}$$

Chapter 1

Fundamental Concepts

At the present stage of human knowledge, quantum mechanics can be regarded as the fundamental theory of atomic phenomena. The experimental data on which it is based are derived from physical events that almost entirely beyond the range of direct human perception. It is not surprising that the theory embodies physical concepts that are foreign to common daily experience.

The most traditional way to introduce the quantum mechanics is to follow the historical development of theory and experiment – Planck's radiation law, the Einstein-Debye's theory of specific heat, the Bohr atom, de Broglie's matter wave and so forth – together with careful analysis of some experiments such as diffraction experiment of light, the Compton effect, and Franck-Hertz effect. In this way we can enjoy the experience of physicists of last century to establish the theory. In this course we do not follow the historical approach. Instead, we start with an example that illustrates the inadequacy of classical concepts in a fundamental way.

1.1 Relation between experimental interpretations and theoretical inferences

Schiff's book has a good introduction to this theory. Please read the relevant chapter in the book after class. Here we just list several experiments which played key roles in development of quantum theory.

Experimental facts

- Electromagnetic wave/light: Diffraction (Young, 1803; Laue, 1912))
- Electromagnetic quanta /light: Black body radiation (Planck, 1900); Photoelectric effect (Einstein, 1904); Compton effect (1923); Combination Principle (Rita-Rydberg, 1908)
- Discrete values for physical quantities: Specific heat (Einstein 1907, Debye 1912); Franck-Hertz experiment (1913); Stern-Gerlach experiment (1922)

Theoretical development

- Maxwell's theory for electromagnetism: Electromagnetic wave (1864)
- Planck's theory for black body radiation: $E = \hbar\omega$: Electromagnetic quanta (1900)
- de Broglie's theory: $P = h/\lambda$: Wave-Particle Duality, (1924)
- Birth of quantum mechanics: Heisenberg's theory (1926); Schrodinger's theory (1926)

1.2 Materials from Britannica Online

1.2.1 Photoelectric effect

The phenomenon in which charge particles are released from a material when it absorbs radiant energy. The photoelectric effect commonly is thought of as the ejection of electrons from the surface of a metal plate when light falls on it. In the broad sense, however, the phenomenon can take place when the radiant energy is in the region of visible or ultraviolet light, X rays, or gamma rays; when the material is a solid, liquid, or gas; and when the particles released are electrons or ions (charged atoms or molecules).

The photoelectric effect was discovered in 1887 by a German physicist, Heinrich Rudolf Hertz, who observed that ultraviolet light changes the lowest voltage at which sparking takes place between given metallic electrodes. At the close of the 19th century, it was established that a cathode ray (produced by an electric discharge in a rarefied-gas atmosphere) consists of discrete particles, called electrons, each bearing an elementary negative charge. In 1900 Philipp Lenard, a German physicist, studying the electrical charges liberated from a metal surface when it was illuminated, concluded that these charges were identical to the electrons observed in cathode rays. It was further discovered that the current (given the name photoelectric because it was caused by light rays), made up of electrons released from the metal, is proportional to the intensity of the light causing it for any fixed wavelength of light that is used. In 1902 it was proved that the maximum kinetic energy of an electron in the photoelectric effect is independent of the intensity of the light ray and depends on its frequency.

The observations that (1) the number of electrons released in the photoelectric effect is proportional to the intensity of the light and that (2) the frequency, or wavelength, of

light determines the maximum kinetic energy of the electrons indicated a kind of interaction between light and matter that could not be explained in terms of classical physics. The search for an explanation led in 1905 to Albert Einstein's fundamental theory that light, long thought to be wavelike, can be regarded alternatively as composed of discrete particles (now called photons), equivalent to energy quanta.

In explaining the photoelectric effect, Einstein assumed that a photon could penetrate matter, where it would collide with an atom. Since all atoms have electrons, an electron would be ejected from the atom by the energy of the photon, with great velocity. The kinetic energy of the electron, as it moved through the atoms of the matter, would be diminished at each encounter. Should it reach the surface of the material, the kinetic energy of the electron would be further reduced as the electron overcame and escaped the attraction of the surface atoms. This loss in kinetic energy is called the work function , symbolized by omega (ω). According to Einstein, each light quantum consists of an amount of energy equal to the product of Planck's universal constant (h) and the frequency of the light (indicated by the Greek ν). Einstein's theory of the photoelectric effect postulates that the maximum kinetic energy of the electrons ejected from a material is equal to the frequency of the incident light times Planck's constant, less the work function. The resulting photoelectric equation of Einstein can be expressed by $E_k = h\nu - \omega$, in which E_k is the maximum kinetic energy of the ejected electron, h is a constant, later shown to be numerically the same as Planck's constant, ν is the frequency of the incident light, and ω is the work function.

The kinetic energy of an emitted electron can be measured by placing it in an electric field and measuring the potential or voltage difference (indicated as V) required to reduce its velocity to zero. This energy is equal to the product of the potential difference and an electron's charge, which is always a constant and is indicated by e; thus, $E_k = eV$.

The validity of the Einstein relationship was examined by many investigators and found to be correct but not complete. In particular, it failed to account for the fact that the emitted electron's energy is influenced by the temperature of the solid. The remedy to this defect was first formulated in 1931 by a British mathematician, Ralph Howard Fowler, who, on the assumption that all electrons with energies greater than the work function would escape, established a relationship between the photoelectric current and the temperature: the current is proportional to the product of the square of the temperature and a function of the incident photon's energy. The equation is $I = \alpha A T^2 \phi(x)$, in which I is the photoelectric current, a and A are constants, and $\phi(x)$ is an exponential series, whose numerical values have been tabulated; the dimensionless value x equals the kinetic energy of the emitted electrons divided by the product of the temperature and the Boltzmann constant of the kinetic theory: $x = (h\nu - \omega)/kT$; in which x is the argument of the exponential series.

1.2.2 Frank-Hertz experiment

in physics, first experimental verification of the existence of discrete energy states in atoms, performed (1914) by the German-born physicists James Franck and Gustav Hertz .

Franck and Hertz directed low-energy electrons through a gas enclosed in an electron tube. As the energy of the electrons was slowly increased, a certain critical electron energy was reached at which the electron stream made a change from almost undisturbed passage through the gas to nearly complete stoppage. The gas atoms were able to absorb the energy of the electrons only when it reached a certain critical value, indicating that within the gas atoms themselves the atomic electrons make an abrupt transition to a discrete higher energy level. As long as the bombarding electrons have less than this discrete amount of energy, no transition is possible and no energy is absorbed from the stream of electrons.

When they have this precise energy, they lose it all at once in collisions to atomic electrons, which store the energy by being promoted to a higher energy level.

1.2.3 Compton effect

increase in wavelength of X rays and other energetic electromagnetic radiations that have been elastically scattered by electrons; it is a principal way in which radiant energy is absorbed in matter. The effect has proved to be one of the cornerstones of quantum mechanics, which accounts for both wave and particle properties of radiation as well as of matter.

The American physicist Arthur Holly Compton explained (1922; published 1923) the wavelength increase by considering X rays as composed of discrete pulses, or quanta, of electromagnetic energy, which he called photons . Photons have energy and momentum just as material particles do; they also have wave characteristics, such as wavelength and frequency. The energy of photons is directly proportional to their frequency and inversely proportional to their wavelength, so lower-energy photons have lower frequencies and longer wavelengths. In the Compton effect, individual photons collide with single electrons that are free or quite loosely bound in the atoms of matter. Colliding photons transfer some of their energy and momentum to the electrons, which in turn recoil. In the instant of the collision, new photons of less energy and momentum are produced that scatter at angles the size of which depends on the amount of energy lost to the recoiling electrons.

Because of the relation between energy and wavelength, the scattered photons have a longer wavelength that also depends on the size of the angle through which the X rays were diverted. The increase in wavelength or Compton shift does not depend on the wavelength of the incident photon.

The Compton effect was discovered independently by the physical chemist Peter

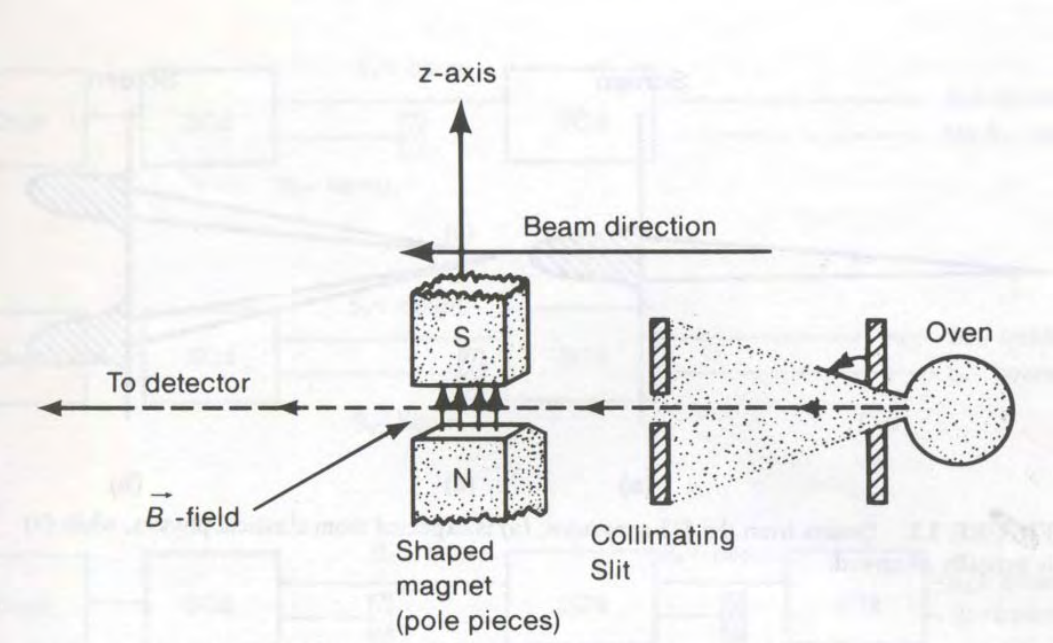


FIGURE 1.1. The Stern-Gerlach experiment.

Figure 1.1: The Stern-Gerlach Experiment

Debye in early 1923.

1.3 The Stern-Gerlach Experiment

We start with the Stern-Gerlach experiment to introduce some basic concepts of quantum mechanics. The two-state problem can be regarded as the most quantum. A lot of important discoveries are related to it. It is worthy studying very carefully. We shall repeat to discuss the problem throughout this course.

1.3.1 The Stern-Gerlach experiment

Oven: silver atoms (Ag) are heated in the oven. The oven has a small hole through which some of the silver atoms escape to form an atomic beam.

Ag: (Electron configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^1$). The outer

shell has only ONE electron ($5s^1$) . The atom has an angular momentum., which is due solely to the spin of 47^{th} electron.

Collimating slit: change the diverging Ag beam to a parallel beam.

Shaped Magnet: N and S are north and south poles of a magnet. The knife-edge of S results in a much stronger magnetic field at the point P than Q . i.e. the magnet generates an inhomogeneous magnetic field.

Role of the inhomogeneous field: to change the direction of the Ag beam. The interaction energy is $E = -\mu \cdot \mathbf{B}$. The force experienced by the atoms is

$$m\vec{a} = \frac{\partial}{\partial z}(\mu \cdot \mathbf{B}) \approx \mu_z \frac{\partial B_z}{\partial z}$$

If the magnetic field is uniform , i.e. $\frac{\partial B_z}{\partial z} = 0.$, the Ag beam will not change its direction. In the field different magnetic moments experience different force, and the atoms with different magnetic moments will change different angles after the beams pass through the shaped magnet. Suppose the length of the shaped magnet L. It takes a time L/v for particles to go though the magnets. The angle is about

$$\frac{a\Delta t}{v} = \frac{\frac{\mu_z}{m}\frac{\partial B_z}{\partial z}\frac{L}{v}}{v} = \frac{\mu_z \frac{\partial B_z}{\partial z} L}{mv^2} = \mu_z \frac{\partial B_z}{\partial z} L/2E_k \propto \mu_z.$$

They will reach at different places on the screen.

Classically: all values of $\mu_z = \mu\cos\theta$ $(0 < \theta < \pi)$ would be expected to realize between $|\mu|$ and $-|\mu|$. It has a continuous distribution.

Experimentally: only two values of z component of $\vec{S}$ are observed (electron spin $\vec{\mu} \propto \vec{S}$)

Consequence: the spin of electron has two discrete values along the magnetic

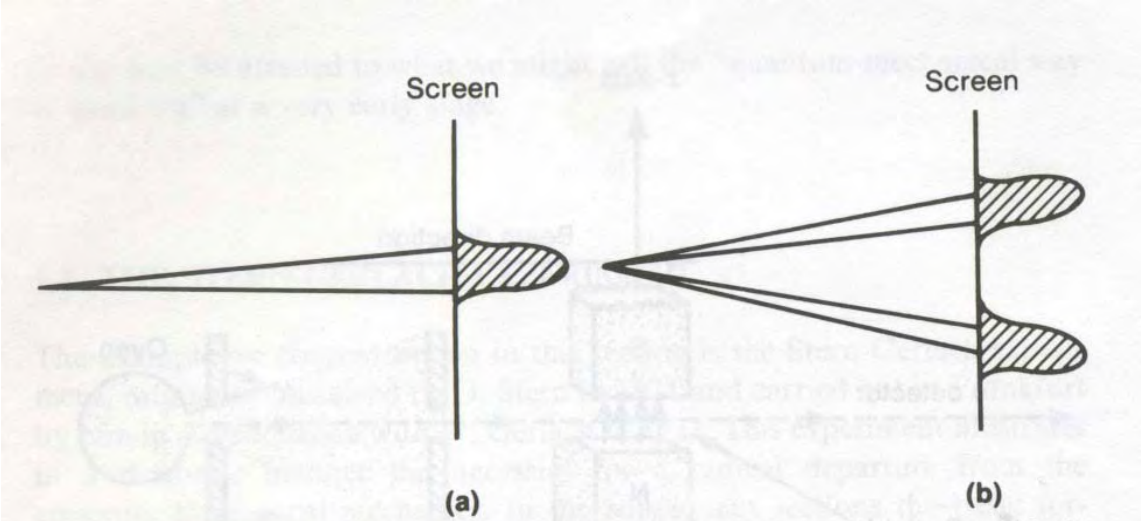


FIGURE 1.2. Beams from the SG apparatus; (a) is expected from classical physics, while (b) is actually observed.

Figure 1.2: Beam from the Stern-Gerlach apparatus: (a) is expected from classical physics, while (b) is actually observed experimentally.

field

$$S = \begin{cases} \hbar/2 \\ -\hbar/2 \end{cases}$$

$$\hbar = 1.0546 \times 10^{-27}\text{erg.s} = 6.5822 \times 10^{-16}\text{eV.s}$$

$----$ Planck's constant divided by 2π

It should be noted that the constant cannot be determined accurately from this experiment.

1.3.2 Sequential Stern-Gerlach Experiment

SG$\hat{z}$ stands for an apparatus with inhomogeneous magnetic field in z direction, and SGx in x direction

Case(a): no surprising!

Case(b): S_z+ beam is made up of 50% S_x+ and 50% S_x-? S_z- beam?

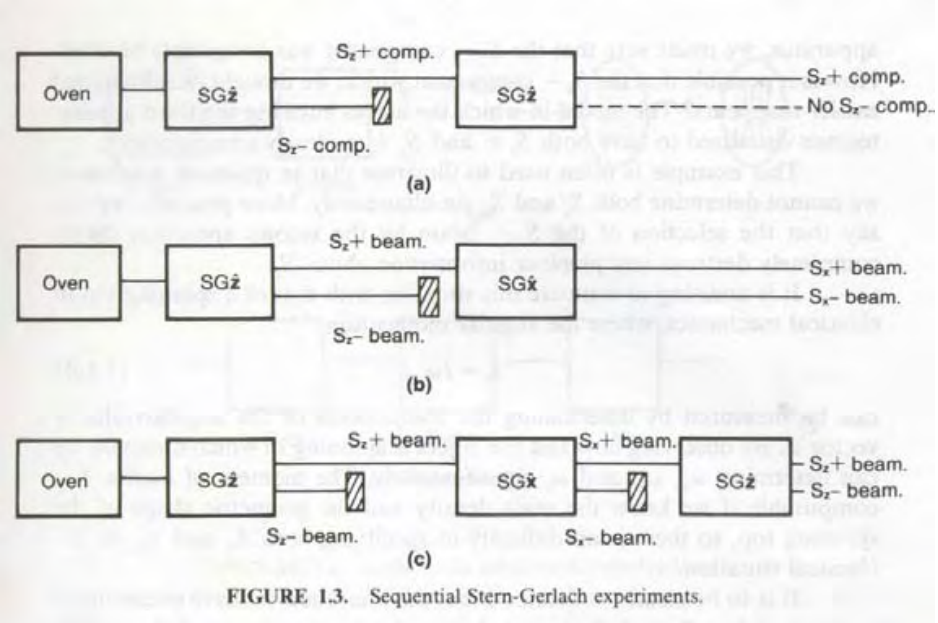


FIGURE 1.3. Sequential Stern-Gerlach experiments.

Figure 1.3: Sequential Stern-Gerlach experiment

Case(c): Since S_z- is blocked at the first step, why is S_x+ beam made up of both S_z+ and S_z- beams?

Consequences of S-G experiment:

- Spin space cannot be described by a 3-dimensional vector.
- The magnetic moment of atom or spin is discrete or quantized.
- We cannot determine both S_z and S_x simultaneously. More precisely, we can say that the selection of S_x+ beam by SG$\hat{\text{x}}$ completely destroys any previous information about S_z.

1.3.3 Analogy with Polarization of Light

It is very helpful if you compare the situation with the analogy of the polarized light through a Polaroid filter. The polarized light wave is described by a complex function,

$$\mathbf{E} = E_0 \hat{\mathbf{x}} \cos(kz - \omega t).$$

Please refer to Sakurai's book, P.6–10.

1.4 Dirac Notation and Operators

The Stern-Gerlach experiment shows that the spin space is not simply a 3-D vector space and lead to consider a complex vector space. There exists a good analogy with polarization of light. (Refer to Sakurai's book). In this section we formulate the basic mathematics of vector spaces as used in quantum mechanics. The theory of linear algebra has been known to mathematician before the birth of quantum mechanics, but the Dirac notation has many advantages. At the early time of quantum mechanics this notation was used to unify Heisenberg's matrix mechanics and Schrodinger's wave mechanics. The notation in this course was first introduced by P. A. M. Dirac.

Ket space: In quantum mechanics, a physical state, for example, a silver atom with definite spin orientation, is represented by a state vector in a complex vector space, denoted by $|\alpha\rangle$, a ket. The state ket is postulated to contain complete information about physical state. The dimensionality of a complex vector space is specified according to the nature of physical system under consideration.

An observable can be represented by **an operator A**

$$\mathbf{A}(|\alpha\rangle) = \mathbf{A}\,|\alpha\rangle$$

Eigenket and eigenvalue:

$$\mathbf{A}(|\alpha\rangle) = a\,|\alpha\rangle$$

Eigenstate: the physical state corresponding to an eigenket, $|\alpha\rangle$.

Two kets can be added to form a new ket: $|\alpha\rangle + |\beta\rangle = |\gamma\rangle$

One of the postulates is that $|\alpha\rangle$ and $c\,|\alpha\rangle$ with the number $c \neq 0$ represent the same physical state.

Bra space: a dual correspondence to a ket space. We postulate that corresponding to every ket there exist a bra. The names come from the word "bracket" → "bra-c-ket".

1. There exists a one-to one correspondence between a ket space and a bra space.

$$|\alpha\rangle \Longleftrightarrow \langle\alpha|$$

2. The bra dual to $c\,|\alpha\rangle$ (c is a complex number)

$$c\,|\alpha\rangle \Longleftrightarrow c^*\,\langle\alpha|$$

Inner product: In general, this product is a complex number.

$$\langle\beta|\alpha\rangle = (\langle\beta|) \cdot (|\alpha\rangle)$$

Two properties of the inner product:

1. $\langle\beta|\alpha\rangle$ and $\langle\alpha|\beta\rangle$ are complex conjugates of each other.

$$\langle\beta|\alpha\rangle = (\langle\alpha|\beta\rangle)^*$$

2. the postulate of positive definite metric.

$$\langle\alpha|\alpha\rangle \geq 0$$

where the equality sign holds only if $|\alpha\rangle$ is a null ket. From a physicist's point of view this postulate is essential for the probabilistic interpretation of quantum mechanics. Question: what happens if we postulate $\langle\alpha|\alpha\rangle \leq 0$?

Orthogonality:

$$\langle\alpha|\beta\rangle = 0.$$

Normalization: all vectors can be normalized!

$$|\tilde{\alpha}\rangle = \left(\frac{1}{\langle\alpha|\alpha\rangle}\right)^{\frac{1}{2}} |\alpha\rangle\,, \qquad \langle\tilde{\alpha}|\tilde{\alpha}\rangle = 1$$

The **norm** of $|\alpha\rangle$: $(\langle\alpha|\alpha\rangle)^{1/2}$

Operator: an operator acts on a ket from the left side, $\mathbf{x}\,|\alpha\rangle$, and the resulting product is another ket. An operator acts on a bra from the right side, $\langle\alpha|\,\mathbf{x}$,and the resulting product is another bra.

- – Equality: $\mathbf{x} = \mathbf{y}$ if $\mathbf{x}\,|\alpha\rangle = \mathbf{y}\,|\alpha\rangle$ for an arbitrary ket
- – Null operator: $\mathbf{x}\,|\alpha\rangle = 0$ for arbitrary $|\alpha\rangle$
- – Hermitian operator: $\mathbf{x} = \mathbf{x}^{\dagger}$
- – $\mathbf{x}\,|\alpha\rangle \longleftrightarrow \langle\alpha|\,\mathbf{x}^{\dagger}$

Multiplication

- – Noncommutative: $\mathbf{xy} \neq \mathbf{yx}$
- – Associative: $\mathbf{x}(\mathbf{yz}) = (\mathbf{xy})\mathbf{z} = \mathbf{xyz}$

– Hermitian adjoint: $(\mathbf{xy})^\dagger = \mathbf{y}^\dagger \mathbf{x}^\dagger$ (Prove it!)

$$\mathbf{y}\,|\alpha\rangle \quad \Rightarrow \quad \langle\alpha|\,\mathbf{y}^\dagger$$

$$\mathbf{xy}\,|\alpha\rangle \quad = \quad \mathbf{x}\,(\mathbf{y}\,|\alpha\rangle) \Rightarrow \left(\langle\alpha|\,\mathbf{y}^\dagger\right)\mathbf{x}^\dagger = \langle\alpha|\,\mathbf{y}^\dagger\mathbf{x}^\dagger$$

Outer product: $|\alpha\rangle\langle\beta|$ is an operator!

The associative axiom of multiplication: the associative property holds as long as we are dealing with "legal" multiplications among kets, bras, and operators.

1. $(|\alpha\rangle\langle\beta|)\cdot|\gamma\rangle = |\alpha\rangle\,(\langle\beta|\,|\gamma\rangle)$;

2. $(\langle\beta|)\cdot(\mathbf{x}\,|\alpha\rangle) = (\langle\beta|\,\mathbf{x})\cdot(|\alpha\rangle) \equiv \langle\beta\,|\mathbf{x}|\,\alpha\rangle$;

3. $\langle\beta\,|\mathbf{x}|\,\alpha\rangle = \langle\beta|\cdot(\mathbf{x}\,|\alpha\rangle) = \{(\langle\alpha|\,\mathbf{x}^\dagger)\cdot|\beta\rangle\}^* \equiv \left\langle\alpha\left|\mathbf{x}^\dagger\right|\beta\right\rangle^*$.

1.5 Base kets and Matrix Representation

1.5.1 Eigenkets of an Observable

The operators for observables must be Hermitian as physical quantities must be real.

1). The eigenvalues of a Hermitian operator $\mathbf{A}$ are real.

Proof. First, we recall the definitions

$$\mathbf{A}\,|a\rangle = a\,|a\rangle \Longleftrightarrow \langle a|\,\mathbf{A}^\dagger = \langle a|\,a^*$$

$$\langle a|\,\mathbf{A}\,|a\rangle = a \Leftrightarrow \langle a|\,\mathbf{A}^\dagger\,|a\rangle = a^*$$

$$\text{If } \mathbf{A} = \mathbf{A}^\dagger \Longrightarrow a = a^*.$$

■

2). The eigenkets of Hermitian A corresponding to different eigenvalues are orthogonal.

Proof.

$$\mathbf{A}\left|a\right\rangle = a\left|a\right\rangle \Longrightarrow \left\langle a'\right|\mathbf{A}\left|a\right\rangle = a\left\langle a'|a\right\rangle$$

$$\left\langle a'\right|\mathbf{A}^{\dagger} = \left\langle a'\right|a' \Longrightarrow \left\langle a'\right|\mathbf{A}\left|a\right\rangle = a'\left\langle a'|a\right\rangle$$

We have

$$(a-a')\left\langle a'|a\right\rangle = 0 \Longrightarrow \left\langle a'|a\right\rangle = 0$$

It is conventional to normalize all eigenkets $|a'\rangle$ of $\mathbf{A}$ so that $\{|a'\rangle\}$ form an orthogonal set: $\langle a"|a'\rangle = \delta_{a',a''}$. ■

1.5.2 Eigenkets as Base kets:

1. All normalized eigenkets of an observable $\mathbf{A}$ form a complete and orthonormal set. $\{\left|a^{(n)}\right\rangle\}$. The number of the eigenkets is equal to the dimensionality of the complex vector space.

2. An arbitrary ket in the ket space can be expanded in terms of the eigenkets of $\mathbf{A}$:

$$\left|\alpha\right\rangle = \sum_n C_n \left|a^{(n)}\right\rangle \Longrightarrow \left\langle a^{(n)}|\alpha\right\rangle = C_n$$

3. The completeness relation (or closure):

$$\sum_n \left|a^{(n)}\right\rangle\left\langle a^{(n)}\right| = 1$$

$$
\begin{aligned}
& (\sum_n \left|a^{(n)}\right\rangle \left\langle a^{(n)}\right|)(\sum_m \left|a^{(m)}\right\rangle \left\langle a^{(m)}\right|) \\
= & \sum_{m.n} \left|a^{(n)}\right\rangle \left\langle a^{(n)} \left|a^{(m)}\right\rangle \right\langle a^{(m)}\right| = \sum_{m.n} \left|a^{(n)}\right\rangle \delta_{mn} \left\langle a^{(m)}\right| \\
= & \sum_n \left|a^{(n)}\right\rangle \left\langle a^{(n)}\right| \Longrightarrow (\sum_n \left|a^{(n)}\right\rangle \left\langle a^{(n)}\right|)(\sum_m \left|a^{(m)}\right\rangle \left\langle a^{(m)}\right| - 1) = 0
\end{aligned}
$$

This relation is very essential to develop the general formalism of quantum mechanics.

4. Projection operator: $P_n = \left|a^{(n)}\right\rangle \left\langle a^{(n)}\right|$

$$P_n \left|\alpha\right\rangle = \left|a^{(n)}\right\rangle \left\langle a^{(n)}\right| \alpha\rangle = C_n \left|a^{(n)}\right\rangle$$

P_n selects that portion of the ket $|\alpha\rangle$ parallel to $\left|a^{(n)}\right\rangle$: $P_n \cdot P_n = P_n$ such that P_n's eigenvalues are either 1 or 0.

$$
\begin{aligned}
P_n \cdot P_n &= (\left|a^{(n)}\right\rangle \left\langle a^{(n)}\right|)(\left|a^{(n)}\right\rangle \left\langle a^{(n)}\right|) \\
&= \left|a^{(n)}\right\rangle \left\langle a^{(n)}|a^{(n)}\right\rangle \left\langle a^{(n)}\right| \\
&= \left|a^{(n)}\right\rangle \left\langle a^{(n)}\right| = P_n
\end{aligned}
$$

1.5.3 Matrix Representation:

Having specified the base kets, we show how to represent an operator, say $\mathbf{X}$, by a square matrix.

$$
\begin{aligned}
\mathbf{X} &= (\sum_n \left|a^{(n)}\right\rangle \left\langle a^{(n)}\right|)\mathbf{X}(\sum_m \left|a^{(m)}\right\rangle \left\langle a^{(m)}\right|) \\
&= \sum_{m.n} \left|a^{(n)}\right\rangle \left\langle a^{(n)}\right| \mathbf{X} \left|a^{(m)}\right\rangle \left\langle a^{(m)}\right| \\
&= \sum_{m.n} (\left\langle a^{(n)}\right| \mathbf{X} \left|a^{(m)}\right\rangle) \left|a^{(n)}\right\rangle \left\langle a^{(m)}\right| = \sum_{m.n} X_{nm} \left|a^{(n)}\right\rangle \left\langle a^{(m)}\right|
\end{aligned}
$$

Let us assume that $\langle a^{(n)}| = (0, \cdots, 0, 1, \cdots)$ and

$$|a^{(n)}\rangle = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ \vdots \end{pmatrix}$$

Thus the outer product of $\langle a^{(m)}|$ and $|a^{(n)}\rangle$ gives a new operator in the form of square matrix,

$$|a^{(n)}\rangle\langle a^{(m)}| = \begin{pmatrix} 0 & \cdots & 0 & \cdots \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

Thus $\mathbf{X}$ can be expressed in a matrix form,

$$\mathbf{X} = \begin{pmatrix} \langle a^{(1)}|\mathbf{X}|a^{(1)}\rangle & \langle a^{(1)}|\mathbf{X}|a^{(2)}\rangle & \cdots \\ \langle a^{(2)}|\mathbf{X}|a^{(1)}\rangle & \langle a^{(2)}|\mathbf{X}|a^{(2)}\rangle & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}.$$

For an operator A which eigenstates are $|a^{(n)}\rangle$

$$\mathbf{A} = \begin{pmatrix} a^{(1)} & 0 & \cdots \\ 0 & a^{(2)} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

Basic Matrix Operations:

1. Transpose: $\mathbf{C} = \mathbf{A}^T \Longrightarrow c_{ij} = a_{ji}$

2. Addition: $\mathbf{C} = \mathbf{A} + \mathbf{B} \Longrightarrow c_{ij} = a_{ij} + b_{ij}$

3. Scalar-matrix multiplication: $\mathbf{C} = \alpha\mathbf{A} \Longrightarrow c_{ij} = \alpha a_{ij}$

4. Matrix-matrix multiplication: $\mathbf{C} = \mathbf{AB} \Longrightarrow c_{ij} = \sum_{k=1}^{r} a_{ik} \cdot b_{ki}$

1.6 Measurements, Observables & The Uncertainty Relation

1.6.1 Measurements

"Measurement" has special meaning in quantum mechanics. It is a physical operation procedure. It is quite different from that in classical physics. In the classic case the measurement reflects the state of an object, such as position, velocity, and energy. The process of measurement does not change the state of the object. For instance we measure your body height, which does not change your body height. In the quantum case the process of measurement changes the state of the object. If we want to measure the spin state of electron we have to let electron go through the Stern-Gerlach apparatus. The magnetic field changes the spin state, and select one of the eigenstates along the direction of the magnetic field. This is not a particular easy subject for a beginner. Let us first read the words of the great master, P. A. M. Dirac, for guidance.

"*A measurement always causes the system to jump into an eigenstate of the dynamic variable that is being measured .*"

—P.A.M. Dirac

Interpretation word by word:

1. Before the measurement of observable A is made, the system is assumed to be repre-

sented by some linear combination

$$|\alpha\rangle = (\sum_n \left|a^{(n)}\right\rangle \left\langle a^{(n)}\right| \alpha\rangle = \sum_n c_n \left|a^{(n)}\right\rangle$$

2. When the measurement is performed, the system is "thrown into" one of the eigenstates, say $\left|a^{(1)}\right\rangle$, of the observable

$$|\alpha\rangle \xrightarrow{\text{A measurement}} \left|a^{(1)}\right\rangle$$

3. **A** measurement usually changes the state. When the measurement causes $|\alpha\rangle$ to change into $\left|a^{(1)}\right\rangle$ it is said that **A** is measured to be $a^{(1)}$!

1.6.2 Spin1/2 system

We are ready to derive the spin 1/2 operator we encounter in the Stern-Gerlach experiment. The eigenvalues of $\mathbf{S}_z$ are $\pm\hbar/2$. We denote the corresponding eigenkets as $|+\rangle$ and $|-\rangle$, respectively,

$$\langle +|+\rangle \equiv \langle -|-\rangle \equiv 1; \quad \langle +|-\rangle = 0.$$

$|+\rangle$ and $|-\rangle$ form a complete (?) and orthonormal (?) set of basis. From the completeness relation: $\mathbf{1} = (|+\rangle\langle +|) + (|-\rangle\langle -|)$, we have

$$\left.\begin{array}{c} \mathbf{S}_z|+\rangle = \frac{\hbar}{2}|+\rangle \\ \mathbf{S}_z|-\rangle = -\frac{\hbar}{2}|-\rangle \end{array}\right\} \Leftrightarrow \left.\begin{array}{c} \mathbf{S}_z|+\rangle\langle +| = \frac{\hbar}{2}|+\rangle\langle +| \\ \mathbf{S}_z|-\rangle\langle -| = -\frac{\hbar}{2}|-\rangle\langle -| \end{array}\right\}$$

$$\mathbf{S}_z(|+\rangle\langle +| + |-\rangle\langle -|) = \frac{\hbar}{2}(|+\rangle\langle +| - |-\rangle\langle -|)$$

$$\mathbf{S}_z = \frac{\hbar}{2}(|+\rangle\langle +| - |-\rangle\langle -|)$$

Let us construct two operators:

$$\mathbf{S}_+ = \hbar|+\rangle\langle -|$$

$$\mathbf{S}_- = \hbar|-\rangle\langle +|$$

From the definition, we get

$$\begin{cases} \mathbf{S}_+ |+\rangle = \hbar |+\rangle \langle -|+\rangle = 0 \\ \mathbf{S}_+ |-\rangle = \hbar |+\rangle \langle -|-\rangle = \hbar |+\rangle \end{cases}$$

$$\begin{cases} \mathbf{S}_- |+\rangle = \hbar |-\rangle \langle +|+\rangle = \hbar |-\rangle \\ \mathbf{S}_- |-\rangle = \hbar |-\rangle \langle +|-\rangle = 0 \end{cases}$$

Let

$$|+\rangle \equiv \begin{pmatrix} 1 \\ \\ 0 \end{pmatrix}; \ |-\rangle \equiv \begin{pmatrix} 0 \\ \\ 1 \end{pmatrix}$$

On the base, we have

$$\mathbf{S}_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ \\ 0 & -1 \end{pmatrix}; \ \mathbf{S}_+ = \hbar \begin{pmatrix} 0 & 1 \\ \\ 0 & 0 \end{pmatrix}; \ \mathbf{S}_- = \hbar \begin{pmatrix} 0 & 0 \\ \\ 1 & 0 \end{pmatrix}$$

1.6.3 Probability Postulate

The probability for jumping into some particular $\left|a^{(n)}\right\rangle$ is given by

$$\text{the probability for } \left|a^{(n)}\right\rangle : \rho_n = \left|\left\langle a^{(n)}|\alpha\right\rangle\right|^2$$

provided that $|\alpha\rangle$ is normalized ($\langle\alpha|\alpha\rangle = 1$). ($|\alpha\rangle = \sum \left|a^{(n)}\right\rangle \left\langle a^{(n)}|\alpha\right\rangle$). **The expectation value** of A with respect to state $|\alpha\rangle$ is defined as

$$\begin{aligned} \langle \mathbf{A} \rangle &\equiv \langle \alpha | \mathbf{A} | \alpha \rangle = \sum_{n.m} \left\langle \alpha | a^{(n)} \right\rangle \left\langle a^{(n)} | \mathbf{A} | a^{(m)} \right\rangle \left\langle \alpha^{(m)} | a \right\rangle \\ &= \sum_n a^{(n)} \times \left| \left\langle \alpha | a^{(n)} \right\rangle \right|^2 = \sum_n a^{(n)} \rho_n \end{aligned}$$

where ρ_n is the probability in the state $\left|a^{(n)}\right\rangle$.

Selective measurement (or filtration)

We imagine a measurement process with a device that selects only one of the eigenket and rejects all others. Mathematically, we can say that such a selective measurement amounts to applying the projection operator.

1.6.4 $\mathbf{S}_x$ and $\mathbf{S}_y$

We are now in the position to determine the eigenkets of $\mathbf{S}_x$ and $\mathbf{S}_y$ and the operators from the results of sequential Stern-Gerlach experiments.(see Fig.1.3)

Case (b): The eigenstates of $\mathbf{S}_x$ and $\mathbf{S}_y$ can be expressed in terms of the eigenstates of $\mathbf{S}_z$. Similar to S_z:

$$\mathbf{S}_x = \frac{\hbar}{2}\left(|S_x+\rangle\langle S_x+| - |S_x-\rangle\langle S_x-|\right)$$

$$\text{From experiment} \implies |\langle +|S_x+\rangle|^2 = |\langle +|S_x-\rangle|^2 = 1/2$$

$$\text{From experiment} \implies |\langle -|S_x+\rangle|^2 = |\langle -|S_x-\rangle|^2 = 1/2$$

$$\implies \begin{cases} |S_x+\rangle = \frac{1}{2^{1/2}}|+\rangle + \frac{1}{2^{1/2}}e^{i\delta_1}|-\rangle \\ |S_x-\rangle = \frac{1}{2^{1/2}}|+\rangle + \frac{1}{2^{1/2}}e^{i\delta_1'}|-\rangle \end{cases}$$

$$\langle S_x + |S_x-\rangle = 0$$

$$\frac{1}{2}\langle +|+\rangle + \frac{1}{2}\langle -|-\rangle e^{-i\delta_1+i\delta_1'} = 0 \Rightarrow \delta_1' = \pi + \delta_1$$

$$\mathbf{S}_x = \frac{\hbar}{2}\left(|S_x+\rangle\langle S_x+| - |S_x-\rangle\langle S_x-|\right)$$

$$= \frac{\hbar}{2}(e^{-i\delta_1}|+\rangle\langle -| + e^{i\delta_1}|-\rangle\langle +|)$$

Likewise,

$$\mathbf{S}_y = \frac{\hbar}{2}(e^{-i\delta_2}|+\rangle\langle -| + e^{i\delta_2}|-\rangle\langle +|)$$

How to determine δ_1 and δ_2?

$$\text{From experiment } |\langle S_y \pm |S_x+\rangle|^2 = |\langle S_y \pm |S_x-\rangle|^2 = 1/2$$

$$\Longrightarrow \quad \delta_1 - \delta_2 = \pm\pi/2$$

We just can determine the difference of δ_1 and δ_2. For convenience we take $\mathbf{S}_x$ to be real such that,

$$\delta_1 = 0 \text{ and } \delta_2 = \pi/2.$$

Therefore,

$$|S_x\pm\rangle = \frac{1}{2^{1/2}}(|+\rangle \pm |-\rangle);$$

$$|S_y\pm\rangle = \frac{1}{2^{1/2}}(|+\rangle \pm i\,|-\rangle)$$

and

$$\mathbf{S}_x = \frac{\hbar}{2}(|+\rangle\langle -| + |-\rangle\langle +|)$$

$$\mathbf{S}_y = \frac{\hbar}{2}(-i\,|+\rangle\langle -| + i\,|-\rangle\langle +|)$$

In the form of matrix.

$$\mathbf{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \mathbf{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \mathbf{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The relations between $\mathbf{S}_x$, $\mathbf{S}_y$ and $\mathbf{S}_\pm$:

$$\mathbf{S}_+ = \mathbf{S}_x + i\mathbf{S}_y$$

$$\mathbf{S}_- = \mathbf{S}_x - i\mathbf{S}_y$$

Define

$$\mathbf{S}_\alpha \equiv \frac{\hbar}{2}\sigma_\alpha$$

where the dimensionless σ_α are called the Pauli matrices:

$$\boldsymbol{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \boldsymbol{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \boldsymbol{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The eigenvalues of these three matrixes are ± 1. (Please check it after class!)

1.6.5 The Algebra of Spin Operators

1. The commutation relations

$$\begin{aligned} [\mathbf{S}_x, \mathbf{S}_y] &= i\hbar \mathbf{S}_z; \\ [\mathbf{S}_y, \mathbf{S}_x] &= -i\hbar \mathbf{S}_z; \\ [\mathbf{S}_i, \mathbf{S}_j] &= i\epsilon_{ijk}\hbar \mathbf{S}_k \end{aligned}$$

$$\begin{pmatrix} \epsilon_{xyz} = \epsilon_{yzx} = \epsilon_{zyx} = 1 \\ \epsilon_{zyx} = \epsilon_{yxz} = \epsilon_{xzy} = -1 \end{pmatrix}$$

   ϵ_{ijk} is an antisymmetric tensor.

2. The anticommutation relations:

$$\{\mathbf{S}_i, \mathbf{S}_j\} = \frac{1}{2}\hbar^2 \delta_{ij}$$

3. The increasing and decreasing operators: $\mathbf{S}_\pm = \mathbf{S}_x \pm i\mathbf{S}_y$

$$\begin{aligned} [\mathbf{S}_z, \mathbf{S}_\pm] &= [\mathbf{S}_z, \mathbf{S}_x] \pm [\mathbf{S}_z, \mathbf{S}_y] = i\mathbf{S}_y \pm i(-i\mathbf{S}_x) \\ &= \pm \mathbf{S}_x + i\mathbf{S}_y \equiv \pm \mathbf{S}_\pm \\ [\mathbf{S}_-, \mathbf{S}_+] &= -2\mathbf{S}_z \end{aligned}$$

4. The square operator of $\vec{S}$

$$\begin{aligned} \mathbf{S}^2 &\equiv \mathbf{S}_x^2 + \mathbf{S}_y^2 + \mathbf{S}_z^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{3}{4}\hbar^2 \\ \frac{3}{4} &= \frac{1}{2} \times \left(1 + \frac{1}{2}\right) \end{aligned}$$

1.6.6 Observable

Compatible Observables: Observables **A** and **B** are defined to be compatible when the corresponding operators commute,

$$[\mathbf{A}, \mathbf{B}] = 0$$

and incompatible when

$$[\mathbf{A}, \mathbf{B}] \neq 0$$

Degeneracy: Suppose there are two or more linear independent eigenkets of A having the same eigenvalues then the eigenvalues of the two eigenkets are said to be degenerate.

If a ket $|\alpha\rangle$ is an eigenket for both A and B, i.e.

$$\mathbf{A}\,|\alpha\rangle = a\,|\alpha\rangle \qquad \mathbf{B}\,|\alpha\rangle = b\,|\alpha\rangle$$

the ket $|\alpha\rangle$ is a simultaneous eigenket of A and B. We can denote it by $|\alpha\rangle = |a, b\rangle$,e.g.

$$\begin{aligned} [\mathbf{S}^2, \mathbf{S}_z] &= 0 \\ \mathbf{S}^2\,|\pm\rangle &= \frac{3}{4}\hbar^2\,|\pm\rangle\,;\ \mathbf{S}_z\,|\pm\rangle = \pm\frac{\hbar}{2}\,|\pm\rangle \\ \mathbf{S}^2(\alpha\,|+\rangle + \beta\,|-\rangle) &= \frac{3}{4}\hbar^2(\alpha\,|+\rangle + \beta\,|-\rangle) \\ \mathbf{S}_z(\alpha\,|+\rangle + \beta\,|-\rangle) &= \frac{\hbar}{2}(\alpha\,|+\rangle - \beta\,|-\rangle) \end{aligned}$$

Theorem 1 *Suppose that A and B are compatible observable, and eigenvalues of A are nondegenerate. Then the matrix elements* $\langle a''|\mathbf{B}|a'\rangle$ *are all diagonal.* ($\mathbf{A}|\alpha\rangle = a|\alpha\rangle$)

Proof. Suppose $\mathbf{A}$ is diagonal on the basis ket $\{|a^{(n)}\rangle\}$

$$\mathbf{A}\left|\alpha^{(n}\right\rangle = a^{(n)}\left|\alpha^{(n)}\right\rangle$$

and all $a^{(n)} \neq a^{(m)}$ if $a \neq m$ A and B are compatible, $[\mathbf{A}, \mathbf{B}] = 0$

$$\begin{aligned} & \left\langle a^{(n)}\left|[\mathbf{A},\mathbf{B}]\right|a^{(m)}\right\rangle \\ = \quad & \left\langle a^{(n)}\left|[\mathbf{AB}-\mathbf{BA}]\right|a^{(m)}\right\rangle \\ = \quad & (a^{(n)}-a^{(m)})\left\langle a^{(n)}\left|\mathbf{B}\right|a^{(m)}\right\rangle = 0 \\ \Longrightarrow \quad & \left\langle a^{(n)}\left|\mathbf{B}\right|a^{(m)}\right\rangle = 0 \quad \text{if } n \neq m \end{aligned}$$

If $\mathbf{A}$ and $\mathbf{B}$ are compatible, we can always diagonalize them on one set of basis ket simultaneously no matter whether A has degenerate eigenvalues! ■

Measurement of $\mathbf{A}$ and $\mathbf{B}$ when $[\mathbf{A}, \mathbf{B}] = 0$

1. Nondegenerate

$$|\alpha\rangle \longrightarrow |a, b\rangle$$

2. Degenerate

$$\begin{aligned} |\alpha\rangle \quad & \longrightarrow \quad \sum_i c_a^{(i)}\left|a', b^{(i)}\right\rangle \\ & \longrightarrow \quad \left|a', b^{(i)}\right\rangle \end{aligned}$$

Whether or not there is degeneracy, A measurements and B measurements do not interfere. We can measure A and B accurately at the same time!

Incompatible Observables

1. Incompatible observables do not have a complete set of simultaneous eigenket.

Proof. Proof: Assume **A** and **B** are incompatible and $\{|a', b'\rangle\}$ is a complete set of simultaneous eigenkets. Then

$$\left.\begin{aligned} \mathbf{AB}\,|a', b'\rangle = \mathbf{A}b'\,|a', b'\rangle = a'b'\,|a', b'\rangle \\ \mathbf{BA}\,|a', b'\rangle = \mathbf{B}a'\,|a', b'\rangle = a'b'\,|a', b'\rangle \end{aligned}\right\}$$

$$(\mathbf{AB} - \mathbf{BA})\,|a', b'\rangle \quad = \quad [\mathbf{A}, \mathbf{B}]\,|a'b'\rangle = 0 \quad \text{for all } \{a'b'\}$$

$$\Longrightarrow \quad [\mathbf{A}, \mathbf{B}] = 0$$

This is in contradiction to the assumption! ■

1. Accidently, there may exist an simultaneous eigenket r a subset of simultaneous eigenket for incompatible A and B.

1.7 Change of Basis

Example 1

Spin 1/2 system:

Basis I:$\{|S_z : +\rangle\,,\ |S_z : -\rangle\}$

$$\mathbf{S}_z = \frac{\hbar}{2}(|S_z : +\rangle\langle S_z : +| - |S_z : -\rangle\langle S_z : -|)$$

$$\mathbf{S}_x = \frac{\hbar}{2}(|S_z : +\rangle\langle S_z : -| - |S_z : -\rangle\langle S_z : +|)$$

$$\mathbf{S}_y = \frac{\hbar}{2}(-i\,|S_z : +\rangle\langle S_z : -| + i\,|S_z : -\rangle\langle S_z : +|)$$

Basis II: $\{|S_x:+\rangle, |S_x:-\rangle\}$

$$\begin{aligned}
\mathbf{S}_x &= \frac{\hbar}{2}(|S_x:+\rangle\langle S_x:+| - |S_x:-\rangle\langle S_x:-|) \\
\mathbf{S}_y &= \frac{\hbar}{2}(|S_x:+\rangle\langle S_x:-| - |S_x:-\rangle\langle S_x:+|) \\
\mathbf{S}_z &= \frac{\hbar}{2}(-i|S_x:+\rangle\langle S_x:-| + i|S_x:-\rangle\langle S_x:+|)
\end{aligned}$$

Connection of two basis

$$|S_x:\pm\rangle = \frac{1}{2^{1/2}}|S_z:+\rangle \pm \frac{1}{2^{1/2}}|S_z:-\rangle$$

$$\begin{pmatrix} |S_x:+\rangle \\ |S_x:-\rangle \end{pmatrix} = \begin{pmatrix} \frac{1}{2^{1/2}} & \frac{1}{2^{1/2}} \\ \frac{1}{2^{1/2}} & -\frac{1}{2^{1/2}} \end{pmatrix} \begin{pmatrix} |S_z:+\rangle \\ |S_z:-\rangle \end{pmatrix}$$

1.7.1 Transformation Operator

Suppose we have two incompatible observables A and B. The ket space can be viewed as being spanned either by the set $\{|a'\rangle\}$or by the set $\{|b'\rangle\}$. i.e. A representation or B representation. Changing the set of base kets is referred to as a change of basis or change of representation. The two bases are connected by a transformation operator.

Theorem 2 *Given two complete and orthogonal sets of base kets, there exist a unitary operator* $\mathbf{U}$ *such that* $\left|b^{(n)}\right\rangle = \mathbf{U}\left|a^{(n)}\right\rangle$.

Unitary operator: $\mathbf{U}\ \mathbf{U}^+ = \mathbf{U}^+\mathbf{U} \equiv 1$

Proof. This theorem is proved by an explicit construction of u: the summation of the out-product of two sets of eigenket forms an operator

$$\mathbf{U} = \sum_k \left|b^{(k)}\right\rangle\left\langle a^{(k)}\right|$$

1)

$$\mathbf{U}\left|a^{(l)}\right\rangle = \sum_k \left|b^{(k)}\right\rangle \underbrace{\left\langle a^{(k)}|a^{(l)}\right\rangle} = \left|b^{(l)}\right\rangle$$

2)

$$\begin{aligned}\mathbf{U}\mathbf{U}^{+} &= \sum_{k,l}\left|b^{(k)}\right\rangle\left\langle a^{(k)}\right|\,a^{(l)}\right\rangle\left\langle b^{(l)}\right| \\ &= \sum_{k,l}\left|b^{(k)}\right\rangle\left\langle b^{(k)}\right| = 1\end{aligned}$$

■

1.7.2 Transformation Matrix

In the matrix representation, the u operator can be expressed in the form of a matrix in the base ket $\{\left|a^{(l)}\right\rangle\}$

$$\mathbf{U} = \{\left\langle a^{(k)}\,|u|\,a^{(l)}\right\rangle\} = \{\left\langle a^{(k)}|b^{(l)}\right\rangle\}$$

For an arbitrary ket in two representations

A:

$$|\alpha\rangle = \sum_n \left|a^{(n)}\right\rangle\left\langle a^{(n)}|\alpha\right\rangle$$

B:

$$|\alpha\rangle = \sum_n \left|b^{(n)}\right\rangle\left\langle b^{(n)}|\alpha\right\rangle$$

Relation of two representations:

$$\begin{aligned}\left\langle b^{(n)}|\alpha\right\rangle &= \sum_k \left\langle b^{(n)}|a^{(k)}\right\rangle\left\langle a^{(k)}|\alpha\right\rangle \\ &= \sum_k \left\langle a^{(n)}\left|\mathbf{U}^{\dagger}\right|a^{(k)}\right\rangle\left\langle a^{(k)}|\alpha\right\rangle\end{aligned}$$

Relation of an operator in two representations

$$\begin{aligned}
& \left\langle b^{(m)} \left| \mathbf{X} \right| b^{(n)} \right\rangle \\
= \quad & \sum_{k,l} \left\langle b^{(n)} | a^{(k)} \right\rangle \left\langle a^{(k)} \left| \mathbf{X} \right| a^{(l)} \right\rangle \left\langle a^{(l)} | b^{(n)} \right\rangle \\
= \quad & \sum_{k,l} \left\langle a^{(m)} \left| \mathbf{U}^{\dagger} \right| a^{(k)} \right\rangle \left\langle a^{(k)} \left| \mathbf{X} \right| a^{(l)} \right\rangle \left\langle a^{(l)} \left| \mathbf{U} \right| a^{(n)} \right\rangle \\
= \quad & \left\langle a^{(m)} \right| \mathbf{U}^{\dagger} \mathbf{X} a^{(l)} \mathbf{U} \left| a^{(n)} \right\rangle \\
\Longrightarrow \quad & \mathbf{X}_b = \mathbf{U}^{\dagger} \mathbf{X}_a \mathbf{U}
\end{aligned}$$

$- - - - - - -$ A similarity transformation

Trace of an operator:

$$\begin{aligned}
T_r(\mathbf{X}) \quad \equiv \quad & \sum_{n} \left\langle a^{(n)} \right| \mathbf{X} \left| \alpha^{(n)} \right\rangle \\
= \quad & \sum_{n.k.l} \left\langle a^{(n)} | b^{(k)} \right\rangle \left\langle b^{(k)} \left| \mathbf{X} \right| b^{(l)} \right\rangle \left\langle b^{(l)} | a^{(n)} \right\rangle \\
= \quad & \sum_{n.k.l} \left\langle b^{(l)} | a^{(n)} \right\rangle \left\langle a^{(n)} | b^{(k)} \right\rangle \left\langle b^{(k)} \left| \mathbf{X} \right| b^{(l)} \right\rangle \\
= \quad & \sum_{k.l} \left\langle b^{(l)} | b^{(k)} \right\rangle \left\langle b^{(k)} \left| \mathbf{X} \right| b^{(l)} \right\rangle \\
= \quad & \sum_{l} \left\langle b^{(l)} \left| \mathbf{X} \right| b^{(l)} \right\rangle
\end{aligned}$$

The trace of X is independent of representation. We can also prove:

$$t_r(xy) = t_r(yx);\ t_r(u^{+}xu) = t_r(x)$$

1.7.3 Diagonalization

When we know the matrix elements of B in the base $\{|a'\rangle\}$, how do we obtain the eigenvalues and eigenket of B:

$$B\left|b^{(l)}\right\rangle = b^l\left|b^{(l)}\right\rangle$$

In the base ket $\{\left|b^{(l)}\right\rangle\}$, the operator is expressed as

$$\begin{aligned}
\mathbf{B}\left|b^{(l)}\right\rangle\left\langle b^{(l)}\right| &= b^l\left|b^{(l)}\right\rangle\left\langle b^{(l)}\right| \\
\mathbf{B}\sum_l\left|b^{(l)}\right\rangle\left\langle b^{(l)}\right| &= \sum_l b^l\left|b^{(l)}\right\rangle\left\langle b^{(l)}\right| \\
\mathbf{B} &= \sum_l b^l\left|b^{(l)}\right\rangle\left\langle b^{(l)}\right|
\end{aligned}$$

In the Dirac bra-ket notation, we rewrite it as

$$\sum_n\left\langle a^{(m)}\left|\mathbf{B}\right|a^{(n)}\right\rangle\left\langle a^{(n)}|b^{(l)}\right\rangle = b^l\left\langle a^{(m)}|b^{(l)}\right\rangle.$$

Furthermore, in the matrix form,

$$\begin{pmatrix} B_{11} & B_{12} & \cdots \\ B_{21} & B_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}\begin{pmatrix} C_1^{(l)} \\ C_2^{(l)} \\ \vdots \end{pmatrix} = b^{(l)}\begin{pmatrix} C_1^{(l)} \\ C_2^{(l)} \\ \vdots \end{pmatrix}$$

where

$$B_{mn} = \left\langle a^{(m)}\left|\mathbf{B}\right|a^{(n)}\right\rangle$$

and

$$C_k^{(l)} = \left\langle a^{(k)}|b^{(l)}\right\rangle$$

As we know from linear algebra, the eigenvalues are determined by

$$\det(\mathbf{B}-\lambda) = 0$$

Example 2

$$\mathbf{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\begin{aligned} \det(\mathbf{S}_x - \lambda I) &= 0 \Rightarrow \det\begin{pmatrix} -\lambda & \frac{\hbar}{2} \\ \frac{\hbar}{2} & \text{-}\lambda \end{pmatrix} = 0 \\ \lambda^2 - \frac{\hbar^2}{4} &= 0 \Rightarrow \lambda = \pm\frac{\hbar}{2} \end{aligned}$$

Eigenvectors?

1.8 Position, Momentum, and Translation

1.8.1 Continuous Spectra

When the eigenvalues of an observable is continuous, the dimensionality of the vector space is infinite. Denote the eigenvalue-eigenket relation by

$$\hat{\xi}\,|\xi\rangle = \xi\,|\xi\rangle$$

We generalize of a vector space with finite dimension to that with infinite dimension

discrete	continuous
$\langle a'|a"\rangle = \delta_{a'a"}$	$\langle \xi'|\xi"\rangle = \delta(\xi' - \xi_\mathrm{J})$
$\sum |a'\rangle\langle a'| = 1$	$\int d\xi\,|\xi\rangle\langle\xi| = 1$
$\|\alpha\rangle = \sum_n \|a^{(n)}\rangle\langle a^{(n)}\|\,\alpha\rangle$	$\|\alpha\rangle = \int d\xi\,|\xi\rangle\langle\xi|\,\alpha\rangle$
$\langle a"\,|\mathbf{A}|\,a'\rangle = a'\delta_{a'a"}$	$\langle \xi"\,|\xi|\,\xi'\rangle = \xi'\delta(\xi' - \xi_\mathrm{J})$

1. The Kronecker symbol δ is replaced by Dirac's δ -function.

2. The discrete sum over the eigenvalues is replaced by an integral over a continuous variable.

1.8.2 Some properties of the $\delta-$function.

1. $\delta(x) = \delta(-x)$

2. $\delta'(x) = -\delta'(-x)$

3. $x\delta(x) = 0$

4. $x\delta'(x) = -\delta(-x)$

5. $\delta(ax) = \frac{1}{a}\delta(-x)$

6. $\delta(x^2 - a^2) = \frac{1}{2}(\delta(a - x) + \delta(a - x))$

7. $\delta(x - a) \cdot f(x) = (\delta(x - a)f(a)$

8. $\int dx\delta(a - x)\delta(b - x) = \delta(a - b)$

Representation of the $\delta-$function

$$\delta(x) = \lim_{g\to\infty} \frac{\sin gx}{\pi x}$$

$$\delta(x) = \lim_{\sigma\to 0} \frac{1}{\pi^{1/2}\sigma} e^{-x^2/\sigma^2}$$

Normalization in terms of the $\delta-$function

$$u_t(r) = \alpha e^{ik_x \cdot x}$$

$$\begin{aligned}\int_{-\infty}^{+\infty} dx u_k^*(r) u_l(r) &= \alpha^2 \int_{-\infty}^{+\infty} e^{-i(k_x - l_x)x} \\ &= \alpha^2 2\pi\delta(k_x - l_x) = \delta(k_x - l_x) \\ \Rightarrow \quad \alpha &= (2\pi)^{1/2}\end{aligned}$$

1.8.3 Position Eigenkets and Position Measurements

To extend the idea of a filtering process to measurements of observables exhibiting continues spectra, we consider the position operator in one dimension. The eigenkets $|x'\rangle$ of the position operator $\hat{\mathrm{x}}$ satisfying

$$\mathbf{x}\,|x'\rangle = x'\,|x'\rangle$$

are postulate to form a complete set. The state ket for an arbitrary physical states can be expanded in terms of $\{|x'\rangle\}$

$$|\alpha\rangle = \int d_{x'}\,|x'\rangle\,\langle x'|\alpha\rangle$$

Suppose we place a very tiny detector that clicks only when the particle is precisely at x' and nowhere else after the detector clicks, we can say the state in question is represented by $|x'\rangle$. In practice the best the detector can do is to locate the particle within a narrow range $(x'_\delta - \frac{\Delta}{2}, x'_\delta + \frac{\Delta}{2})$ (Δ is very small). When the detector clicks, the state ket changes abruptly as follows

$$|\alpha\rangle = \int_{-\infty}^{\infty} d_{x'}\,|x'\rangle\,\langle x'|\alpha\rangle \xrightarrow{\text{measurement}} \int_{x_\delta - \frac{\Delta}{2}}^{x_\delta + \frac{\Delta}{2}} d_{x'}\,|x'\rangle\,\langle x'|\alpha\rangle$$

Assume that $\langle x'|\alpha\rangle$ does not change appreciably within the narrow interval, the probability that the detector clicks is given by

$$|\langle x_0|\alpha\rangle|^2\,\Delta$$

Obviously

$$\int_{-\infty}^{+\infty} |\langle x|\alpha\rangle|^2 \, dx = 1 \quad = \langle \alpha|\alpha\rangle \, .$$

In the wave mechanics, the physical state is represented by a wave function. Thus $\langle x|\alpha\rangle$ is the wave function for the state $|\alpha\rangle$

Wave function in position space: $\langle x'|\alpha\rangle$ in $|\alpha\rangle = \int d_{x'} \, |x'\rangle \, \langle x'|\alpha\rangle$ is the wave function in the position space. We assume that the position eigenkets $|x'\rangle$ are complete. It can be three dimensional, i.e. x' in $|x'\rangle$ stand for three components of the position vectors. In this word the position is an observable, and $[x_i, x_j] = 0$.

1.8.4 Translation

Suppose we start with a state that is well located around x', and introduce an translation operator $\mathbf{T}(l)$ such that

$$\mathcal{T}(l) \, |x\rangle = |x + l\rangle \, .$$

Several properties of $\mathbf{T}(l)$:

1. $\mathbf{T}(l = 0) = 1$
2. $\mathbf{T}(l_1)\mathcal{T}(l_2) = \mathbf{T}(l_1 + l_2)$
3. $\mathbf{T}(-l)\mathbf{T}(l) = 1 \Longleftrightarrow \mathbf{T}(-l) = \mathbf{T}^{-1}(l)$
4. $\mathbf{T}(-l)^{+}\mathbf{T}(l) = 1$

From the definition we have

$$\langle x| \, \mathbf{T}(l)^{\dagger} \quad = \quad \langle x + l|$$

$$\left\langle x \left| \mathbf{T}(l)^{\dagger}\mathbf{T}(l) \right| x \right\rangle \quad = \quad \langle x + l|x + l\rangle = \langle x|x\rangle$$

We now consider an infinitesimal translation $l = \delta x \to 0$. We demonstrate that if $\mathbf{T}(\delta x)$ is taken to be

$$\mathbf{T}(\delta x) \approx 1 - i\mathbf{K}\delta x + 0((\delta x)^2)$$

where $\mathbf{K}$ is an Hermitian operator $\mathbf{K}^\dagger = \mathbf{K}$. then all properties listed are satisfied.

Let us check them..

1. $\delta x = 0$:

$$\mathbf{T}(\delta x = 0) = 1$$

2. $\mathbf{T}(\delta x_1)\mathbf{T}(\delta x_2) = \mathbf{T}(\delta x_1 + \delta x_2)$:

$$(1 - iK\delta x_1)(1 - iK\delta x_2)$$

$$= \quad 1 - iK(\delta x_1 + \delta x_2) + 0(\delta x_1 \delta x_2)$$

3. $\mathbf{T}(-\delta x)\mathbf{T}(\delta x) = 1$

$$(1 + iK\delta x)(1 - iK\delta x) = 1 - iK^2(\delta x)^2 = 1$$

4. $\mathbf{T}(\delta x)^\dagger \mathbf{T}(\delta x) = 1$

$$\begin{aligned}(1 - i\mathbf{K}\delta x)^\dagger(1 - i\mathbf{K}\delta x) &= (1 + i\mathbf{K}^\dagger\delta x)(1 - i\mathbf{K}\delta x) \\ &= 1 + i(\mathbf{K}^\dagger - \mathbf{K})\delta x + 0((\delta x)^2)\end{aligned}$$

Commutation relation of $\mathbf{x}$ and $\mathbf{K}$:

$$\begin{aligned}
\mathbf{xT}(\delta x)\,|x\rangle \quad &= \quad \mathbf{x}\,|x+\delta x\rangle = (x+\delta x)\,|x+\delta x\rangle \\
\mathbf{T}(\delta x)\mathbf{x}\,|x\rangle \quad &= \quad \mathbf{T}(\delta x)x\,|x\rangle = x\mathbf{T}(\delta x)\,|x\rangle = x\,|x+\delta x\rangle \\
&\Longrightarrow \quad (\mathbf{xT}(\delta x)-\mathbf{T}(\delta x)\mathbf{x})\,|x\rangle = \delta x\,|x+\delta x\rangle \\
&\Longrightarrow \quad (-i\mathbf{xK}\delta x + i\mathbf{Kx}\delta x)\,|x\rangle = \delta x\,|x+\delta x\rangle \approx \delta x\,|x\rangle \\
&\Longrightarrow \quad [\mathbf{x},\mathbf{K}] = i
\end{aligned}$$

$\hat{\mathrm{x}}$ and K do not commute with each other!

Momentum Operator in the Position Basis.

Translation Operator for an infinitesimal small displacement is defined as ($\mathbf{T}(\delta x) = 1 - i\mathbf{K}\delta x$). Let $\mathbf{T}(\delta x)$ act on an arbitrary state

$$\begin{aligned}
|\alpha\rangle \quad &\rightarrow \quad \mathbf{T}(\delta x)\,|\alpha\rangle = \int dx\mathbf{T}(\delta x)\,|x\rangle\,\langle x|\alpha\rangle = \int dx\,|x+\delta x\rangle\,\langle x|\alpha\rangle \\
&= \quad \int dx\,|x\rangle\,\langle x-\delta x|\alpha\rangle \qquad\qquad x+\delta_x \rightarrow x \\
&= \quad \int dx\,|x\rangle\,(\langle x|\alpha\rangle - \frac{\partial}{\partial x}\,\langle x|\alpha\rangle\,\delta x) = \int dx\,|x\rangle\,(1-\delta x\frac{\partial}{\partial x})\,\langle x|\alpha\rangle \\
\text{also} \quad &\Longrightarrow \quad \int dx\,|x\rangle\,\langle x|\,(1-i\mathbf{K}\delta x)\,|\alpha\rangle \\
&= \quad \int dx\,|x\rangle\,(\langle x|\alpha\rangle - i\mathbf{K}\,\langle x|\alpha\rangle\,\delta x) \Longrightarrow K = -i\frac{\partial}{\partial x}
\end{aligned}$$

Consider an ideal wave function

$$\langle x|\alpha\rangle = \frac{1}{(2\pi)^{1/2}}e^{+i\hat{P}x/\hbar}$$

which has the momentum P

$$\mathbf{K}\,\langle x|\alpha\rangle = \frac{\mathbf{P}}{\hbar}\,\langle x|\alpha\rangle$$

The physical significance of K is that $\hat{\mathrm{K}}$ is an operator for the momentum with a proportionality factor. The factor is the Planck's constant over $2\pi : \hbar = h/2\pi$

L. de Broglie's relation (1924):

$$\frac{2\pi}{\lambda} = \frac{p}{\hbar}$$

de Broglie wave is also called matter wave, any aspect of the behavior or properties of a material object that varies in time or space in conformity with the mathematical equations that describe waves. By analogy with the wave and particle behavior of light that had already been established experimentally, the French physicist Louis de Broglie suggested (1924) that particles might have wave properties in addition to particle properties. Three years later the wave nature of electrons was detected experimentally. Objects of everyday experience, however, have a computed wavelength much smaller than that of electrons, so their wave properties have never been detected; familiar objects show only particle behavior. De Broglie waves play an appreciable role, therefore, only in the realm of subatomic particles. The response of the wave properties of a particle to an external force follows a basic law of quantum mechanics that, in its mathematical form, is known as the Schrödinger equation.

The momentum operator in the position space

$$\mathbf{P} = -i\hbar\frac{\partial}{\partial x}.$$

The commutation relation:

$$\begin{aligned}
[\mathbf{x},\mathbf{p}] &= i\hbar \\
[\mathbf{x},\mathbf{p}]f(x) &= (\mathbf{xp}-\mathbf{px})f(x) = -i\hbar x\frac{\partial}{\partial x}f(x) + i\hbar\frac{\partial}{\partial x}(xf(x)) \\
&= -i\hbar x\frac{\partial}{\partial x}f(x) + i\hbar x\frac{\partial}{\partial x}f(x) + i\hbar f(x)
\end{aligned}$$

Therefore

$$[\mathbf{x},\mathbf{p}]f(x) = i\hbar f(x)$$

1.9 The Uncertainty Relation

The commutation relation $[\mathbf{x},\mathbf{p}] = i\hbar$ shows that the position and the momentum are incompatible. This relation leads to the famous uncertainty relation

$$\left\langle(\Delta\mathbf{x})^2\right\rangle\left\langle(\Delta\mathbf{p})^2\right\rangle \geq \hbar^2/4$$

Let A ad B be observables. Define $\Delta\mathbf{A} \equiv \mathbf{A} - \langle\mathbf{A}\rangle$. The expectation value of $\left\langle(\Delta\mathbf{A})^2\right\rangle$ is known as the dispersion of A. For any pair of operators, A and B, we have

$$\left\langle(\Delta\mathbf{A})^2\right\rangle\left\langle(\Delta\mathbf{B})^2\right\rangle \geq \left|\langle[\mathbf{A},\mathbf{B}]\rangle\right|^2/4.$$

The uncertainty relation can be understood from the postulate of measurement.

Proof.

$$\begin{aligned}
\left\langle(\Delta\mathbf{A})^2\right\rangle &= \left\langle(\mathbf{A}-\langle\mathbf{A}\rangle)^2\right\rangle = \left\langle\mathbf{A}^2 - 2\mathbf{A}\langle\mathbf{A}\rangle + \langle\mathbf{A}\rangle^2\right\rangle \\
&= \left\langle\mathbf{A}^2\right\rangle - \langle\mathbf{A}\rangle^2
\end{aligned}$$

1) The Schwarz inequality

$$\langle\alpha|\alpha\rangle\cdot\langle\beta|\beta\rangle \geq \left|\langle\alpha|\beta\rangle\right|^2$$

where the equality only holds if $|\alpha\rangle = |\beta\rangle$.

$$\left.\begin{array}{c} (\langle\alpha| + \lambda^* \langle\beta|)(|\alpha\rangle + \lambda |\beta\rangle) \geq 0 \\ \text{take} \qquad \lambda = -\frac{\langle\beta|\alpha\rangle}{\langle\beta|\beta\rangle} \end{array}\right\}$$

$$\Longrightarrow \quad \langle\alpha|\alpha\rangle \langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$$

To simplify the problem, we can take $\langle\alpha|\alpha\rangle = \langle\beta|\beta\rangle = 1$ and $|\langle\alpha|\beta\rangle|^2 \leq 1$. Let

$$|\alpha\rangle = \Delta\mathbf{A}\,|\rangle$$

$$|\beta\rangle = \Delta\mathbf{B}\,|\rangle$$

$$\Longrightarrow \left\langle(\Delta\mathbf{A})^2\right\rangle \left\langle(\Delta\mathbf{B})^2\right\rangle \geq |\langle\Delta\mathbf{A}\Delta\mathbf{B}\rangle|^2$$

where we have used the hermiticity of A and B since they are observables

2)

$$\begin{aligned} \Delta\mathbf{A}\Delta\mathbf{B} &= \frac{1}{2}(\Delta\mathbf{A}\Delta\mathbf{B} - \Delta\mathbf{B}\Delta\mathbf{A}) \\ &\quad + \frac{1}{2}(\Delta\mathbf{A}\Delta\mathbf{B} + \Delta\mathbf{B}\Delta\mathbf{A}) \\ &= \frac{1}{2}[\Delta\mathbf{A}, \Delta\mathbf{B}] + \frac{1}{2}\{\Delta\mathbf{A}, \Delta\mathbf{B}\} \\ &= \frac{1}{2}[\mathbf{A}, \mathbf{B}] + \frac{1}{2}\{\Delta\mathbf{A}, \Delta\mathbf{B}\} \end{aligned}$$

Anti-Hermitian of $[\mathbf{A}, \mathbf{B}]$:

$$\begin{aligned} [\mathbf{A}, \mathbf{B}]^\dagger &= (\mathbf{AB} - \mathbf{BA})^\dagger \\ &= (\mathbf{AB})^\dagger - (\mathbf{BA})^\dagger \\ &= \mathbf{B}^\dagger\mathbf{A}^\dagger - \mathbf{A}^\dagger\mathbf{B}^\dagger \\ &= -[\mathbf{A}, \mathbf{B}] \end{aligned}$$

Hermitian of $\{\Delta\mathbf{A}, \Delta\mathbf{B}\}$

$$(\{\Delta\mathbf{A}, \Delta\mathbf{B}\})^{+} = \{\Delta\mathbf{A}, \Delta\mathbf{B}\}$$

3) a. The Hermitian operator has only purely real expectation value

$$\begin{aligned}
\mathbf{H}^{\dagger} &= \mathbf{H}, \mathbf{H}\left|h\right\rangle = h\left|h\right\rangle \\
\left\langle h\right|\mathbf{H}^{\dagger} &= h^{*}\left\langle h\right| \\
&\Longrightarrow \begin{cases} \left\langle h\left|\mathbf{H}\right|h\right\rangle = h \\ \left\langle h\left|\mathbf{H}^{\dagger}\right|h\right\rangle = h^{*} \end{cases} \Longrightarrow h = h^{*}
\end{aligned}$$

b. The anti-Hermitian operator has only purely imaginary expectation value

$$\begin{aligned}
\mathbf{A}^{\dagger} &= -\mathbf{A}, \\
\mathbf{A}\left|a\right\rangle &= a\left|a\right\rangle, \left\langle a\right|\mathbf{A}^{\dagger} = a^{*}\left\langle a\right| \\
\left\langle a\left|\mathbf{A}\right|a\right\rangle &= a, \left\langle a\left|\mathbf{A}^{\dagger}\right|a\right\rangle = a^{*} \\
&\Longrightarrow a = -a^{*}
\end{aligned}$$

Therefore

$$\begin{aligned}
\left\langle \Delta\mathbf{A}\Delta\mathbf{B}\right\rangle &= \frac{1}{2}\left\langle [\mathbf{A}, \mathbf{B}]\right\rangle + \frac{1}{2}(\left\langle \{\Delta\mathbf{A}, \Delta\mathbf{B}\}\right\rangle) \\
&= +i\,\mathrm{Im}\left\langle \Delta\mathbf{A}\Delta\mathbf{B}\right\rangle + \mathrm{Re}\left\langle \Delta\mathbf{A}\Delta\mathbf{B}\right\rangle \\
\left|\left\langle \Delta\mathbf{A}\Delta\mathbf{B}\right\rangle\right|^{2} &= \frac{1}{4}(\left\langle [\mathbf{A}, \mathbf{B}]\right\rangle)^{2} + \frac{1}{4}(\left\langle \{\Delta\mathbf{A}, \Delta\mathbf{B}\}\right\rangle)^{2} \\
&\geq \frac{1}{4}(\left\langle [\mathbf{A}, \mathbf{B}]\right\rangle)^{2} \\
\left\langle (\Delta\mathbf{A})^{2}\right\rangle\left\langle (\Delta\mathbf{B})^{2}\right\rangle &\geq \frac{1}{4}(\left\langle [\mathbf{A}, \mathbf{B}]\right\rangle)^{2}
\end{aligned}$$

$$[\mathbf{x}, \mathbf{p}] = i\hbar$$

$$\left\langle (\Delta \mathbf{x})^2 \right\rangle \left\langle (\Delta \mathbf{p})^2 \right\rangle \geq \hbar^2/4$$

■

Since the position and momentum operators are incompatible, $[\mathbf{x}, \mathbf{p}] \neq 0$, we cannot find a complete set of simultaneous eigenkets for x and p such that the two observables can be measured at the same time. For instance for an eigenstate of $\mathbf{x}$, $\mathbf{x}\left|x\right\rangle = x\left|x\right\rangle$, it is not an eigenstate of the momentum. It can be spanned in the momentum space,

$$\mathbf{p}\left|x\right\rangle = \mathbf{p}\int dp\left|p\right\rangle\left\langle p\right|\left|x\right\rangle = \int dp\left\langle p|x\right\rangle p\left|p\right\rangle .$$

You may have an expectation value.

Example 3

A plane wave with a momentum p_0:

$$\phi_{p_0}(x) = \frac{1}{(2\pi\hbar)^{1/2}}\exp[ip_0 x]$$

The probability to find x is a constant in the whole space, $\left|\phi_{p_0}(x)\right|^2 = \frac{1}{2\pi\hbar}$.

Example 4

A particle at $x = x_0$:

$$\phi_{x_0}(x) = \delta(x - x_0)$$

In the momentum space,

$$\begin{aligned}\phi_{x_0}(x) &= \delta(x-x_0) \\ &= \int \frac{dp}{2\pi\hbar} e^{ip(x-x_0)}\end{aligned}$$

Example 5

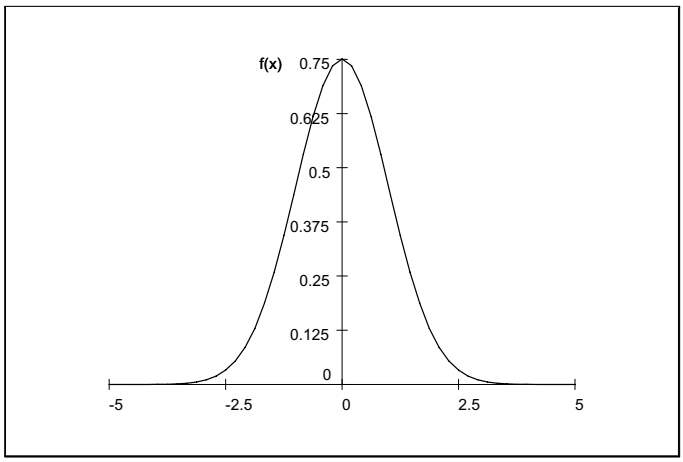
A Gaussian wave package:

$$\phi(x) = \frac{1}{\pi^{1/4}x_0^{1/2}} \exp[-x^2/2x_0^2]$$

The particle is mainly confined in the regime, $\delta x \sim x_0$. In the k space,

$$\begin{aligned}\phi(p) &= \frac{1}{(2\pi)^{1/2}} \int \phi(x) e^{-ipx/\hbar} dx \\ &= \frac{1}{(2\pi)^{1/2}} \int \frac{1}{\pi^{1/4}x_0^{1/2}} \exp[-x^2/2x_0^2 - ipx/\hbar] dx \\ &= \frac{1}{(2\pi)^{1/2}} \int \frac{1}{\pi^{1/4}x_0^{1/2}} \exp[-\frac{1}{2}\left(\frac{x}{x_0} + \frac{ipx_0}{\hbar}\right)^2] dx \\ &\quad \exp[-\frac{1}{2}\left(\frac{px_0}{\hbar}\right)^2] \\ &= \frac{\sqrt{2}\pi^{1/4}x_0^{1/2}}{(2\pi)^{1/2}} \int \frac{1}{\pi^{1/2}\sqrt{2}x_0} \exp[-\frac{1}{2}\left(\frac{x}{x_0} + \frac{ipx_0}{\hbar}\right)^2] dx \\ &\quad \exp[-\frac{1}{2}\left(\frac{px_0}{\hbar}\right)^2] \\ &= \frac{x_0}{\pi^{1/4}x_0^{1/2}} \exp[-p^2x_0^2/2\hbar^2]\end{aligned}$$

The particle is mainly confined in the regime, $\delta p \sim \hbar/x_0$. Thus $\delta x \delta p \sim \hbar$.



Example 6

Momentum Determination Experiment

We assume that the particle is an atom in an excited state, which will give off a photon that has the frequency ν_0 if the atom is at rest. Because of the Doppler effect, the motion of the atom toward the observer with speed ν means that the observed frequency is given approximately by

$$\nu = \nu_0(1 + \frac{v}{c}) \Longrightarrow v = c(\frac{\nu}{\nu_0} - 1)$$

Accurate measurement of the momentum mv by measurement of the frequency ν requires a relatively long time τ; the minimum error in the frequency measurement can be shown to be $\Delta\nu \approx 1/\tau$. The instant at which the photon is emitted is uncertain by τ, at this instant, the momentum of the atom decreases by $\hbar\nu/c$, and its velocity decreases by $\hbar\nu/mc$. This makes the subsequent position of the atom uncertain by the amount $\Delta x \approx \frac{\hbar v}{mc} \cdot \tau$.Since the later the photon is emitted,

the longer the atom has the higher velocity and the farther it will have traveled. This position uncertainty arises entirely because of the finiteness of τ. If τ were zero, and we knew the velocity and the velocity change on emission of photon, we would know where the atom is at each instant; it is because τ is finite that we do not know when the velocity changed and hence where the atom is later times. The momentum uncertainty is obtained:

$$\begin{aligned} \Delta p_x &\approx m\Delta v \approx mc(\frac{\nu}{\nu_0} - 1) \\ &\approx \frac{mc}{\nu_0}\Delta\nu \approx \frac{mc}{\nu_0 c} \end{aligned}$$

In the nonrelativistic case considered here $v/c << 1 \implies \nu \approx \nu_0$ Therefore

$$\Delta x \cdot \Delta p \sim \hbar$$

Example 7

2×2 matrix: Suppose a 2×2 matrix X is written as

$$\begin{aligned} X &= a_0\sigma_0 + a \cdot \sigma \qquad (a_0 \text{ and } a_i \text{ are real}) \\ &= \begin{pmatrix} a_0 & 0 \\ 0 & a_0 \end{pmatrix} + \begin{pmatrix} 0 & a_x \\ a_x & 0 \end{pmatrix} \\ &\quad + \begin{pmatrix} 0 & -ia_y \\ ia_y & 0 \end{pmatrix} + \begin{pmatrix} a_z & 0 \\ 0 & -a_z \end{pmatrix} \\ &= \begin{pmatrix} a_0 + a_z & a_x - ia_y \\ a_x + ia_y & a_0 - a_z \end{pmatrix} \end{aligned}$$

Eigenvalues of X:

$$\det(X - \lambda I) = 0$$

$$\det \begin{pmatrix} a_0 + a_z - \lambda & a_x - ia_y \\ a_x + ia_y & a_0 - a_z - \lambda \end{pmatrix}$$

$$= (a_0 + a_z - \lambda)(\ a_0 - a_z - \lambda) - (a_x - ia_y)(a_x + ia_y)$$

$$= (a_0 - \lambda)^2 - a_z^2 - a_x^2 - a_y^2 = 0$$

$$\implies \lambda_\pm = a_0 \pm \left(a_x^2 + a_y^2 + a_z^2\right)^{1/2}$$

Chapter 2

Quantum Dynamics

This chapter is devoted exclusively to the dynamic development of state kets and/or observables. In other words, we are concerned here with the quantum mechanical analogue of Newton's equation of motion.

2.1 Time Evolution and the Schrödinger Equation

2.1.1 Time Evolution Operator

We now discuss how a physical state evolves with time. Suppose we have a physical system whose state ket at t_0 is represented by $|\alpha\rangle$. Let us denote the ket corresponding to the state at some later time t by

$$|\alpha, t_0 : t\rangle$$

Our main task is to study the time evolution of a state ket:

$$|\alpha\rangle = |\alpha, t_0 : t_0\rangle \Longrightarrow |\alpha, t_0 : t\rangle$$

As in the case of translation, we assume that the two kets are connected by the time-evolution operator

$$|\alpha, t_0 : t\rangle = U(t, t_0)\,|\alpha\rangle$$

Several properties of U:

1. The identity

$$U(t_0, t_0) = 1$$

2. The unitarity

$$U^{\dagger}(t, t_0)U(t, t_0) = 1$$

3. The composition:

$$U(t_2, t_0) = U(t_2, t_1)U(t_1, t_0)$$

Because time is assumed to be continuous, we consider an infinitesimal time-evolution operator

$$|\alpha, t_0; t_0 + \delta t\rangle = U(t_0 + \delta t, t_0)\,|\alpha\rangle$$

As

$$\lim_{\delta t \to 0} U(t_0 + \delta t, t_0) = 1$$

we expand the operator in terms of δt

$$\begin{aligned} U(t_0 + \delta t, t_0) &= U(t_0, t_0) + \frac{\partial}{\partial t}U(t, t_0)|_{t=t_0}\delta t + ... \\ &= 1 - i\hat{\Omega}\delta t + ... \end{aligned}$$

Just like the operator K in the translation operator $\mathcal{T}(l)$, $\hat{\Omega}$ is a Hermitian operator.

What's the physical meaning of $\hat{\Omega}$?

We consider a simple example. In the position space

$$\begin{array}{ccc} \langle x|\alpha, t_0, t\rangle & = & \langle x|U(t_1 t_0)|\alpha\rangle \\ \Downarrow & & \tilde{\tilde{\tilde{}}}\Downarrow \\ \frac{1}{(2\pi)^{1/2}} e^{i(kx-\omega(t-t_0))} & & \tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{}}}}}}}} \frac{1}{(2\pi)^{1/2}} e^{ikx} \end{array}$$

$$t \to t_0 + \delta t \Longrightarrow \Omega = \omega$$

In the old quantum theory, the time-frequency ω is postulated to be related to energy

$$E = \hbar\omega \quad \text{(Planck-Einstein Relation)}$$

In the classical mechanics, the energy is related to the Hamiltonian operator $\hat{\mathrm{H}}$, which is also the generator of time-evolution. It is then natural to relate or define $\hat{\Omega}$ to the Hamiltonian operator $\hat{\mathrm{H}}$:

$$\hat{\Omega} = \hat{H}/\hbar$$

Thus

$$U(t_0 + \delta t, t_0) = 1 - i\frac{\hat{H}}{\hbar}\delta t + ...$$

2.1.2 The Schrodinger Equation.

We are now in the position to derive the fundamental differential equation for the time-evolution operator. $U(t, t_0)$ and a physical state $|\alpha\rangle$. From the composition property of

U,

$$\begin{aligned} U(t+\delta t, t_0) &= U(t+\delta t, t)U(t, t_0) \\ &= \left(1 - i\frac{\hat{H}}{\hbar}\delta t\right) U(t, t_0) \end{aligned}$$

$$\frac{U(t+\delta t, t_0) - U(t, t_0)}{\delta t} = -\frac{i}{\hbar} H U(t, t_0)$$

Take $\delta t \to 0^+$, we obtain

$$i\hbar\frac{\partial}{\partial t} U(t, t_0) = H U(t, t_0)$$

Multiplying a state ket from the right sides

$$\begin{aligned} i\hbar\frac{\partial}{\partial t} U(t, t_0)\,|\alpha\rangle &= H U(t, t_0)\,|\alpha\rangle \\ i\hbar\frac{\partial}{\partial t}\,|\alpha, t_0; t\rangle &= H\,|\alpha, t_0; t\rangle \end{aligned}$$

The formal solutions to the Schrodinger equation for the time-evolution operator $U(t, t_0)$

Case A: The Hamiltonian operator is independent of time,

$$\begin{aligned} i\hbar\frac{\partial}{\partial t} U(t, t_0) &= H U(t, t_0) \\ i\hbar\frac{\frac{\partial}{\partial t} U(t, t_0)}{U(t, t_0)} &= H \\ i\hbar\frac{\partial}{\partial t} \ln U(t, t_0) &= H \\ \ln U(t, t_0) - \ln U(t_0, t_0) &= -\frac{i}{\hbar}\int_{t_0}^{t} H dt \end{aligned}$$

$$U(t, t_0) = \exp[-\frac{i}{\hbar} H(t - t_0)]$$

Case B: The Hamiltonian $\hat{H}$ is time-dependent but the $\hat{H}'s$ at different times commute

$$\int_{t_0}^{t} dt \ln U(t, t_0) = -\frac{i}{\hbar}\int_{t_0}^{t} dt H(t)$$

$$U(t,t_0) = \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt H(t)\right]$$

Case C: The Hamiltonian $\hat{H}$ is time-dependent but the $\hat{H}'$s at different times do not commute, i.e.

$$[H(t_1), H(t_2)] \neq 0$$

$$\begin{aligned} U(t,t_0) &= 1 - \frac{i}{\hbar}\int_0^t dt_1 H(t_1) + \frac{(-i)^2}{\hbar^2}\int_{t_{10}}^{t} dt_1 \int_{t_0}^{t_1} dt_2 H(t_1)H(t_2) + ... \\ &= 1 + \sum_{n=1}^{\infty}(\frac{-i}{\hbar})^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 ... \int_{t_0}^{t_n - 1} dt_n \times H(t_1)H(t_2)...H(t_n) \end{aligned}$$

Energy Eigenkets:

To be able to evaluate the effect of time-evolution operator on a general ket $|\alpha\rangle$, we consider a special base ket used in expanding $|\alpha\rangle$. Assume that we know all energy eigenkets of an time-independent H with eigenvalues E_n

$$H\left|a^{(n)}\right\rangle = E_n\left|a^{(n)}\right\rangle$$

$\{\left|a^{(n)}\right\rangle\}$ forms a complete and orthogonal set of base kets. Therefore

$$\begin{aligned} U(t,t_0) &= \exp(-\frac{iH}{\hbar}(t-t_0)) \\ &= \sum_{n.m}\left|a^{(m)}\right\rangle\left\langle a^{(m)}\right| e^{-i\frac{H}{\hbar}(t-t_0)}\left|a^{(n)}\right\rangle\left\langle a^{(n)}\right| \\ &= \sum_{n.} e^{-i\frac{E_n}{\hbar}(t-t_0)}\left|a^{(n)}\right\rangle\left\langle a^{(n)}\right|. \end{aligned}$$

Once the expansion of the initial ket $|\alpha\rangle$ in terms of $\{\left|a^{(n)}\right\rangle\}$ is known,

$$|\alpha\rangle = \sum_{n.}\left|a^{(n)}\right\rangle\left\langle a^{(n)}\right|\alpha\rangle = \sum_n C_n\left|a^{(n)}\right\rangle.$$

The time-evolution operator enables us to solve any initial time problem,

$$\begin{aligned} |\alpha, t_0; t\rangle &= e^{-i\frac{H}{\hbar}(t-t_0)}|\alpha\rangle \\ &= \sum_{n.} C_n e^{-i\frac{E_n}{\hbar}(t-t_0)}\left|a^{(n)}\right\rangle. \end{aligned}$$

In other words

$$C_n(t=t_0)=C_n \rightarrow C_n(t)=C_n e^{-i\frac{E_n}{\hbar}(t-t_0)}.$$

The phase of $C_n(t)$ changes with time, but its modulus remains unchanged. If all eigenvalues are not degenerate, the relative phases of C_n do vary with time and the state ket varies with time.

A special case: if the initial state happens to be one of energy eigenkets, say $|\alpha\rangle = \left|a^{(n)}\right\rangle$, we have

$$|\alpha, t_0; t\rangle = e^{-i\frac{E_n}{\hbar}(t-t_0)}\left|a^{(n)}\right\rangle.$$

The state remains unchanged. Thus the basic task in quantum dynamics is reduced to find a complete set of energy eigenket and eigenvalues. It is very helpful if we can find a maximal set of commuting observables Â,

B, Ĉ,...which also commute with the Hamiltonian

$$[\hat{A},\hat{B}]=[\hat{B},\hat{C}]=[\hat{A},\hat{C}]=...=0$$

$$[\hat{A},\hat{H}]=[\hat{B},\hat{H}]=[\hat{C},\hat{H}]=...=0$$

In the case, the energy eigenket can be characterized by the indices $\{a,b,c...\}\equiv\{k\}$ For example,

$$\begin{cases} \hat{A}\,|k\rangle = a\,|k\rangle\,, \\ \hat{B}\,|k\rangle = b\,|k\rangle\,,.. \\ \hat{H}\,|k\rangle = E_k\,|k\rangle \end{cases}$$

Therefore it is of fundamental importance to find a complete set of mutually compatible observables that also commute with H.

2.1.3 Time Dependence of Expectation Value: Spin Precession.

It is instructive to study how the expectation value of an observable changes as a function of time. To end this we treat an example here: spin precession. We start with a Hamiltonian of a spin 1/2 system with magnetic moment $\mu = e\hbar/am_ec$ subjected to an external magnetic field $\vec{B} = B\hat{Z}$

$$H = -\frac{e}{m_e c}\vec{S}\cdot\vec{B} = -\frac{eB}{m_e c}\vec{S}_z = \omega\vec{S}_z$$

As

$$\vec{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

then the corresponding eigenvalues of $\hat{\mathrm{H}}$ are

$$E_\pm = \pm\frac{\hbar}{2}\omega \quad (= S_z\omega).$$

Since the Hamiltonian is time-independent, the time-evolution operator for the state ket

$$U(t,0) = e^{-i\omega\hat{S}_z t/\hbar}$$

The eigenkets of $\hat{S}_z$ are

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{for } S_z = +\frac{\hbar}{2}$$

$$|-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{for } S_z = -\frac{\hbar}{2}$$

$$\Longrightarrow H|\pm\rangle = \pm\frac{1}{2}\hbar\omega\ |\pm\rangle$$

i.e., $|\pm\rangle$ are also the energy eigenkets with eigenvalues $\pm\hbar\omega/2$. Suppose at $t = 0$

$$|\alpha\rangle = C_+|+\rangle + C_-|-\rangle$$

At a later time t,

$$\begin{aligned} |\alpha, t_0 : t\rangle &= U(t, t_0)\,|\alpha\rangle \\ &= C_+ e^{-\frac{i\omega t}{2}}\,|+\rangle + C_- e^{+\frac{i\omega t}{2}}\,|-\rangle \end{aligned}$$

Specifically, (1) Let us suppose the initial state $|\alpha\rangle$ is the spin up state $|+\rangle$,i,e. $C_+ = 1$ and $C_- = 0$, then

$$|\alpha, t_0 : t\rangle = e^{-i\frac{\omega t}{2}}\,|+\rangle$$

This is a stationery state ! (2) Suppose the initial state $|\alpha\rangle$ is the spin state $|S_x+\rangle$:

$$|S_x+\rangle = \frac{1}{2^{1/2}}\,|+\rangle + \frac{1}{2^{1/2}}\,|-\rangle$$

At a later time t

$$|\alpha, t_0 : t\rangle = \frac{1}{2^{1/2}} e^{-i\frac{\omega t}{2}}\,|+\rangle + \frac{1}{2^{1/2}} e^{i\frac{\omega t}{2}}\,|-\rangle$$

The probability for the system to be found in the state $|S_x\pm\rangle = \frac{1}{\sqrt{2}}\,(|+\rangle \pm |-\rangle)$

$$\begin{aligned} &\langle S_x + |\alpha, t_0 : t\rangle \\ = \;& \frac{1}{2^{1/2}}(\langle +| + \langle -|)\frac{1}{2^{1/2}}(e^{-i\frac{\omega t}{2}}\,|+\rangle + e^{i\frac{\omega t}{2}}\,|-\rangle) \\ = \;& \frac{1}{2}(e^{-i\frac{\omega t}{2}} + e^{i\frac{\omega t}{2}}) = \cos\frac{\omega t}{2} \end{aligned}$$

$$\begin{aligned} |\langle S_x + |\alpha, t_{0:} t\rangle|^2 &= \cos^2\frac{\omega t}{2} \\ \langle S_x - |\alpha, t_{0:} t\rangle &= -i\sin\frac{\omega t}{2} \\ |\langle S_x - |\alpha, t_{0:} t\rangle|^2 &= \sin^2\frac{\omega t}{2} \end{aligned}$$

The total probability is conserved.

$$|\langle S_x + |\alpha, t_{0:} t\rangle|^2 + |\langle S_x - |\alpha, t_{0:} t\rangle|^2 = 1$$

The expectation value of S_x is

$$\begin{aligned}\langle S_x\rangle &= \langle \alpha, t_{0:}t\,|S_x|\,\alpha, t_{0:}t\rangle \\ &= \frac{\hbar}{2}\left|\langle S_x + |\alpha, t_{0:}t\rangle\right|^2 - \frac{\hbar}{2}\left|\langle S_x - |\alpha, t_{0:}t\rangle\right|^2 \\ &= \frac{\hbar}{2}\cos\omega t\end{aligned}$$

Similarly, we have

$$\begin{aligned}\langle S_y\rangle &= \frac{\hbar}{2}\sin\omega t \\ \langle S_z\rangle &= 0\end{aligned}$$

Question: what happens if we take $\vec{B} = B\hat{x}$?

2.2 The Schrodinger versus the Heisenberg Picture

2.2.1 Unitary operators

Unitary operators are used for many purposed in quantum mechanics. It satisfies that $U^\dagger U = 1$. Under the unitary transformation that changes the state kets it is important to keep in mind that the inner product of a state bra and a state ket remains unchanged,

$$\langle\alpha|\beta\rangle = \left\langle\alpha|U^\dagger U|\beta\right\rangle.$$

Another mathematical observation is that

$$\left(\langle\alpha|\,U^\dagger\right)X\left(U\,|\beta\rangle\right) = \langle\alpha|\left(U^\dagger X U\right)|\beta\rangle$$

that follows from the associative axiom of multiplication. This identity suggests two different approaches to evaluate the expectation values of physical observables under the unitary transformation.

2.2.2 Two Approaches

When we are concerned with a time-dependent of a physical observable $\hat{X}$ there are two approaches:

Approach I:

$$\begin{aligned} |\alpha\rangle &\rightarrow |\alpha, t_0 : t\rangle = U(t, t_0)\,|\alpha, t_0\rangle \\ \left\langle \hat{X} \right\rangle_{tI} &\rightarrow \langle \alpha, t_0 : t|\, \hat{X}\, |\alpha, t_0 : t\rangle \\ &= \left\langle \alpha \left| U^{+} X U \right| \alpha \right\rangle \end{aligned}$$

Approach II:

$$\begin{aligned} |\alpha\rangle &\rightarrow |\alpha\rangle \\ \hat{X} &\rightarrow U^{+} X U \equiv \hat{X}(t) \\ \left\langle \hat{X} \right\rangle_{tII} &= \langle \alpha\, |X(t)|\, \alpha \rangle \\ &= \left\langle \alpha \left| U^{+} X U \right| \alpha \right\rangle \end{aligned}$$

The expectation values of two approaches are the same!

$$\left\langle \hat{X} \right\rangle_{tI} = \left\langle \hat{X} \right\rangle_{tII}.$$

Approach I (The Schrodinger Picture): The state ket varies with time $|\alpha\rangle \rightarrow U\,|\alpha\rangle$

while operators do not change. Recall the Schrodinger equation for the wave function, i.e., the state.

Approach II (The Heisenberg Picture): The operators vary with time $X \rightarrow U^{+}XU$ while the ket does not change. Recall the Heisenberg equation for operators.

We denote the operator $X^{(H)}$ in the Heisenberg picture. $U(t) = U(t, t_0)$. The relation of an observable in two pictures

$$X^{(H)}\,(t) = U^{+}(t)X^{(S)}U(t)$$

The state ket

$$\begin{aligned} |\alpha, t_0 : t\rangle_H &= |\alpha, t_0 = 0\rangle\,; \\ |\alpha, t_0 : t\rangle_S &= U(t)\,|\alpha, t_0 = 0\rangle = U(t)\,|\alpha, t_0 : t\rangle_H \end{aligned}$$

2.2.3 The Heisenberg Equation of Motion.

We now derive the fundamental equation of motion in the Heisenberg picture. Assume that $\hat{X}^{(S)}$ does not depend explicitly on time

$$\begin{aligned} \frac{d}{dt}X^{(H)} &= \frac{d}{dt}\left[U^{+}(t)\hat{X}^{(S)}\,U(t)\right] \\ &= \left(\frac{d}{dt}U^{+}(t)\right)\hat{X}^{(S)}\,U(t) + U^{+}(t)X^{(S)}\frac{d}{dt}U(t) \\ &= -\frac{1}{i\hbar}U^{+}(t)\hat{H}\hat{X}^{(S)}\,U(t) + \frac{1}{i\hbar}U^{+}(t)\hat{X}^{(S)}\,\hat{H}U(t) \\ &= +\frac{1}{i\hbar}U^{+}(t)\hat{X}^{(S)}\,U(t)U^{+}(t)\hat{H}U(t) - \frac{1}{i\hbar}U^{+}(t)\hat{H}U(t)U^{+}(t)X^{(S)}U(t) \\ &= \frac{1}{i\hbar}[\hat{X}^{(H)}\,, \hat{H}^{(H)}] \end{aligned}$$

$$i\hbar\frac{d}{dt}X^{(H)} = [X^{(H)}\,, H^{(H)}]$$

This is the Heisenberg equation of motion! In the case that $\hat{H}$ is time-independent or the $\hat{H}$'s at different times commutes we have

$$\hat{H}^{(H)} = U^{+}\hat{H}U = \hat{H}$$

Thus

$$i\hbar\frac{d}{dt}X^{(H)} = [X^{(H)}, \hat{H}]$$

2.2.4 How to construct a Hamiltonian

1. For a physical system with classical analogue we assume the Hamiltonian to be of the same form as in classical physics; we merely replace the classical x_i' and p_i' by the corresponding operators $\hat{x}_i$ and $\hat{p}_i$ in quantum mechanics. With this assumption we can reproduce the correct classical equation in the classical limit. It is required that the Hamiltonian in quantum mechanics should be Hermitian.

2. When the physical system in question has no classical analogues, we can only guess the structure of the Hamiltonian. We try various forms until we get the Hamiltonian that leads to results agreeing with empirical observation.

Two useful formulas:

$$[\hat{x}_i, F(\hat{p})] = i\hbar\frac{\partial}{\partial p_i}F$$

and

$$[\hat{p}, G(\hat{x})] = -i\hbar\frac{\partial}{\partial x_i}G$$

where F and G are functions that can be expanded in powers of $p_i's$ and $x_i's$ respectively.

Example 1

A free particle: The Hamiltonian to describe the motion of a free particle of mass m is taken to be of the same form as in classical mechanics:

$$H = \frac{p^2}{2m} = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2)$$

We look at the observables x_i and p_i (they are operators, NOT numbers)

$$\frac{d}{dt}p_i = \frac{1}{i\hbar}[p_i, H] = 0$$

$$\frac{d}{dt}x_i = \frac{1}{i\hbar}[x_i, H] = \frac{p_i}{m} = \frac{p_i(0)}{m}$$

So

$$x_i(t) = x_i(0) + \frac{p_i(0)}{m}t$$

We know

$$[x_i(0), x_j(0)] = 0$$

but

$$[x_i(t), x_i(0)] = -i\frac{\hbar}{m}t$$

Example 2

A particle in a potential.

$$H = \frac{p^2}{2m} + V(x)$$

The Heisenberg equation of motion leads to

$$\frac{dp_i}{dt} = \frac{1}{i\hbar}[p_i, V(x)] = -\frac{\partial}{\partial x_i}V(x)$$

$$\frac{dx_i}{dt} = \frac{1}{i\hbar}[x_i, H] = \frac{p_i}{m}$$

Furthermore,

$$\frac{d^2x_i}{dt^2} = \frac{1}{i\hbar}[\frac{dx_i}{dt}, H] = \frac{1}{i\hbar}[\frac{p_i}{m}, H] \equiv \frac{1}{m}\frac{dp_i}{dt}$$

$$\frac{d^2x_i}{dt^2} \quad = \quad -\nabla V(x)$$

Newtonian Equation?

The expectation value of this equation is known as the Ehrenfest theorem. It has the classical mechanics analogue. The reason is that the Planck constant disappears in the equation.

2.3 Simple Harmonic Oscillator.

2.3.1 Eigenvalue and eigenstates

We consider a simple harmonic oscillator in a one-dimensional case. The basic Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{m}{2}\omega^2 x^2$$

where x and p are Hermitian since they are physically dynamic variables. The quantum condition is

$$[x, p] = xp - px = i\hbar$$

As the first step to solve the problem, we evaluate the commutator basket of x and p with H

$$[x, H] = \frac{1}{2m}[x, p^2] = \frac{i\hbar}{m}p$$

$$[p, H] = \frac{m\omega^2}{2}[p, x^2] = -i\hbar m\omega^2 x$$

Adding the two equations, we have

$$\begin{aligned}[x + i\gamma p, H] &= \gamma\hbar m\omega^2 x + \frac{i\hbar}{m}p \\ &= \gamma\hbar m\omega^2(x + i\frac{1}{\gamma}\frac{1}{m^2\omega^2}p)\end{aligned}$$

where γ is a constant. Here we take

$$\gamma = \pm\frac{1}{m\omega}$$

We have

$$[x \pm i\frac{1}{m\omega}p, H] = \pm\hbar\omega(x \pm i\frac{1}{m\omega}p)$$

As

$$[x + i\frac{1}{m\omega}p, x - i\frac{1}{m\omega}p] = \frac{2\hbar}{m\omega}$$

we take

$$a = \left(\frac{m\omega}{2\hbar}\right)^{1/2}(x + i\frac{1}{m\omega}p);\ a^+ = \left(\frac{m\omega}{2\hbar}\right)^{1/2}(x - i\frac{1}{m\omega}p)$$

such that

$$[a, a^+] = 1.$$

Furthermore,

$$a^+a = \frac{m\omega}{2\hbar}(x - i\frac{1}{m\omega}p)(x + i\frac{1}{m\omega}p) = \frac{H}{m\omega} - \frac{1}{2}$$

Thus

$$H = \hbar\omega(\hat{N} + \frac{1}{2})$$

where

$$\hat{N} = a^+a,$$

Obviously,

$$[H, \hat{N}] = 0 \qquad i.e.$$

N and H can be diagonalized simultaneously. We denote the eigenkets of N by its eigenvalues n. So

$$\hat{N}\,|n\rangle = n\,|n\rangle$$

and

$$H\,|n\rangle = (n + \frac{1}{2})\hbar\omega\,|n\rangle$$

What's n?

We first note that

$$[a, N] = aa^{+}a - a^{+}aa = [a, a^{+}]a = a$$

$$[a^{+}, N] = -a^{+}$$

As a result,

$$\begin{aligned} \hat{N}a^{+}\,|n\rangle &= \left\{[\hat{N}, a^{+}] + a^{+}\hat{N}\right\}|n\rangle \\ &= (n+1)a^{+}\,|n\rangle \end{aligned}$$

Likewise,

$$\hat{N}a\,|n\rangle = (n-1)a\,|n\rangle$$

Thus $a^{+}\,|n\rangle$ is also an eigenket of $\hat{N}$ with eigenvalue $n+1$ (increased by one). $a\,|n\rangle$ is an eigenket of $\hat{N}$ with eigenvalue $n-1$ (decreased by one). So we call a the decreasing operator and a^{+} the increasing operator. From the point of view of energy, the increase (decrease) of n by one amounts to the creation (annihilation) of one quantum unit of energy. Hence the terms "creation and annihilation operator" for a^{+} and a are deemed appropriate. Since

$a\,|n\rangle$ is an eigenket with $n-1$. We write

$$\begin{aligned} a\,|n\rangle &= C_n\,|n-1\rangle \\ (\langle n|\,a^+)(a\,|n\rangle) &= \langle n-1|\,(C_n^* C_n)\,|n-1\rangle \\ &\Downarrow \\ \langle n\,|a^+ a|\,n\rangle &= n = |C_n|^2 \geq 0 \end{aligned}$$

We take C_n real. then,

$$a\,|n\rangle = n^{1/2}\,|n-1\rangle$$

Likewise,

$$a^+\,|n\rangle = (n+1)^{1/2}\,|n+1\rangle$$

Suppose we keep on applying a to both sides of eq.(1),

$$a^2\,|n\rangle = [n(n-1)]^{1/2}\,|n-2\rangle$$

$$a^3\,|n\rangle = [n(n-1)(n-2)]^{1/2}\,|n-3\rangle$$

The sequence of the eigenket must terminate at $n=0$ as $n \geq 0$. If n is a non-integer, the sequence shall not terminate and leads to eigenkets with negative eigenvalues. This is in contradiction with $n \geq 0$. To conclude n is a nonnegative integer. The lowest energy state, i.e. the ground state of the oscillator is

$$E_{n=0} = \frac{1}{2}\hbar\omega$$

The eigenstate	eigenvalue
$\|0\rangle$	$\frac{1}{2}\hbar\omega$
$\|1\rangle = a^+ \|0\rangle$	$\frac{3}{2}\hbar\omega$
$\|2\rangle = \frac{1}{2^{1/2}}(a^+)^2 \|0\rangle$	$\frac{3}{2}\hbar\omega$
$\|3\rangle = \frac{1}{(3!)^{1/2}}(a^+)^3 \|0\rangle$	$\frac{7}{2}\hbar\omega$
$\vdots$	$\vdots$
$\|n\rangle = \frac{1}{(n!)^{1/2}}(a^+)^n \|0\rangle$	$(n+\frac{1}{2})\hbar\omega$

Position and Momentum

$$x = \left(\frac{\hbar}{2m\omega}\right)^{1/2}(a+a^+)$$

$$p = i\left(\frac{m\hbar\omega}{2}\right)^{1/2}(-a+a^+)$$

From the orthonormality conditions

$$\langle n'|a|n\rangle = n^{1/2}\delta_{n'n-1}$$

$$\langle n'|a^+|n\rangle = [n+1]^{1/2}\,\delta_{n'n+1}$$

In the matrix form,

$$a = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 2^{1/2} & 0 & \cdots \\ 0 & 0 & 0 & 3^{1/2} & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$a^{+} = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ 1 & 0 & 0 & 0 & \cdots \\ 0 & 2^{1/2} & 0 & 0 & \cdots \\ 0 & 0 & 3^{1/2} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

The matrix elements of x and p are

$$\begin{aligned} \langle n' \left| x \right| n \rangle &= \left(\frac{\hbar}{2m\omega} \right)^{1/2} \\ &\quad \left(n^{1/2} \delta_{n'n-1} + (n-1)^{1/2} \delta_{n'n+1} \right) \\ \langle n' \left| p \right| n \rangle &= i \left(\frac{m\omega\hbar}{2} \right)^{1/2} \\ &\quad \left(-n^{1/2} \delta_{n'n-1} + (n-1)^{1/2} \delta_{n'n+1} \right) \end{aligned}$$

In the Position Representation: the wave function

We first derive $\langle x|0\rangle$

$$\begin{aligned} a \left| 0 \right\rangle &= 0 \\ \Longrightarrow \quad & \langle x \left| a \right| 0 \rangle = 0 \\ \Longrightarrow \quad & \int dx' \langle x \left| a \right| x' \rangle \langle x' \left| 0 \right\rangle = 0 \end{aligned}$$

Recall

$$a = \left(\frac{m\omega}{2\hbar} \right)^{1/2} (x + i \frac{p}{m\omega})$$

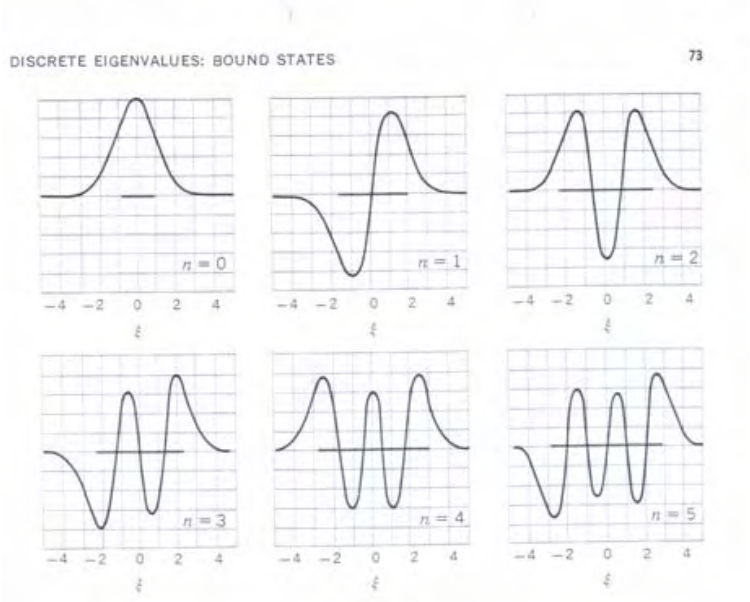


Figure 2.1: Energy eigenfunctions for the first six states of the harmonic oscillator.

$$\begin{aligned}
\langle x\,|\hat{x}|\,x'\rangle &= x\delta(x-x') \\
\langle x\,|p|\,x'\rangle &= -i\hbar\delta(x-x')\frac{\partial}{\partial x} \\
&\Longrightarrow \quad (x+\frac{\hbar}{m\omega}\frac{d}{dx})\,\langle x|0\rangle = 0
\end{aligned}$$

Take $\hbar/m\omega = x_0^2$. The solution of the equation is

$$\langle x|0\rangle = \frac{1}{\pi^{\frac{1}{4}}x_0^{1/2}}\exp(-\frac{1}{2}\frac{x^2}{x_0^2})$$

In general

$$\begin{aligned}
\langle x|n\rangle &= \left\langle x\left|\frac{(a^+)^n}{(n!)^{1/2}}\right|0\right\rangle = \left\langle x\left|\frac{(a^+)^n}{(n!)^{1/2}}\right|x\right\rangle\langle x|0\rangle \\
&= \frac{x_0^{-\frac{n+1}{2}}}{\pi^{\frac{1}{4}}\,(2^n n!)^{1/2}}(x-x_0\frac{d}{dx})^n e^{-\frac{1}{2}\frac{x^2}{x_0^2}}
\end{aligned}$$

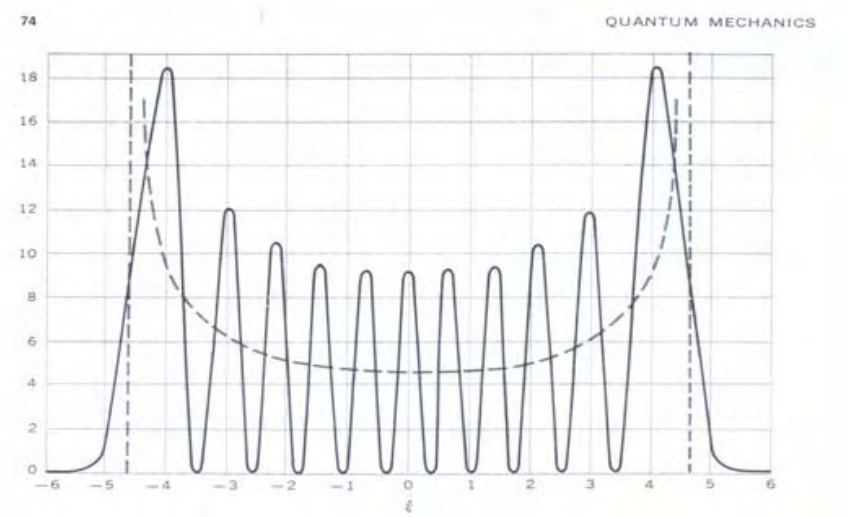


Figure 2.2: The position probability density for the state n=10 of a harmonic oscillator (solid curve) and for a classical oscillator of the same total energy (dashed line).

2.3.2 Time Development of the Oscillator

So far we have not discussed the time evolution of oscillator state ket or observables like a and p. Everything we did is supposed to hold at some instant of time, say $t = 0$. Now we come to see the time evolution of x and p. In the Heisenberg picture,

$$\begin{aligned} \frac{dp}{dt} &= \frac{1}{i\hbar}[p, H] = -m\omega^2 x; \\ \frac{dx}{dt} &= \frac{1}{i\hbar}[x, H] = \frac{p}{m}. \end{aligned}$$

$$\begin{aligned} \frac{d^2p}{dt^2} &= \frac{1}{i\hbar}[\frac{dp}{dt}, H] = \frac{1}{i\hbar}[-m\omega^2 x, H] = -\omega^2 p; \\ \frac{d^2x}{dt^2} &= \frac{1}{i\hbar}[\frac{dx}{dt}, H] = \frac{1}{i\hbar}[\frac{p}{m}, H] = -\omega^2 x; \end{aligned}$$

Equivalently,

$$\begin{aligned}
\frac{da}{dt} &= -i\omega a \Longrightarrow a(t) = a(0)e^{-i\omega t} \\
\frac{da^+}{dt} &= i\omega a^+ \Longrightarrow a^+(t) = a^+(0)e^{i\omega t} \\
x(t) + \frac{i}{m\omega}p(t) &= (x(0) + i\frac{p_{(0)}}{m\omega})e^{-i\omega t} \\
x(t) - \frac{i}{m\omega}p(t) &= (x(0) - i\frac{p_{(0)}}{m\omega})e^{i\omega t} \\
x(t) &= x(0)\cos\omega t + \frac{1}{m\omega}p(0)\sin\omega t \\
p(t) &= -m\omega x(0)\sin\omega t + p(0)\cos\omega t
\end{aligned}$$

For any energy eigenket, we have

$$\begin{cases}
\langle n\,|x(t)|\,n\rangle = 0 \\
\langle n\,|p(t)|\,n\rangle = 0
\end{cases}$$

For a superposition of energy eigenstates such as

$$|\alpha\rangle = C_0\,|0\rangle + C_1\,|1\rangle$$

we have

$$\begin{aligned}
\langle\alpha\,|x(t)|\,\alpha\rangle &= \left[\frac{\hbar}{2m\omega}(C_0^*C_1e^{i\omega t} + C_0C_1^*e^{-i\omega t})\right]^{1/2} \\
&= 2^{1/2}X_0\,|C_0C_1|\cos(\omega t + \delta)
\end{aligned}$$

2.3.3 The Coherent State

How can we construct a superposition of energy eigenstates that most closely imitates the classical oscillator? In wave-function language, we want a wave packet that bounces back

and forth without spreading in shape. It turns out that a coherent state does the desired job.

A coherent state:

$$a\,|\lambda\rangle = \lambda\,|\lambda\rangle$$

Properties of $|\lambda\rangle$

1. The coherent state $|\alpha\rangle = \sum_{n=0}^{\infty} f(n)\,|n\rangle$

   $|f(n)|^2$ is of the Poisson type about some mean value $\bar{n}$

$$|f(n)|^2 = (\frac{\bar{n}^n}{n!}\exp(-\bar{n}))$$

2. It can be obtained by translating the oscillator ground state by some finite distance.

3. It satisfies the minimum uncertainty relation at all time

$$\left\langle (\Delta x(t))^2 \right\rangle \left\langle (\Delta P(t))^2 \right\rangle = \hbar^2/4$$

4. $\lambda = (\bar{n})^{1/2}$

2.4 Schrodinger Wave Equation: Simple Harmonic Oscillator

The Schrodinger equation (see p66 in Schiff's book)

$$H\Psi = \left(\frac{p^2}{2m} + \frac{m}{2}\omega^2 x^2\right)\Psi = E\Psi$$

To solve the problem we first introduce the dimensionless variable $\xi = x/x_0$,

$$\left(-\frac{\hbar^2}{2mx_0^2}\frac{d^2}{d\xi^2} + \frac{m}{2}\omega^2 x_0^2\xi^2\right)\Psi = E\Psi$$

$$\left(-\frac{d^2}{d\xi^2} + \frac{m^2\omega^2}{\hbar^2}x_0^4\xi^2\right)\Psi = \frac{2mx_0^2}{\hbar^2}E\Psi$$

$$\left(-\frac{d^2}{d\xi^2} + \xi^2\right)\Psi = \frac{2E}{\hbar\omega}\Psi = \lambda\Psi$$

We take

$$x_0^2 = \frac{\hbar}{m\omega}.$$

As the potential approach infinite when x$\rightarrow +\infty$ we require the wavefunction approach to zero. From the equation we have

$$\Psi \rightarrow \xi^n e^{-\xi^2/2}.$$

We assume

$$\Psi \rightarrow H(\xi)e^{-\xi^2/2}.$$

Then

$$H^{''} - 2\xi H^{'} + (\lambda - 1)H = 0$$

The solutions are the Hermite polynomials,

$$H_n^{''} - 2\xi H_n^{'} + 2nH_n = 0$$

such that

$$\lambda = 2n + 1; E_n = (n + \frac{1}{2})\hbar\omega \quad n = 0, 1, 2, ...$$

Alternatively, we may write the Hamiltonian in the form

$$\left(-\frac{d^2}{d\xi^2} + \xi^2\right)\Psi = \lambda\Psi$$

$$\frac{1}{2}\left[\left(\xi + \frac{d}{d\xi}\right)\left(\xi - \frac{d}{d\xi}\right) + \left(\xi - \frac{d}{d\xi}\right)\left(\xi + \frac{d}{d\xi}\right)\right]\Psi = \lambda\Psi$$

$$\begin{aligned} a &= \frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right); a^\dagger = \frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right) \\ [a, a^\dagger] &= 1 \end{aligned}$$

$$\left(2a^\dagger a + 1\right)\Psi = \lambda\Psi$$

The ground state

$$a\Psi_0 = 0.$$

2.5 Propagators and Feynman Path Integrals

2.5.1 Propagators in Wave Mechanics.

Time-evolution problem with a time-independent Hamiltonian can be solved once we expand the initial ket in terms of the eigenkets of an observable that commute with H.

$$\begin{aligned} & |\alpha, t_0, t\rangle \\ = \;& \exp(-\frac{i}{\hbar}H(t-t_0))\,|\alpha, t_0\rangle \\ = \;& \sum_{\{a'\}} \exp(-\frac{i}{\hbar}H(t-t_0))\,|a'\rangle\,\langle a'\,|\alpha, t\,\rangle \\ = \;& \sum_{\{a'\}} \exp(-\frac{i}{\hbar}E_{a'}(t-t_0))\,|a'\rangle\,\langle a'\,|\alpha, t\,\rangle \end{aligned}$$

Multiplying both sides by $\langle x|$ on the left, we have

$$\begin{aligned}
& \langle x|\alpha, t_0 : t\rangle \\
= & \sum_{a'} \exp(-\frac{i}{\hbar} E_{a'}(t-t_0)) \langle x|a'\rangle \langle a'|\alpha, t\rangle \\
= & \int dx' \sum_{a'} \exp(-\frac{i}{\hbar} E_{a'}(t-t_0)) \langle x|a'\rangle \langle a'|x'\rangle \langle x'|\alpha, t_0\rangle \\
= & \int dx' K(x,t,x',t_0') \langle x'|\alpha, t_0\rangle
\end{aligned}$$

where

$$K(x,t,x',t_0') = \sum_{a'} \langle x|a'\rangle \langle a'|x'\rangle e^{-\frac{i}{\hbar}E_{a'}(t-t_0)}$$

Denote by $\psi_\alpha(x,t)$ the wave-function

$$\psi_\alpha(x,t) \equiv \langle x|\alpha, t_0 : t\rangle$$

we have

$$\psi_\alpha(x,t) \equiv \int dx' K(x,t,x',t_0')\psi_\alpha(x',t)$$

We call the kernel of the integral operator K as the propagator in the wave mechanics. In any given problem the propagator depends only on the potential and is independent of the initial and final wave-function. It can be constructed once the energy eigenvalues and eigen functions are given. Clearly the time evolution of the wave function is completely predicted if K is known and $\psi_\alpha(x',t)$ is given initially. The only peculiar feature, if any, is that when a measurement intervenes, the wave function changes abruptly in an uncontrollable way„ into one of the eigen functions of observable being measured.

Two Properties of K:

1. For $t > t_0$, K satisfies the Schrodinger's time-dependent wave equation in the variables

x' an t with x and t_0 fixed.

$$i\hbar\frac{\partial}{\partial t}K(x,t,x',t_0') = HK(x,t,x',t)$$

2.

$$\lim_{t\to t_0} K(x,t,x',t_0') = \delta(x-x')$$

Proof.

$$\lim_{t\to t_0} K(x,t,x',t_0') = \lim_{t\to t_0}\sum_{a'}\langle x|a'\rangle\langle a'|x'\rangle\, e^{-i\frac{E_{a'}}{\hbar}(t-t_0)}$$

$$= \lim_{t\to t_0}\sum_{a'}\langle x|a'\rangle\langle a'|x'\rangle = \langle x|x'\rangle = \delta(x-x')$$

The propagator K is simply the Green's function for the time-dependent wave equation satisfying

$$(-\frac{\hbar^2}{2m}\nabla^2 + V_{(x)} - i\hbar\frac{\partial}{\partial t})K(x,t,x',t_0') = -i\hbar\delta(x-x')\delta(t-t_0) \tag{2.1}$$

With the boundary condition

$$K(x,t,x',t_0') = 0 \quad \text{for} \quad t < t_0$$

The δ-function $\delta(t-t_0)$ is needed on the right hand side of the Eq.(2.1) because K varies discontinuously at $t = t_0$. ■

Example 3

A free particle in 1D

The Hamiltonian is expressed as

$$H = \frac{1}{2m}\hat{P}^2$$

The momentum $\hat{\mathrm{P}}$ commutes with H. Hence $|P\rangle$ is a simultaneous eigenket of the operators $\hat{\mathrm{P}}$ and $\hat{\mathrm{H}}$.

$$\begin{aligned} \hat{P}\,|P\rangle &= P\,|P\rangle \\ \hat{H}\,|P\rangle &= \frac{P^2}{2m}\,|P\rangle \end{aligned}$$

Thus

$$\begin{aligned} & K(x,t,x',t_0') \\ = & \sum_p \langle x|p\rangle\,\langle p|x'\rangle \exp\left[-i\frac{p^2}{2m\hbar}(t-t_0)\right] \\ = & \int \frac{dp}{2\pi\hbar}\exp\left[i\frac{px}{\hbar}-i\frac{px'}{\hbar}-\frac{p^2}{2m\hbar}(t-t_0)\right] \\ = & \int_{-\infty}^{+\infty}\frac{dp'}{2m\hbar}\exp\left[-i\frac{t-t_0}{2m\hbar}(P-\frac{m(x-x')}{t-t_0})^2+i\frac{m(x-x')^2}{2\hbar(t-t_0)}\right] \\ = & \lim_{\alpha\to 0^+}\int_{-\infty}^{+\infty}\frac{dp}{2m\hbar}\exp\left[-\alpha\,|p|-i\frac{t-t_0}{2m\hbar}(P-\frac{m(x-x')}{t-t_0})^2+i\frac{m(x-x')^2}{2\hbar(t-t_0)}\right] \\ = & \left[\frac{m}{2\pi i\hbar(t-t_0)}\right]^{1/2}\exp(i\frac{m(x-x')^2}{2\hbar(t-t_0)}) \end{aligned}$$

Certain space and time integral derivable from K are of considerable.

Without loss of generality, we set $t=0$ in the following

(1) $x = x'$

$$\begin{aligned} G(t) &= \int dx K(x,t,x,0) \\ &= \int dx \sum_a \langle x|a\rangle \langle a|x\rangle e^{-i\frac{E_a t}{\hbar}} \\ &= \int dx \sum_a \langle a|x\rangle \langle x|a\rangle e^{-i\frac{E_a t}{\hbar}} \\ &= \sum_a \langle a|a\rangle e^{-i\frac{E_a t}{\hbar}} \\ &= T_r(e^{-iHt/\hbar}) \end{aligned}$$

(2) Let us consider the Laplace-Fourier transform of G(t).

$$\begin{aligned} \tilde{G}(E) &\equiv -i\int_0^\infty dt G(t) e^{iEt/\hbar - \varepsilon t/\hbar} \quad (\varepsilon \to 0^+) \\ &= -i\int_0^\infty dt \sum_a e^{-i(E-E_a+i\varepsilon)t/\hbar} \\ &= \sum_a \frac{1}{E - E_a + i\varepsilon} \qquad (\varepsilon \to 0^+) \end{aligned}$$

The complete energy spectrum is exhibited as simply poles of $\tilde{G}(E)$ in the complex plane.

2.5.2 Propagator as a Transition Amplitude.

To gain further insight into the physical meaning of the propagator, we rewrite it in an alternative form, which is related the concept of transition amplitude.

$$\begin{aligned} K(x,t,x',0) &= \sum_a \langle x|a\rangle \langle a|x'\rangle e^{-iE_a(t-t_0)/\hbar} \\ &= \sum_a \left\langle x \left| e^{-\frac{iE_a t}{\hbar}} \right| a \right\rangle \left\langle x \left| e^{\frac{iE_a t_0}{\hbar}} \right| x' \right\rangle \\ &= \sum \left\langle x \left| e^{-\frac{iHt}{\hbar}} \right| a \right\rangle \left\langle a \left| e^{\frac{iHt_0}{\hbar}} \right| x' \right\rangle \\ &= \langle x,t|x',t_0\rangle \end{aligned}$$

Where $|x,t\rangle$ and $|x',t_0\rangle$ are to be understood as an eigenket and of the position operators in the Heisenberg picture. Roughly speaking, $\langle x,t|x',t_0\rangle$ is the amplitude for the particle to go from a space-time point (x',t_0) to another one (x,t)

Path Integral as the Sum Over Paths

Without loss of generality we restrict ourselves to one-dimensional problem. The entire time interval between $t^i = t_1$ and $t^f = t_N$ is divided into N-1 equal parts.

$$t_j - t_{j-1} = \Delta t = \frac{t_N - t_1}{N-1} \qquad (j = 1, ...N)$$

Exploiting the composition property we obtain

$$\begin{aligned} &\langle x_N,t_N|x_1,t_1\rangle \\ = &\int dx_{N-1} \int dx_{N-2} ... \int dx_2 \\ &\times \langle x_N,t_N|x_{N-1},t_{N-1}\rangle \langle x_{N-1},t_{N-1}|x_{N-2},t_{N-2}\rangle \\ &... \langle x_2,t_2|x_1,t_1\rangle \end{aligned}$$

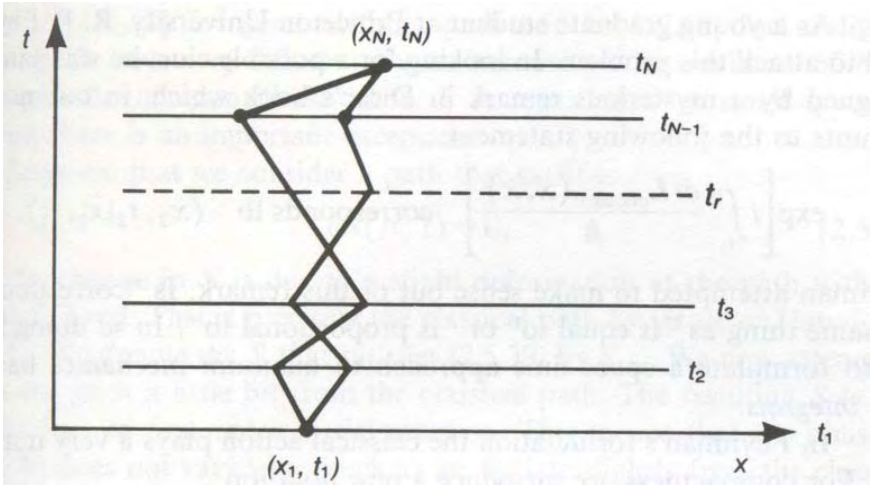


Figure 2.3: Paths in x-t plane.

Before proceeding further, it is profitable to review here how paths appear in classical mechanics. Suppose we have a particle subjected to a force field, say gravitional field,.

$$V_{(x)} \quad \Leftrightarrow \quad mgx$$

$$(x_1, t_1) \quad \Leftrightarrow \quad (h, 0)$$

$$(x_N, t_N) \quad \Leftrightarrow \quad (0, \left(\frac{2h}{g}\right)^{1/2})$$

The classical Lagrangian is written as

$$L_c(x, x') = \frac{1}{2}m\left(\frac{dx}{dt}\right)^2 - V(x)$$

According to Hamiltonian's principle, the unique path is determined by minimizing the action

$$\delta \int_{t_1}^{t_N} dt L_c(x, x) = 0$$

Feynman's Formalism

The basic difference between classical mechanics and quantum mechanics should be apparent: In classical mechanics, a definite path in x-t plane is associated with the

particle's motion; in contrast, in quantum mechanics all possible paths must play roles including those which do not bear any resemblance to the classical path.. Yet the difference should disappear when $\hbar \to 0$. To formulate Feynman's approach, let us go back to $\langle x_n, t_n | x_{n-1}, t_{n-1} \rangle$ with $\Delta t = t_n - t_{n-1}$ $(\Delta t \to 0)$. We write

$$\langle x_n, t_n | x_{n-1}, t_{n-1} \rangle = \frac{1}{w(\Delta t)} \exp(i \frac{S(n, n-1)}{\hbar})$$

where

$$S(n, n-1) = \int_{t_{n-1}}^{t_n} dt L_c(x, x)$$

and w(Δt) is determined by

$$\langle x_n, t_n | x_{n-1}, t_{n-1} \rangle \,|_{t_n = t_{n-1}} = \delta(x_n - x_{n-1})$$

Because at any given time the position kets in the Heisenberg picture form a complete set, it is legitimate to insert the identity operator written as

$$\int dx \, |x, t\rangle \, \langle x, t| = 1$$

at any time we desire. For example,

$$\begin{aligned} \left\langle x^f, t^f | x^i, t^i \right\rangle &= \int dx \left\langle x^f, t^f | x, t \right\rangle \left\langle x, t | x^i, t^i \right\rangle \\ &= \int dx dx' \left\langle x^f, t^f | x', t' \right\rangle \left\langle x', t' | x, t \right\rangle \left\langle x, t | x^i, t^i \right\rangle \\ &= \ ... \end{aligned}$$

and so on. If we somehow guess the form of $\langle x_2, t_2 | x_1, t_1 \rangle$ for a finite time interval by compounding the appropriate transition amplitude for infinitesimal time interval. This property leads to formulate a space-time approach to quantum mechanics. Our task is to

evaluate the $\Delta t \to 0$ limit of S(n,n-1). As $\Delta t \to 0$,

$$\begin{aligned} S(n,n-1) &= \int_{t_{n-1}}^{t_n} dt(\frac{1}{2}m\dot{x}^2 - V(x)) \\ &= \Delta t(\frac{1}{2}m(\frac{x_n - x_{n-1}}{\Delta t})^2 - V(\frac{x_n - x_{n-1}}{2})) \end{aligned}$$

For a free-particle case, $V = 0$,

$$\langle x_n, t_n | x_{n-1}, t_{n-1} \rangle \,|_{t_n = t_{n-1}} = \delta(x_n - x_{n-1})$$

we obtain

$$\frac{1}{w(\Delta t)} = \Big(\frac{m}{2\pi i\hbar\Delta t}\Big)^{1/2}$$

where we have used

$$\int_{-\infty}^{\infty} \Big(\frac{m}{2\pi i\hbar\Delta t}\Big)^{1/2} e^{i\frac{m}{2\pi i\hbar\,\Delta t}\xi^2} d\xi = 1$$

and

$$\lim_{\Delta t \to 0} \Big(\frac{m}{2\pi i\hbar\Delta t}\Big)^{1/2} e^{i\frac{m}{2\pi i\hbar\,\Delta t}\xi^2} = \delta(\xi)$$

To summarize, as $\Delta t \to 0$, we obtain

$$\langle x_n, t_n | x_{n-1}, t_{n-1} \rangle = \Big(\frac{m}{2\pi i\hbar\Delta t}\Big)^{1/2} e^{i\frac{W(n,n-1)}{\hbar}}$$

The final expression for the transition amplitude with $t_N - t_1$ is

$$\begin{aligned} & \langle x_N, t_N | x_1, t_1 \rangle \\ = & \lim_{N \to +\infty} (\frac{m}{2\pi i\hbar\Delta t})^{\frac{N-1}{2}} \int dx_{N-1} dx_{N-2} ... dx_2 \prod_{n=2}^{N} e^{i\frac{W(n,n-1)}{\hbar}} \\ \equiv & \int_{x_1}^{x_N} \mathcal{D}(x(t_1)) e^{i\int_{t_1}^{t_N} L_c(x,x)dt/\hbar} \end{aligned}$$

This is Feynman's path integral!

2.6 The Gauge Transformation and Phase of Wave Function

2.6.1 Constant Potential

In classical mechanics, it is well known that the zero point of potential energy is of no physical significance. The force that appears in Newton's second law depends only on the gradient of the potential; an additive constant is clearly irrelevant. e.g.

$$m\frac{d\vec{v}}{dt} = f : \quad \begin{matrix} mg & -eE \\ -\bigtriangledown\phi_g & -\bigtriangledown\phi_e \end{matrix}$$

when $\phi \rightarrow \phi + \phi_0$

$$m\frac{d\vec{v}}{dt} = f \rightarrow m\frac{d\vec{v}}{dt} = f$$

Let us look at the time evolution of a Schrodinger picture state ket subject to some potential

$$\begin{aligned} V_{(x)} &\implies V_{(x)} + V_0 \\ H &= \frac{P^2}{2m} + V(x) \implies H = \frac{P^2}{2m} + V(x) + V_0 \\ |\alpha, t_0 : t\rangle &\implies \widetilde{|\alpha, t_0 : t\rangle} =? \end{aligned}$$

To be precise we consider a time-independent H

$$|\alpha, t_0 : t\rangle = e^{-i\frac{H}{\hbar}(t-t_0)} \ |\alpha, t_0\rangle$$

Thus

$$\widetilde{|\alpha, t_0 : t\rangle} = e^{-i\frac{V_0(t-t_0)}{\hbar}} \ |\alpha, t_0 : t\rangle$$

For a stationary state, if the time-dependence computed with V(x) is

$$e^{-iE(t-t_0)/\hbar}$$

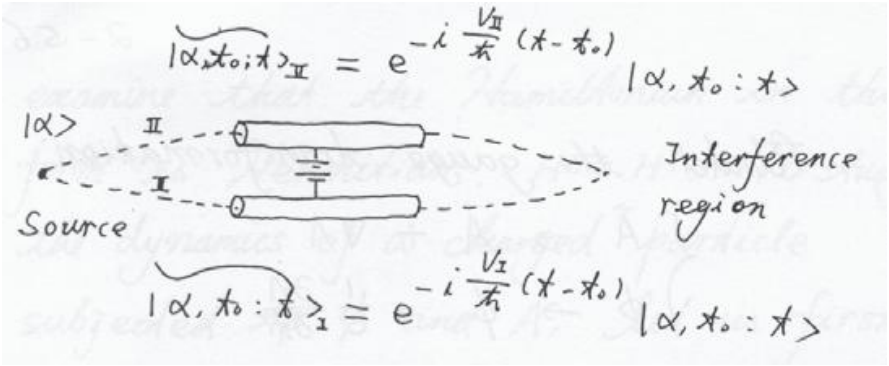


Figure 2.4: Quantum-mechanical interference to detect a potential difference.

then the corresponding time dependence computed with $V(x) + V_0$ is

$$e^{-i(E+V_0)(t-t_0)/\hbar}$$

Even though the choice of the absolute scale of the potential is arbitrary, potential difference are of non-trivial physical significance and in fact, can be detected in a very striking way. A beam of charged particles is split into two parts, each of which enters a metallic cage. A particle in the beam can be visualized as a wave packet whose dimension is much smaller than the dimension of the cage. Inside the cage the potential is spatially uniform. Hence the particle in the cage experience no force. If we desire, a finite potential difference between the two cages can be maintained by turning on a switch. The final state which the two beams reach at interference region is

$$|f\rangle = \frac{1}{2^{1/2}} |\alpha, t_0 : t\rangle_I + \frac{1}{2^{1/2}} |\alpha, t_0 : t\rangle_{II}$$

Thus

$$\langle f|f\rangle = 1 + \cos(V_I - V_{II})t/\hbar$$

This is an observable effect! This is a purely quantum mechanical effect and has no classical analogue.

2.6.2 Gauge Transformation in Electromagnetism

We first recall the Maxwell's equations

$$\begin{cases} \nabla \cdot D = 4\pi\rho; \\ \nabla \times H = \frac{4\pi}{c} J + \frac{1}{c}\frac{\partial D}{\partial t}; \\ \nabla \cdot B = 0; \\ \nabla \times E = -\frac{1}{c}\frac{\partial D}{\partial t} \end{cases}$$

$$D = E + 4\pi P$$

$$H = B - 4\pi M$$

We introduce a scalar potential ϕ and a vector potential $\vec{A}$

$$\begin{cases} \vec{B} = \bigtriangledown \times \vec{A} \\ \vec{E} = - \bigtriangledown \phi - \frac{1}{c}\frac{\partial}{\partial t}\vec{A} \end{cases}$$

Then the Maxwell's equations are reduced to

$$\begin{cases} \bigtriangledown^2 \phi - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\phi = -4\pi\rho \\ \bigtriangledown^2 \vec{A} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\phi = -\frac{4\pi}{c} J \end{cases}$$

with

$$\bigtriangledown \vec{A} + \frac{1}{c}\frac{\partial \phi}{\partial t} = 0$$

Under the gauge transformation.

$$\begin{cases} \vec{A} \to \vec{A} + \bigtriangledown \Lambda \\ \phi \to \phi - \frac{1}{c}\frac{\partial \Lambda}{\partial t} \end{cases}$$

with

$$\bigtriangledown^2 \Lambda - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\Lambda = 0$$

the Maxwell's equations keep unchanged! In quantum mechanics, the Hamiltonian for a particle of electric charge e ($e < 0$ for electron in Sakurai's book) , subjected to the electromagnetic field is taken from classical physics to be

$$\begin{aligned} H &= \frac{1}{2m}(p - \frac{e}{c}A)^2 + e\phi \\ &= \frac{1}{2m}(p^2 - \frac{e}{c}pA - \frac{e}{c}Ap + \frac{e^2}{c^2}A^2) + e\phi \\ &\neq \frac{1}{2m}(p^2 - \frac{2e}{c}pA + \frac{e^2}{c^2}A) + e\phi \end{aligned}$$

because p and A do not commute, $[p, A] \neq 0$. It is straightforward to examine that the Hamiltonian in this form is Hermitian, $H = H^+$. To study the dynamics of a charged particle subjected to ϕ and A, let us first proceed in the Heisenberg picture:

$$\frac{d}{dt}x_i = \frac{1}{i\hbar}[x_i, H] = \frac{1}{m}(p_i - \frac{e}{c}A_i)$$

where $i = x, y, z$. Define

$$\pi \equiv m\frac{d\vec{x}}{dt} = p - \frac{e}{c}A$$

We call that p is canonical momentum and $\vec{\pi}$ is kinetic (or mechanical) momentum. The commutation relation of π_i and π_j is

$$\begin{aligned} [\pi_i, \pi_j] &= -\frac{i\hbar e}{c}(\frac{\partial}{\partial x_i}A_j - \frac{\partial}{\partial x_i}A_j) \\ &= -i\frac{\hbar e}{c}\epsilon_{ijk}(\bigtriangledown \times \mathbf{A})_k \end{aligned}$$

Hence the Hamiltonian can be rewritten as

$$H = \frac{\pi^2}{2m} + e\phi$$

We now study the Schrodinger's equation with ϕ and A in the position space.

$$\begin{aligned} & \left\langle x \left| (p - \frac{e}{c}A(x))^2 \right| \alpha, t_0 : t \right\rangle \\ = & \int dx_1 \int dx_2 \left\langle x \left| (p - \frac{e}{c}A(x)) \right| x_1 \right\rangle \left\langle x_1 \left| (p - \frac{e}{c}A(x)) \left| x_2 \right\rangle \right\langle x_2 \right| \alpha, t_0 : t \right\rangle \\ = & (-i\hbar \bigtriangledown - \frac{e}{c}A(x))^2 \left\langle x | \alpha, t_0 : t \right\rangle \end{aligned}$$

Thus the Schrodinger's equation is derived as

$$[\frac{1}{2m}(-i\hbar \bigtriangledown - \frac{e}{c}A_{(x)})^2 + e\phi] \left\langle x | \alpha, t_0 : t \right\rangle = i\hbar \frac{\partial}{\partial t} \left\langle x | \alpha, t_0 : t \right\rangle$$

Denote

$$\varphi(x) \equiv \left\langle x | \alpha, t_0 : t \right\rangle$$

and

$$\rho = \varphi^*(x)\varphi(x)$$

The time derivative of the density is

$$\frac{\partial}{\partial t}\rho = (\frac{\partial}{\partial t}\varphi^*)\varphi + \varphi^* \frac{\partial}{\partial t}\varphi = - \bigtriangledown \cdot \mathbf{j}$$

$$\frac{\partial}{\partial t}\rho + \bigtriangledown \cdot \mathbf{j} = \mathbf{0}$$

where

$$\mathbf{j} = \frac{\hbar}{m} I_m(\varphi^* \bigtriangledown \varphi) - \frac{e}{mc} A \left|\varphi\right|^2$$

For

$$\begin{aligned} \varphi &= \varrho^{1/2} e^{is/\hbar} \\ j &= \frac{\rho}{m}(\bigtriangledown s - \frac{e}{c}A) \end{aligned}$$

2.6.3 The Gauge Transformation

In quantum mechanics, we consider the gauge transformation

$$\begin{cases} \phi \to \phi \\ A \to A + \bigtriangledown \Lambda \end{cases}$$

e.g. Consider a uniform magnetic field in z direction

$$\vec{B} = B\hat{z} = (\frac{\partial}{\partial x}A_y - \frac{\partial}{\partial y}A_x)\hat{z}$$

To derive the field, we can choose

(1). $A_x = -\frac{1}{2}By,\ \ A_y = \frac{1}{2}Bx,$

(2). $A_x = -By,\ \ A_y = 0.$

These two vector potentials are connected by a gauge transformation

$$A \to A + \bigtriangledown(\frac{Bxy}{2})$$

Let us denote by $|\alpha\rangle$ the state ket in the presence of A, and $|\tilde{\alpha}\rangle$ the state ket in the presence of . The Schrodinger's equations for these two state kets are

$$[\frac{1}{2m}(p - \frac{e}{c}A)^2 + e\phi]\,|\alpha, t_0 : t\rangle = i\hbar\frac{\partial}{\partial t}\,|\alpha, t_0 : t\rangle$$

$$[\frac{1}{2m}(p - \frac{e}{c}A - \frac{e}{c}\bigtriangledown\Lambda)^2 + e\phi]|\widetilde{\alpha, t_0 : t}\rangle = i\hbar\frac{\partial}{\partial t}|\widetilde{\alpha, t_0 : t}\rangle$$

What's the relation of $|\alpha, t_0 : t\rangle$ and $|\widetilde{\alpha, t_0 : t}\rangle$?

We come to construct an operator $\mathcal{G}$ such that

$$|\tilde{\alpha}\rangle = \mathcal{G}\,|\alpha\rangle$$

with $\mathcal{G}\mathcal{G}^\dagger$=1.

$$\mathcal{G}^\dagger[\frac{1}{2m}(p - \frac{e}{c}A - \frac{e}{c}\bigtriangledown\Lambda)^2 + e\phi]\mathcal{G}\,|\alpha, t_0 : t\rangle = i\hbar\frac{\partial}{\partial t}\,|\alpha, t_0 : t\rangle$$

We require

(1). $\langle\alpha|x|\alpha\rangle = \langle\tilde{\alpha}|x|\tilde{\alpha}\rangle$:

$$\mathcal{G}^{\dagger} x \mathcal{G} = x$$

(2). $\left\langle\alpha|p - \frac{e}{c}A|\alpha\right\rangle = \left\langle\tilde{\alpha}|p - \frac{e}{c}\tilde{A}|\tilde{\alpha}\right\rangle$:

$$\begin{aligned}
\mathcal{G}^{\dagger}\left(p - \frac{e}{c}A - \frac{e}{c}\bigtriangledown\Lambda\right)\mathcal{G} &= \left(p - \frac{e}{c}A\right) \\
\mathcal{G}^{\dagger}[p, \mathcal{G}] &= +\frac{e}{c}\bigtriangledown\Lambda \\
\mathcal{G}^{\dagger}(-i\hbar\nabla\mathcal{G}) &= +\frac{e}{c}\bigtriangledown\Lambda \\
-i\hbar\nabla\ln\mathcal{G} &= +\frac{e}{c}\bigtriangledown\Lambda \\
\mathcal{G} &= \exp\left[i\frac{e}{\hbar c}\Lambda\right]
\end{aligned}$$

Therefore, if we take

$$|\tilde{\alpha}\rangle = e^{i\frac{e}{\hbar c}\Lambda}|\alpha\rangle$$

then

$$\begin{aligned}
& e^{-i\frac{e}{\hbar c}\Lambda}\left(\frac{1}{2m}(p - \frac{e}{c}A - \frac{e}{c}\bigtriangledown\Lambda)^2 + e\phi\right)e^{i\frac{e}{\hbar c}\Lambda} \\
= \quad & \frac{1}{2m}(p - \frac{e}{c}A)^2 + e\phi
\end{aligned}$$

The two wave-function are related via

$$\varphi(x,t) = e^{i\frac{e}{\hbar c}\Lambda}\varphi(x,t)$$

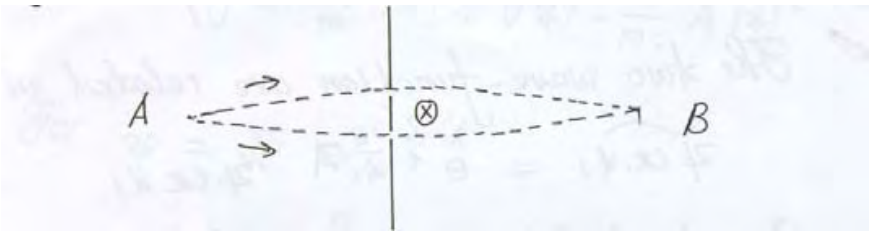


Figure 2.5:

In the form $\varphi = \rho^{1/2} \exp[iS/\hbar]$,we have

$$\begin{aligned} A &\rightarrow A + \nabla\Lambda \\ \rho &\rightarrow \rho \\ S &\rightarrow S + \frac{e}{c}\Lambda \end{aligned}$$

2.6.4 The Aharonov-Bohm Effect

Consider a particle of charge e going above or below a very long impenetrable cylinder, as shown in Fig.

Inside the cylinder is a magnetic field parallel to the cylinder axis, taken to be normal to the plane of Fig. So the particle paths above and below enclose a magnetic flux.

Assume the magnetic field

$$B = \begin{cases} B\hat{z} & \text{if } \rho < \rho_a \\ 0 & \text{if } \rho > \rho_a \end{cases}$$

Hence the particle does not experience the Lorentz force outside cylinder.

$$A = \begin{cases} (0, \frac{1}{2}B\rho, 0), & \text{if } \rho < \rho_a \\ (0, \frac{1}{2\rho}B\rho_a^2, 0), & \text{if } \rho > \rho_a \end{cases}$$

Our object is to study how the probability of finding the particle in the interference region $\vec{B}$ depends on the magnetic flux. For pedagogical reason we prefer to use the Feynman path-integral method to attack this problem.

In the presence of the magnetic field, the Lagrangian can be obtained

$$L_c^{(0)} = \frac{1}{2}m(\frac{dx}{dt})^2 \rightarrow \frac{1}{2}m(\frac{dx}{dt})^2 + \frac{e}{c}\frac{d\vec{x}}{dt}\vec{A}$$

The corresponding change in the action is given by

$$\begin{aligned} S^{(0)}(n,n-1) \quad &\rightarrow \quad S^{(0)}(n,n-1) + \frac{e}{c}\int_{t_{n-1}}^{t_n} dt\frac{d\vec{x}}{dt}\vec{A} \\ &= S^{(0)}(n,n-1) + \frac{e}{c}\int_{x_{n-1}}^{x_n} d\vec{l}\cdot\vec{A} \end{aligned}$$

where $d\vec{l}$ is the differential line element along the path segment. So when we consider the entire contribution from x_1 to x_n.We have

$$\begin{aligned} &\prod_n \exp(iS^{(0)}(n,n-1)/\hbar) \\ \Longrightarrow \quad &\prod_n \exp(iS^{(0)}(n,n-1)/\hbar)\exp(\frac{ie}{\hbar c}\int_{x_{n-1}}^{x_n}\vec{A}\cdot d\vec{l}) \end{aligned}$$

The entire transition amplitude is

$$\int_{above} D_{[x_{(t)}]}e^{i\frac{S^{(0)}(N,1)}{\hbar}} \times e^{i\frac{e}{\hbar c}\int_{x_1}^{x_n} A\cdot d\vec{l}_{above}} + \int_{below} D_{[x_{(t)}]}e^{i\frac{S^{(0)}(N,1)}{\hbar}} \times e^{i\frac{e}{\hbar c}\int_{x_1}^{x_n} A\cdot d\vec{l}_{below}}$$

The probability for finding the particle in the interference region B depends on the modulus square of the entire transition amplitude and hence on the phase difference between the contribution from the paths going above and below. i.e.

$$\rho \propto 1 + \cos(\varphi_1 - \varphi_2)$$

where

$$\begin{aligned}
\varphi_1 - \varphi_2 &= \frac{e}{\hbar c}\left\{\int_{x_1}^{x_n} A\cdot d\vec{l}_{above} - \int_{x_1}^{x_n} \vec{A}\cdot d\vec{l}_{below}\right\} \\
&= \frac{e}{\hbar c}\oint A\cdot d\vec{l} \\
&= \frac{e}{\hbar c}\iint \nabla\times A\cdot d\vec{a} \\
&= \frac{e}{\hbar c}\phi_B
\end{aligned}$$

where ϕ_B stands for the magnetic flux inside the impenetrable cylinder. This means that as we change the magnetic field strength, there is a sinusoidal component in the probability for observing the particle in region B with a period given by a fundamental unit of magnetic flux, namely

$$\frac{2\pi\hbar c}{|e|} = 4.135\times 10^{-7} \quad \text{Gauss-cm}^2$$

2.7 Interpretation of Wave Function.

2.7.1 What's $\Psi_\alpha(x)$?

Since

$$|\alpha, t_0 : t\rangle = \int d_x\, |x\rangle \langle x|\alpha, t_0 : t\rangle = \int d_x\, |x\rangle\, \Psi_\alpha(x,t)$$

$\Psi_\alpha(x,t)$ is regarded as an expansion coefficient of $|\alpha, t_0 : t\rangle$ in terms of the position eigenkets $\{|x\rangle\}$. The quantity

$$\rho(x,t) = |\Psi_\alpha(x,t)|^2$$

is defined as the probability density. So $\rho(x,t)dx$ is the probability that the particle appears in a narrow range round x at time t. This is the so-called the probabilistic interpretation of

wave function.

The Continuity Equation.

$$\begin{aligned} & \frac{\partial}{\partial t}\rho(x,t) \\ = \; & (\frac{\partial}{\partial t}\Psi^*(x,t))\Psi(x,t) + \Psi^*(x,t)(\frac{\partial}{\partial t}\Psi(x,t)) \\ = \; & -\frac{1}{i\hbar}(H^*\Psi^*)\Psi + \Psi^*\frac{1}{i\hbar}H\Psi \end{aligned}$$

Assume

$$\begin{aligned} H &= -\frac{\hbar^2}{2m}\nabla^2 + V \\ \frac{\partial}{\partial\rho}\rho(x,t) &= i\frac{1}{2m}\hbar(\Psi^*(\nabla^2\Psi) - \Psi(\nabla^2\Psi^*)) + \frac{1}{i\hbar}(V - V^*)\Psi^*\Psi \end{aligned}$$

As

$$\begin{aligned} \Psi^*\nabla^2\Psi &= \nabla(\Psi^*\nabla\Psi) - (\nabla\Psi^*)(\nabla\Psi) \\ \Psi\nabla^2\Psi^* &= \nabla(\Psi\nabla\Psi^*) - (\nabla\Psi)(\nabla\Psi^*) \\ \frac{\partial}{\partial t}\rho &= i\frac{\hbar}{2m}\nabla(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) + \frac{1}{\hbar}I_m(V)\cdot\rho \\ \frac{\partial}{\partial t}\rho + \nabla\cdot\mathbf{j} &= \frac{1}{\hbar}I_m(V)\cdot\rho \\ \mathbf{j} &= -\frac{i\hbar}{2m}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) = \frac{\hbar}{m}I_m(\Psi^*\nabla\Psi) \end{aligned}$$

——The probability flux.

When V is purely real, we have

$$\frac{\partial}{\partial t}\rho + \nabla\cdot\mathbf{j} = 0$$

This is the conservation law for probability. When V is complex, which is often used for nuclear reaction for particles absorbed by nuclei, it is accounted for the disappearance of

particles. Except for the probability density, the wave function contains more physics than expected. Let us write it as

$$\Psi(x,t) = \rho(x,t)^{1/2} \exp[iS(x,t)/\hbar]$$

with $\rho > 0$ and S real.

$$\begin{aligned} \Psi^* \nabla \Psi &= \rho^{1/2} \nabla \rho^{1/2} + \frac{i}{\hbar} \rho \nabla S \\ \\ \Longrightarrow \quad \mathbf{j} &= \frac{\rho}{m} \nabla S \end{aligned}$$

The spatial variation of the phase of the wave function characterizes the probability flux; the stronger the phase variation, the more intense the flux. The direction of $\mathbf{j}$ at some point x is seen to be normal to the surface of a constant that goes through that point. Since $\mathbf{j}$ is a flux, $\mathbf{j}$ can be rewritten as

$$\mathbf{j} = \rho(\nabla S/m) \equiv \rho \mathbf{v}$$

This physical meaning is still unclear. It is not a velocity traditionally!

2.7.2 The Classical Limit

Substituting $\Psi = \rho^{1/2} e^{iS/\hbar}$ into a Schrodinger equation leads to

$$\begin{aligned} & -\frac{\hbar^2}{2m}(\nabla^2 \rho^{1/2} + \frac{2i}{\hbar} \nabla \rho^{1/2} \cdot \nabla S) - \frac{1}{\hbar^2} \rho^{1/2} |\nabla S|^2 + (\frac{i}{\hbar}) \rho^{1/2} \nabla^2 S + \rho^{1/2} V \\ = \quad & i\hbar(\frac{\partial \rho^{1/2}}{\partial t} + \frac{i}{\hbar} \rho^{1/2} \frac{\partial S}{\partial t}) \end{aligned}$$

Taking $\hbar \to 0$, we obtain

$$\frac{1}{2m} |\nabla S(x,t)|^2 + V(x) + \frac{\partial}{\partial t} S(x,t) = 0$$

This is the Hamilton-Jacobi equation in classical mechanics. In this sense, the Schrodinger equation goes back to the classical mechanics in the limit $\hbar \to 0$. In the classical mechanics

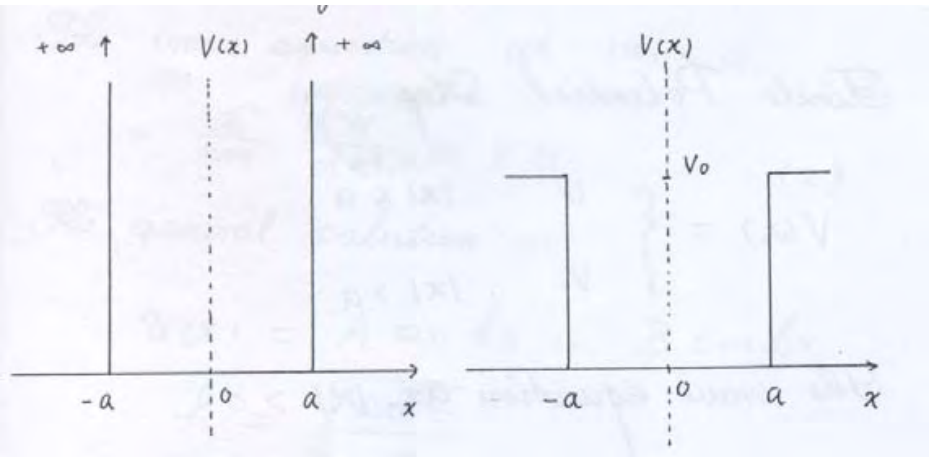


Figure 2.6: One-dimensional square well potential with (a) perfectly rigid walls (b) finite potential.

$S(x,t)$ stands for Hamiltonian principal function. In a stationary state with time dependent $e^{-iE_t/\hbar}$, the Hamilton's principle function S is separable

$$S(x,t) = W(x) - Et$$

2.8 Examples

2.8.1 One dimensional square well potential

Perfect rigid wall

$$V(x) = \begin{cases} 0, & |x| \leq a \\ +\infty, & |x| > a \end{cases}$$

Since the potential is infinite at $|x| > a$ the wave function must vanish at the points $x = \pm a$. The wave function for $|x| \leq a$ is simply

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} = Eu.$$

Introduce a dimensionless quantity $x = \xi a$,

$$\frac{d^2}{d\xi^2}u = -\frac{2ma^2}{\hbar^2}Eu = -\alpha^2 u$$

where $\alpha = (2ma^2E/\hbar^2)^{1/2}$. The general solution is

$$u(\xi) = A\sin\alpha\xi + B\cos\alpha\xi.$$

Application of the boundary conditions at $x = \pm a$, i.e., $\xi = 1$, gives

$$A\sin\alpha + B\cos\alpha = 0$$

$$-A\sin\alpha + B\cos\alpha = 0$$

There are two possible classes of solution

(1). $A = 0$ and $\cos\alpha = 0$

$$\alpha = (n + \frac{1}{2})\pi \tag{2.2}$$

$$u = B\cos\alpha\xi = B\cos\frac{(2n+1)\pi x}{2a} \tag{2.3}$$

$$E = \frac{\hbar^2}{2m}\frac{\alpha^2}{a^2} = \frac{(2n+1)^2\pi^2\hbar^2}{8ma^2} \tag{2.4}$$

(2) $B = 0$ and $\sin\alpha = 0$

$$\alpha = n\pi \tag{2.5}$$

$$u = A\sin\alpha\xi = A\sin\frac{n\pi x}{a} \tag{2.6}$$

$$E = \frac{\hbar^2}{2m}\frac{\alpha^2}{a^2} = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{2.7}$$

Finite potential step

$$V(x) = \begin{cases} 0, & |x| \le a \\ V_0, & |x| > a \end{cases}$$

The wave equation at $|x| < a$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} = Eu$$

The wave equation at $|x| > a$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + V_0 u = Eu$$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} = (E - V_0)u$$

The general solution for $E < V_0$

$$u(x) = \begin{cases} Ce^{-\beta x}, & x > a \\ De^{+\beta x}, & x < a \end{cases}$$

where $\beta = [2m(V_0 - E)]^{1/2}/\hbar$.

For $E > V_0$

$$u(x) = \begin{cases} C_1 \sin kx + D_1 \cos kx, & x > a \\ C_2 \sin kx + D_2 \cos kx, & x < a \end{cases}$$

The wave equation at $|x| < a$ is the same as that in the rigid wall potential, and the general solution is.

$$u(\xi) = A \sin kx + B \cos kx.$$

where $k = (2mE/\hbar^2)^{1/2}$. We now impose on the solutions (1) and (2) the requirements that u and du/dx be continuous at x=$\pm a$.

$$\begin{aligned} A \sin ka + B \cos ka &= Ce^{-\beta a} \\ kA \sin ka - kB \cos ka &= \beta Ce^{-\beta a} \\ -A \sin ka + B \cos ka &= De^{-\beta a} \\ A \sin ka + B \cos ka &= \beta De^{-\beta a} \end{aligned}$$

from which we obtain

$$\begin{aligned} 2A\sin ka &= (C-D)e^{-\beta a} \\ 2kA\cos ka &= -\beta(C-D)e^{-\beta a} \\ 2B\cos ka &= (C+D)e^{-\beta a} \\ 2kB\sin ka &= \beta(C+D)e^{-\beta a} \end{aligned}$$

Two classes of solutions

(1) A=0 and C=D

$$k\tan ka = \beta$$

(2) B=0 and C=-D

$$k\cot ka = -\beta$$

Parity

The Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} + V(x)u(x) = Eu(x)$$

If the potential is symmetric about $x = 0$, $V(x) = V(-x)$, we have

$$-\frac{\hbar^2}{2m}\frac{d^2u(-x)}{dx^2} + V(x)u(-x) = Eu(-x)$$

The u(x) and u(-x) are solutions of the same wave equation with the same eigenvalues E. Addition or subtraction these two equations gives $u(x) \pm u(-x)$, the solution of the Schrodinger equation. To simplify the notation, $u(x) = \pm u(-x)$. Such wave function are

said to have even or odd parity. Note that

$$\cos x = \cos(-x)$$

$$\sin x = -\sin(-x)$$

2.8.2 A charged particle in a uniform magnetic field

Consider a charged particle in a uniform magnetic field. Assume the particle is confined in a two-dimensional plane, and the magnetic field is perpendicular to the plane, say along the z direction. The Hamiltonian is given by

$$H = \frac{1}{2m}(p - \frac{e}{c}A)^2$$

with

$$\vec{B} = B\hat{z} = (\frac{\partial}{\partial x}A_y - \frac{\partial}{\partial y}A_x)\hat{z}$$

To derive the field, we can choose

(1). $A_x = -By, \;\; A_y = 0.$

(2). $A_x = -\frac{1}{2}By, \;\; A_y = \frac{1}{2}Bx.$

Case (1): $A_x = -By, \;\; A_y = 0.$

$$\begin{aligned} H &= \frac{1}{2m}\left[(p_x - \frac{e}{c}A_x)^2 + (p_y - \frac{e}{c}A_y)^2\right] \\ &= \frac{1}{2m}\left[(p_x - \frac{eB}{c}y)^2 + (p_y)^2\right] \end{aligned}$$

Notice that $[p_x, H] = 0$, i.e. p_x is a good quantum number. The general form of the wavefunction is

$$\Psi = \phi(y)e^{ip_0 x}$$

The Schrodinger equation $H\Psi = E\Psi$ is reduced to

$$\frac{1}{2m}\left[(p_0 - \frac{eB}{c}y)^2 + (p_y)^2\right]\phi(y) = E\phi(y)$$

Alternatively

$$\left[\frac{p_y^2}{2m} + \frac{e^2B^2}{2mc^2}(y - y_0)^2\right]\phi(y) = E\phi(y)$$

with $y_0 = \frac{cp_0}{eB}$. Thus the problem is reduced to the simple harmonic oscillator.

(2). $A_x = -\frac{1}{2}By, \quad A_y = \frac{1}{2}Bx.$

$$\begin{aligned} H &= \frac{1}{2m}\left[(p_x - \frac{e}{c}A_x)^2 + (p_y - \frac{e}{c}A_y)^2\right] \\ &= \frac{1}{2m}\left[(p_x - \frac{eB}{2c}y)^2 + (p_y + \frac{eB}{2c}x)^2\right] \end{aligned}$$

In this case both p_x and p_y are not good quantum numbers. We cannot solve this problem like in the case (1). Take

$$\begin{aligned} \pi_x &= p_x - \frac{eB}{2c}y; \\ \pi_y &= p_y + \frac{eB}{2c}x \end{aligned}$$

$$[\pi_x, \pi_y] = -2i\hbar\frac{eB}{2c} = -i\frac{\hbar eB}{c}$$

$$\begin{aligned} H &= \frac{1}{2m}\left[\pi_x^2 + \pi_y^2\right] \\ &= \frac{1}{4m}\left[(\pi_x + i\pi_y)(\pi_x - i\pi_y) + (\pi_x - i\pi_y)(\pi_x + i\pi_y)\right] \end{aligned}$$

$$[\pi_x - i\pi_y, \pi_x + i\pi_y] = \frac{2\hbar eB}{c}$$

Take

$$\begin{aligned} a &= \sqrt{\frac{c}{2\hbar eB}}(\pi_x - i\pi_y) \\ a^\dagger &= \sqrt{\frac{c}{2\hbar eB}}(\pi_x + i\pi_y) \end{aligned}$$

Thus $[a, a^\dagger] = 1$.

$$\begin{aligned} H &= \frac{\hbar eB}{2mc}\left(a^\dagger a + aa^\dagger\right) \\ &= \frac{\hbar eB}{mc}\left(a^\dagger a + \frac{1}{2}\right) \Leftrightarrow \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) \end{aligned}$$

Chapter 3

Theory of Angular Momentum

This chapter is concerned with a systematic treatment of angular momentum and related topics.

3.1 Rotation and Angular Momentum

We consider the rotation in the space of a physical system in a state represented by a ket $|\alpha\rangle$ or the wave function $\varphi_\alpha(\mathbf{r})$. We describe a rotation by a linear operator R, which is so defined that any vector $\mathbf{r}$ is rotated into the new vector $R\,\mathbf{r}$. The rotation changes the ket $|\alpha\rangle$ into the new ket $|\alpha'\rangle$ or change the wave function $\varphi_\alpha(\mathbf{r})$ into the wave function $\varphi_{\alpha'}(\mathbf{r}')$, which means

$$\varphi_{\alpha'}(R\mathbf{r}) = \varphi_\alpha(\mathbf{r})$$

$$\left\langle \mathbf{r} \left| \mathcal{D}^+(R)\mathcal{D}(R) \right| \alpha \right\rangle = \langle \mathbf{r}|\alpha\rangle$$

$$\langle R\mathbf{r}|\alpha'\rangle = \langle \mathbf{r}|\alpha\rangle$$

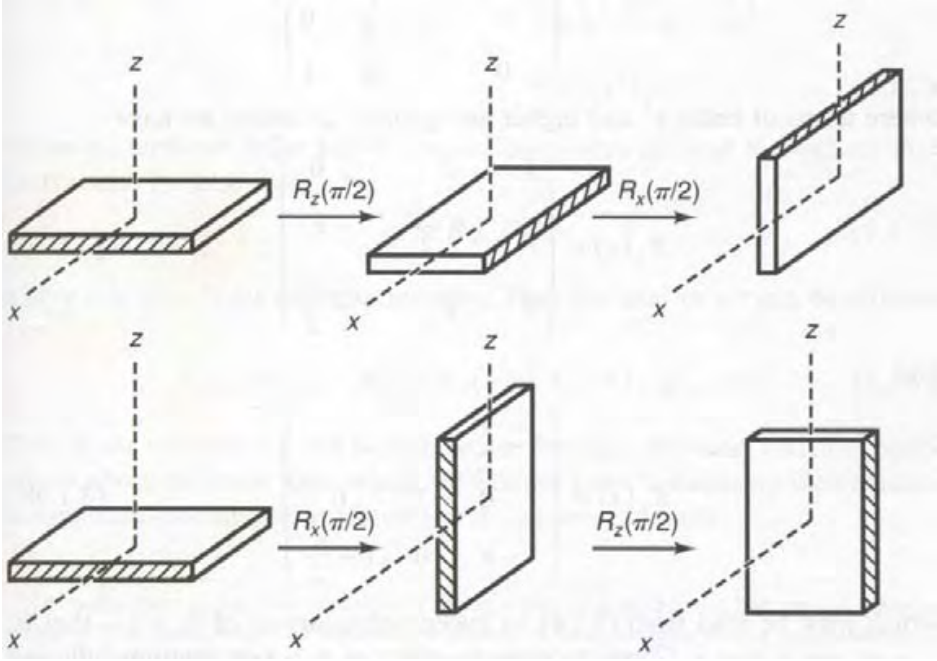


Figure 3.1: Example to illustrate the noncommunativity of finite rotation.

3.1.1 Finite versus infinitesimal rotation

From elementary physics, we know that

(1) Rotations about the same axis commute.

$$R_z(\frac{\pi}{6})R_z(\frac{\pi}{3}) = R_z(\frac{\pi}{3})R_z(\frac{\pi}{6}) = R_z(\frac{\pi}{3}+\frac{\pi}{6})$$

(2). Rotation about different axes do not commute.

$$R_x(\frac{\pi}{2})R_z(\frac{\pi}{2}) \neq R_z(\frac{\pi}{2})R_x(\frac{\pi}{2})$$

Consider a vector $\mathbf{V}$ with three components V_x, V_y and V_z. When we rotate the vector , we obtain a new vector, $\mathbf{V}_R$ with V_{Rx}, V_{Ry},and V_{Rz}. These two vectors are

connected by a 3×3 matrix

$$\begin{pmatrix} V_{Rx} \\ V_{Ry} \\ V_{Rz} \end{pmatrix} = \begin{pmatrix} R_{xx} & R_{xy} & R_{xz} \\ R_{yx} & R_{yy} & R_{yz} \\ R_{zx} & R_{zy} & R_{zz} \end{pmatrix} \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix}$$

The requirement that V_R be real when V are real means that the elements of R are real. The length of the vector V and V_R do not change, which means

$$(V_{Rx}, V_{Ry}, V_{Rz}) \begin{pmatrix} V_{Rx} \\ V_{Ry} \\ V_{Rz} \end{pmatrix} = V_x^2 + V_y^2 + V_z^2$$

$$V_R^T V_R = V^T R^T R V = V^T V$$

$$R^T R = R R^T = 1$$

where "T" stands for a transpose of a matrix: $R_{ij}^T = R_{ji}$. To be definite we consider a rotation about $z_$axis by an angle ϕ

$$V_{Rz} = V_z$$

$$V_{Rx} = V_x \cos\phi - V_y \sin\phi \, (= V_0 \cos(\phi + \varphi))$$

$$V_{Ry} = V_x \sin\phi + V_y \cos\phi \, (= V_0 \sin(\phi + \varphi))$$

where $V_x = V_0 \cos\varphi$ and $V_y = V_0 \sin\varphi$. In the matrix form, we obtain

$$R_z(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Similarly

$$R_x(\phi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & -\sin\phi \\ 0 & \sin\phi & \cos\phi \end{pmatrix}$$

$$R_y(\phi) = \begin{pmatrix} \cos\phi & 0 & \sin\phi \\ 0 & 1 & 0 \\ -\sin\phi & 0 & \cos\phi \end{pmatrix}$$

We are particularly interested in an infinitesimal form, from which a great deal can be learned about the structure of R. Take $\sin\phi \approx \phi$, $\cos\phi \approx 1 - \frac{\phi^2}{2}$, we have

$$\begin{aligned} R_x(\phi) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-\varepsilon^2/2 & -\varepsilon \\ 0 & \varepsilon & 1-\varepsilon^2/2 \end{pmatrix} \\ &= 1 + O(\varepsilon) + O(\varepsilon^2) + ... \end{aligned}$$

$$R_y(\phi) = \begin{pmatrix} 1-\varepsilon^2/2 & 0 & \varepsilon \\ 0 & 1 & 0 \\ -\varepsilon & 0 & 1-\varepsilon^2/2 \end{pmatrix}$$

$$R_z(\phi) = \begin{pmatrix} 1-\varepsilon^2/2 & -\varepsilon & 0 \\ \varepsilon & 1-\varepsilon^2/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Elementary matrix manipulation lead to

$$R_x(\varepsilon)R_y(\varepsilon) - R_y(\varepsilon)R_x(\varepsilon) = R_z(\varepsilon^2) - 1.$$

If we just remain the quantities of first order in ε , any two rotations about different axes commute because $R_z(\varepsilon^2) \approx 1$

In quantum mechanics

Because rotations affect physical systems, the state ket corresponding to a rotated system is expected to look different from the state ket corresponding to the original system. Given a rotation operator $\vec{R}$, characterized by a 3×3 matrix R, we associated with an operator $\mathcal{D}(R)$ in the appropriate ket space such that

$$|\alpha\rangle_R = \mathcal{D}(R)\,|\alpha\rangle$$

where $|\alpha\rangle_R$ and $|\alpha\rangle$ stand for the kets of the rotated and unrotated systems, respectively. To construct the rotation operator, it is again fruitful to examine first its properties under an infinitesimal rotation

$$\mathcal{D}(\hat{n}d\phi) = 1 - i\frac{\hat{J}\cdot\hat{n}}{\hbar}d\phi$$

we define J_k the k- component of the angular momentum. A finite rotation can be obtained by compounding successively infinitesimal rotation about the same axis

$$\begin{aligned}
\mathcal{D}_z(\phi) &= \lim_{N\to+\infty}[\mathcal{D}_z(\frac{\phi}{N})]^N \\
&= \lim_{N\to+\infty}(1 - i\frac{J_z}{\hbar}\cdot\frac{\phi}{N})^N \\
&= \left[\lim_{N\to+\infty}(1 - i\frac{J_z}{\hbar}\cdot\frac{\phi}{N})^{N\hbar/(-iJ_z\phi)}\right]^{-i\frac{J_z}{\hbar}\phi} \\
&= \exp(-i\frac{J_z}{\hbar}\phi)
\end{aligned}$$

$$\text{Definition: } \lim_{x\to+\infty}(1+\frac{1}{x})^x \equiv e$$

In order to obtain the angular momentum commutator relations we need more concepts. For every R, there exists a rotation operator $\mathcal{D}(R)$ in the appropriate ket space

$$R \Longrightarrow \mathcal{D}(R)$$

We postulate that $\mathcal{D}(R)$ has the same group properties as R.

1. Identity:

$$R \cdot 1 = R \Longrightarrow \mathcal{D}(R) \cdot \mathcal{D}(0) = \mathcal{D}(R)$$

2. Closure:

$$R_1 \cdot R_2 = R_3 \Longrightarrow D(R_1)D(R_2) = D(R_3)$$

3. Inverse:

$$RR^{-1} = 1 \Longrightarrow \mathcal{D}(R)\mathcal{D}(R^{-1}) = \mathcal{D}(0) = 1$$

4.Associativity:

$$R_1(R_2R_3) \quad = \quad (R_1R_2)R_3$$

$$\mathcal{D}(R_1)\mathcal{D}(R_2R_3) \quad = \quad \mathcal{D}(R_1R_2)\ \mathcal{D}(R_3)$$

As

$$R_x(\varepsilon)R_y(\varepsilon) - R_y(\varepsilon)R_z(\varepsilon) = R_z(\varepsilon^2) - 1$$

we examine

$$\mathcal{D}_x(\varepsilon)\mathcal{D}_y(\varepsilon) - \mathcal{D}_y(\varepsilon)\mathcal{D}_x(\varepsilon)$$

$$= \quad (1 - i\frac{J_x\varepsilon}{\hbar} - \frac{J_x^2\varepsilon^2}{2\hbar^2})(1 - i\frac{J_y\varepsilon}{\hbar} - \frac{J_y^2\varepsilon^2}{2\hbar^2})$$

$$-(1 - i\frac{J_y\varepsilon}{\hbar} - \frac{J_y^2\varepsilon^2}{2\hbar^2})(1 - i\frac{J_x\varepsilon}{\hbar} - \frac{J_x^2\varepsilon^2}{2\hbar^2})$$

$$= \quad -[J_x, J_y]\varepsilon^2/\hbar^2 = 1 - \mathcal{D}_z(\varepsilon^2)$$

$$\mathcal{D}_z(\varepsilon^2) \quad = \quad 1 - i\frac{J_z}{\hbar}\varepsilon^2$$

$$\Longrightarrow \quad [J_x, J_y] = i\hbar J_z$$

Similarly, we obtain

$$[J_i, J_j] = i\hbar\epsilon_{ijk}J_k$$

or

$$\vec{J} \times \vec{J} = i\hbar\vec{J}$$

Comparing with a conventional vector $\mathbf{v}$

$$\mathbf{v} \times \mathbf{v} = 0.$$

3.1.2 Orbital angular momentum

If the vector $\vec{\phi}$ is of infinitesimal length and only quantities of first order in $\vec{\phi}$ are retained, the relation $V_R = RV$ may be written

$$V_R = V + \vec{\phi} \times \vec{V}$$

where

$$R = \begin{pmatrix} 1 & -\phi_z & \phi_y \\ \phi_z & 1 & -\phi_x \\ -\phi_y & \phi_x & 1 \end{pmatrix}$$

To derive the formula we have used the infinitesimal rotation, for example,

$$\begin{aligned} R_z(\phi) &= \begin{pmatrix} \cos\phi_z & -\sin\phi_z & 0 \\ \sin\phi_z & \cos\phi_z & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &= 1 + \begin{pmatrix} 0 & -\phi_z & 0 \\ \phi_z & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{aligned}$$

and the infinitesimal rotation about any axis are commutable.

Now we wish to find a transformation $|\alpha\rangle_R$ that changes the ket $|\alpha\rangle$ into the ket $|\alpha\rangle_R$

$$\begin{aligned} |\alpha\rangle_R &= \mathcal{D}(\phi)\,|\alpha\rangle \\ \Longrightarrow\quad & \langle r|\,\mathcal{D}^{+}(\phi)\,|\alpha\rangle_R = \langle r\,|\alpha\,\rangle \\ \Longrightarrow\quad & \langle Rr\,|\alpha\,\rangle_R = \langle r\,|\alpha\,\rangle \\ \Longrightarrow\quad & \langle r\,|\alpha\,\rangle_R = \left\langle R^{-1}r\,|\alpha\,\right\rangle \end{aligned}$$

Thus we have

$$\begin{aligned} \mathcal{D}(\vec{\phi})\varphi_\alpha(r) &= \varphi_\alpha(R^{-1}r) \\ &\approx \varphi_\alpha(r-\phi\times r) \\ &\approx \varphi_\alpha(r)-(\phi\times r)\cdot\bigtriangledown\varphi_\alpha(r) \\ \Longrightarrow\quad & \mathcal{D}(\vec{\phi}) = 1-\frac{i}{\hbar}\hat{L}\cdot\phi+\cdots \end{aligned}$$

where

$$\hat{L} = r\times\hat{P}$$

$$\begin{aligned} L_x &= yP_z - zP_y (= -i\hbar(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y})) \\ L_y &= zP_x - xP_z (= -i\hbar(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z})) \\ L_z &= xP_y - yP_x (= -i\hbar(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x})) \end{aligned}$$

These operators satisfy

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k$$

3.1.3 Rotation operator for spin 1/2

We have already checked that

$$[S_i, S_j] = i\hbar\epsilon_{ijk}S_k$$

Consider a rotation by a finite angle ϕ about the z-axis. If the ket of a spin 1/2 system before rotation is given by $|\alpha\rangle$, the ket after rotation is given by

$$|\alpha\rangle_R = \mathcal{D}_z(\phi)\,|\alpha\rangle$$

with

$$\mathcal{D}_z(\phi) = e^{-i\frac{S_z}{\hbar}\phi}$$

To see the physical meaning of $\mathcal{D}_z(\phi)$, we compute

$$\begin{aligned}
& \mathcal{D}_z^+(\phi) S_x \mathcal{D}_z(\phi) \\
= \;& e^{i\frac{S_z}{\hbar}\phi} S_x e^{-i\frac{S_z}{\hbar}\phi} = e^{i\frac{S_z}{\hbar}\phi}\frac{\hbar}{2}\left(|+\rangle\langle -| + |-\rangle\langle +|\right) e^{-i\frac{S_z}{\hbar}\phi} \\
= \;& \frac{\hbar}{2}\left(e^{i\frac{\phi}{2}}|+\rangle\langle -|\, e^{i\frac{\phi}{2}} + e^{-i\frac{\phi}{2}}|-\rangle\langle +|\, e^{-i\frac{\phi}{2}}\right) \\
= \;& \frac{\hbar}{2}[(|+\rangle\langle -| + |-\rangle\langle +|)\cos\phi + i\,(|+\rangle\langle -| - |-\rangle\langle +|)\sin\phi] \\
= \;& S_x\cos\phi - S_y\sin\phi
\end{aligned}$$

$$\mathcal{D}_z^\dagger(\phi)\begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix}\mathcal{D}_z(\phi) = \begin{pmatrix} S_x\cos\phi - S_y\sin\phi \\ S_x\sin\phi + S_y\cos\phi \\ S_z \end{pmatrix}$$

$$= \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix}$$

Compare with

$$V_R = RV.$$

3.1.4 Spin precession revisited

The Hamiltonian is

$$\begin{aligned} H &= -\frac{e}{mc}\mathbf{S}\cdot\mathbf{B} \\ &= \omega\mathbf{S}_z \end{aligned}$$

where $\omega = |e|\,B/mc$. The time evolution operator is given by

$$U(t) = \exp\left[-iHt/\hbar\right] = \exp\left[-i\sigma_z\omega t/2\right].$$

For an arbitrary state $|\alpha\rangle$, at a later time t

$$\begin{aligned} |\alpha,t\rangle &= U(t)\,|\alpha\rangle \\ &= U(t)(|+\rangle\langle+| + |-\rangle\langle-|)\,|\alpha\rangle \\ &= e^{-i\omega t/2}\,|+\rangle\langle+|\alpha\rangle + e^{+i\omega t/2}\,|-\rangle\langle-|\alpha\rangle \end{aligned}$$

The operators change as

$$\begin{aligned} \langle\mathbf{S}_x\rangle_t &= \langle\mathbf{S}_x\rangle_{t=0}\cos\omega t - \langle\mathbf{S}_y\rangle_{t=0}\sin\omega t \\ \langle\mathbf{S}_y\rangle_t &= \langle\mathbf{S}_y\rangle_{t=0}\cos\omega t + \langle\mathbf{S}_x\rangle_{t=0}\sin\omega t \\ \langle\mathbf{S}_z\rangle_t &= \langle\mathbf{S}_z\rangle_{t=0} \end{aligned}$$

Conclusion: the period for the state ket is twice as long as the period for spin precession:

$$\tau_{\text{precession}} = 2\pi/\omega;$$

$$\tau_{\text{state ket}} = 4\pi/\omega.$$

3.2 Rotation Group and the Euler Angles

3.2.1 The Group Concept

The branch of mathematics that is appropriate for a full treatment of symmetry is the theory of groups. Here we give a few basic definitions: A set of objects a,b,c... form a group if a process can be defined that enables us to combine any two of the objects, such as a and b, to form an object ab, and if the following conditions are satisfied:

1. All results of combination, such as a,b, are members of the group.
2. The group contains an identity or unit member e that has the properties $ae = ea = a$, where a is any member of the group.
3. Each member a has an inverse a^{-1} also in the group, such that $aa^{-1} = a^{-1}a = e$.
4. Group combination is associative, so that

$$a(bc) = (ab)c$$

The members of the group are called elements. Though we frequently refer to the combination as "multiplication", this does not mean ordinary multiplication. For example, the set of integers, positive, negative, and zero, form a group if the law of combination is ordinary addition.

A group is abelian if multiplication is commutative, so that $ab = ba$ for all pair of elements. Otherwise the group is non-abelian.

Two groups are said to be isomorphic to each other if there is a unique one-to-one correspondence between elements of the two groups such that products of corresponding elements correspond to each other.

Examples:

(1). The elements are 1 and -1 and the law of combination is multiplication.

(2). $\{e, a, a^2 ... a^N = e\}$: a is the root of $x^N = 1$.

3.2.2 Orthogonal Group

We discussed rotations of a vector. The rotated vector and unrotated vector are connected by a 3×3 real and orthogonal matrix

$$V_R = RV$$

All rotation matrices form a group.

1. Combination of two R_1 and R_2 is a new matrix $R_1 R_2$
2. Identity: $R = 1$
3. The inverse matrix: $R^T = R^{-1}$ and $R^T R = RR^T = I$
4. Associativity:$(R_1 R_2)R_3 = R_1(R_2 R_3)$

This group is named SO(3), where S stands for special, O stands for orthogonal, 3 for three dimension. If the vector is n-dimensional, the R form a SO(n) group.

3.2.3 "Special"?

Consider

$$R_z(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Its determinant is

$$\det(R_z(\phi)) = 1$$

In fact,

$$\det(R) = 1 \Longrightarrow \text{“}S\text{”}$$

-1 is not one of elements in SO(n). We postulate that $\mathcal{D}(R)$ has the same group properties of R. The determinant of $\mathcal{D}(R)$ is

$$\begin{aligned} \det[\mathcal{D}(R)] &= \det\left(\exp[-i\frac{\vec{J}\cdot\vec{n}}{\hbar}\phi]\right) \\ &= \exp\left[\det(-i\frac{\vec{J}\cdot\vec{n}}{\hbar}\phi)\right] = 1 \end{aligned}$$

since

$$\det[J_k] = 0.$$

3.2.4 Unitary Unimodular Group

Another rotation we discussed is for the spin 1/2 system, where the rotation matrices are 2×2. We can write a unitary unimodular matrix as

$$u(a,b) = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}$$

where a and b are complex satisfying $|a|^2 + |b|^2 = 1$. All these matrices form a group.

(1) Closure:

$$u(a_1, b_1)u(a_2, b_2) = u(a_1a_2 - b_1b_2^*, a_1b_2 + a_2^*b_1)$$

where

$$|a_1a_2 - b_1b_2|^2 + |a_1b_2 + a_2^*b_1|^2 = 1$$

(2) Identity:

$$u(1,0) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

(3) Inverse:

$$u^+(a,b)u(a,b) = 1$$

(4) Associative: multiplications of matrices are associative.

If we set

$$\begin{aligned} \mathrm{Re}(a) &= \cos\frac{\phi}{2} \\ \mathrm{Re}(b) &= -n_y \sin\frac{\phi}{2} \\ \mathrm{Im}(a) &= -n_z \sin\frac{\phi}{2} \\ \mathrm{Im}(b) &= -n_x \sin\frac{\phi}{2} \end{aligned}$$

the $u(a,b)$ can be rewritten as

$$u(a,b) \Longrightarrow e^{-i\frac{\sigma\cdot\vec{n}}{2}\phi}$$

As $\det[u(a,b)] = 1$, this group is called SU(2) group. SU(2) and SO(3) have a two-to-one correspondence: In SU(2). a rotation by 2π produces -1. a rotation by 4π produces 1. In SO(3) , a rotation 2π produces 1. More generally, U(a,b) and U(-a,-b) correspond to one matrix in R (in SO(3)).

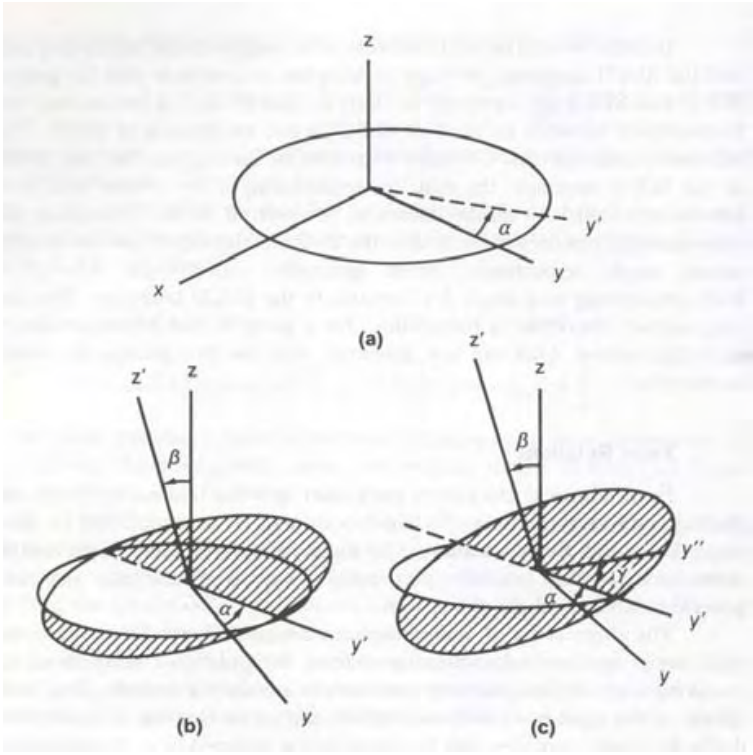


Figure 3.2: Euler rotations.

3.2.5 Euler Rotations

Three steps:

$$\text{(a)} \quad : \quad \mathrm{R}_z(\alpha) \;\; \mathrm{y} \rightarrow y'$$

$$\text{(b)} \quad : \quad \mathrm{R}_{y'}(\beta) \;\; \mathrm{z} \rightarrow z'$$

$$\text{(c)} \quad : \quad \mathrm{R}_{z'}(\gamma) \;\; \mathrm{y'} \rightarrow y''$$

In terms of 3×3 orthogonal matrices the product of the three operations can be written as

$$R(\alpha, \beta, \gamma) \equiv R_{z'}(\gamma) R_{y'}(\beta) R_z(\alpha)$$

There appear both rotations about body axes and about the space-fixed axes. This is rather inconvenient! It is desirable to express the body-axis rotations in terms of space-fixed axis

rotation. Fortunately, we have

$$\begin{aligned} R_{y'}(\beta) &= R_z(\alpha)R_y(\beta)R_z^{-1}(\alpha) \\ R_{z'}(\gamma) &= R_{y'}(\beta)R_z(\gamma)R_{y'}^{-1}(\beta) \end{aligned}$$

Therefore,

$$R(\alpha,\beta,\gamma) = R_z(\alpha)R_y(\beta)R_z(\gamma)$$

As an example we calculate $\mathcal{D}(\alpha,\beta,\gamma)$ for a spin 1/2 system.

$$\begin{aligned} D(\alpha,\beta,\gamma) &= D_z(\alpha)D_y(\beta)D_z(\gamma) \\ &= e^{-i\frac{\sigma_3}{2}\alpha}e^{-i\frac{\sigma_2}{2}\beta}e^{-i\frac{\sigma_3}{2}\gamma} \end{aligned}$$

Recall that

$$\exp(-i\frac{\vec{\sigma}\cdot\vec{n}}{2}\phi) = \cos\frac{\phi}{2} - i\vec{\sigma}\cdot\vec{n}\sin\frac{\phi}{2}$$

To prove the identity we use the $(\vec{\sigma}\cdot\vec{n})^2 = 1$.

$$\begin{aligned} D(\alpha,\beta,\gamma) = &\begin{pmatrix} \cos\frac{\alpha}{2} - i\sin\frac{\alpha}{2} & 0 \\ 0 & \cos\frac{\alpha}{2} + i\sin\frac{\alpha}{2} \end{pmatrix} \\ &\cdot \begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix} \cdot \begin{pmatrix} \cos\frac{\gamma}{2} - i\sin\frac{\gamma}{2} & 0 \\ 0 & \cos\frac{\gamma}{2} + i\sin\frac{\gamma}{2} \end{pmatrix} \\ = &\begin{pmatrix} e^{-i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} & -e^{-i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} \\ e^{-i\frac{\alpha-\gamma}{2}}\sin\frac{\beta}{2} & e^{-i\frac{\alpha+\gamma}{2}}\cos\frac{\beta}{2} \end{pmatrix} \end{aligned}$$

3.3 Eigenvalues and Eigenkets of Angular Momentum

The commutation relation between three components of $\vec{J}$ are already derived:

$$[J_x, J_y] = i\hbar J_z$$

$$[J_y, J_z] = i\hbar J_x$$

$$[J_z, J_x] = i\hbar J_y$$

These relation are often rewritten in a more compact form

$$J \times J = i\hbar J$$

In this section we work out the eigenvalues and eigenkets of angular momentum. To this end, we introduce a new set of operators:

$$(1).\ J^2 = J_x J_x + J_y J_y + J_z J_z$$

$$(2).\ J_\pm = J_x \pm i J_y \quad [\mathrm{J}_+ = (\mathrm{J}_-)^+]$$

J^2 commutes with all three J_k $(k = x, y, z)$

$$[J^2, J_k] = 0$$

As J_x, J_y and J_z do not commute, we cannot diagonalize J_x , J_y and J_z simultaneously. However we can choose one J_k to be diagonalized with J^2. By convention, we choose J_z . We denote the eigenvalues of $J^2$and J_z by a and b, respectively

$$J^2 |a, b\rangle = a |a, b\rangle$$

$$J_z |a, b\rangle = b |a, b\rangle$$

To determine the values of a and b, it is convenient to work with the ladder operator, $J_{\pm}$.

$$\begin{aligned}
[J_z, J_y] &= -i\hbar J_x \\
[J_z, J_x] &= i\hbar J_y \\
[J_z, J_y] &= -i\hbar J_x \\
[J_z, J_x + iJ_y] &= \hbar(J_x + iJ_y)
\end{aligned}$$

The commutation relations become

$$\begin{aligned}
[J_z, J_{\pm}] &= \pm\hbar J_{\pm} \\
[J_+, J_-] &= 2\hbar J_z \\
[J_{\pm}, J^2] &= 0
\end{aligned}$$

First of all , we have

$$\begin{aligned}
\left\langle a', b' \left| J^2 \right| a, b \right\rangle &= a\delta_{aa'}\delta_{bb'}; \\
\left\langle a', b' \left| J_z \right| a, b \right\rangle &= b\delta_{aa'}\delta_{bb'}
\end{aligned}$$

Then

$$\begin{aligned}
J_z J_{\pm} |a, b\rangle &= \{[J_z, J_{\pm}] + J_{\pm} J_z\} |a, b\rangle \\
&= (\pm\hbar J_{\pm} + bJ_{\pm}) |a, b\rangle \\
&= (b \pm \hbar) J_{\pm} |a, b\rangle
\end{aligned}$$

From this relation, we conclude

$$J_{\pm} |a, b\rangle = C_{\pm}(a, b) |a, b \pm \hbar\rangle .$$

Note that the bra of $J_\pm |a,b\rangle$ are

$$\langle a,b| J_\mp = \langle a, b \pm \hbar| C_\pm^*(a,b)$$

$$\langle a,b| J_\mp J_\pm |a,b\rangle = |C_\pm(a,b)|^2$$

J^2 can be expressed in terms of $\mathrm{J}_\pm$ and J_z

$$J^2 = \frac{1}{2}(J_+J_- + J_-J_+) + J_z^2$$

$$= J_-J_+ + J_z^2 + J_z\hbar = J_+J_- + J_z^2 - J_z\hbar$$

$$a = |C_+(a,b)|^2 + b(b+\hbar) = |C_-(a,b)|^2 + b(b-\hbar)$$

$$|C_+(a,b)|^2 = a - b(b+\hbar) \geq 0$$

$$|C_-(a,b)|^2 = a - b(b-\hbar) \geq 0$$

If $|a,b\rangle$ is one of eigenkets, then

$$J_\pm |a,b\rangle = C_\pm(a,b)\,|a, b\pm\hbar\rangle$$

If $C_+(a,b)$ or $C_-(a,b)$ is not equal to zero, $|a, b\pm\hbar\rangle$ is also one of eigenkets suppose that we keep on applying $J_\pm$ to both side of the equation above. We can obtain numerical eigenkets with smaller and smaller or larger and larger $b \pm n\hbar$ until the sequence terminates at some $b_{\max}$ and $b_{\min}$ such that

$$\begin{cases} C_+(a, b_{\max}) = 0 \\ C_-(a, b_{\min}) = 0 \end{cases}$$

So

$$|C_+(a,b_{\max})|^2 = a - b_{\max}(b_{\max}+\hbar) = 0$$

$$|C_-(a,b_{\max})|^2 = a - b_{\min}(b_{\min}-\hbar) = 0$$

$$a = b_{\max}(b_{\max}+\hbar) = b_{\min}(b_{\min}-\hbar)$$

$$\implies b_{\max} = -b_{\min}$$

Clearly, we must be able to reach $|a, b_{\max}\rangle$ by applying J_+ successively to $|a, b_{\min}\rangle$ a finite number of times. i.e.

$$|a, b_{\max}\rangle \propto (J_+)^n |a, b_{\min}\rangle$$

$$\propto |a, b_{\min} + n\hbar\rangle$$

We obtain

$$b_{\max} = b_{\min} + n\hbar$$

As a result,

$$b_{\max} = \frac{n}{2}\hbar$$

and

$$a = \frac{n}{2}(\frac{n}{2}+1)\hbar^2$$

It is conventional to define

$$b_{\max} = -b_{\min} = \frac{n}{2}\hbar = j\hbar$$

and

$$|a, b\rangle \implies |j, m\rangle$$

such that

$$J^2 |j, m\rangle = j(j+1)\hbar^2 |j, m\rangle$$

$$J_z |j, m\rangle = m\hbar |j, m\rangle$$

with $m = -j, -j+1, ...j$.

Take $C_{\pm}(a,b)$ real, we have

$$J_+ |j,m\rangle = [j(j+1) - m(m+1)]^{1/2} \hbar |j.m+1\rangle ;$$

$$J_- |j,m\rangle = [j(j+1) - m(m-1)]^{1/2} \hbar |j.m-1\rangle .$$

The eigenkets $\{|j,m\rangle\}$ form a basis for angular momentum operator

$$\langle jm\ |j',m'\rangle = \delta_{jj'}\delta_{mm'}.$$

In the form of matrix, elements of $J_{\pm}$

$$\langle j'm'\,|J_{\pm}|\,jm\rangle = \hbar\,[j(j+1) - m(m\pm 1)]^{1/2}\,\delta_{jj'}\delta_{m'm\pm 1}.$$

As a result,

$$\langle j'm'\,|J_x|\,jm\rangle = \left\langle j'm' \left| \frac{J_+ + J_-}{2} \right| jm \right\rangle$$

$$= \frac{\hbar}{2}\,[j(j+1) - m(m+1)]^{1/2}\,\delta_{jj'}\delta_{m'm+1}$$

$$+\frac{\hbar}{2}\,[j(j+1) - m(m-1)]^{1/2}\,\delta_{jj'}\delta_{m'm-1}$$

$$\langle j'm'\,|J_y|\,jm\rangle$$

$$= \frac{\hbar}{2i}\,[j(j+1) - m(m+1)]^{1/2}\,\delta_{jj'}\delta_{m'm+1}$$

$$-\frac{\hbar}{2i}\,[j(j+1) - m(m-1)]^{1/2}\,\delta_{jj'}\delta_{m'm-1}$$

$$\langle jm'\,|J_z|\,jm\rangle = m\hbar\delta_{mm'};$$

$$\left\langle jm' \left| J^2 \right| jm \right\rangle = j(j+1)\hbar^2\delta_{mm'}$$

Our choice of a representation in which J^2 and J_z are diagonal has led to discrete sequences of values for the corresponding labels j and m. The infinite matrices thus obtained are most conveniently handled by breaking them up into an infinite set of finite matrices, each of which is characterized by a particular value of j and has $2j+1$ rows and columns.

(1) $j = 1/2$: $m = \pm 1/2$

$$J_x = \tfrac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad J_y = \tfrac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$J_z = \tfrac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad J^2 = \tfrac{3}{4}\hbar^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

(2) $j = 1, m = \pm 1, 0$

$$J_x = \tfrac{\hbar}{2^{1/2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad J_y = \tfrac{\hbar}{2^{1/2}}\begin{pmatrix} 0 & -i & 0 \\ -i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

$$J_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 - 1 & \end{pmatrix} \qquad J^2 = 2\hbar^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

(3) $j = \frac{3}{2}, m = \pm\frac{3}{2}, \pm\frac{1}{2}$

$$J_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 3^{1/2} & 0 & 0 \\ 3^{1/2} & 0 & 2 & 0 \\ 0 & 2 & 0 & 3^{1/2} \\ 0 & 0 & 3^{1/2} & 0 \end{pmatrix}$$

$$J_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i3^{1/2} & 0 & 0 \\ -i3^{1/2} & 0 & -2i & 0 \\ 0 & 2i & 0 & -i3^{1/2} \\ 0 & 0 & i3^{1/2} & 0 \end{pmatrix}$$

$$J_z = \frac{\hbar}{2}\begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}$$

$$J^2 = \frac{15}{4}\hbar^2\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

3.3.1 Representation of Rotation Operator

Have obtained the matrix elements of J_z and $J_\pm$, we are now in position to study the matrix elements of rotation operator $\mathcal{D}($

$$\text{R})\mathcal{D}^{(j)}_{mm'}(R) = \left\langle jm' \left| e^{-iJ\cdot\hat{n}\phi/\hbar} \right| jm \right\rangle \text{Since } [J^2, J_k] = 0, \text{ we have}$$

$$[\mathcal{D}(R), J^2] = 0$$

So $\mathcal{D}(R)\left|j,m\right\rangle$ is still an eigenket of J^2 with the same eigenvalue $j(j+1)\hbar^2$

$$J^2\mathcal{D}(R)\left|jm\right\rangle = j(j+1)\hbar^2\mathcal{D}(R)\left|jm\right\rangle$$

We just consider the matrix elements of $\mathcal{D}(R)$ with the same j. For every j there are $2j+1$ values of m. $\mathcal{D}(R)$ should be a $(2j+1)\times(2j+1)$ square matrix. For a rotated ket

$$D(R)\left|jm\right\rangle = \sum_{m'}\left|jm'\right\rangle\left\langle jm'\right|D(R)\left|jm'\right\rangle = \sum_{m'} D^{(j)}_{mm'}(R)\left|jm'\right\rangle$$

As is well known, the Euler angles may be used to characterize the most general rotation. We have

$$\begin{aligned} D^{(j)}_{mm'}(\alpha,\beta,\gamma) &= \left\langle jm' \left| e^{-i\frac{J_z}{\hbar}\alpha} e^{-i\frac{J_y}{\hbar}\beta} e^{-i\frac{J_z}{\hbar}\gamma} \right| jm \right\rangle \\ &= e^{i(m'\alpha - m\gamma)} \left\langle jm' \left| e^{-i\frac{J_y}{\hbar}\beta} \right| jm \right\rangle \end{aligned}$$

For $j = 1/2$

$$J_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\left\{ \left\langle jm' \left| e^{-i\frac{J_y}{\hbar}\beta} \right| jm \right\rangle \right\} = \begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix}$$

To derive the matrix we can make use of the identity: $(J_y/\hbar)^2 = 1/4$.

For $j = 1$,

$$J_y = \frac{\hbar}{2^{1/2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

$$\{ \left\langle jm' \left| e^{-i\frac{J_y}{\hbar}\beta} \right| jm \right\rangle \} = \begin{pmatrix} \cos^2\frac{\beta}{2} & -\frac{1}{2^{1/2}}\sin\beta & \sin^2\frac{\beta}{2} \\ \frac{1}{2^{1/2}}\sin\beta & \cos\beta & -\frac{1}{2^{1/2}}\sin\beta \\ \sin^2\frac{\beta}{2} & \frac{1}{2^{1/2}}\sin\beta & \cos^2\frac{\beta}{2} \end{pmatrix}$$

To derive the matrix we can make use of the identity: $(J_y/\hbar)^3 = J_y/\hbar$.

3.4 Schwinger Oscillator Model.

There exists a very interesting connection between the algebra of angular momentum and the algebra of two independent simple harmonic oscillators. Let us consider two types of

oscillator: plus and minus type. The creation and annihilation operator are denoted by $a_{\pm}$ and $a_{\pm}^{+}$, respectively,

$$[a_+, a_+^+] = 1, [a_-, a_-^+] = 1$$

These two oscillators are uncoupled,

$$[a_+, a_-^+] = [a_-, a_+^+] = 0$$

Define the number operators

$$\begin{aligned} N_+ &= a_+^+ a_+ \\ N_- &= a_-^+ a_- \end{aligned}$$

We have

$$\begin{aligned} [N_+, a_+] &= -a_+ \\ [N_-, a_-] &= -a_- \\ [N_+, a_+^+] &= a_+^+ \\ [N_-, a_-^+] &= a_-^+ \end{aligned}$$

Since $[N_+, N_-] = 0$, we define the simultaneous eigenket of N_+ and N_- by $|n_+, n_-\rangle$ such that

$$|n_+, n_-\rangle = \left(\frac{(a_+^+)^{n_+}}{(n_+!)^{1/2}} \right) \left(\frac{(a_-^+)^{n_-}}{(n_-!)^{1/2}} \right) |0, 0\rangle$$

with

$$\begin{aligned} a_{\pm}\left|0,0\right\rangle &= 0 \\ a_{+}^{+}\left|n_{+},n_{-}\right\rangle &= (n_{+}+1)^{1/2}\left|n_{+}+1,n_{-}\right\rangle \\ a_{-}\left|n_{+},n_{-}\right\rangle &= (n_{-})^{1/2}\left|n_{+},n_{-}-1\right\rangle \end{aligned}$$

We define

$$\begin{aligned} J_{+} &\equiv \hbar a_{+}^{+}a_{-};\ J_{-}\equiv\hbar a_{-}^{+}a_{+} \\ J_{z} &\equiv \frac{\hbar}{2}(a_{+}^{+}a_{+}-a_{-}^{+}a_{-}) = \frac{1}{2\hbar}[J_{+},J_{-}] = \frac{\hbar}{2}(N_{+}-N_{_}) \end{aligned}$$

We can prove that these operators satisfy the angular momentum relations

$$[J_{z},J\pm] = \pm\hbar J_{\pm}$$

Define the total number operator N by

$$N = N_{+}+N_{-},$$

we can prove

$$\begin{aligned} J^{2} &= J_{z}^{2}+\frac{1}{2}(J_{+}J_{-}+J_{-}J_{+}) \\ &= \frac{N}{2}(\frac{N}{2}+1)\hbar^{2}. \end{aligned}$$

Therefore, we have

$$\begin{aligned}
J^2 \left|n_+, n_-\right\rangle &= \hbar^2 \frac{n_+ + n_-}{2}\left(\frac{n_+ + n_-}{2} + 1\right)\left|n_+, n_-\right\rangle \\
J_+ \left|n_+, n_-\right\rangle &= \hbar a_+^+ a_- \left|n_+, n_-\right\rangle \\
&= \hbar\left[(n_+ + 1)n\right]^{1/2}\left|n_+ + 1, n_- - 1\right\rangle \\
J_- \left|n_+, n_-\right\rangle &= \hbar\left[n_+(n_- + 1)\right]^{1/2}\left|n_+ - 1, n_- + 1\right\rangle \\
J_z \left|n_+, n_-\right\rangle &= \frac{\hbar}{2}(n_+ - n_-)\left|n_+, n_-\right\rangle
\end{aligned}$$

These expression can be reduced to the familiar forms for angular momentum provided that

$$\begin{aligned}
n_+ &\implies j + m \\
n_- &\implies j - m
\end{aligned}$$

$$\left|n_+, n_-\right\rangle \Longrightarrow |j, m\rangle = \frac{(a_+^+)^{j+m}}{\left[(j+m)!\right]^{1/2}} \frac{(a_-^+)^{j-m}}{\left[(j-m)!\right]^{1/2}} |0, 0\rangle$$

So we can check

$$\begin{aligned}
J^2 \left|j, m\right\rangle &= j(j+1)\hbar^2 \left|j, m\right\rangle \\
J_+ \left|j, m\right\rangle &= \left[j(j+1) - m(m-1)\right]^{1/2}\hbar\left|j, m+1\right\rangle \\
J_- \left|j, m\right\rangle &= \left[j(j+1) - m(m-1)\right]^{1/2}\hbar\left|j, m-1\right\rangle \\
J_z \left|j, m\right\rangle &= m\hbar\left|j, m\right\rangle
\end{aligned}$$

3.4.1 Spin 1/2 system

We define the spin 1/2 operators $S_\pm$ and S_z in terms of the creation and annihilation operators a_σ^+ and $a_\sigma(\sigma =\uparrow,\downarrow)$. For $S = 1/2$,

$$n_\uparrow + n_\downarrow = 2s = 1.$$

We have two eigenkets for S_z

$$\begin{aligned} |+\rangle &= a_\uparrow^+ |0\rangle \\ |-\rangle &= a_\downarrow^+ |0\rangle \end{aligned}$$

The operators are expressed as

$$\begin{aligned} S_+ &= \hbar a_\uparrow^+ a_\downarrow \\ S_- &= \hbar a_\downarrow^+ a_\uparrow \\ S_z &= \frac{\hbar}{2}(a_\uparrow^+ a_\uparrow - a_\downarrow^+ a_\downarrow) \end{aligned}$$

Since $[a_\uparrow, a_\uparrow^+] = [a_\downarrow, a_\downarrow^+] = 1$, we usually call a and a^+ the boson operators. In the case of $S = 1/2$, $a_\sigma^2 = (a_\sigma^+)^2 = 0$. So they are called hard-core bosons since no two bosons can be occupied at the same site. (Please check whether the commutation relations still hold if

$$\begin{aligned} \left\{a_\uparrow, a_\uparrow^+\right\} &= a_\uparrow a_\uparrow^+ + a_\uparrow^+ a_\uparrow = 1 \\ \left\{a_\downarrow, a_\downarrow^+\right\} &= 1. \\ \left\{a_\downarrow, a_\uparrow^+\right\} &= 0. \end{aligned}$$

i.e., a are fermionic operators.)

3.4.2 Two-spin–1/2 system

We now consider two-spin-1/2 system: S_1 and S_2. For each $S_i (i = 1, 2)$, we have

$$|i+\rangle = a_{i\uparrow}^{+} |0\rangle$$

$$|i-\rangle = a_{i\downarrow}^{+} |0\rangle$$

There are four possible configurations for combination of two spins

$$|1+2+\rangle = |1+\rangle \otimes |2+\rangle = a_{1\uparrow}^{+} a_{2\uparrow}^{+} |0\rangle$$

$$|1+2-\rangle = |1+\rangle \otimes |2-\rangle = a_{1\uparrow}^{+} a_{2\downarrow}^{+} |0\rangle$$

$$|1-2+\rangle = |1-\rangle \otimes |2+\rangle = a_{1\downarrow}^{+} a_{2\uparrow}^{+} |0\rangle$$

$$|1-2-\rangle = |1-\rangle \otimes |2-\rangle = a_{1\downarrow}^{+} a_{2\downarrow}^{+} |0\rangle$$

We are now in a position to construct eigenstates of the total spin

$$S = S_1 + S_2$$

and its z_- component

$$S_z = S_1^z + S_2^z.$$

We first examine the two kets: $|1+, 2+\rangle$ and $|1-, 2-\rangle$.

$$S_z |1+, 2+\rangle = (S_{1z} + S_{2z}) |1+, 2+\rangle$$

$$= \hbar |1+, 2+\rangle$$

$$S^2 |1+, 2+\rangle = 2\hbar^2 |1+, 2+\rangle$$

We denote

$$|s = 1, m = 1\rangle = |1+, 2+\rangle = a_{1\uparrow}^{+} a_{2\uparrow}^{+} |0\rangle$$

Similarly,

$$|s=1, m=-1\rangle = |1-, 2-\rangle = a^+_{1\downarrow} a^+_{2\downarrow} |0\rangle$$

Recall that

$$J_- |j, m\rangle$$

$$= \left[j(j+1) - m(m-1)\right]^{1/2} \hbar \, |j, m-1\rangle$$

$$|s=1, m=0\rangle$$

$$= \frac{1}{2^{1/2}\hbar} S_- |s=1, m=1\rangle$$

$$= \frac{1}{2^{1/2}} (a^+_{1\uparrow} a^+_{2\downarrow} + a^+_{1\downarrow} a^+_{2\uparrow}) |0\rangle$$

We have obtained three eigenkets for S and S_z. There should exist another eigenket since there are four possible configurations for two spins. The fourth eigenket must be a combination of $|1+, 2-\rangle$ and $|1-, 2+\rangle$

$$|\alpha\rangle = a |1+, 2-\rangle + b |1 - 2+\rangle$$

It is easy to check

$$S_z |\alpha\rangle = 0$$

We make use of property of orthogonality of eigenkets

$$\langle s=1, m=0 \, | \alpha \rangle = 0$$

From this equation, we obtain

$$a = -b \Longrightarrow a = -b = \frac{1}{2^{1/2}}$$

Furthermore,

$$S^2 |\alpha\rangle = 0 \Longrightarrow |\alpha\rangle = |s=0, m=0\rangle$$

$$\frac{1}{2^{1/2}}(a^+_{1\uparrow}a^+_{2\downarrow} - a^+_{1\downarrow}a^+_{2\uparrow})\,|0\rangle$$

3.4.3 Explicit Formula for Rotation Matrices.

Schwinger's scheme can be used to derive in a very simple way, a closed formula for rotation matrices. We apply the rotation operator $\mathcal{D}(R)$ to $|jm\rangle$. In the Euler angle rotation the only non-trivial rotation in the second one about y- axis . So

$$\begin{aligned}\mathcal{D}(R) &= \mathbf{D}(\alpha,\beta,\gamma)_{\alpha=\gamma=0}\\ &= e^{-iJ_y\beta/\hbar}\end{aligned}$$

Applying $\mathcal{D}(R)$ on $|j,m\rangle$, we have

$$\begin{aligned}&\mathcal{D}(R)\,|jm\rangle\\ =\;& \mathcal{D}(R)\frac{(a^+_+)^{j+m}}{[(j+m)!]^{1/2}}\frac{(a^+_-)^{j-m}}{[(j-m)!]^{1/2}}\,|0\rangle\\ =\;& \frac{[D(R)a^+_+D^{-1}_{(R)}]^{j+m}}{[(j+m)!]^{1/2}}\frac{[D(R)a^+_-D^{-1}_{(R)}]^{j-m}}{[(j-m)!]^{1/2}}\mathcal{D}(R)\,|0\rangle\end{aligned}$$

$$J_y = \frac{1}{2i}(J_+ - J_-) = \frac{1}{2i}(a^+_+a_- - a^+_-a_+)$$

We have

$$J_y\,|0\rangle = 0$$

and

$$\mathcal{D}(R)\,|0\rangle = |0\rangle$$

We come to calculate

$$f_\pm(\beta) = \mathcal{D}(R)a^+_\pm\mathcal{D}^{-1}(R) = e^{-i\frac{J_y}{\hbar}\beta}a^+_\pm e^{+i\frac{J_y}{\hbar}\beta}$$

$$\begin{aligned}\frac{d}{d\beta}f_+(\beta) &= -i\frac{1}{\hbar}e^{-i\frac{J_y}{\hbar}\beta}[J_y, a_+^+]e^{i\frac{J_y}{\hbar}\beta} \\ &= \frac{1}{2}e^{-i\frac{J_y}{\hbar}\beta}a_-^+e^{i\frac{J_y}{\hbar}\beta} \\ &= \frac{1}{2}f_-(\beta)\end{aligned}$$

Similarly

$$\frac{d}{d\beta}f_-(\beta) = -\frac{1}{2}f_+(\beta)$$
$$\frac{d^2}{d\beta^2}f_\pm(\beta) + (\frac{1}{2})^2 f_\pm(\beta) = 0$$

The solutions are

$$f_\pm(\beta) = \cos\frac{\beta}{2}\tilde{C}_{1\pm} + \sin\frac{\beta}{2}\tilde{C}_{2\pm}$$

The boundary conditions are

$$f_\pm(\beta)|_{\beta=0} = a_\pm^+ \Rightarrow \tilde{C}_{1\pm} = a_\pm^+$$

$$\frac{d}{d\beta}f_\pm(\beta)\Big|_{\beta=0} = \pm\frac{1}{2}f_\mp(\beta)|_{\beta=0} \Longrightarrow \tilde{C}_{2\pm} = \pm a_\mp^+$$

We have

$$f_\pm(\beta) = \cos\frac{\beta}{2}a_\pm^+ \pm \sin\frac{\beta}{2}a_\mp^+$$

$$\mathcal{D}(R)\begin{pmatrix} a_+^+ \\ a_-^+ \end{pmatrix}\mathcal{D}^{-1}(R) = \begin{pmatrix} \cos\frac{\beta}{2} & \sin\frac{\beta}{2} \\ -\sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix}\begin{pmatrix} a_+^+ \\ a_-^+ \end{pmatrix}$$

Recalling the binomial theorem,

$$(x+y)^n = \sum_{n=0}^{N}\frac{N!}{n!(N-n)!}x^n y^{N-n}$$

$$\begin{aligned}\mathcal{D}(R)\,|jm\rangle &= \frac{[\cos\frac{\beta}{2}a_+^+ + \sin\frac{\beta}{2}a_-^+]^{j+m}}{[(j+m)!]^{1/2}} \times \frac{[\cos\frac{\beta}{2}a_-^+ - \sin\frac{\beta}{2}a_+^+]^{j-m}}{[(j-m)!]^{1/2}}\,|0\rangle \\ &= \sum_{m'} d^{(j)}_{m'm}(\beta)\,|jm'\rangle\end{aligned}$$

$$d^{(j)}_{m'm} = \sum_k (-1)^{k-m+m'} \frac{[(j+m)!(j-m)!(j+m')!(j-m')!]^{1/2}}{(j+m-k)!k!(j-k-m')!(k-m+m')}$$
$$\times (\cos\frac{\beta}{2})^{2j-2k+m-m'} (\sin\frac{\beta}{2})^{2k-m+m'}$$

Notice that $d^{(j)}_{m'm}(\beta) = \langle jm'| \mathcal{D}(R) |jm\rangle$.

3.5 Combination of Angular Momentum and Clebsh-Gordan Coefficients

One of the important problems in quantum theory is the combination of the angular momenta associated with two parts of a system (such as the spin and orbital angular momenta of one electron) to form the angular momentum of the whole system. The addition of two vectors $\vec{v}_1$ and $\vec{v}_2$ forms a triangle. The third vector $\vec{v} = \vec{v}_1 + \vec{v}_2$. The maximal value of v is $v_1 + v_2$ and the minimal value of $\vec{v}$ is $|v_1 - v_2|$. We start with two commuting angular momentum operators J_1 and J_2 : all components of J_1 commute with all components of J_2.The orthonormal eigenkets of J_1^2 and J_{1z} are $|j_1 m_1\rangle$ and J_2 has no effect on them. Similarly, $|j_2 m_2\rangle$ are the eigenkets of J_2^2 and J_{2z}, and J_1 has no effect on them. Denote

$$|j_1 j_2 m_1 m_2\rangle = |j_1 m_1\rangle \otimes |j_2 m_2\rangle$$

we have

$$\begin{aligned} J_1^2 \left|j_1 j_2 m_1 m_2\right\rangle &= j_1(j_1+1)\hbar^2 \left|j_1 j_2 m_1 m_2\right\rangle \\ J_{1z} \left|j_1 j_2 m_1 m_2\right\rangle &= m_1 \hbar \left|j_1 j_2 m_1 m_2\right\rangle \\ J_2^2 \left|j_1 j_2 m_1 m_2\right\rangle &= j_2(j_2+1)\hbar^2 \left|j_1 j_2 m_1 m_2\right\rangle \\ J_{2z}^2 \left|j_1 j_2 m_1 m_2\right\rangle &= m_2 \hbar \left|j_1 j_2 m_1 m_2\right\rangle . \end{aligned}$$

The infinitesimal rotation operator that affects both subspaces is written as

$$(I_1 - i\frac{J_1 \cdot \vec{n}\delta\phi}{\hbar}) \otimes (I_2 - i\frac{J_2 \cdot \vec{n}\delta\phi}{\hbar}) = I_1 \otimes I_2 - i\frac{J_1 \otimes I_2 + J_2 \otimes I_1}{\hbar} \cdot \vec{n}\delta\phi$$

So we define the total angular momentum

$$J = J_1 \otimes I_2 + I_1 \otimes J_2 \equiv J_1 + J_2$$

It is noted that

$$J \times J = i\hbar J$$

Since J^2, J_1^2, J_2^2 and J_z are compatible, we denote their simultaneous eigenkets by

$$\left|j_1 j_2 j m\right\rangle \equiv \left|j m\right\rangle$$

Recall that there are $(2j_1+1)$ eigenkets $\left|j_1 m_1\right\rangle$ and $(2j_2+1)$ eigenkets $\left|j_2 m_2\right\rangle$. Therefore there are $(2j_1+1) \times (2j_2+1)$ kets

$$\left|j_1 j_2 m_1 m_2\right\rangle \equiv \left|j_1 m_1\right\rangle \otimes \left|j_2 m_2\right\rangle (\equiv \left|m_1, m_2\right\rangle)$$

These kets form a complete and orthogonal set of basis:

$$\sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} \left|m_1, m_2\right\rangle \left\langle m_1, m_2\right| = 1$$

The connection between $|jm\rangle$ and $|m_1, m_2\rangle$ is

$$|jm\rangle = \sum_{m_1 m_2} |m_1, m_2\rangle \langle m_1, m_2|jm\rangle$$

$\{\langle m_1, m_2|jm\rangle\}$ are the Clebsh-Gordan coefficients. Note that

$$(J_z - J_{1z} - J_{2z}) |jm\rangle = 0$$

$$(m - m_1 - m_2) \langle m_1, m_2|jm\rangle = 0$$

It is apparent that $\langle m_1, m_2|jm\rangle$ is zero unless $m = m_1 + m_2$. The largest value of m is $j_1 + j_2$ and this occurs only when $m_1 = j_1$ and $m_2 = j_2$. Therefore the largest j is $j_1 + j_2$, and that there is only such a state

$$|j_1 + j_2 \; j_1 + j_2\rangle = |j_1, j_2\rangle$$

$$|j = j_1 + j_2 \; m = j_1 + j_2\rangle = |m_1 = j_1, m_2 = j_2\rangle$$

The next largest value of m is $j_1 + j_2 - 1$ and this occurs twice: when (1) $m_1 = j_1$ and $m_2 = j_2 - 1$. and (2)$m_1 = j_1 - 1$ and $m_2 = j_2$. One of the two linear independent combination of these two states ($m = j_1 + j_2 - 1$) must be associated with the new state with $j = j_1 + j_2$ and $m = j_1 + j_2 - 1$. Since for each j value there must be values of m ranging from $j_1 + j_2$ to $-j_1 - j_2$. The other combination is associated with $j = j_1 + j_2 - 1$. By an extension of this argument we can see that each j value, ranging from $j_1 + j_2$ to $|j_1 - j_2|$ by integer steps, appears just once. Each j value is associated with $2j + 1$ combinations of the original kets

$$\sum_{j=|j_1 - j_2|}^{j_1 + j_2} (2j + 1) = (2j_1 + 1)(2j_2 + 1)$$

which is equal to the number of $|m_1, m_2\rangle$ as expected.

3.5.1 Clebsch-Gordan coefficients

The Clebsch-Gordan coefficients form a unitary matrix. Furthermore the matrix elements are taken to be real by convention. An immediate consequence is $\langle jm|m_1, m_2\rangle = \langle m_1, m_2|jm\rangle$. The orthogonality conditions of the matrix are

(1). $\langle m_1, m_2|m_1', m_2'\rangle = \delta_{m_1 m_1'}\delta_{m_2 m_2'}$

$$\sum_{j.m} \langle m_1, m_2|jm\rangle \langle jm|m_1', m_2'\rangle = \delta_{m_1 m_1'}\delta_{m_2 m_2'}$$

(2). $\langle jm|j'm'\rangle = \delta_{jj'}\delta_{mm'}$

$$\sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} \langle jm|m_1, m_2\rangle \langle m_1, m_2|j'm'\rangle = \delta_{jj'}\delta_{mm'}$$

(3). $\langle jm|m_1, m_2\rangle \neq 0$ only if $m = m_1 + m_2$

Recursion Relations

We apply $J_\pm$ to the left side of Eq.

$$|jm\rangle = \sum_{m_1'=-j_1}^{j_2} \sum_{m_2'=-j_2}^{j_2} |m_1', m_2'\rangle \langle m_1', m_2'|jm\rangle$$

$$J_+ |jm\rangle$$

$$= \sum_{m_1'=-j_1}^{j_2} \sum_{m_2'=-j_2}^{j_2} (J_{1+} + J_{2+}) |m_1', m_2'\rangle \langle m_1', m_2'|jm\rangle$$

$$[j(j+1) - m(m+1)]^{1/2} |jm+1\rangle$$

$$= \sum [j_1(j_1+1) - m_1'(m_1'+1)]^{1/2} |m_1'+1, m_2'\rangle \langle m_1', m_2'|jm\rangle$$

$$+ \sum [j_2(j_2+1) - m_2(m_2+1)]^{1/2} |m_1', m_2'+1\rangle \langle m_1', m_2'|jm\rangle$$

Multiplying $\langle m_1, m_2|$ from the left side

$$[j(j+1) - m(m+1)]^{1/2} \langle m_1, m_2 | j \; m+1 \rangle$$

$$= [j_1(j_1+1) - m_1(m_1+1)]^{1/2} \langle m_1 - 1, m_2 | jm \rangle$$

$$+ [j_2(j_2+1) - m_2(m_2+1)]^{1/2} \langle m_1, m_2 - 1 | jm \rangle$$

Similarly,

$$[j(j+1) - m(m-1)]^{1/2} \langle m_1, m_2 | jm-1 \rangle$$

$$= [j_1(j_1+1) - m_1(m_1-1)]^{1/2} \langle m_1 + 1, m_2 | jm \rangle$$

$$+ [j_2(j_2+1) - m_2(m_2+1)]^{1/2} \langle m_1, m_2 + 1 | jm \rangle$$

Construction Procedure

Combination of the two recursion relations and the orthogonality conditions can leads to all Clebsch-Gordan coefficients . We start with the sector with the largest value of m :

(1) $m = j_1 + j_2$, $j = j_1 + j_2$

$$\langle j_1, j_2 | j_1 + j_2 \;\; j_1 + j_2 \rangle = 1$$

(2) $m = j_1 + j_2 - 1$

$$\text{(a) } m_1 = j_1, \; m_2 = j_2 - 1$$

$$\text{(b) } m_1 = j_1 - 1, \;\; m_2 = j_2$$

$$j = j_1 + j_2$$

$$j = j_1 + j_2 - 1$$

$$| \; j_1 + j_2 \;\; j_1 + j_2 \; \rangle = |j_1, j_2\rangle$$

$$[(j_1 + j_2 \;)(j_1 + j_2 + 1) - ((j_1 + j_2 \;)(j_1 + j_2 - 1)]^{1/2}$$

$$\times |j_1 + j_2 \;\; j_1 + j_2 - 1\rangle$$

$$= \quad [j_1(j_1 + 1) - j_1(j_1 - 1)]^{1/2} \, |j_1 - 1 \; , \; j_2\rangle$$

$$+ [j_2(j_2 + 1) - j_2(j_2 - 1)]^{1/2} \, |j_1 \; , \; j_2 - 1\rangle$$

$$\langle j_1 - 1, j_2 | j_1 + j_2 \;\; j_1 + j_2 \;\; - 1\rangle \quad = \quad \left(\frac{j_1}{j_1 + j_2}\right)^{1/2}$$

$$\langle j_1, j_2 - 1 | j_1 + j_2 \;\; j_1 + j_2 \;\; - 1\rangle \quad = \quad \left(\frac{j_2}{j_1 + j_2}\right)^{1/2}$$

$\langle m_1, m_2 | j_1 + j_2 - 1, \;\; j_1 + j_2 - 1 \; \rangle$

These two coefficients are determined by the orthogonality conditions

$$\langle j, j - 1 | j - 1, j \;\; - 1\rangle = 0$$

$$\langle j_1 + j_2, j_1 + j_2 \;\; - 1 | j_1 j_2 - 1\rangle \, \langle j_1 j_2 - 1 | j_1 + j_2 - 1, j_1 + j_2 \;\; - 1\rangle$$

$$+ \langle j_1 + j_2, j_1 + j_2 \;\; - 1 | j_1 - 1 \;\; j_2\rangle \, \langle j_1 - 1 \;\; j_2 | j_1 + j_2 - 1, j_1 + j_2 \;\; - 1\rangle = 0$$

$$\left(\frac{j_2}{j_1 + j_2}\right)^{1/2} \langle j_1, j_2 - 1 | j_1 + j_2 - 1, \;\; j_1 + j_2 \;\; - 1\rangle$$

$$+ \left(\frac{j_1}{j_1 + j_2}\right)^{1/2} \langle j_1 - 1, j_2 | j_1 + j_2 - 1, \;\; j_1 + j_2 \;\; - 1\rangle = 0$$

$$x \quad = \quad \left(\frac{j_1}{j_1 + j_2}\right)^{1/2}$$

$$y \quad = \quad \left(\frac{j_2}{j_1 + j_2}\right)^{1/2}$$

$$\begin{cases} \langle j_1 + j_2 - 1,\ j_1 + j_2\ - 1 | j_1 + j_2 - 1, j_1 + j_2 - 1 \rangle = 1 \\ x^2 + y^2 = 1 \end{cases}$$

$$\begin{cases} \langle j_1 j_2 - 1 | j_1 + j_2 - 1, j_1 + j_2 - 1 \rangle = + \left(\frac{j_1}{j_1 + j_2} \right)^{1/2} \\ \langle j_1 - 1\ j_2 | j_1 + j_2 - 1, j_1 + j_2 - 1 \rangle = - \left(\frac{j_2}{j_1 + j_2} \right)^{1/2} \end{cases}$$

The convention here is that the first matrix element, which has the form $\langle j_1, j - j_1 | j, j \rangle$, is real and positive.

(3) $m = j_1 + j_2 - 2$

$$\text{(a) } m_1 = j_1 \quad m_2 = j_2 - 2$$

$$\text{(b) } m_1 = j_1 - 1 \quad m_2 = j_2 - 1$$

$$\text{(c) } m_1 = j_1 - 2 \quad m_2 = j_2$$

$$j = j_1 + j_2$$

$$j = j_1 + j_2 - 1$$

$$j = j_1 + j_2 - 2$$

$\langle m_1, m_2 | j_1 + j_2,\ m \rangle$ and $\langle m_1, m_2 | j_1 + j_2 - 1,\ m \rangle$ are determined by the recursion relations and the coefficients in (2). The coefficients $\langle m_1, m_2 | j_1 + j_2 - 2,\ m \rangle$ are determined by the orthogonality conditions.

In this construction procedure, the only difficult part is the use of orthogonally, which becomes progressively more complicated as the rank of the submatrix increases. However it needs be employed only once for each submatrix, and it is easier to work out an example with particular numerical values for j_1 and j_2 than the general case just considered.

(a) $J_- \left|j_1 + j_2, j_1 + j_2 - 1\right\rangle$

$$\langle j_1 j_2 - 2 | j_1 + j_2, j_1 + j_2 - 2\rangle = \left[\frac{j_2(2j_2 - 1)}{(j_1 + j_2)(2j_1 + 2j_2 - 1)}\right]^{\frac{1}{2}}$$

$$\langle j_1 - 1 j_2 - 1 | j_1 + j_2, j_1 + j_2 - 2\rangle = \left[\frac{4j_1 j_2}{(j_1 + j_2)(2j_1 + 2j_2 - 1)}\right]^{\frac{1}{2}}$$

$$\langle j_1 - 2 j_2 | j_1 + j_2, j_1 + j_2 - 2\rangle = \left[\frac{j_1(2j_1 - 1)}{(j_1 + j_2)(2j_1 + 2j_2 - 1)}\right]^{\frac{1}{2}}$$

(b) $J_- \left|j_1 + j_2 - 1,\ j_1 + j_2 - 1\right\rangle$

$$\begin{aligned}
\langle j_1 j_2 - 2 | j_1 + j_2 - 1, j_1 + j_2 - 2\rangle &= \left[\frac{j_1(2j_2 - 1)}{(j_1 + j_2)(j_1 + j_2 - 1)}\right]^{\frac{1}{2}} \\
\langle j_1 - 1 j_2 - 1 | j_1 + j_2 - 1, j_1 + j_2 - 2\rangle &= \frac{j_1 - j_2}{[(j_1 + j_2)(j_1 + j_2 - 1)]^{\frac{1}{2}}} \\
\langle j_1 - 2 j_2 | j_1 + j_2 - 1, j_1 + j_2 - 2\rangle &= -\left[\frac{j_2(2j_1 - 1)}{(j_1 + j_2)(j_1 + j_2 - 1)}\right]^{\frac{1}{2}}
\end{aligned}$$

3.6 Examples

3.6.1 Two spin-1/2 systems

3.6.2 Spin-orbit coupling

PROBLEM

1. Find the eigenvalues and eigenvectors of $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. Suppose an electron is in the spin state $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$. If S_y is measured, what is the probability of the result $\hbar/2$?

2. Let $\mathbf{n}$ be a unit vector in a direction specified by the polar angles (θ, ϕ). Show that the component of the angular momentum in the direction $\mathbf{n}$ is

$$\begin{aligned} \mathbf{L}_n &= \sin\theta\cos\phi\mathbf{L}_x + \sin\theta\sin\phi\mathbf{L}_y + \cos\theta\mathbf{L}_z \\ &= \frac{1}{2}\sin\theta\left(e^{-i\phi}\mathbf{L}_+ + e^{i\phi}\ \mathbf{L}_-\right) + \cos\mathbf{L}_z. \end{aligned}$$

If the system is in simultaneously eigenstates of $\mathbf{L}^2$ and $\mathbf{L}_z$ belonging to the eigenvalues $l(l+1)\hbar^2$ and $m\hbar$, i.e., $|l, m\rangle$,

(a) what are the possible results of a measurement of $\mathbf{L}_n$?

(b) what are the expectation values of $\mathbf{L}_n$ and $\mathbf{L}_n^2$?

3. Obtain an explicit expression for

$$U_R(\boldsymbol{\phi}) = \exp(-i\boldsymbol{\phi}\mathbf{n}\cdot\mathbf{S}/\hbar)$$

in the form of a 2×2 matrix when $\mathbf{S}$ is the spin operator with $S = 1/2$. Let the unit vector $\mathbf{n}$ have the polar angles θ and ϕ. Show explicitly that your matrix for $U_R(\boldsymbol{\phi})$ is unitary and that it is equal to -1 when $\phi = 2\pi$.

4. Prove a sequence of Euler rotations represented by

$$\begin{aligned} & D(1/2)(\alpha,\beta,\gamma) \\ = \ & \exp\left(-i\frac{\alpha}{2}\sigma_3\right)\exp\left(-i\frac{\beta}{2}\sigma_2\right)\exp\left(-i\frac{\gamma}{2}\sigma_3\right) \\ = \ & \begin{pmatrix} e^{-i(\alpha+\gamma)/2}\cos\frac{\beta}{2} & e^{-i(\alpha-\gamma)/2}\sin\frac{\beta}{2} \\ e^{-i(\alpha-\gamma)/2}\sin\frac{\beta}{2} & e^{i(\alpha+\gamma)/2}\cos\frac{\beta}{2} \end{pmatrix}. \end{aligned}$$

Because of the group properties of rotations, we expect that this sequence of operations is equivalent to a single rotation about some axis by an angle ϕ. Find ϕ.

5. Calculate the matrix of Clebsch-Gordan coefficients in the case of $j_1 = 1/2$ and $j_2 = 1/2$. According to the matrix, write explicitly the eigenstates of the total angular momentum and its z component in terms of (j_1, m_1) and (j_2, m_2).

6. Use the raising or lowering operator to find the following Clebsch-Gordan coefficients

$$\left|\frac{3}{2}, \frac{1}{2}\right\rangle = a\,|1,1\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle + b\,|1,0\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle .$$

Chapter 4

Symmetries in Physics

Symmetry is a fundamental attribute of the natural world that enables an investigator to study particular aspects of physical systems by themselves. For example, the assumption that space is homogeneous, or possesses translational symmetry, leads to the conclusion that the linear momentum of a closed isolated system does not change as the system moves. This makes it possible to study separately the motion of the center of mass and the internal motion of the system. A systematic treatment of the symmetry properties and the conservation law is useful in solving more complicated problems. It provides a deeper insight into the structure of physics.

In this chapter we consider the geometrical symmetries that may be associated with the displacements of a physical system in space and time, with its rotation and inversion in space, and with the reversal of the sense of progression of time.

4.1 Symmetries and Conservation Laws

4.1.1 Symmetry in Classical Physics

An alternative way to describe a classical system is to introduce Lagrangian $\mathcal{L}$:

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i} - \frac{\partial \mathcal{L}}{\partial q_i} = 0$$

which is called the Lagrange equation. For a conservative system,

$$\mathcal{L} = \mathcal{T} - \mathcal{V}$$

where

$$\mathcal{V} = \mathcal{V}(q_1, q_2, ...q_N).$$

For example, the Lagrangian for a harmonic oscillator is

$$\mathcal{L} = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2.$$

From the Lagrange equation, we obtain

$$m\ddot{x} = -kx.$$

This is the Newtonian equation of motion! When the potential is related to velocity or generalized velocity, the Lagrangian is constructed in a different way. For instance, the Lagrangian for a charged particle subjected to an electromagnetic field

$$\mathcal{L} = \mathcal{T} - q\phi + \frac{q}{c}A \cdot v.$$

If the Lagrangian is unchanged under displacement in the general sense,

$$q_i \rightarrow q_i + \delta q_i$$

i.e.,

$$\frac{\partial \mathcal{L}}{\partial q_i} = 0,$$

from the Lagrange equation, it follows that

$$\frac{dP_i}{dt} = 0$$

where that canonical momentum is defined as

$$P_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i}.$$

In other words, the canonical momentum is conserved, i.e. the law of conservation.

4.1.2 Symmetry in Quantum Mechanics

In quantum mechanics, we have learned to associate a unitary operator, say U, with an operation like translation and rotation. It has become customary to call U a symmetry operator regardless of whether the physical system itself possesses the symmetry to U. When we say that a system possesses that symmetry to U, which implies that

$$U^{\dagger} H U = H$$

For a continuous symmetry, we take an infinitesmal displacement ε and expand the operator,

$$U = 1 - \frac{i\varepsilon}{\hbar} G$$

where G is the Hermitian generator of the symmetry operator. Thus,

$$[G, H] = 0.$$

By virtue of the Heisenberg equation of motion, we have

$$\frac{dG}{dt} = 0.$$

Hence G is a constant of the motion. In the language of quantum mechanics, we say that G and H can be diagonalized simultaneously. Suppose $|g\rangle$ an eigenstate of G. Then, the state at a later time

$$|g, t_0, t\rangle = U(t, t_0)\,|g\rangle$$

is also an eigenstate of G.

Proof.

$$\begin{aligned} G\,|g, t_0, t\rangle &= GU(t, t_0)\,|g\rangle \\ &= U(t, t_0)G\,|g\rangle \\ &= gU(t, t_0)\,|g\rangle\,. \end{aligned}$$

■

4.1.3 Degeneracy

Suppose that

$$[H, U] = 0$$

for the symmetry operator U and $|n\rangle$ is an energy eigenket with eigenvalue E_n. Then, $U\,|n\rangle$ is also an eigenket of H with the same energy eigenvalue.

Proof.

$$\begin{aligned} HU\,|n\rangle &= UH\,|n\rangle \\ &= E_n U\,|n\rangle\,. \end{aligned}$$

Suppose $|n\rangle$ and $U\,|n\rangle$ represent two different kets. Then these two states with the same energy are said to be degenerated. ■

Remark 3 *The proof is very trivial, but the concept play a far more important role in quantum mechanics.*

4.1.4 Symmetry and symmetry breaking

If $|n\rangle$ is non-degenerated, $U|n\rangle$ and $|n\rangle$ must represent the same physical state although they can differ a trivial phase factor, i.e.,

$$U|n\rangle = e^{i\delta}|n\rangle .$$

In the case, we say that the state $|n\rangle$ also possesses the symmetry. If

$$U|n\rangle \neq e^{i\delta}|n\rangle ,$$

we say that the symmetry is spontaneously broken in the state although the Hamiltonian possesses the symmetry. The spontaneous symmetry breaking occurs when the state is degenerated. The spontaneous broken symmetry is one of the most important concepts in modern physics, from elementary particle physics to condensed matter physics.

Example 1

for a hydrogen atom problem,

$$H = \frac{1}{2m}P^2 + V(r).$$

The Hamiltonian is rotational invariant

$$[D(R), H] = 0.$$

One of eigenstates is denoted by $|n, j, m\rangle$ with E_n. Then

$$D(R)|n, j, m\rangle = \sum_{m'} D^{(j)}_{mm'}|n, j, m'\rangle$$

is also an eigenket of H with the same energy E_n. For each pair of n and j there are $2j+1$ values of m:

$$m = -j, -j+1, ..., j$$

Therefore $|n, j, m\rangle$ should be at least $(2j+1)$-fold degenerated.

Example 2

Two-spin Problem

The Hamiltonian for two spins S_1 and S_2 is written as

$$H = J\mathbf{S}_1 \cdot \mathbf{S}_2.$$

Denote the eigenstate for H by $|S_{tot}, M\rangle$

$$\begin{aligned} H\,|S_{tot}, M\rangle &= \frac{J}{2}\left[(\mathbf{S}_1+\mathbf{S}_2)^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2\right]|S_{tot}, M\rangle \\ &= \frac{J}{2}\left[S_{tot}\left(S_{tot}+1\right) - 2s(s+1)\right]|S_{tot}, M\rangle \end{aligned}$$

The total spin can be

$$S_{tot} = 2s, 2s-1, ..., 0.$$

As the M can be taken to be

$$M = -S_{tot}, -S_{tot}+1, ..., S_{tot}.$$

and the eigenvalue of H is independent of M, so the state $|S_{tot}, M\rangle$ is $(2S_{tot}+1)$-fold degenerated.

The ground state energy:

(1) Antiferromagnetic $J > 0$, $S_{tot} = 0$

$$E_g = -s(s+1)J$$

(2) Ferromagnetic $J < 0$, $S_{tot} = 2s$

$$E_g = s^2 J$$

SU(2) symmetry: When the system is rotated the rotation operator

$$U = e^{i\frac{(\mathbf{S}_1+\mathbf{S}_2)\cdot n}{\hbar}\phi}$$

As

$$[H, \mathbf{S}] = 0,$$

we have

$$U^\dagger H U = H.$$

For the ground state

(1) $J > 0$, $S_{tot} = 0$

$$U\,|S=0, M=0\rangle = |S=0, M=0\rangle$$

The state also possesses the SU(2) symmetry.

(2)$J < 0$, $S_{tot} = 2s$

$$U\,|S=2s, M=0\rangle \neq |S=2s, M=0\rangle$$

The ground state is $(4s+1)$-fold degenerate. The symmetry is spontaneously broken.

4.1.5 Summary: symmetries in physics

Space Translation	$r \rightarrow r + \delta r$	Momentum
Time evolution	$t \rightarrow t + \delta t$	Energy
Rotation	$r \rightarrow r'$	Angular Momentum
Space Inversion	$r \rightarrow -r$	Parity
Time reversal	$t \rightarrow -t$	Charge conjugate
Permutation	$(12) \rightarrow (21)$	Quantum Statistics
Gauge	$\Psi \rightarrow e^{i\theta}\Psi$	Charge

Space translation

$$U_r^\dagger(\rho) r U_r(\rho) = r + \rho$$

$$U_r^\dagger(\rho) = \exp[-i\frac{\mathbf{P}}{\hbar} \cdot \rho]$$

$$U_r^\dagger(\rho) H U_r(\rho) = H$$

$$[P, H] = 0$$

Time evolution

$$U_t^\dagger(\tau) t U_t(\tau) = t + \tau$$

$$U_t^\dagger(\tau) = \exp[-i\frac{\mathbf{H}}{\hbar}\tau]$$

$$U_t^\dagger(\tau) H U_t(\tau) = H$$

$$|\alpha(t)\rangle = \exp\left[-iHt/\hbar\right]|\alpha(0)\rangle$$

Rotation

$$r' = Rr$$

$$|\alpha\rangle_R = \mathcal{D}(R)\,|\alpha\rangle$$

$$\mathcal{D}(R) = \exp\left[-i\phi\frac{\mathbf{J}\cdot\mathbf{n}}{\hbar}\right]$$

$$\mathcal{D}^\dagger(R)H\mathcal{D}(R) = H$$

$$[J, H] = 0$$

Gauge Invariance

$$H\Psi = i\hbar\frac{\partial}{\partial t}\Psi$$

This symmetry is related to the conservation of "charge", i.e., the number of the particles.

4.2 Discrete Symmetries

In this section we consider two symmetry operators that can be considered to be discrete

4.2.1 Parity

The parity operation, as applied to transformation on the coordinate system, changes a right-handed (RH) system into a left-handed (LH) system. Let us denote the parity operator Π, which satisfies

$$\begin{cases} |\alpha\rangle \to \Pi\,|\alpha\rangle \\ \Pi^\dagger x \Pi = -x \\ \{x, \Pi\} = 0 \\ \Pi^\dagger\Pi = 1 \end{cases}$$

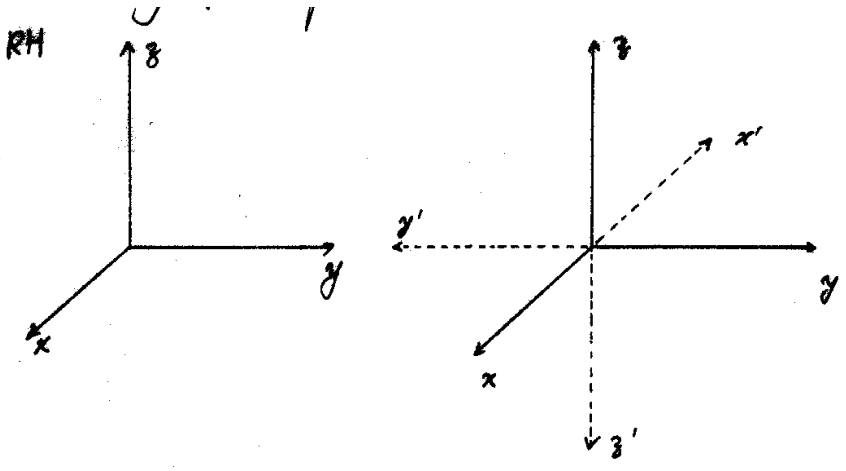


Figure 4.1:

$$\Pi^{\dagger}\Pi = 1 -> \Pi^{\dagger} = \Pi^{-1} = \Pi$$

The physical meaning is that under this operation

$$V = (x, y, z) \Rightarrow V' = (-x, -y, -z)$$

$$V' = RV$$

where

$$R = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

How does an eigenket of the position operator transform under parity?Assume

$$\hat{x}\,|x\rangle = x\,|x\rangle$$

$$\Pi\hat{x}\,|x\rangle = x\Pi\,|x\rangle$$

$$-\hat{x}\Pi\,|x\rangle = x\Pi\,|x\rangle$$

$$\hat{x}\,(\Pi\,|x\rangle) = -x\,(\Pi\,|x\rangle)$$

Thus we conclude that

$$\Pi |x\rangle = e^{-i\delta} |-x\rangle .$$

Applying the parity operation twice

$$\Pi^2 \hat{x} = \Pi (-\hat{x}\Pi) = \hat{x}\Pi^2$$

and

$$\hat{x}\Pi^2 |x\rangle = \Pi^2 \hat{x} |x\rangle = x\Pi^2 |x\rangle$$

Thus

$$\Pi^2 = 1.$$

Therefore its eigenvalue can be only +1 or -1.

4.2.2 The Momentum Operator

Space translation followed by parity is equivalent to parity followed by translation in the opposite direction:

$$\begin{aligned} \Pi\mathcal{T}(dx) |x\rangle &= \Pi |x + dx\rangle \\ &= \lambda |-x - dx\rangle \\ &= \mathcal{T}(-dx)\lambda |-x\rangle \\ &= \mathcal{T}(-dx)\Pi |x\rangle \end{aligned}$$

Since

$$\mathcal{T}(dx) = 1 - i\frac{P}{\hbar}dx + ...,$$

it follows that

$$\Pi P = -P\Pi$$

or

$$\{\Pi, P\} = 0.$$

4.2.3 The Angular Momentum

Define

$$\mathcal{L} = x \times P,$$

then

$$\Pi\mathcal{L} = \mathcal{L}\Pi.$$

For 3×3 matrices, we have

$$R^{(parity)} R^{(rotation)} = R^{(r)} R^{(p)}$$

where

$$R^{(p)} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

which implies that parity and rotation operation commute. Therefore

$$\Pi D(R) = D(R)\Pi.$$

$$D(R) = 1 - iJ \cdot n\varepsilon/\hbar + \cdots$$

$$\Pi J = J\Pi$$

$$\Pi S = S\Pi$$

$$\Pi L = L\Pi$$

Let us now look at the parity property of wave function whose state ket is $|\alpha\rangle$:

$$\Psi(x) = \langle x|\alpha\rangle\,.$$

Suppose $|\alpha\rangle$ the eigenket of parity

$$\Pi\,|\alpha\rangle = \lambda\,|\alpha\rangle\,. \quad (\lambda = \pm 1)$$

Then

$$\begin{aligned} \langle x|\,\Pi\,|\alpha\rangle &= \lambda\,\langle x\,|\alpha\rangle \\ \langle -x\,|\alpha\rangle &= \lambda\,\langle x\,|\alpha\rangle \\ \Psi(-x) &= \lambda\Psi(x) \end{aligned}$$

The wave function is also parity.

Example 3

Solution for a square-well potential

$$-\frac{\hbar^2}{2m}\frac{d^2U(x)}{dx^2} = EU(x)$$

with $|x| \leq a$. In the replacement $x \to -x$,

$$-\frac{\hbar^2}{2m}\frac{d^2U(-x)}{dx^2} = EU(-x)$$

Thus if U(x) is one solution, U(-x) must be also one solution. The solutions are

$$U(x) = e^{\pm ik\cdot x/\hbar}$$

where $k^2 = 2mE/\hbar^2$. We can construct

Odd Parity: $U(x) - U(-x) = U_{odd}(x)$

Even Parity: $U(x) + U(-x) = U_{even}(x)$

$\sin kx/\hbar$ and $\cos kx/\hbar$

Example 4

Simple harmonic oscillator: The basic Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2.$$

We have

$$\Pi^\dagger H \Pi = H$$

and

$$\left.\begin{array}{l} \Pi^\dagger \mathbf{x} \Pi = -\mathbf{x} \\ \Pi^\dagger \mathbf{p} \Pi = -\mathbf{p} \end{array}\right\} \Rightarrow \left\{\begin{array}{l} \Pi^\dagger a^\dagger \Pi = -a^\dagger \\ \Pi^\dagger a \Pi = -a \end{array}\right.$$

The eigenkets are

$$|n\rangle = \frac{1}{n!}\left(a^\dagger\right)^n |0\rangle$$

The ground state wave function is

$$\langle x|0\rangle = \frac{1}{\pi^{1/2}x_0}\exp\left[-\frac{1}{2}\frac{x^2}{x_0^2}\right]$$

So

$$\langle x|0\rangle = \langle -x|0\rangle$$

How about $\langle x|n\rangle$?

$$\langle x|\Pi|n\rangle = (-1)^n \langle x|n\rangle .$$

$$\langle -x||n\rangle = (-1)^n \langle x|n\rangle$$

At $x = 0$, we have $\langle x = 0|n\rangle = 0$ for odd n.

Example 5

Double well potential

Let us now look at the parities of energy eigenstates.

Theorem 4 *Suppose* $[H, \Pi] = 0$ *and* $|n\rangle$ *is an eigenstate of* H *with eigenvalue* E_n

$$H|n\rangle = E_n|n\rangle$$

then (a) if $|n\rangle$ *is nondegenerate,* $\Pi|n\rangle$ *is also a parity eigenket; (b) if* $|n\rangle$ *is degenerate,* $\Pi|n\rangle$ *may not be a parity eigenket.*

Proof. *We can construct two states*

$$\frac{1}{2^{1/2}}(1 \pm \Pi)|n\rangle .$$

■

4.2.4 Lattice Translation

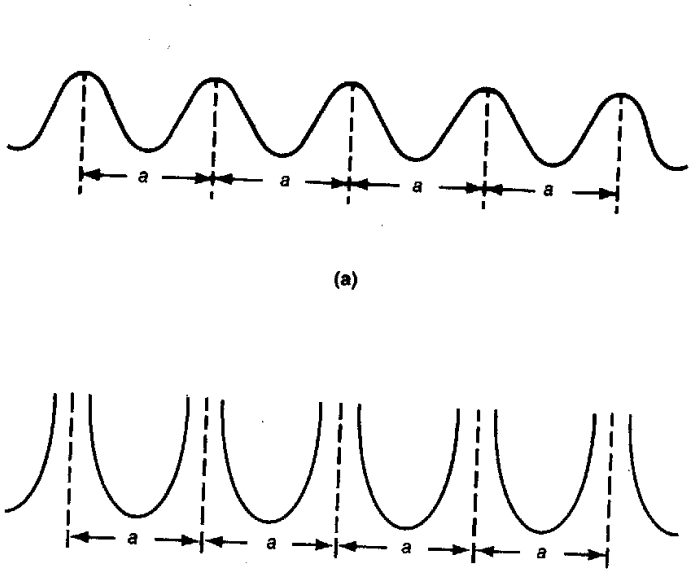


FIGURE (a) Periodic potential in one-dimension with periodicity a. (b) The periodic potential when the barrier height between two adjacent lattice sites becomes infinite.

(from Sakurai, 1994)

Consider a periodic potential in one dimension:

$$V(x \pm a) = V(x).$$

We introduce a translational operator $\tau(a)$ such that

$$\tau^{\dagger}(a) x \tau(a) \quad = \quad x + a;$$

$$\tau^{\dagger}(a) V(x) \tau(a) \quad = \quad V(x + a).$$

Thus the Hamiltonian is invariant under the translation

$$\tau^{\dagger}(a) H \tau(a) = H.$$

As τ is unitary, we have

$$H\tau = \tau H.$$

τ and H commute with each other. So τ can be diagonalized with H simultaneously. τ is unitary, but not hermitian. We expect the eigenvalue to be a complex number of modulus

1. Denote $|n\rangle$ a state ket in which the particle is localized at the nth site. When τ is applied to it

$$\tau(a)\,|n\rangle = |n+1\rangle\,.$$

To construct an eigenket for τ, we consider a linear combination

$$|\theta\rangle = \sum_{n=-\infty}^{+\infty} e^{in\theta}\,|n\rangle\,.$$

This state is an eigenstate for τ :

$$\begin{aligned}
\tau(a)\,|\theta\rangle &= \sum_{n=-\infty}^{+\infty} e^{in\theta}\tau(a)\,|n\rangle = \sum_{n=-\infty}^{+\infty} e^{in\theta}\,|n+1\rangle \\
&= e^{-i\theta}\sum_{n=-\infty}^{+\infty} e^{i(n+1)\theta}\,|n+1\rangle \\
\tau(a)\,|\theta\rangle &= e^{-i\theta}\,|\theta\rangle
\end{aligned}$$

A more realistic example:

$$\begin{aligned}
\langle n|\,H\,|n\rangle &= E_0 \\
\langle n|\,H\,|n\pm 1\rangle &= -t
\end{aligned}$$

and all other elements are equal to zero. That is

$$\begin{aligned}
H\,|n\rangle &= E_0\,|n\rangle - t\,|n+1\rangle - t\,|n-1\rangle \\
H &= \sum_n \{E_0\,|n\rangle\,\langle n| - t\,|n+1\rangle\,\langle n| - t\,|n-1\rangle\,\langle n|\} \\
H\,|\theta\rangle &= \sum_n \{E_0\,|n\rangle\,\langle n| - t\,|n+1\rangle\,\langle n| - t\,|n-1\rangle\,\langle n|\}\,|\theta\rangle \\
&= (E_0 - 2t\cos\theta)\,|\theta\rangle
\end{aligned}$$

4.3 Permutation Symmetry and Identical Particles

4.3.1 Identical particles

Identical particles cannot be distinguished by means of any inherent properties, since otherwise they could not be identical in all respect. In classical mechanics the existence of sharply definable trajectories for individual particles makes it possible in principles to distinguish between particles that are identical except for their path since each particle can be followed during the course of an experiment. In quantum mechanics, the finite size and the spreading of the wave packets that can describe individual particles often make it impossible to distinguish between identical particles because of their positions, especially if they interact with each others to an appreciable extent.

Distinguishable and indistinguishable identical particles

Two identical particles are indistinguishable if the wave functions for the two particles overlap, and distinguishable if the wave functions do not overlap.

Permutation Symmetry

Let us consider the Hamiltonian of a system of two identical particles.

$$H = \frac{1}{2m}P_1^2 + \frac{1}{2m}P_2^2 + V_{pair}(|x_1 - x_2|) + V_{ext}(x_1) + V_{ext}(x_2)$$

Symmetry: to exchange the positions of two particles: $1 \Leftrightarrow 2$, the Hamiltonian is invariant

$$H \Longleftrightarrow H.$$

Define the permutation operator

$$P_{12} \left|x_1\right\rangle_1 \otimes \left|x_2\right\rangle_2 \quad = \quad \left|x_2\right\rangle_1 \otimes \left|x_1\right\rangle_2$$

$$P_{12}^{\dagger} H(x_1, x_2) P_{12} \quad = \quad H(x_2, x_1).$$

Clearly

$$P_{12} \quad = \quad P_{21}$$

$$P_{12}^2 \quad = \quad 1$$

Consider a state ket for two particles:

$$\left|k\right\rangle_1 \otimes \left|k'\right\rangle_2$$

$$P_{12} \left|k\right\rangle_1 \otimes \left|k'\right\rangle_2 = \left|k'\right\rangle_1 \otimes \left|k\right\rangle_2$$

We can construct two states

$$\frac{1}{2}\left[\left(\left|k\right\rangle_1 \otimes \left|k'\right\rangle_2 \pm \left|k'\right\rangle_1 \otimes \left|k\right\rangle_2\right)\right]$$

which are eigenstates of P_{12} with eigenvalues ± 1, respectively.

Our consideration can be extended to a system made up of many identical particles

$$P_{ij} \left|x_1, x_2, \cdots x_i \cdots, x_j, \cdots, x_N\right\rangle$$

$$= \quad \left|x_1, x_2, \cdots xj \cdots, x_i, \cdots, x_N\right\rangle$$

Clearly

$$P_{12}^2 = 1$$

just as before, and the allowed eigenvalues of P_{ij} are ± 1. It is important to note that, in general

$$[P_{ij}, P_{lm}] \neq 0.$$

Connection between spin and statistics

Half-odd-integer spin particles are fermions: electrons, protons, $\cdots$

Integer spin particles are boson: mesons, ^{4}He nucleus,$\cdots$

Although the allowed values of P_{ij} are ± 1, system containing N identical particles are either totally symmetrical or antisymmetric under the interchange of any pair.

Boson:

$$P_{ij} \left| N\ bosons \right\rangle = \left| N\ bosons \right\rangle$$

Fermions

$$P_{ij} \left| N\ fermions \right\rangle = - \left| N\ fermions \right\rangle$$

It is empirical fact that a mixed symmetry does not occur.

The exclusion principle

An immediate consequence of the electron being a fermion is that the electrons must satisfy the Pauli exclusion principle, which states that no two electrons can occupy the same state.

Let us consider a system containing N electrons without interaction

$$H(1, 2, , \cdots, N) = H_0(1) + H_0(2) + \cdots + H_0(N).$$

Assume $U_\alpha(n)$ are the wave functions of $H_0(n)$ with energy ε_α

$$H_0(n) U_\alpha(n) = \varepsilon_\alpha U_\alpha(n).$$

The product of N one-particle eigen functions are the energy eigen wave function of total system..

$$\begin{aligned} U(1,2,\cdots,N) &= U_\alpha(1)U_\beta(n)\cdots U_\gamma(N) \\ HU &= (\varepsilon_\alpha+\varepsilon_\beta+\cdots+\varepsilon_\gamma)U. \end{aligned}$$

As electrons are fermions, we have to express the wave function in an antisymmetric form. One way is to express as a determinant of the U's

$$\begin{aligned} & U_A(1,2,\cdots,N) \\ = \quad & \det\begin{pmatrix} U_\alpha(1) & U_\alpha(2) & \cdots & U_\alpha(N) \\ U_\beta(1) & U_\beta(2) & \cdots & U_\beta(N) \\ \vdots & \vdots & \ddots & \vdots \\ U_\gamma(1) & U_\gamma(2) & \cdots & U_\gamma(N) \end{pmatrix}. \end{aligned}$$

This function is antisymmetric and satisfies the Schrodinger equation with energy

$$\varepsilon_\alpha+\varepsilon_\beta+\cdots+\varepsilon_\gamma.$$

If two or more of the U's are the same,

$$U_A(1,2,\cdots,N)=0$$

which is the so-called Pauli exclusion principle.

To simplify the notation we introduce the creation and annihilation operator $c^\dagger$

and c such that

$$\begin{aligned} H_0 c_\alpha^\dagger |0\rangle &= \varepsilon_\alpha c_\alpha^\dagger |0\rangle \\ c_\alpha |0\rangle &= 0 \\ c_\alpha c_\alpha^\dagger + c_\alpha^\dagger c_\alpha &= 1 \\ c_\alpha^\dagger c_\beta^\dagger + c_\beta^\dagger c_\alpha^\dagger &= 0 \end{aligned}$$

The Shcrodinger equation can be reduced to

$$H |U_A\rangle = (\varepsilon_\alpha + \varepsilon_\beta + \cdots + \varepsilon_\gamma) |U_A\rangle$$

with

$$|U_A\rangle = c_\alpha^\dagger c_\beta^\dagger \cdots c_\gamma^\dagger |0\rangle .$$

Example 6

Two-particle problem

A system contains two particles, which is described by the Hamiltonian

$$H = H_1 + H_2$$

where

$$\begin{aligned} H_1 &= \frac{1}{2m_1} P_1^2 + \frac{1}{2} k_1 x_1^2 \\ H_2 &= \frac{1}{2m_2} P_2^2 + \frac{1}{2} k_2 x_2^2 \end{aligned}$$

(1) $m_1 \neq m_2$, $k_1 \neq k_2$

(2) $m_1 = m_2$, $k_1 = k_2$

4.4 Time Reversal

In this section we study a discrete symmetry, called time reversal. The terminology was first introduced by E. Wigner in 1932.

4.4.1 Classical cases

Let us first look at the classical case: a motion of particle sujected to a certain force. Its trajectory is given by the Newtonian equation of motion,

$$m\frac{d^2\mathbf{r}}{dt^2} = -\nabla V(r).$$

If $\mathbf{r}(t)$ is the soltion of the equation, then $\mathbf{r}(-t)$ is also the solution of the equation. In another word, when we make a transformation $t \to -t$, the Newtonian equation of motion keeps unchanged. Of course we should notice the change of the boundary condition or initial conditions for the problem.

Maxwell equations:

4.4.2 Antilinear Operators

4.4.3 Antiunitary operators

4.4.4 T for a zero spin particle

4.4.5 T for a nonzero spin particle

Chapter 5

Approximation Methods for Bound States

As in the case of classical mechanics, there are relatively few physically interesting problems in the quantum mechanics which can be solved exactly. Approximation methods are therefore very important in nearly all the applications of the theory. In this chapter we shall develop several approximation methods.

Approximation methods can be conveniently divided into two groups, according to whether the Hamiltonian of the system is time-independent or time-dependent.

5.1 The Variation Method

The variation method can be used for the approximate determination of the lowest or ground-state energy level of a system when there is no closely related problem that is capable of

exact solution, so that the perturbation method is inapplicable.

5.1.1 Expectation value of the energy

We attempt to estimate the ground state energy by considering a trial ket, $\left|\tilde{0}\right\rangle$, or a trial wave function. To this end we first prove a theorem of a great of importance. We define the expectation value $\bar{H}$ such that

$$\bar{H} = \frac{\left\langle\tilde{0}\right| H \left|\tilde{0}\right\rangle}{\left\langle\tilde{0}|\tilde{0}\right\rangle}.$$

Then we can prove the following

Theorem 5 *The expectation value of a trial state ket is always not less than the ground state energy*

$$\bar{H} \geq E_0.$$

Proof. *We can always imagine that any trial state can be expanded as*

$$\left|\tilde{0}\right\rangle = \sum_k |k\rangle \left\langle k|\tilde{0}\right\rangle$$

where $|k\rangle$ is an exact eigenket of H. The expectation value

$$\begin{aligned}
\bar{H} &= \frac{\left\langle\tilde{0}\right| H \left|\tilde{0}\right\rangle}{\left\langle\tilde{0}|\tilde{0}\right\rangle} \\
&= \frac{\sum_{k,l} \left\langle\tilde{0}|k\right\rangle \langle k|H|l\rangle \left\langle l|\tilde{0}\right\rangle}{\left\langle\tilde{0}|\tilde{0}\right\rangle} \\
&= \frac{\sum_k \left\langle\tilde{0}|k\right\rangle \left\langle k|\tilde{0}\right\rangle E_k}{\left\langle\tilde{0}|\tilde{0}\right\rangle} \\
&\geq \frac{\sum_k \left\langle\tilde{0}|k\right\rangle \left\langle k|\tilde{0}\right\rangle E_0}{\left\langle\tilde{0}|\tilde{0}\right\rangle} = E_0.
\end{aligned}$$

In the last step we use the property $E_k \geq E_0$. ■

The variation method does not tell us what kind of trial state ket are to estimate the ground state energy. Quite often we must appeal to physical intuition. In practice, we characterize the trial state ket by one or more parameters λ_n can compute $\bar{H}$ as a function of λ_n. Then we minimize the $\bar{H}$ by setting the derivatives with respect to the parameters zero

$$\frac{\partial \bar{H}}{\partial \lambda_n} = 0.$$

The result of the variation method is an upper limit for the ground state energy of the system, which is likely to be close if the form of the trial state ket or the trial wave function resembles that of the eigenfunction. Thus it is important to make use of any available information or physical intuition in choosing the trial function.

5.1.2 Particle in a one-dimensional infinite square well

We attempt to estimate the ground state energy of the infinite-well (one-dimensional box) problem defined by

$$V = \begin{cases} 0, \text{ for } |x| < a \\ +\infty, \text{ for } x > a. \end{cases}$$

The exact solution are, of course, well known:

$$\begin{aligned} \langle x|0\rangle &= \frac{1}{a^{1/2}} \cos\left(\frac{\pi x}{2a}\right), \\ E_0 &= \left(\frac{\hbar^2}{2m}\right)\left(\frac{\pi^2}{4a^2}\right). \end{aligned}$$

But suppose we did not know these. Evidently the wave function must vanish at $x = \pm a$. Further the ground state should has even parity. The simplest analytic wave function that satisfies both requirements is

$$\langle x|0\rangle = a^2 - x^2.$$

There is no variational parameter. We can compute $\tilde{H}$ as follows

$$\begin{aligned}\tilde{H} &= \frac{\int dx \langle 0|x\rangle \frac{p^2}{2m} \langle x|0\rangle}{\int dx \langle 0|x\rangle \langle x|0\rangle} \\ &= \frac{10}{\pi^2} E_0 \approx 1.0132 E_0.\end{aligned}$$

A much better result can be obtained if we use a more general trial function

$$\langle x|0\rangle = a^\gamma - x^\gamma.$$

where γ is regarded a variational wave parameter. Straightforward algebra gives

$$\tilde{H} = \frac{(\gamma+1)(2\gamma+1)}{2\gamma-1} \frac{\hbar^2}{4ma^2},$$

which has a minimum at

$$\gamma = \frac{1+6^{1/2}}{2} \approx 1.72,$$

This gives

$$\tilde{H} = \frac{5+26^{1/2}}{\pi^2} E_0. \approx 1.00298 E_0$$

The state with an odd parity?

$$\langle x|0\rangle = x\left(a^\gamma - x^\gamma\right).$$

5.1.3 Ground State of Helium Atom

We use the variation method with a simple trial function to obtain an upper limit for the energy of the ground state of the helium atom. The helium atom consists of a nucleus of charge $+2e$ surrounded by two electrons, we find that its Hamiltonian is

$$\begin{aligned}H &= -\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right) \\ &\quad -2e^2\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{e^2}{r_{12}} \\ &= H_1 + H_2 + V_{12}\end{aligned}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are two position vectors of two electrons with respect to the nucleus as origin, and $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$. If we neglect the interaction energy $\frac{e^2}{r_{12}}$ between the two electrons, the ground state wave function of H would be product of two normalized hydrogenic wave functions

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{Z^3}{\pi a_0^3} e^{-(Z/a_0)(r_1+r_2)} \tag{5.1}$$

with $a_0 = \hbar^2/\mu e^2$ and $Z = 2$.

Why $Z = 2$?

We shall use Eq.(5.1) as the trial wave function and permit Z to be the variation parameter. The kinetic energy of each electron is

$$E_{k1} = \int d\mathbf{r}_1 d\mathbf{r}_2 \Psi^*(\mathbf{r}_1, \mathbf{r}_2) \left(-\frac{\hbar^2}{2m}\nabla_1^2\right) \Psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{e^2 Z^2}{2a_0}.$$

The Coulomb energy of each electron is

$$E_{C1} = \int d\mathbf{r}_1 d\mathbf{r}_2 \Psi^*(\mathbf{r}_1, \mathbf{r}_2) \left(-\frac{2e^2}{r_1}\right) \Psi(\mathbf{r}_1, \mathbf{r}_2) = -\frac{2e^2 Z}{a_0}.$$

The interaction energy of two electrons is

$$E_{int} = \int d\mathbf{r}_1 d\mathbf{r}_2 \Psi^*(\mathbf{r}_1, \mathbf{r}_2) \left(\frac{e^2}{r_{12}}\right) \Psi(\mathbf{r}_1, \mathbf{r}_2) = -\frac{5e^2 Z}{8a_0}.$$

Here we make use of the formula

$$\frac{1}{r_{12}} = \frac{1}{r_1} \sum_{l=0}^{\infty} \left(\frac{r_2}{r_1}\right)^l P_l(\cos\theta), \quad r_1 > r_2$$

$$\frac{1}{r_{12}} = \frac{1}{r_2} \sum_{l=0}^{\infty} \left(\frac{r_1}{r_2}\right)^l P_l(\cos\theta), \quad r_2 > r_1$$

where P_l is the spherical harmonics and θ is the angle of there two vectors.

Totally, the expectation value of the Hamiltonian is

$$\begin{aligned}\tilde{H} &= \frac{e^2Z^2}{a_0} - \frac{4e^2Z}{a_0} + \frac{5e^2Z}{8a_0} \\ &= \frac{e^2}{a_0}\left(Z^2 - \frac{27}{8}Z\right) \\ &= \frac{e^2}{a_0}\left[\left(Z - \frac{27}{16}\right)^2 - \left(\frac{27}{16}\right)^2\right].\end{aligned}$$

The expectation is minimized at

$$Z = 27/16 \approx 1.69.$$

and

$$\tilde{H} = -\left(\frac{27}{16}\right)^2 \frac{e^2}{a_0} = -2.85\frac{e^2}{a_0}.$$

The experimental value for a helium atom is $2.904e^2/a_0$, so our estimation is about 1.9 high.

5.2 Stationary Perturbation Theory: Nondegenerate Case

5.2.1 Statement of the Problem

In this section we shall discuss the Rayleigh-Schrodinger perturbation theory, which analyses the modifications of discrete energy levels and the corresponding eigenfunctions of a system when a perturbation is applied.

We consider a time independent Hamiltonian H such that it can be split into two parts, namely

$$H = H_0 + V.$$

The perturbation theory is based on the assumption that when V=0, both the exact eigenvalues $E_n^{(0)}$ and the exact energy eigenkets $\left|n^{(0)}\right\rangle$ of H_0 are know

$$H_0 \left|n^{(0)}\right\rangle = E_n^{(0)} \left|n^{(0)}\right\rangle .$$

We are required to find approximate eigenkets and eigenvalues for the full Hamiltonian problem

$$(H_0 + V) \left|n\right\rangle = E_n \left|n\right\rangle .$$

In general, V is not the full potential operator. We expect that the V is not very "large" and should not change the eigenvalues and eigenkets of H_0 very much.

It is customary to introduce a parameter λ such that we solve

$$(H_0 + \lambda V) \left|n\right\rangle = E_n \left|n\right\rangle$$

instead of the original one. We take $0 \leq \lambda \leq 1$. The case of $\lambda = 0$ corresponds to the unperturbed problem and the case of $\lambda = 1$ corresponds to the full strength problem we want to solve.

5.2.2 The Two-State Problem

Before we embark on a systematic presentation of the basic method, let us see how the expansion in λ might indeed be valid in the exactly soluble two-state problem we have encountered many times already. Suppose we have a Hamiltonian that can be written as

$$\begin{aligned} H &= H_0 + \lambda V \\ &= E_1^{(0)} \left|1^{(0)}\right\rangle \left\langle 1^{(0)}\right| + E_2^{(0)} \left|2^{(0)}\right\rangle \left\langle 2^{(0)}\right| + \lambda V_{12} \left|1^{(0)}\right\rangle \left\langle 2^{(0)}\right| + \lambda V_{21} \left|2^{(0)}\right\rangle \left\langle 1^{(0)}\right| \end{aligned}$$

where $E_n^{(0)}$ and $\left|n^{(0)}\right\rangle$ are the exact eigenvalues and eigenstates for H_0.The index "0" stands for the unperturbed problem. We can also express the Hamiltonian by a square matrix

$$H = \begin{pmatrix} E_1^{(0)} & \lambda V_{12} \\ \lambda V_{21} & E_2^{(0)} \end{pmatrix}.$$

What is the eigenvalues of H?

$$E_1 = \frac{E_1^{(0)} + E_2^{(0)}}{2} + \left[\left(\frac{E_1^{(0)} - E_2^{(0)}}{2}\right)^2 + \lambda^2 V_{12}V_{21}\right]^{1/2};$$

$$E_2 = \frac{E_1^{(0)} + E_2^{(0)}}{2} - \left[\left(\frac{E_1^{(0)} - E_2^{(0)}}{2}\right)^2 + \lambda^2 V_{12}V_{21}\right]^{1/2}.$$

So this problem can be solved exactly. Let us suppose λV is small compared with the relevant energy scale, the difference of the energy eigenvalues of the unperturbed problem:

$$\lambda \left|V_{12}\right| \ll \left|E_1^{(0)} - E_2^{(0)}\right|$$

Using the formula

$$(1+x)^{1/2} = 1 + \frac{1}{2}x - \frac{1}{8}x^2 + \cdots, \tag{5.2}$$

we obtain the expansion of the energy eigenvalues in terms of λ

$$E_1 = E_1^{(0)} + \frac{\lambda^2 V_{12}V_{21}}{E_1^{(0)} - E_2^{(0)}} + \cdots;$$

$$E_2 = E_2^{(0)} - \frac{\lambda^2 V_{12}V_{21}}{E_1^{(0)} - E_2^{(0)}} + \cdots.$$

As the expansion in Eq.(5.2) holds for $x < 1$, the expansion is available in the case of small V.

5.2.3 Formal Development of Perturbation$\cdots$

We are dealing with the perturbation of a bound state. The assumption that V is small compared with the energy scale suggests that we expand the perturbed eigenvalues and

eigenkets as power series in V. This is most conveniently accomplished in the terms of the parameter λ such that the zero, first, etc., powers of λ correspond to the zero, first, etc., orders of the perturbation calculation.

The perturbed wave function and energy level are written

$$\begin{aligned} |n\rangle &= \left|n^{(0)}\right\rangle + \lambda \left|n^{(1)}\right\rangle + \lambda^2 \left|n^{(2)}\right\rangle + \cdots ; \\ E_n &= E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots \end{aligned}$$

and are substituted into the wave equation to give

$$\begin{aligned} & (H_0 + \lambda V)\left(\left|n^{(0)}\right\rangle + \lambda \left|n^{(1)}\right\rangle + \lambda^2 \left|n^{(2)}\right\rangle + \cdots\right) \\ = \quad & \left(E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots\right) \times \left(\left|n^{(0)}\right\rangle + \lambda \left|n^{(1)}\right\rangle + \lambda^2 \left|n^{(2)}\right\rangle + \cdots\right). \end{aligned}$$

Since the Equation is supposed to be valid for a continuous range of λ, we can equate the coefficients of equal powers of λ on the both sides to obtain a series of equations that represent successively higher orders of the perturbation.

$$\left(H_0 - E_n^{(0)}\right)\left|n^{(0)}\right\rangle = 0 \tag{5.3}$$

$$\left(H_0 - E_n^{(0)}\right)\left|n^{(1)}\right\rangle = (E_n^{(1)} - V)\left|n^{(0)}\right\rangle \tag{5.4}$$

$$\left(H_0 - E_n^{(0)}\right)\left|n^{(2)}\right\rangle = (E_n^{(1)} - V)\left|n^{(1)}\right\rangle + E_n^{(2)}\left|n^{(0)}\right\rangle \tag{5.5}$$

$$\left(H_0 - E_n^{(0)}\right)\left|n^{(3)}\right\rangle = (E_n^{(1)} - V)\left|n^{(2)}\right\rangle + E_n^{(2)}\left|n^{(1)}\right\rangle + E_n^{(3)}\left|n^{(0)}\right\rangle \tag{5.6}$$

$$\vdots$$

Zero-order perturbation

The Eq. (5.3) means that $\left|n^{(0)}\right\rangle$ is one of the unperturbed eigenkets, as expected. We can obtain it directly by taking $\lambda = 0$. The eigenvalue is $E_n^{(0)}$. Since we are dealing

with the perturbation of a bound state, the state ket $\left|n^{(0)}\right\rangle$ is discrete. It is assumed to be nondegenerate as well, although others of unperturbed eigenkets may be degenerate or continuously distributed in energy.

First-order perturbation

Multiplying an eigen bra of the unperturbed Hamiltonian from the left hand on both sides of the Eq.(5.4), we obtain

$$\left\langle n^{(0)}\right| \left(H_0 - E_n^{(0)}\right) \left|n^{(1)}\right\rangle = \left\langle n^{(0)}\right| \left(E_n^{(1)} - V\right) \left|n^{(0)}\right\rangle \tag{5.7}$$

$$\left\langle m^{(0)}\right| \left(H_0 - E_n^{(0)}\right) \left|n^{(1)}\right\rangle = \left\langle m^{(0)}\right| \left(E_n^{(1)} - V\right) \left|n^{(0)}\right\rangle \tag{5.8}$$

where $m \neq n$. The Eq. (5.7) gives

$$E_n^{(1)} = \left\langle n^{(0)}\right| V \left|n^{(0)}\right\rangle = V_{nn}.$$

It is convenient to calculate $\left|n^{(1)}\right\rangle$ by expanding it in terms of the unperturbed eigenkets

$$\left|n^{(1)}\right\rangle = \sum_m c_m^{(1)} \left|m^{(0)}\right\rangle$$

where the summation runs over all possible eigenkets of H_0. To simplify the notation, we define

$$V_{mn} = \left\langle m^{(0)}\right| V \left|n^{(0)}\right\rangle$$

From the Eq.(5.5),

$$\begin{aligned} \left(H_0 - E_n^{(0)}\right) \sum_m c_m^{(1)} \left|m^{(0)}\right\rangle &= \left(E_n^{(1)} - V\right) \left|n^{(0)}\right\rangle \\ \sum_m c_m^{(1)} \left(E_m^{(0)} - E_n^{(0)}\right) \left|m^{(0)}\right\rangle &= \left(E_n^{(1)} - V\right) \left|n^{(0)}\right\rangle \end{aligned}$$

multiplying $\left\langle m^{(0)}\right|$ from the left hand side, we obtain

$$c_m^{(1)} = \frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}} \ .$$

Second-order perturbation

The second-order correction to the energy is

$$E_n^{(2)} = \left\langle n^{(0)} \right| V \left| n^{(1)} \right\rangle = \sum_{m \neq n} \frac{V_{mn} V_{nm}}{E_n^{(0)} - E_m^{(0)}}.$$

Similarly, we expand $\left|n^{(2)}\right\rangle$ in terms of the unperturbed eigenkets

$$\left|n^{(2)}\right\rangle = \sum_m c_m^{(2)} \left|m^{(0)}\right\rangle.$$

To calculate $c_m^{(2)}$, we apply $\left\langle m^{(0)}\right|$ from the left hand on both side of the Equation and obtain

$$\left\langle m^{(0)} \right| \left(H_0 - E_n^{(0)}\right) \left|n^{(2)}\right\rangle = \left\langle m^{(0)} \right| \left(E_n^{(1)} - V\right) \left|n^{(1)}\right\rangle + \left\langle m^{(0)} \right| E_n^{(2)} \left|n^{(0)}\right\rangle.$$

That is

$$c_m^{(2)} = \frac{1}{E_m^{(0)} - E_n^{(0)}} \left\{ \left\langle m^{(0)} \right| \left(E_n^{(1)} - V\right) \left|n^{(1)}\right\rangle + \left\langle m^{(0)} \right| E_n^{(2)} \left|n^{(0)}\right\rangle \right\}.$$

Summary

In short, the explicit expression for the energy expansion is

$$E_n = E_n^{(0)} + \lambda V_{nn} + \lambda^2 \sum_{m \neq n} \frac{V_{nm} V_{mn}}{E_n^{(0)} - E_m^{(0)}} + \cdots.$$

The expansion of the perturbed eigenket is as follows

$$\begin{aligned}
|n\rangle \quad = \quad & \left|n^{(0)}\right\rangle \\
& + \lambda \sum_{m \neq n} \frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}} \left|m^{(0)}\right\rangle \\
& + \lambda^2 \sum_{m \neq n} \sum_{l \neq n} \frac{V_{ml}}{E_m^{(0)} - E_n^{(0)}} \frac{V_{\mathrm{ln}}}{E_l^{(0)} - E_n^{(0)}} \left|m^{(0)}\right\rangle \\
& - \lambda^2 \sum_{l \neq n} \frac{V_{mn}}{E_l^{(0)} - E_n^{(0)}} \frac{V_{nn}}{E_l^{(0)} - E_n^{(0)}} \left|m^{(0)}\right\rangle \\
& + \cdots.
\end{aligned}$$

Remark 6 *The state ket $|n\rangle$ is not normalized. A normalized state ket should be*

$$\frac{1}{\langle n|n\rangle}|n\rangle$$

Example 1

Two-state problem

5.3 Application of the Perturbation Expansion

To illustrate the perturbation method we developed in the last lecture, let us look at several examples. All examples can be solved analytically. We can compare the perturbation results with the exact results.

5.3.1 Simple harmonic oscillator

The first two examples concern a simple harmonic oscillator whose unperturbed Hamiltonian is the usual one

$$H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2.$$

As we already know the Hamiltonian can be solved in this way

$$H_0 = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$$

where

$$a^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(x - i\frac{p}{m\omega}\right)$$

$$a = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(x + i\frac{p}{m\omega}\right)$$

with the eigenvalues

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right).$$

Example 2

$V_0 = \frac{\varepsilon}{2}m\omega^2x^2$

This problem can be solved exact in this way:

$$H = H_0 + V_0$$

$$= \frac{p^2}{2m} + \frac{1}{2}m(1+\varepsilon)\omega^2x^2.$$

The eigenvalues are

$$E_n = \hbar(1+\varepsilon)^{1/2}\omega\left(n + \frac{1}{2}\right).$$

In the perturbation approach, we just concern the ground state energy.

The first order perturbation is

$$E_1 = \langle 0|\, V_0\, |0\rangle = \varepsilon\,\langle 0|\,\frac{1}{2}m\omega^2x^2\,|0\rangle = \frac{\varepsilon}{4}\hbar\omega$$

The second order perturbation is

$$E_2 = \sum_{k\neq 0}\frac{|\langle k|\, V_0\, |0\rangle|^2}{E_0 - E_k} = \frac{|\langle 2|\, V_0\, |0\rangle|^2}{E_0 - E_2} = -\frac{\varepsilon^2}{16}\hbar\omega$$

Thus the perturbation correction to the ground state energy is

$$\triangle E = \hbar\omega\left(\frac{\varepsilon}{4} - \frac{\varepsilon^2}{16} + 0(\varepsilon^3)\right).$$

Compare it with the exact result

Example 3

$V_0 = \lambda x$

This problem can also be solved exactly:

$$\begin{aligned} H &= H_0 + V_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \lambda x \\ &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2(x - x_0)^2 - \frac{1}{2}m\omega^2 x_0^2 \end{aligned}$$

where

$$x_0 = -\frac{\lambda}{m\omega^2}.$$

Making a replacement, $y = x - x_0$ and $\partial_x = \partial_y$, we have

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dy^2} + \frac{1}{2}m\omega^2 y^2 - \frac{1}{2}m\omega^2 x_0^2.$$

The eigenvalues are

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) - \frac{\lambda^2}{2m\omega^2}.$$

The first order perturbation is

$$E_1 = \langle 0| V_0 |0\rangle = 0$$

The second order perturbation is

$$\begin{aligned} E_2 &= \sum_{k\neq 0} \frac{|\langle k| V_0 |0\rangle|^2}{E_0 - E_k} \\ &= \frac{|\langle 1| V_0 |0\rangle|^2}{E_0 - E_1} \\ &= -\frac{\lambda^2}{2m\omega^2}. \end{aligned}$$

5.3.2 Atomic hydrogen

The Schrodinger equation for a hydrogen atom is

$$(-\frac{\hbar^2}{2\mu}\nabla^2 - \frac{Ze^2}{r})\Phi = E\Phi$$

In the spherical coordinates,

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}.$$

The wave function can be written as

$$\Phi = R(r)Y_{lm}(\theta,\phi)$$

where $Y_{lm}(\theta,\phi)$ is a spherical harmonic. (See Schiff, P.76 or Sakurai, P. 454). It is the eigenfunction for orbital angular momentum operators

$$L^2Y_{lm}(\theta,\phi) = l(l+1)\hbar^2Y_{lm}(\theta,\phi)$$

$$L^zY_{lm}(\theta,\phi) = m\hbar Y_{lm}(\theta,\phi)$$

The Schrodinger equation is reduced to

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{l(l+1)}{r^2}\right) - \frac{Ze^2}{r}\right]R = ER.$$

The solution of this equation is

$$E_n = -\frac{\mu Z^2e^4}{2\hbar^2n^2} = -\frac{Z^2e^2}{2a_0n^2}$$

where $n = n' + l + 1$ and $a_0 = \hbar^2/\mu e^2$. The first three radial functions are

$$R_{10} = \left(\frac{Z}{a_0}\right)^{3/2} 2e^{-Zr/a_0}$$

$$R_{20} = \left(\frac{Z}{2a_0}\right)^{3/2}\left(2 - \frac{Zr}{a_0}\right)e^{-Zr/2a_0}$$

$$R_{21} = \left(\frac{Z}{6a_0}\right)^{3/2}\frac{Zr}{a_0}e^{-Zr/2a_0}$$

Degeneracy

$n = 1$: the ground state is nondegenerate

$n = 2$: the first excited state is four-fold degenerate. (1) $l = 0$ and $m = 0$; (2) $l = 1$ and $m = -1$

Example 4

Gravitational energy shift

Let consider an ordinary hydrogen atom (proton + electron) whose unperturbed Hamiltonian is

$$H_0 = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{Ze^2}{r}$$

where $\mu = m_e M_p/(m_e + M_p)$ is the reduced mass. Now the proton and electron interact not only through the electrostatic potential, but also by means of the gravational interaction. The perturbation due to the gravitational force is

$$V = -G\frac{m_e M_p}{r}$$

where G is the gravitational constant. The ground state wave function of atomic hydrogen is

$$\Phi = R_{10}(r)Y_{00}(\theta, \phi)$$

where

$$Y_{00}(\theta, \phi) = \left(\frac{1}{4\pi}\right)^{1/2}$$

To first order in the perturbation theory, the energy shift of the ground

state of atomic hydrogen due to this perturbation is

$$\begin{aligned} E_1^{(1)} &= \langle 0| V_0 |0\rangle \\ &= \int d\mathbf{r} \left|Y_{00}(\theta,\phi)R_{10}(r)\right|^2 V(r) \\ &= \int_0^{\pi} d\theta \sin\theta \int_0^{2\pi} d\phi \int_0^{\infty} dr r^2 \left|Y_{00}(\theta,\phi)R_{10}(r)\right|^2 V(r) \\ &= \int_0^{\infty} dr r^2 \frac{4}{a_0^3} e^{-r/a_0} \left(-G\frac{m_e M_p}{r}\right) = -G\frac{m_e M_p}{a_0} \end{aligned}$$

The ground state energy is

$$E_1^{(0)} = -\frac{e^2}{2a_0}.$$

The relative energy shift is

$$\frac{E_1^{(1)}}{E_1^{(0)}} = \frac{2Gm_e M_p}{e^2} \approx 8.7 \times 10^{-40}.$$

Needless to say, it is not necessary to calculate higher order correction in the present case.

5.4 Stationary Perturbation Theory: Degenerate Case

Until now we have assumed that the perturbed state differs slightly from an unperturbed bound state. The perturbation method for a nondegenerate case we developed fails when the unperturbed state are degenerate.

5.4.1 Revisited two-state problem

Starting from the two-state Hamiltonian

$$H = \begin{pmatrix} E_1^{(0)} & \lambda V_{12} \\ \lambda V_{21} & E_2^{(0)} \end{pmatrix},$$

we consider the special case of $E_1^{(0)} = E_2^{(0)}$, that is, the two states are energy degenerate. In fact, this problem can be solved exactly; the energy eigenvalues are,

$$E_1 = E_1^{(0)} + \lambda (V_{12} V_{21})^{\frac{1}{2}}; \tag{5.9}$$

$$E_2 = E_1^{(0)} - \lambda (V_{12} V_{21})^{\frac{1}{2}}. \tag{5.10}$$

However we cannot get this result by using the nondegenerate perturbation theory. A blind application of the nondegenerate perturbation formula obviously runs into difficulty because

$$E_1 = E_1^{(0)} + \frac{\lambda^2 V_{12} V_{21}}{E_1^{(0)} - E_2^{(0)}} + \cdots;$$

$$E_2 = E_2^{(0)} - \frac{\lambda^2 V_{12} V_{21}}{E_1^{(0)} - E_2^{(0)}} + \cdots.$$

become singular if V_{12} is nonvanishing and $E_1^{(0)} = E_2^{(0)}$. So we must modify the method of the nondegenerate case to accommodate such a situation. One way to avoid the catastrophe is to choose our base kets in such a way that λV has no off-diagonal matrix element. In the two-state case, we choose a new base ket

$$\left| \tilde{n}^{(0)} \right\rangle = a_n \left| 1^{(0)} \right\rangle + b_n \left| 2^{(0)} \right\rangle$$

the transformed perturbation becomes

$$\lambda \tilde{V} = \lambda \begin{pmatrix} (V_{12} V_{21})^{1/2} & 0 \\ 0 & -(V_{12} V_{21})^{1/2} \end{pmatrix}.$$

The solution to the coefficients a_n and b_n are

$$\begin{aligned} \frac{b_1}{a_1} &= \frac{(V_{12}V_{21})^{1/2}}{V_{21}}; \\ \frac{b_2}{a_2} &= -\frac{(V_{12}V_{21})^{1/2}}{V_{12}} \end{aligned}$$

and the state should be normalized

$$|a_n|^2 + |b_n|^2 = 1.$$

The transformation matrix is

$$U = \begin{pmatrix} a_1 & b_1 \\ a_2 & b_2 \end{pmatrix}.$$

In this way the degeneracy of the perturbed state is removed. We can consider the perturbation correction according to the nondegenerate perturbation theory. Note that we choose the perturbation potential is diagonal when the unperturbed state is degenerate. The following problem is left as an exercise:

$$V = \begin{pmatrix} \lambda V_{11} & \lambda V_{12} \\ \lambda V_{21} & \lambda V_{22} \end{pmatrix}$$

as a perturbation to a two-fold degenerate state.

5.4.2 The basic procedure of degenerate perturbation theory

We see from the two-state example that the degeneracy can be removed by choosing a new set of base kets. Here we present a more detailed approach. Suppose now that there are two states, $|n\rangle$ and $|m\rangle$, that have the same unperturbed energy. Then we cannot apply the nondegenerate perturbation formula when $E_m = E_n$ unless it happens that $V_{mn} = 0$. We

first consider the case in which $V_{mn} \neq 0$. the initial state is not specified by its unperturbed energy; the state may be $|n\rangle$ or $|m\rangle$ or any linear combination of them. Let us suppose that the perturbation V removes the degeneracy in some order, so that for finite λ there are two states that have different energy. We start from the perturbation equations in the last lecture

$$\left(H_0 - E_n^{(0)}\right)\left|n^{(0)}\right\rangle = 0 \tag{5.11}$$

$$\left(H_0 - E_n^{(0)}\right)\left|n^{(1)}\right\rangle = (E_n^{(1)} - V)\left|n^{(0)}\right\rangle. \tag{5.12}$$

Out of infinite number of combinations of the two states we choose the particular pair which depends on V. From the Eq.(5.11), we obtain

$$|\alpha\rangle = c_m\left|m^{(0)}\right\rangle + c_n\left|n^{(0)}\right\rangle;$$

$$E_\alpha^{(0)} = E_m^{(0)} = E_n^{(0)}.$$

Substitute the combined state into the Eq.(5.12) and take the inner product of this equation successively with $\left|n^{(0)}\right\rangle$ and $\left|m^{(0)}\right\rangle$, we obtain

$$\left(V_{mm} - E_\alpha^{(1)}\right)c_m + V_{mn}c_n = 0$$

$$\left(V_{nn} - E_\alpha^{(1)}\right)c_n + V_{nm}c_m = 0.$$

The two solutions of this equation are

$$E_\alpha^{(1)} = \frac{1}{2}(V_{mm} + V_{nn}) \pm \frac{1}{2}\left[(V_{mm} - V_{nn})^2 + 4\left|V_{mn}\right|^2\right]^{1/2}$$

These two solutions are equal if and only if

$$V_{mm} = V_{nn}$$

$$V_{mn} = 0.$$

In this case we say the degeneracy is not removed in the first order perturbation and we have to consider the second order perturbation. On the other hand if either or both of two equations are not satisfied, the two valued of $E_\alpha^{(1)}$ are distinct, and each can be used to calculate c_m and c_n. In this case, we can use the nondegenerate perturbation theory to determine the higher order perturbation. The coefficients $c_l^{(1)}$ are determined by

$$c_l^{(1)}(E_l^{(0)} - E_m^{(0)}) = -V_{lm}c_m - V_{\ln}c_l$$

for $l \neq m, n$ if we assume that $c_m^{(1)} = c_n^{(1)} = 0$.

How to solve triplet degenerate problem**?**

The basic procedure of the degenerate perturbation theory:

(1) Identify degenerate unperturbed eigenkets and construct the perturbation matrix V, a $g \times g$ matrix if the degeneracy is g-fold.

(2) Diagonalization the perturbation matrix by solving, as usual, the appropriate secular equation.

(3) Identify the roots of secular equation with the first-order energy shifts; the base kets that diagonalize the V matrix are the correct zero-order kets to which the perturbed kets approach in the limit $\lambda \to 0$;

(4) For higher orders use the formulas of the corresponding nondegenerate perturbation theory except in the summations, where we exclude all contributions from the unperturbed kets in the degenerate subspace.

5.4.3 Example: Zeeman Effect

The change in the energy levels of an atom caused by a uniform external magnetic field is called the Zeeman effect. We now consider the change of first order in the field strength for

a hydrogen atom

A constant magnetic field can be represented by the vector potential

$$\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r}$$

since $\mathbf{B} = \bigtriangledown \times \mathbf{A}$. The energy related to the vector potential is

$$\begin{aligned} \triangle H &= -\frac{ie\hbar}{\mu c}\mathbf{A} \cdot \bigtriangledown + \frac{e^2}{2\mu c}\mathbf{A}^2 \\ &= \frac{e}{2\mu c}\mathbf{B} \cdot \mathbf{L} + \frac{e^2}{8\mu c^2}B^2 r^2 \sin^2\theta \end{aligned}$$

where $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, θ is the angle between $\mathbf{r}$ and $\mathbf{H}$, and e is a positive quantity. Since we wish to work only to the first order in $\mathbf{B}$ we can put

$$V = \frac{e}{2\mu c}\mathbf{B} \cdot \mathbf{L}.$$

The energy eigenfunctions of the unperturbed hydrogen atom are usually chosen to be eigenstates of L_z with the eigenvalues $m\hbar$. We choose the magnetic field is in the z-direction, then the first order perturbation is

$$E_1^{(0)} = \langle m| V |m\rangle = \frac{e}{2\mu c}Bm\hbar.$$

So the degeneracy of the $2l + 1$ states is removed in first order.

(1). s-wave: $l = 0$, and $m = 0$;

(2). p-wave: $l = 1$, and $m = -1$, 0, and 1.

5.4.4 Example: First Order Stark Effect in Hydrogen

The change in the energy levels of an atom cause by a uniform external electric field of strength E is called *the Stark effect*. The perturbation V is now the extra energy of the

nucleus and electron in the external field and is ready shown to be

$$V = eEr\cos\theta$$

where the polar axis and **E** are in the direction of positive z and e is again a positive quantity. In a hydrogen atom the Coulomb potential is rotationally invariant. The wave function for any spherically symmetric ponetial energy, when expressed in spherical harmonics, have even or odd parity according as the azimuthal quantum number l is even or odd. Since the perturbation is odd parity with respect to inversion, the ground state has even parity and has no first-order Stark effect. The first excited state ($n = 2$) of hydrogen is four fold degenerate; the quantum numbers l and m have the value $(0,0)$, $(1,-1)$, $(1,0)$, $(1,1)$. Since the perturbation V commutes with the z-component of angular momentum,

$$[L_z, V] = 0,$$

we obtain

$$(m_i - m_k)\left\langle l, m_i\right| V \left|l', m_k\right\rangle = 0.$$

The nonvanishing matrix elements of V are

$$\begin{aligned} V_1 &= \langle 1,0|\, V\, |0,0\rangle = \langle 0,0|\, V\, |1,0\rangle \\ &= eE\int d\mathbf{r} u^*_{210}(\mathbf{r}) r\cos\theta u_{200}(\ \mathbf{r}) \\ &= \frac{eE}{16a_0^4}\int_{-1}^{+1}\cos^2\theta d\cos\theta\int_0^\infty dr(2-\frac{r}{a_0})e^{-r/a0} \\ &= -3eEa_0. \end{aligned}$$

The first order energy correction is determined by the secular equation

$$\begin{vmatrix} -E_1 & V_1 & 0 & 0 \\ V_1 & -E_1 & 0 & 0 \\ 0 & 0 & -E_1 & 0 \\ 0 & 0 & 0 & -E_1 \end{vmatrix} = 0.$$

The four roots of the secular equation are

$$E_1 = \begin{cases} -|V_1| \\ 0 \\ 0 \\ +|V_1| \end{cases},$$

so that half of the four fold degeneracy is removed in the first order.

5.5 The Wentzel-Kramers-Brillouin (WKB) approximation

5.6 Time-dependent Problem: Interacting Picture and Two-State Problem

When the Hamiltonian depends on the time, there are no stationary solution of the Schrödinger equation. Thus our identification of a bound state with a discrete energy level and stationary eigenket must be modified.

5.6.1 Time-dependent Potential and Interacting Picture

We consider a Hamiltonian H such that is can be split into two parts,

$$H = H_0 + V(t),$$

where H_0 does not contain time explicitly. The problem of H_0 or $V(t) = 0$ is assumed to be solved completely, i.e.,

$$H_0 \left|n\right\rangle = E_n \left|n\right\rangle .$$

Assume $V(t) = 0$ at $t = 0$. the state ket is given by

$$\left|\alpha\right\rangle = \sum_n c_n(0) \left|n\right\rangle .$$

In the system of H_0, the state ket at a later time will evolve into

$$\left|\alpha\right\rangle = \sum_n c_n(0) e^{-iE_n t/\hbar} \left|n\right\rangle .$$

Our question is how the state ket of H (not H_0) changes as time goes on.

Now we must work with the time-dependent Schrodinger equation

$$i\hbar \frac{\partial}{\partial t} \left|\alpha(t)\right\rangle = \left(H_0 + V(t)\right) \left|\alpha(t)\right\rangle . \tag{5.13}$$

Our procedure consists in expressing

$$\left|\alpha(t)\right\rangle = \sum_n c_n(t) e^{-iE_n t/\hbar} \left|n\right\rangle . \tag{5.14}$$

Substituting Eq. (5.14) into Eq. (5.13), we obtain

$$i\hbar \frac{\partial}{\partial t} c_k = \sum_n \left\langle k\right| V \left|n\right\rangle c_n e^{iE_{kn} t/\hbar} \tag{5.15}$$

where the Bohr frequency is defined as

$$\omega_{kn} = \frac{E_k - E_n}{\hbar}.$$

This equation is exactly equivalent to the original problem.

Interaction picture

Two kinds of changes have been made in going from Eq. (5.13). First, we have changed the representation from specified in terms of the coordinates to being specified in terms of the unperturbed energy eigenvalues. Second, we have changed from the Schrodinger to the interaction picture.

$$\begin{aligned} \langle k| V_I |n\rangle &= \langle k| e^{iH_{0S}t/\hbar} V_S e^{-iH_{0S}t/\hbar} |n\rangle \\ &= \langle k| V_S |n\rangle e^{-iE_{kn}t/\hbar}. \end{aligned}$$

5.6.2 Time-dependent Two-State Problem

Exact soluble problem of time-dependent potential are rather rare. However, a two state problem with sinusoidal oscillating potential can be solved exactly.

The Problem is defined by

$$\begin{aligned} H_0 &= E_1 |1\rangle\langle 1| + E_2 |2\rangle\langle 2| \ \ (E_2 > E_1) \\ V(t) &= \gamma e^{i\omega t} |1\rangle\langle 2| + \gamma e^{-i\omega t} |2\rangle\langle 1|. \end{aligned}$$

In the interaction picture, the Eq. (5.15) can be written as

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = \begin{pmatrix} 0 & \gamma e^{i\triangle\omega t} \\ \gamma e^{-i\triangle\omega t} & 0 \end{pmatrix} \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix}$$

The equation is reduced to

$$i\hbar \frac{\partial}{\partial t} c_1(t) = \gamma e^{i\triangle\omega t} c_2(t) \tag{5.16}$$

$$i\hbar \frac{\partial}{\partial t} c_2(t) = \gamma e^{-i\triangle\omega t} c_1(t) \tag{5.17}$$

where $\triangle\omega = \omega + E_1 - E_2$.

How to solve this equation?

From Eq. (5.16) we have

$$c_2(t) = (\gamma e^{i\triangle\omega t})^{-1} i\hbar \frac{\partial}{\partial t} c_1(t)$$

Substituting c_2 into Eq.(5.17),

$$i\hbar \frac{\partial}{\partial t}\left[(\gamma e^{i\triangle\omega t})^{-1} i\hbar \frac{\partial}{\partial t} c_1(t)\right] = \gamma e^{-i\triangle\omega t} c_1(t)$$

$$-\frac{\partial^2}{\partial t^2} c_1 + i\Delta\omega \frac{\partial}{\partial t} c_1 = \frac{\gamma^2}{\hbar^2} c_1$$

Assume $c_1 = c\exp[i\lambda t]$, we have

$$\lambda^2 - \Delta\omega\lambda = \gamma^2/\hbar^2;$$

$$\lambda = \frac{1}{2}\left(\Delta\omega \pm \sqrt{\Delta\omega^2 + \gamma^2/\hbar^2}\right)$$

So the general solutions are

$$c_1 = \alpha_+ e^{\frac{i}{2}(\triangle\omega + \omega_R)t} + \alpha_- e^{\frac{i}{2}(\triangle\omega - \omega_R)t}$$

$$c_2 = -\frac{\hbar}{2\gamma}(\triangle\omega + \omega_R)\alpha_+ e^{-\frac{i}{2}(\triangle\omega - \omega_R)t} - \frac{\hbar}{2\gamma}(\triangle\omega - \omega_R)\alpha_- e^{-\frac{i}{2}(\triangle\omega + \omega_R)t}$$

α are two coefficients and determined by the initial conditions and

$$\omega_R = \left[\frac{4\gamma^2}{\hbar^2} + (\omega + \omega_{12})^2\right]^{1/2}.$$

If initially, at t=0, only the lower is populated so that

$$c_1(0) = 1, \text{ and } c_2(0) = 0$$

then the probability for being found in each of the two states is given by

$$|c_2(t)|^2 = \frac{\gamma^2}{\gamma^2 + (\omega + \omega_{12})^2\hbar^2/4} \times \sin^2\left(\frac{1}{2}\omega_R t\right),$$

$$|c_1(t)|^2 = 1 - |c_2(t)|^2$$

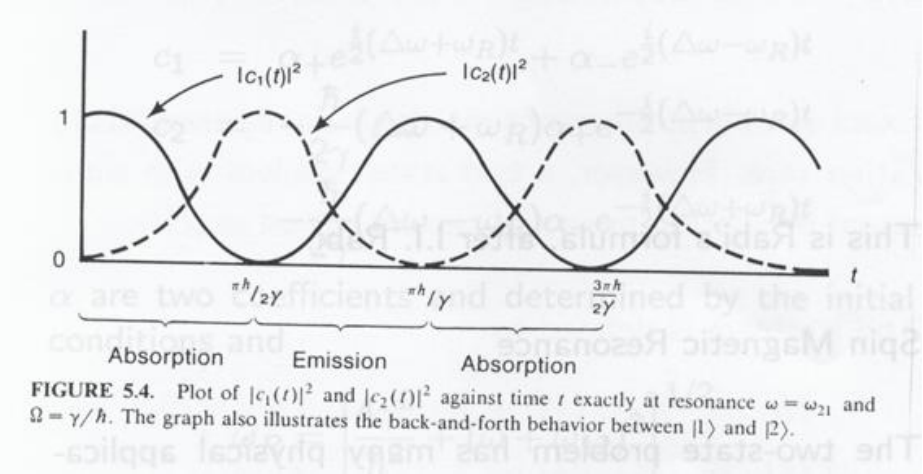


FIGURE 5.4. Plot of $|c_1(t)|^2$ and $|c_2(t)|^2$ against time t exactly at resonance $\omega = \omega_{21}$ and $\Omega = \gamma/\hbar$. The graph also illustrates the back-and-forth behavior between $|1\rangle$ and $|2\rangle$.

Figure 5.1:

This is Rabi's formula, after I.I. Rabi.

Spin Magnetic Resonance

The two-state problem has many physical applications: Spin magnetic resonance, maser etc. Consider a spin 1/2 system subjected to a t-independent uniform magnetic field in the z-direction and, in addition, a t-dependent magnetic field rotating in the xy plane.

$$B = B_0\hat{z} + B_1(\hat{x}\cos\omega t + \hat{y}\sin\omega t)$$

with B_0 and B_1 constant.

We treat the effect of the uniform t-independent field as H_0 and the effect of the rotating field as $V(t)$.

$$\begin{aligned} H0 &= -\frac{e\hbar B_0}{2m_e c}\left(|+\rangle\langle+| - |-\rangle\langle-|\right) \\ V(t) &= -\frac{e\hbar B_1}{2m_e c}\left[\cos\omega t\left(|+\rangle\langle-| + |-\rangle\langle+|\right) + \sin\omega t\left(-i\,|+\rangle\langle-| + i\,|-\rangle\langle+|\right)\right] \end{aligned}$$

Four Nobel Prize winners who took advantage of resonance in two-level systems

- Rabi (1944): on molecular beams and nuclear magnetic resonance;

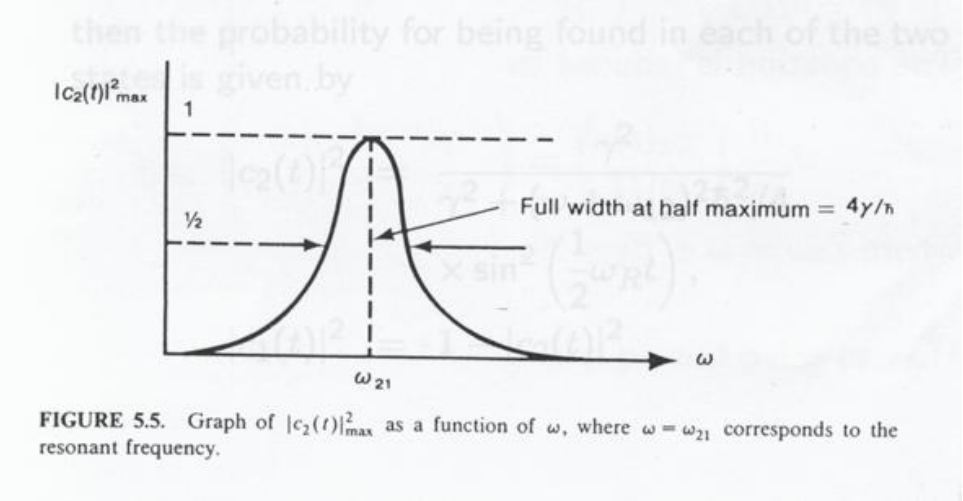


FIGURE 5.5. Graph of $|c_2(t)|^2_{max}$ as a function of ω, where $\omega = \omega_{21}$ corresponds to the resonant frequency.

Figure 5.2:

- Bloch and Purcell (1952): on B field in atomic nuclei and nuclear magnetic moments;
- Townes, Basov, and Prochorov (1964): on masers, lasers, and quantum optics;
- Kastler (1966): on optical pumping

5.7 Time-dependent Perturbation Problem

5.7.1 Perturbation Theory

We now return to Eq. (5.3), replace V by λV, and express the c_n as the power series in λ

$$c_n = c_n^{(0)} + \lambda c_n^{(1)} + \lambda^2 c_n^{(2)} + \cdots .$$

The substitution yields the set of equations

$$\begin{aligned} \frac{\partial}{\partial t} c_n^{(0)} &= 0 \\ i\hbar \frac{\partial}{\partial t} c_n^{(s+1)} &= \sum_k \langle n| V |k\rangle \, c_k^{(s)} e^{+iE_{nk}t/\hbar}. \end{aligned}$$

The zero-order coefficient are constant in time. We shall assume that all except one of the $c_n^{(0)}$, say $n = m$, are zero, so that the system is initially in a definite unperturbed energy state. Thus the solutions to the zero order coefficients are

$$c_n^{(0)} = \langle n|m\rangle = \delta_{mn}.$$

Integration of the first-order equation gives

$$c_n^{(1)} = (i\hbar)^{-1} \int_{-\infty}^{t} \langle n| V(t) |m\rangle e^{iE_{nm}t/\hbar} dt \tag{5.18}$$

The integral constant has been chosen in such a way that $c_n^{(1)}$ vanish at $t = t_0$. To first order in the perturbation, the transition probability corresponding to the transition $m \to n$, (*that is, the probability that the system, initially in the state m, be found at time t in the state* $m \neq n$) is therefore

$$P_{mn} = \left|c_n^{(1)}\right|^2, \;\; n \neq m.$$

It is also worth noting that for $t > t_0$ the coefficient c_m of the state m is given to first order in the perturbation by

$$\begin{aligned} c_m(t) &\approx c_m^{(0)}(t) + c_m^{(1)}(t) \\ &\approx 1 + (i\hbar)^{-1} \int_{-\infty}^{t} \langle m| V(t) |m\rangle \, dt \\ &\approx \exp\left[-\frac{i}{\hbar} \int_{-\infty}^{t} \langle m| V(t) |m\rangle \, dt\right] \end{aligned}$$

So the principal effect of the perturbation on the initial state is to change the phase.

5.7.2 Time-independent perturbation

The result take particular simple form if the perturbation V is independent of time, except for being switched on suddenly at a given time. We then obtain

$$\begin{aligned} c_m^{(1)} &= -\frac{i}{\hbar}\langle m|\, V\, |m\rangle\, t \\ c_n^{(1)} &= \frac{\langle n|\, V\, |m\rangle}{\hbar}\frac{1-e^{iE_{nm}t/\hbar}}{E_{nm}} \end{aligned}$$

Hence

$$c_m e^{-iE_m t/\hbar}\, |m\rangle \approx e^{(E_m+V_{mm})t/\hbar}\, |m\rangle$$

This is in agreement with the result using the stationary perturbation theory. the first order transition probability from m to n is given by

$$P_{mn}^{(1)} = 2\left(\frac{\langle n|\, V\, |m\rangle}{\hbar}\right)^2 \left(\frac{\sin\left(E_{mn}t/2\right)}{E_{nm}}\right)^2$$

It is worth noting that this is valid for nondegenerate case.

5.7.3 Harmonic perturbation

Eq. (5.18) takes a particularly simple form if the perturbation V depends on harmonically on the time except for being turned on at one time and off at a latter time. We shall call these two times 0 and t_0, respectively, and assume that we can write

$$\langle k|\, V(t)\, |m\rangle = \langle k|\, V\, |m\rangle \sin\omega t$$

where $\langle k|\, V\, |m\rangle$ is time independent. The first order amplitude at any time t at or after t_0

$$c_n^{(1)} = -\frac{\langle n|\, V\, |m\rangle}{i\hbar}\left(\frac{e^{i(\omega_{nm}+\omega)t_0}-1}{\omega_{nm}+\omega} - \frac{e^{i(\omega_{nm}-\omega)t_0}-1}{\omega_{nm}-\omega}\right)$$

The structure of Eq. (**??**) suggests that the amplitude is appreciable only when the denominator of one or the other of the two terms is particularly zero. The first term is important

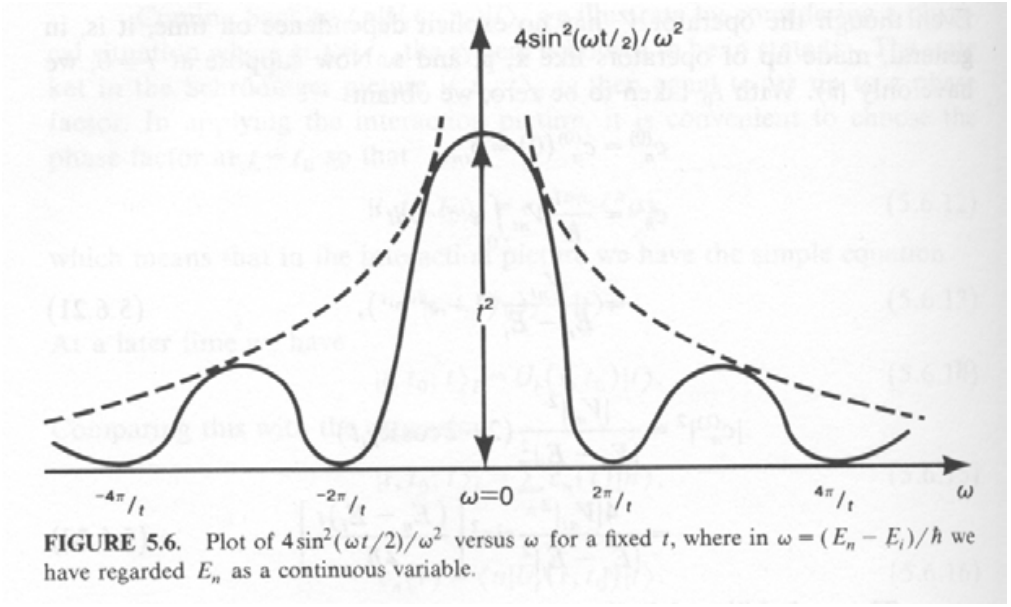


FIGURE 5.6. Plot of $4\sin^2(\omega t/2)/\omega^2$ versus ω for a fixed t, where in $\omega = (E_n - E_i)/\hbar$ we have regarded E_n as a continuous variable.

Figure 5.3:

when $\omega \approx -\omega_{nm}$ and the second term is important when $\omega \approx -\omega_{nm}$. For the present, we specialize to a situation in which the initial state m is a discrete bound state and the final state n is one of a continuous set of dissociated states. The first order probability of finding the system in the state $|n\rangle$ after the perturbation is removed is

$$\left|c_n^{(1)}(t > t_0)\right|^2 = \frac{4\left|\langle n|\, V\, |m\rangle\right|^2}{\hbar^2} \times \frac{\sin^2\left[(\omega_{nm} - \omega)\, t_0/2\right]}{(\omega_{nm} - \omega)^2}. \tag{5.19}$$

5.7.4 The Golden Rule

The factor $\sin^2\left[(\omega_{nm} - \omega)\, t_0/2\right] / (\omega_{nm} - \omega)^2$ is plotted in Figure. the height of the main peak increases in proportional to t_0^2. Thus if there is a group of states $|n\rangle$ that have energy nearly equal to $En+\hbar\omega$, and for which $|\langle n|\, V\, |m\rangle|$ is roughly independent of n, the probability of finding a system in one or another of these states is proportional to t_0.

The transition probability per unit time is given by integrating Eq. (5.19) over

n and dividing by t_0

$$w = \frac{1}{t_0} \int \left| c_n^{(1)}(t > t_0) \right|^2 \rho(n) dE_n$$

where $\rho(n)dE_n$ is the number of final states with energies between E_n and $E_n + dE_n$. the concept of an energy density $\rho(n)$ of final state is sensible, since we are considering the case in which the transition is to one or another of a continuous set of dissociated states. We now take advantage of the fact that the breadth of the main peak in Sinc$x$ becomes small as t_0 becomes large, and we regard $|\langle n| V |m\rangle|$ and $\rho(n)$ as quantities sufficiently independent of En so that they can be taken outside in the integral. The probability is approximately written as

$$w = \frac{2\pi}{\hbar} \rho(n) \left| \langle n| V |m\rangle \right|^2$$

where we have made use of the result

$$\int_{-\infty}^{+\infty} \frac{\sin^2 x}{x^2} dx = \pi.$$

This formula, first obtained by P. A. Dirac, was later dubbed by E. Fermi "The Golden Rule" of perturbation theory.

Chapter 6

Collision Theory

Problems for which the energy eigenvalues are continuously distributed usually arise in connection with the collision of a particle with a force field. In a collision problem the energy is specified in advance, the behavior of the wave function at great distance is found in terms of it. This asymptotic behaviors can then be related to the amount of scattering of the particle by the force. There are so few systems of physical interest for which exact solutions can be found that approximation methods play an important part in applications of the theory. Various methods that are useful in scattering problems are considered in this chapter.

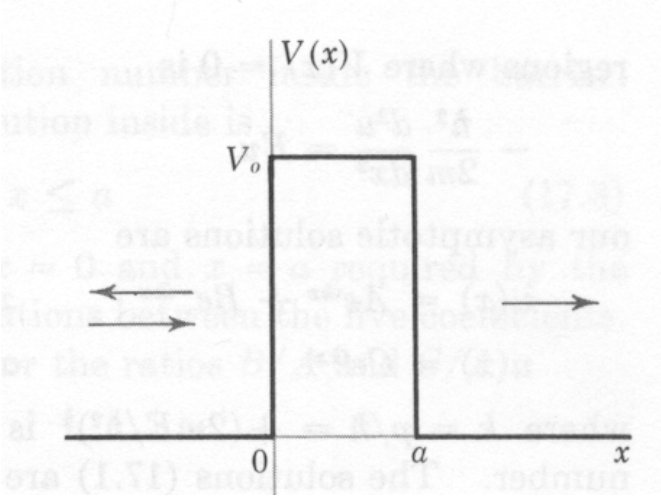


Figure 6.1:

6.1 Collisions in one- and three-dimensions

6.1.1 One-dimensional square potential barriers

We consider first the one-dimensional collision of a particle with the square potential barrier. In this problem we are interested in a particle that approaches from the region of negative x and is reflected or transmitted by the carrier. In the corresponding classical problem, the particle is always reflected if its energy is less than that of the top of the barrier, and it is always transmitted if the energy is great. We shall see that, in the quantum problem, both reflection and transmission occur with finite probability for most energies of the particle.

Asymptotic behaviors

We are interested in representing a particle that approaches from the left with energy $E > 0$ and may be turned back by the potential barrier or penetrate through it. Thus the asymptotic behavior in the region where $V(x) = 0$ is as follows: for $x < 0$ we want the wave function to represent a particle moving to the left (reflected particle) as well as to the right (incident particle): for $x > a$, we want the wave function to represent only a

particle moving to the right (transmitted particle).

The wave function in the region where $V(x) = 0$ is

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}u = Eu.$$

Our asymptotic solution are

$$\begin{aligned} u(x) &= Ae^{ikx} + Be^{-ikx}, \quad x < 0 \\ u(x) &= Ce^{ikx}, \qquad\quad x > a \end{aligned}$$

where

$$k = p/\hbar = \left(\frac{2mE}{\hbar^2}\right)^{1/2}$$

Normalization

Recall the definition of the possibility current density

$$J = \frac{\hbar}{2im}\left[\Psi^*\nabla\Psi - (\nabla\Psi^*)\,\Psi\right].$$

The possibility current densities at $x < 0$ and $x > a$ are

$$\begin{aligned} J(x) &= \frac{\hbar k}{m}\left(|A|^2 - |B|^2\right),\ x < 0 \\ J(x) &= \frac{\hbar k}{m}|C|^2,\ x > a. \end{aligned}$$

The two currents are independent of the position and should be equal due to the conversation of the practice.

Scattering coefficients

The character of the solution inside the potential barrier depends on whether E is greater or less than the potential barrier V_0.

The case $E > V_0$

The solution in the potential barrier is

$$u(x) = Fe^{i\alpha x} + Ge^{-i\alpha x}, \;\; 0 < x < a$$

where

$$\alpha = \left(\frac{2m\,(E - V_0)}{\hbar^2} \right)^{1/2}.$$

The continuity of u and $\partial u/\partial x$ at $x = 0$ and $x = a$ required by the boundary condition provides four relations between the five coefficients. At $x = 0$,

$$\begin{aligned} A + B &= F + G \\ k(A - B) &= \alpha(F - G) \end{aligned}$$

At $x = a$,

$$\begin{aligned} Fe^{i\alpha a} + Ge^{-i\alpha a} &= Ce^{ika} \\ \alpha\left(Fe^{i\alpha a} + Ge^{-i\alpha a}\right) &= kCe^{ika} \end{aligned}$$

We can eliminate F and G and solve for the ratios B/A and C/A.

$$\begin{aligned} \frac{B}{A} &= \frac{\left(k^2 - \alpha^2\right)\left(1 - e^{2i\alpha a}\right)}{(k+\alpha)^2 - (k-\alpha)^2 e^{2i\alpha a}} \\ \frac{C}{A} &= \frac{4k\alpha\left(1 - e^{i(\alpha - k)a}\right)}{(k+\alpha)^2 - (k-\alpha)^2 e^{2i\alpha a}} \end{aligned}$$

The reflection coefficient is

$$\left|\frac{B}{A}\right|^2 = \left[1 + \frac{4E(E - V_0)}{V_0^2 \sin^2 \alpha a}\right]^{-1}.$$

The transmission coefficient is

$$\left|\frac{C}{A}\right|^2 = \left[1 + \frac{V_0^2 \sin^2 \alpha a}{4E(E - V_0)}\right]^{-1}.$$

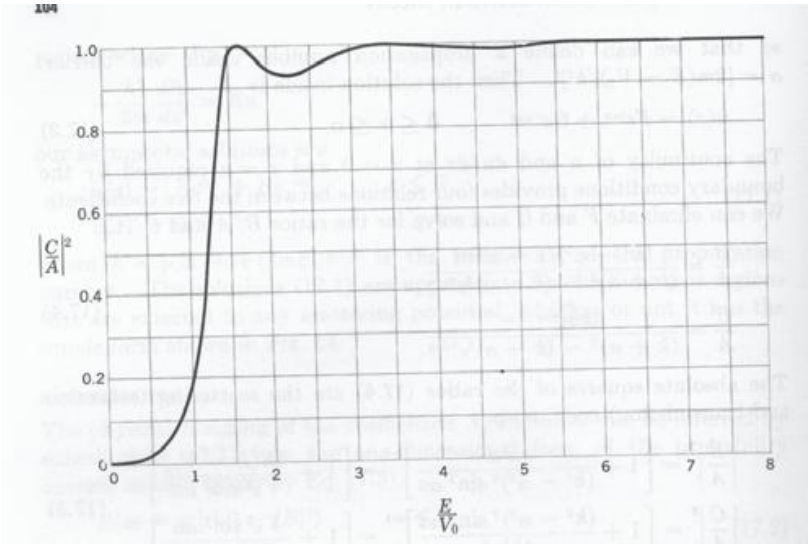


Figure 6.2: The transmission coefficient of a square barrier.

The case $E < V_0$

The reflection and transmission coefficients for $0 < E < V_0$ are obtained by replace α by $i\beta$ in the wave function in the potential barrier.

$$\beta = \left(\frac{2m\,(V_0 - E)}{\hbar^2}\right)^{1/2}.$$

The reflection coefficient is

$$\left|\frac{B}{A}\right|^2 = \left[1 + \frac{4E(V_0 - E)}{V_0^2 \sinh^2 \alpha a}\right]^{-1}.$$

The transmission coefficient is

$$\left|\frac{C}{A}\right|^2 = \left[1 + \frac{V_0^2 \sinh^2 \alpha a}{4E(V_0 - E)}\right]^{-1}.$$

6.2 Collision in three dimensions

Scattering cross section

The angular distribution of particles scattered by a fixed center of force or by other particles is conveniently described in terms of a *scattering cross section.* Suppose that we bombard a group of n particles or scattering centers with a parallel flux of N particles per unit time and count the number of incident particles that emerge per unit time in a small solid angle $\triangle\omega_0$ centered about a direction that has polar angles θ_0 and ϕ_0 with respect to the bombarding direction as polar axis. This number will be proportional to N, n and $\triangle\omega_0$ provided that the flux is small enough so that there is no interference between bombarded particles and no appreciable diminution of the bombarded particles by their recoil out of the target region, and provided also that the bombarded particles are far enough apart so that each collision process involves only one of them.

The different scattering cross section $\sigma_0(\theta_0,\phi_0)$: the number of incident particles that emerge per unit time in $\triangle\omega_0$ can be written

$$nN\sigma_0(\theta_0,\phi_0)\triangle\omega_0.$$

The total scattering cross section:

$$\sigma_0 = \int \sigma_0(\theta_0,\phi_0)d\omega_0.$$

For a collision of a particle with a fixed scattering center, the definition of the differential scattering cross section is equally valid in the laboratory and center-of-mass coordinate systems, since a scattering center that is fixed has an infinite effective mass and so that the center of mass of the system does not move. For a collision between two particles of finite mass, however, the differential cross section applies in general only to the laboratory coordinate system and to the observation of the scattered incident particle. It does not describe in the observation of the recoil bombarded particle in the laboratory system, although it is of course possible to obtain a differential cross section for the recoil particle from $\sigma_0(\theta_0,\phi_0)$.

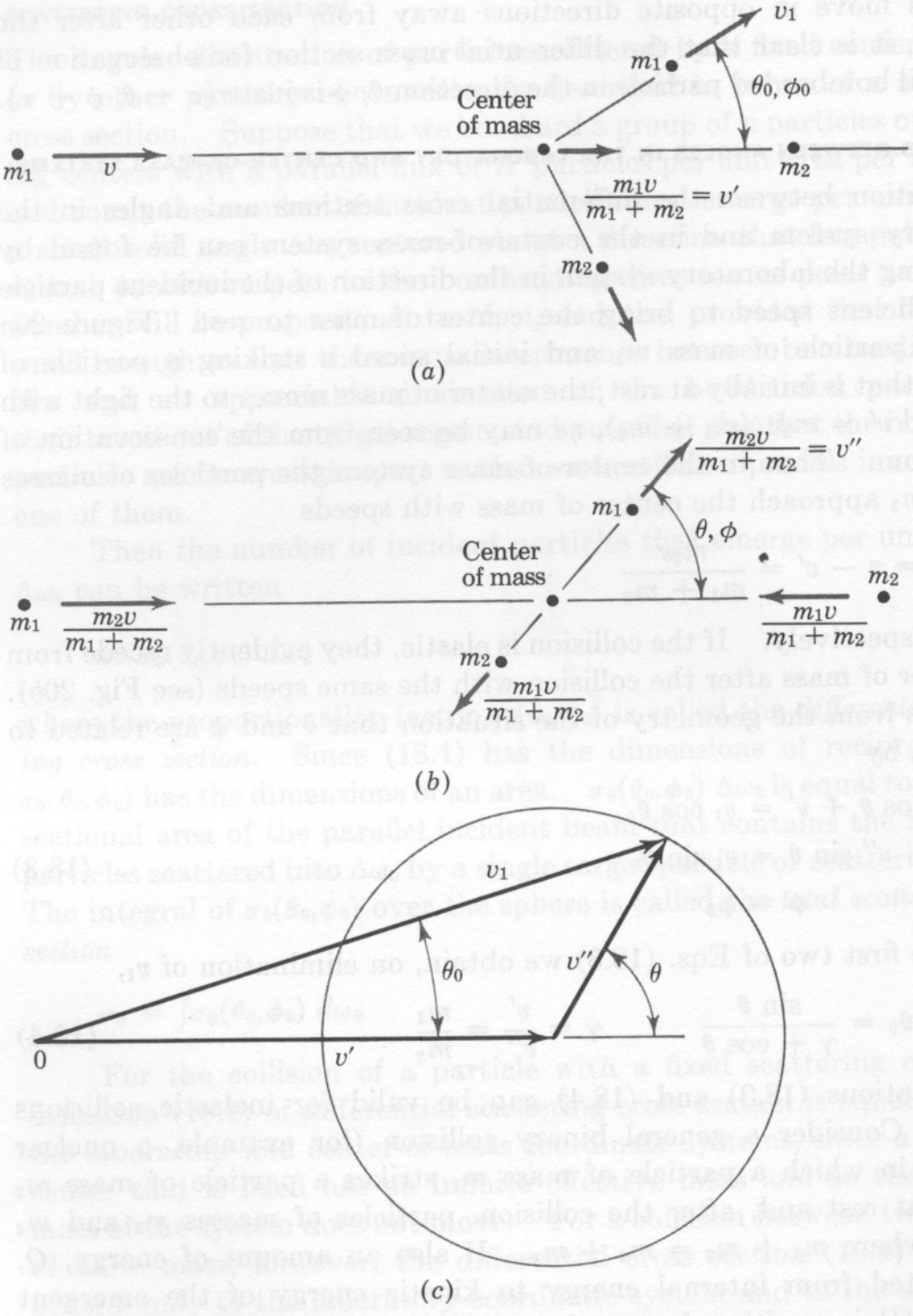


Fig. 20 (*a*) Laboratory coordinate system, in which the target particle of mass m_2 is initially at rest. (*b*) Center-of-mass coordinate system, in which the center of mass is initially and always at rest. (*c*) Vector addition of velocity of center of mass in laboratory system ($\mathbf{v}'$) to velocity of observed particle in center-of-mass system ($\mathbf{v}''$) to give velocity observed in laboratory system ($\mathbf{v}_1$); if $v'' < v'$, θ_0 cannot exceed the angle $\sin^{-1}(v''/v')$.

Figure 6.3:

Relation between angles in the laboratory and center-of-mass systems

the relation between the differential cross section and angles in the laboratory system and in the center-of-mass system can be found by translating the laboratory system in the direction of the incident particle with sufficient speed to bring the center of mass to rest. Assume that a particle of mass m_1 and initial speed v strikes a particle of mass m_2 that is initially at rest. The center of mass moves with the speed

$$v' = \frac{m_1}{m_1 + m_2} v.$$

Thus in the center-of-mass system the speeds of two particles are $v'' = v - v'$ and v'. If the collision is elastic, they evidently recede from the center of mass after the collision with the same speed. Thus θ_0,ϕ_0 and θ,ϕ are related by

$$\begin{aligned} v'' \cos\theta + v' &= v_1 \cos\theta_0 \\ v'' \sin\theta &= v_1 \sin\theta_0 \\ \phi &= \phi_0 \end{aligned}$$

From these Eqs., we obtain

$$\begin{aligned} \tan\theta_0 &= \frac{\sin\theta}{\gamma + \cos\theta} \\ \gamma &= \frac{v'}{v''} = \frac{m_1}{m_2} \end{aligned}$$

Relation between cross sections

The relation between the cross section in the laboratory and center-of-mass coordinate systems can be obtained from the definitions, which imply that the same number of particles are scattered into differential solid angle $d\omega_0$ about θ_0, ϕ_0 as are scattered into

$d\omega$ about θ, ϕ.

$$\sigma_0(\theta_0, \phi_0) \sin\theta_0 d\theta_0 d\phi_0 = \sigma(\theta, \phi) \sin\theta d\theta d\phi.$$

With the help of the relation θ_0, ϕ_0 and θ, ϕ, we obtain

$$\sigma_0(\theta_0, \phi_0) = \frac{\left(1 + \gamma^2 + 2\gamma\cos\theta\right)^{1/2}}{|1 + \gamma\cos\theta|}\sigma(\theta, \phi).$$

It should be noted that the total cross section is the same for both laboratory and center-of-mass systems and also for both the outgoing particles, since the total number of collision that takes place is independent of the mode of description of the process.

Dependence on γ

For $\gamma < 1$, θ_0 increase from 0 to π as θ increase from 0 to π. For $\gamma = 1$, $\theta_0 = \theta/2$ and varies from 0 to $\pi/2$ as θ varies from 0 to π; in this case

$$\sigma_0(\theta_0, \phi_0) = 4\cos\theta_0 \sigma(2\theta_0, \phi_0)$$

and no particle appear in the backward hemisphere in the laboratory system. For $\gamma > 1$, θ_0 first increase from 0 to a maximum value $\cos^{-1}(-1/\gamma)$, which is less than $\pi/2$, as θ increases from 0 to $\cos^{-1}$(-1/γ); θ_0 then decreases to 0 as θ increases further to π. In this case $\sigma_0(\theta_0, \phi_0)$ is usually infinite at the maximum value of θ_0, although this singularity gives a finite contribution to the total cross section; no particles appear beyond the maximum θ_0 in the laboratory system.

6.3 Scattering by Spherically Symmetric Potentials

In this section, we assume that the potential V is a function only of r, and we find the connection between the solution separated in spherical polar coordinate and the asymptotic

form.

Asymptotic behaviors

The differential scattering cross section in the center-of-mass coordinate system can be found from

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + V\right)u = Eu$$

where $\mu = m_1 m_2/(m_1 + m_2)$. The scattering is determined by the asymptotic form of u in the region where $V = 0$

$$u = A[e^{ikz} + \frac{1}{r}f(\theta,\phi)e^{ikr}] \tag{6.1}$$

where $k = \mu v/\hbar$ and v is the speed of the incident particle. The probability current density J is given by

$$\mathbf{J}(r) = \frac{\hbar}{2\mu i}\left[\Psi^\dagger\left(\nabla\Psi\right) - \left(\nabla\Psi^\dagger\right)\Psi\right]$$

The gradient operator can be expressed in polar coordinates as

$$\nabla = \frac{\partial}{\partial r}\hat{\mathbf{r}} + \frac{1}{r}\frac{\partial}{\partial\theta}\hat{\boldsymbol{\theta}} + \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\hat{\boldsymbol{\phi}}.$$

Since the second and third terms are small when r is large, the current for large r is in the radial direction and

$$J_r = \frac{\hbar k}{\mu}\left|f(\theta,\phi)\right|^2/r^2$$

The number of scattered particles entering the solid angle (or detector) per unit time is

$$\begin{aligned} N d\omega &= J_r r^2 d\omega \\ &= \frac{\hbar k}{\mu}\left|f(\theta,\phi)\right|^2 d\omega. \end{aligned}$$

From the definition of the cross section, it follows

$$\sigma(\theta,\phi) = \left|f(\theta,\phi)\right|^2.$$

Differential cross section

The asymptotic behavior of the wave function determines the differential scattering cross section but cannot itself be found without solving the wave equation throughout all space. In the spherical polar coordinate,

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial^2\phi}\right]u=(E-V)u.$$

The radial and angular parts of the solution can be separated by taking

$$u(r,\theta,\phi)=R(r)Y_{lm}(\theta,\phi)$$

where

$$Y_{lm}(\theta,\phi)=N_{lm}P_l^m(\cos\theta)e^{im\phi}$$

is the spherical harmonic. The problem now possesses symmetry about the polar axis, so that u, f, and σ are independent of the angle ϕ. That is, we just consider the case of $m=0$. In the case the $\mathrm{P}_l^{m=0}$ is reduced to the Legendre polynomials. Thus, the general solution can then be written as a sum of products of radial function and Legendre polynomials,

$$\begin{aligned} u &= \sum_{l=0}^{\infty}(2l+1)i^l R_l(r)P_l(\cos\theta) \\ &= \sum_{l=0}^{\infty}(2l+1)i^l r^{-1}\chi_l(r)P_l(\cos\theta) \end{aligned}$$

where P_l is the Legendre polynomial of order l, and χ_l satisfies

$$\frac{d^2\chi_l}{d^2r}+\left[k^2-U(r)-\frac{l(l+1)}{r^2}\right]\chi_l=0$$

where

$$\begin{aligned} k &= \left(\frac{2\mu E}{\hbar^2}\right)^{1/2} \\ U(r) &= \frac{2\mu V(r)}{\hbar^2}\to 0,\ \text{as } r\to+\infty \end{aligned}$$

In the limit of r$\rightarrow +\infty$, the solution χ_l is one of the form

$$\chi_l \propto e^{\pm ikr} \rightarrow A_l \sin(kr + \delta_l')$$

In some specialized problem, U(r) can be neglected for r greater than some distance a, and a may be small enough so that the l term in not negligible. The general form for $R_l(r)$ has the form

$$\begin{aligned} R_l(r) &= e^{i\delta_l} \left[\cos\delta_l j_l\left(kr\right) - \sin\delta_l n_l(kr)\right] \\ &\longrightarrow \frac{e^{i\delta_l}}{kr}\sin(kr - \frac{l}{2}\pi + \delta_l),\ r \rightarrow \infty. \end{aligned} \tag{6.2}$$

Here j_l is the special Bessel function;

$$\begin{aligned} j_l(\rho) &= \left(\frac{\pi}{2\rho}\right)^{1/2} J_{l+1/2}(\rho) \\ &\rightarrow \frac{1}{\rho}\cos(\rho - \frac{l+1}{2}\pi),\ \rho \rightarrow \infty \\ &\rightarrow \frac{\rho^l}{(2l+1)!!},\ \rho \rightarrow 0 \end{aligned}$$

n_l is the special Neumann function;

$$\begin{aligned} n_l(\rho) &= (-1)^{l+1}\left(\frac{\pi}{2\rho}\right)^{1/2} J_{-l-1/2}(\rho) \\ &\rightarrow \frac{1}{\rho}\sin(\rho - \frac{l+1}{2}\pi),\ \rho \rightarrow \infty \\ &\rightarrow -\frac{(2l-1)!!}{\rho^{l+1}},\ \rho \rightarrow 0. \end{aligned}$$

To identify the form of f, we require an expansion of $e^{ikr\cos\theta}$ in Legendre polynomials;

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty}(2l+1)i^l j_l(kr)P_l(\cos\theta).$$

Comparison of Eq.(6.1) with the general form $R_l(r)$ gives

$$\begin{aligned} & e^{ikz} + r^{-1} f(\theta, \phi) e^{ikr} \\ = & \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos\theta) + r^{-1} f(\theta, \phi) e^{ikr} \\ = & \sum_{l=0}^{\infty} (2l+1) i^l A_l (kr)^{-1} \sin(kr - \frac{l\pi}{2} + \delta_l) P_l(\cos\theta). \end{aligned}$$

A_l are the coefficient for different l, and should take the form

$$A_l = e^{i\delta_l}.$$

Thus it gives

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)(e^{2i\delta_l} - 1) P_l(\cos\theta).$$

Thus the differential cross section is

$$\begin{aligned} \sigma(\theta) &= |f(\theta)|^2 \\ &= \frac{1}{k^2} \left| \sum_{l=0}^{\infty} (2l+1)(e^{2i\delta_l} - 1) P_l(\cos\theta) \right|^2 \end{aligned}$$

Total elastic cross section

The total elastic cross section is given by

$$\begin{aligned} \sigma &= 2\pi \int_0^{\pi} \sigma(\theta) \sin\theta d\theta \\ &= \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l. \end{aligned}$$

Here we make use of the orthogonality property of the Legendre polynomials

$$\int_{-1}^{+1} d\cos\theta P_l(\cos\theta) P_{l'}(\cos\theta) = \frac{2}{2l+1} \delta_{ll'}.$$

The total cross section can also be related to $f(0)$. it follows from the generating function for the Legendre polynomials that $P(l) = 1$ for all l, so that

$$f(0) = \frac{1}{i2k} \sum_{l=0}^{\infty} (2l+1) \left(e^{2i\delta_l} - 1 \right)$$

Comparison with the total cross section shows

$$\sigma = \frac{2\pi}{ik} \left[f(0) - f^*(0) \right] = \frac{4\pi}{k} \operatorname{Im} f(0).$$

This relation is known as the optical theorem.

The physical interpretation of the optical theorem is as follows: In order for scattering to take place, particles must be removed in an amount proportional to σ from the incident beam, so that its intensity is smaller behind the scattering region ($\theta \approx 0$) than in front of it. This can occur only by the interference between two terms in the asymptotic expression of the wave function.

Phase shifts

The angle δl is called the phase shift of the lth partial wave, since according to Eq.(6.2) it is the difference in phase between the asymptotic forms of the actual radial function $R_l(kr)$ and the radial function $j_l(kr)$ in the absence of the scattering potential. the phase shifts completely determine the scattering, and the scattering cross section vanishes when each of δ_l is 0^o or 180^o.

6.4 Applications

6.4.1 Scattering by a square well

In general, for a given potential, phase shifts are calculated from a numerical solution of the radial equations. In a few cases an analytical solution is possible, in particular for scattering

by an attractive square well, for which the reduced potential $U(r)$ is

$$U(r) = \begin{cases} -U_0(<0), & r < a; \\ 0, & r > a. \end{cases}$$

Inside the well ($r < a$) the radial equation is

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + K^2\right] R_l(Kr) = 0$$

where we set $K^2 = k^2 + U_0$. The regular solution of this equation is

$$R_l^I(Kr) = A_l j_l(Kr),\ r < a.$$

In the exterior region, the radial equation is

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2\right] R_l(kr) = 0$$

The general solution is

$$R_l^E(kr) = B_l\left[j_l(kr) - \tan\delta_l n_l(kr)\right],\ r > a. \tag{6.3}$$

The solutions for $r < a$ and $r > a$ can be joined smoothly at $r = a$ by requiring that

$$R_l^I(Ka) = R_l^E(ka);$$

$$\left.\frac{dR_l^I(Kr)}{dr}\right|_{r=a} = \left.\frac{dR_l^E(kr)}{dr}\right|_{r=a}$$

Eliminating the normalization constants gives

$$\tan\delta_l(k) = \frac{kj_l'(ka)j_l(Ka) - Kj_l(ka)j_l'(Ka)}{kn_l'(ka)j_l(Ka) - Kn_l(ka)j_l'(Ka)}.$$

At low energies, the scattering is dominated by the $l = 0$ wave. Using the formula

$$j_0(\rho) = \frac{\sin\rho}{\rho}$$

$$n_0(\rho) = -\frac{\cos\rho}{\rho}$$

we have

$$\tan\delta_0(k) = \frac{k\tan Ka - K\tan ka}{K + k\tan ka\tan Ka}.$$

In the low-energy limit, $ka \ll 1$,

$$\delta_0(k) = -ka\left(1 - \frac{\tan Ka}{Ka}\right)$$

Then the $l = 0$ partial cross section is

$$\begin{aligned}\sigma_{l=0} &= \frac{4\pi}{k^2}\sin^2\delta_0 \\ &\approx 4\pi a^2\left(1 - \frac{\tan Ka}{Ka}\right)^2\end{aligned}$$

6.4.2 Scattering by a hard-sphere potential

Another simple, but interesting example is the hard-sphere potential

$$U(r) = \begin{cases} +\infty, & r < a; \\ 0, & r > a. \end{cases}$$

Since the scattered particle cannot penetrate into the region $r < a$, the wave function in the exterior region must vanish at $r = a$. Since the scattered particle cannot penetrate into the region $r < a$, the wave function in the exterior region, given by Eq.(6.3), must vanish at $r = a$, from which

$$\tan\delta_l(k) = \frac{j_l(ka)}{n_l(ka)}.$$

In the low-energy limit, $ka \ll 1$,

$$\begin{aligned}\tan\delta_l(k) &= \frac{(ka)^l}{(2l+1)!!}\Big/\left[-\frac{(2l-1)!!}{(ka)^{l+1}}\right] \\ &= -\frac{(ka)^{2l+1}}{(2l+1)!!(2l-1)!!}\end{aligned}$$

Hence $|\tan\delta_l(k)|$ quickly decreases as l increases. As a result, the low-energy scattering is always dominated by the s-wave. Since $j_0(\rho) = \sin\rho/\rho$ and $n_0(\rho) = -\cos\rho/\rho$, we have

$$\delta_0 = -ka.$$

So the cross section is

$$\delta_0 = 4\pi a^2.$$

At high energies ($ka >> 0$), we find

$$\delta_l = \frac{l\pi}{2} - ka$$

so that

$$\begin{aligned} \delta_{tot} &\approx \frac{4\pi}{k^2}\sum_{l=0}^{l_{\max}}(2l+1)\sin^2(\frac{2\pi}{2} - ka) \\ &\approx 2\pi a^2. \end{aligned}$$

It is interesting to compare this result with that obtained from classical mechanics.

6.5 Approximate Collision Theory

See Sakurai's book: section 7.1, 7.2, and 7.3

6.5.1 The Lippman-Schwinger Equation

Let us begin with the time-independent formulation of scattering processes. The Hamiltonian is written as

$$H = H_0 + V = \frac{P^2}{2m} + V.$$

H_0 describes the particle is far away from the scattering center. We have two Schrodinger equations in the absence and presence of V:

$$H_0 |\phi\rangle = E |\phi\rangle$$

$$(H_0 + V) |\Psi\rangle = E |\Psi\rangle$$

When $V \to 0$, $|\Psi\rangle \to |\phi\rangle$. We assume the two equations have the same energy eigenvalue. Combining the two equations

$$(E - H_0) |\Psi\rangle = V |\Psi\rangle + (H_0 - E) |\phi\rangle$$

If $(E - H_0)^{-1}$ exist, we have

$$|\Psi\rangle = (E - H_0)^{-1} V |\Psi\rangle + |\phi\rangle$$

Unfortunately, the operator $(E - H_0)^{-1}$ is singular. To avoid the difficulty, we introduce an infinitesmal complex $i\varepsilon$ ($\varepsilon \to 0^+$) such that $E \to E + i\varepsilon$. In this way the equation becomes

$$\left|\Psi^{(+)}\right\rangle = |\phi\rangle + \frac{1}{E - H_0 + i\varepsilon} V \left|\Psi^{(+)}\right\rangle \tag{6.4}$$

In the position space, Eq.(6.4) is reduced to

$$\begin{aligned} \langle \mathbf{x} \left|\Psi^{(+)}\right\rangle &= \langle \mathbf{x} |\phi\rangle + \int d\mathbf{x}' \langle \mathbf{x}| \frac{1}{E - H_0 + i\varepsilon} |\mathbf{x}'\rangle \langle \mathbf{x}'| V \left|\Psi^{(+)}\right\rangle \\ &= \langle \mathbf{x} |\phi\rangle + \frac{2m}{\hbar^2} \int d\mathbf{x}' G(\mathbf{x}, \mathbf{x}') \langle \mathbf{x}'| V \left|\Psi^{(+)}\right\rangle \end{aligned}$$

We evaluate the kernel of integral $G(\mathbf{x}, \mathbf{x}')$.

$$\begin{aligned}
G(\mathbf{x}, \mathbf{x}') &= \frac{\hbar^2}{2m} \langle \mathbf{x} | \frac{1}{E - H_0 + i\varepsilon} | \mathbf{x}' \rangle \\
&= \frac{\hbar^2}{2m} \int d\mathbf{p} \langle \mathbf{x} | \mathbf{p} \rangle \langle \mathbf{p} | \frac{1}{E - H_0 + i\varepsilon} | \mathbf{p} \rangle \langle \mathbf{p} | \mathbf{x}' \rangle \\
&= \frac{\hbar^2}{2m} \int d\mathbf{p} \langle \mathbf{x} | \mathbf{p} \rangle \langle \mathbf{p} | \frac{1}{E - p^2/2m + i\varepsilon} | \mathbf{p} \rangle \langle \mathbf{p} | \mathbf{x}' \rangle \\
&= \frac{\hbar^2}{2m} \int d\mathbf{p} \langle \mathbf{x} | \mathbf{p} \rangle \frac{1}{E - p^2/2m + i\varepsilon} \langle \mathbf{p} | \mathbf{x}' \rangle \\
&= \frac{\hbar^2}{2m} \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \frac{\exp[i\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}')/\hbar]}{E - p^2/2m + i\varepsilon}
\end{aligned}$$

where we have used

$$\begin{aligned}
\langle \mathbf{x} | \mathbf{p} \rangle &= (2\pi\hbar)^{-3/2} \exp[i\mathbf{p} \cdot \mathbf{x}/\hbar] \\
\langle \mathbf{p} | \mathbf{x} \rangle &= (2\pi\hbar)^{-3/2} \exp[-i\mathbf{p} \cdot \mathbf{x}/\hbar].
\end{aligned}$$

Take $E = \hbar^2 k^2/2m$ and $p = \hbar q$,

$$\begin{aligned}
G(\mathbf{x}, \mathbf{x}') &= \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{\exp[i\mathbf{q} \cdot (\mathbf{x} - \mathbf{x}')]}{k^2 - q^2 + i\varepsilon} \\
&= \int \frac{dq q^2 d\phi \sin\theta d\theta}{(2\pi)^3} \frac{\exp[iq |\mathbf{x} - \mathbf{x}'| \cos\theta]}{k^2 - q^2 + i\varepsilon} \\
&= \frac{i}{4\pi^2 |\mathbf{x} - \mathbf{x}'|} \int_0^{+\infty} dq q \frac{\exp[iq |\mathbf{x} - \mathbf{x}'|] - \exp[-iq |\mathbf{x} - \mathbf{x}'|]}{k^2 - q^2 + i\varepsilon} \\
&= -\frac{1}{4\pi} \frac{\exp[ik |x - x'|]}{|x - x'|}
\end{aligned}$$

In the last step we used the residue theorem:

$$\begin{aligned}
\oint \frac{dz}{z - z_0} &= 2\pi i \\
\oint_c f(z) dz &= 2\pi i \sum a_{-1 z_i} = 2\pi i (\text{sum of enclosed residues}).
\end{aligned}$$

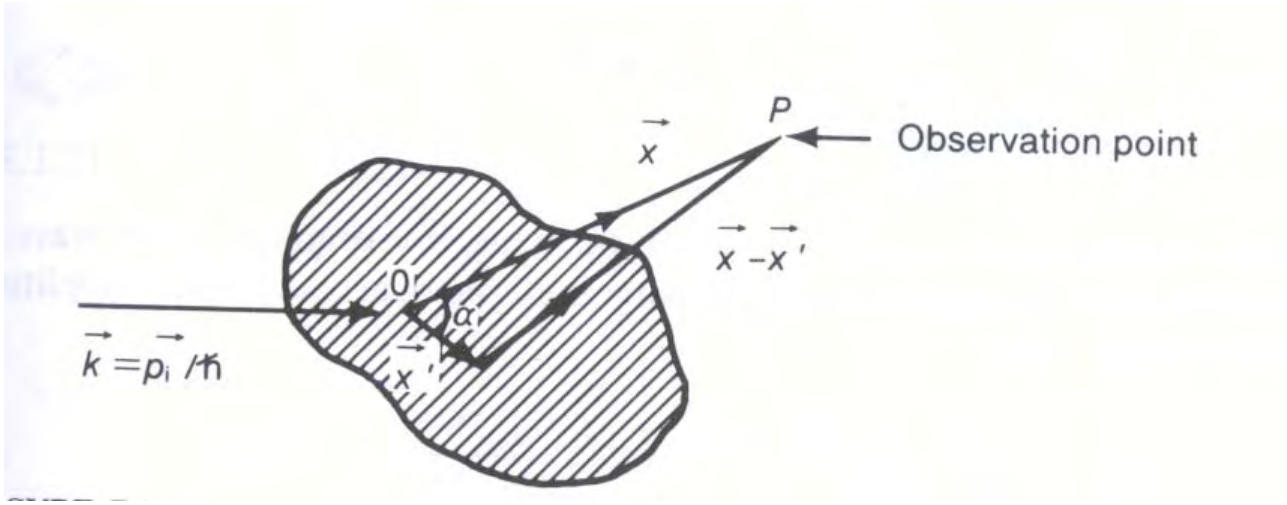


Figure 6.4:

The equation becomes

$$\langle \mathbf{x} \left| \Psi^{(+)} \right\rangle = \langle \mathbf{x} \left| \phi \right\rangle - \frac{2m}{\hbar^2} \int dx' \frac{e^{+ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|} \langle \mathbf{x}' | V \left| \Psi^{(+)} \right\rangle .$$

Assume that V is a local potential,

$$\langle \mathbf{x}' | V | \mathbf{x}'' \rangle = V(x')\delta(\mathbf{x}'-\mathbf{x}'')$$

$$\langle \mathbf{x} \left| \Psi^{(+)} \right\rangle = \langle \mathbf{x} \left| \phi \right\rangle - \frac{2m}{\hbar^2} \int dx' \frac{e^{+ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|} V(x') \langle \mathbf{x}' \left| \Psi^{(+)} \right\rangle .$$

As the observation point is far away from the scatterer,

$$|\mathbf{x}| = r \gg |\mathbf{x}'| = r'$$

$$|\mathbf{x}-\mathbf{x}'| = (r^2 - 2rr'\cos\alpha + r'^2)^{1/2}$$

$$= r(1 - \frac{r'}{r}\cos\alpha + ...)$$

From this approximation, we have

$$\frac{e^{+ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|} \approx \frac{e^{ikr}}{r} e^{-i\mathbf{k}\cdot\mathbf{r}'}.$$

So,

$$\langle \mathbf{x} \left| \Psi^{(+)} \right\rangle \rightarrow \langle \mathbf{x} \left| \phi \right\rangle - \frac{2m}{\hbar^2} \frac{e^{ikr}}{r} \int d\mathbf{x}\prime e^{-i\mathbf{k}\cdot\mathbf{r}'} V(x') \langle \mathbf{x}' \left| \Psi^{(+)} \right\rangle .$$

Comparing with the asymptotic form of the wave function,

$$\langle \mathbf{x} \left| \Psi^{(\pm)} \right\rangle \rightarrow \frac{1}{(2\pi)^{3/2}} \left[e^{i\mathbf{k}\bullet\mathbf{r}} + \frac{e^{ikr}}{r} f(\mathbf{k}', \mathbf{k}) \right]$$

We have

$$f(k', k) = -\frac{2m\pi}{\hbar^2} \int d\mathbf{x}' \frac{\exp[-ikx']}{(2\pi)^{3/2}} V(x') \langle \mathbf{x}' \left| \Psi^{(+)} \right\rangle$$

6.5.2 The Born Approximation

The formula contains the unknown wave function. We have to introduce the approximation.

$$\begin{aligned} \left| \Psi^{(+)} \right\rangle &= |\phi\rangle + \frac{1}{E - H_0 + i\varepsilon} V \left| \Psi^{(+)} \right\rangle \\ &= |\phi\rangle + \frac{1}{E - H_0 + i\varepsilon} V \left(|\phi\rangle + \frac{1}{E - H_0 + i\varepsilon} V \left| \Psi^{(+)} \right\rangle \right) \\ &= |\phi\rangle + \frac{1}{E - H_0 + i\varepsilon} V |\phi\rangle + ... \end{aligned}$$

Assume the effect of the scattering is not very strong, we replace $\langle \mathbf{x}' \left| \Psi^{(+)} \right\rangle$ by $\langle \mathbf{x}' \left| \phi \right\rangle$ in the integral,

$$\langle \mathbf{x}' \left| \Psi^{(+)} \right\rangle \rightarrow \langle \mathbf{x}' \left| \phi \right\rangle = \exp[-i\mathbf{k} \cdot \mathbf{x}'].$$

This is the first-order Born approximation. The amplitude is

$$f(k', k) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} \int d\mathbf{x}' e^{i(\mathbf{k}-\mathbf{k}')\bullet\mathbf{x}'} V(\mathbf{x}')$$

which is the Fourier transform of the potential except for a constant.

For a spherical symmetric potential, assume $\left| \mathbf{k} - \mathbf{k}' \right| = q = 2k \sin\theta/2$. ($k = k\prime$ as

the energy is conserved.)

$$\begin{aligned} f &= -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int_0^{2\pi} drr^2 \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta e^{iqr\cos\theta} V(r) \\ &= -\frac{2m}{\hbar^2 q}\int_0^{+\infty} drrV(r)\sin qr \end{aligned}$$

6.5.3 Application: from Yukawa potential to Coloumb potential

As an illustration of the Born approximation, we consider the Yukawa potential

$$U(r) = U_0 \frac{e^{-\mu r}}{\mu r}$$

$$f(\mathbf{k}', \mathbf{k}) = -\int drU(r)\frac{r\sin qr}{q} = -U_0 \frac{1}{q^2+\mu^2}$$

where

$$q = |\mathbf{k}' - \mathbf{k}|$$

$$\begin{aligned} \int drrV(r)\sin qr &= \frac{U_0}{\mu}\int_0^{+\infty} dre^{-\mu r}\sin qr \\ &= \frac{U_0}{\mu}\int_0^{+\infty} dre^{-\mu r}\frac{e^{iqr}-e^{-iqr}}{2i} \\ &= \frac{U_0}{i2\mu}\left(\frac{1}{\mu - iq} - \frac{1}{\mu + iq}\right) \\ &= \frac{U_0 q}{q^2+\mu^2}. \end{aligned}$$

So the differential cross section is

$$\sigma(\theta) = \left(\frac{2mU_0}{\mu\hbar}\right)^2 \frac{1}{[2k^2(1-\cos\theta)+\mu^2]}.$$

When $\alpha = 0$, the Yukawa potential is reduced to the Coloumb potential, $U_0/\mu \to ZZ'e^2$. We obtain

$$\begin{aligned}\sigma(\theta) &= \frac{\left(2mZZ'e^2\right)^2}{\hbar^4}\frac{1}{16k^4\sin^4\frac{\theta}{2}} \\ &= \left(\frac{ZZ'e^2}{E}\right)^2\frac{1}{16k^4\sin^4\frac{\theta}{2}}\end{aligned}$$

This is the Rutherford scattering cross section. From Rutherford formula we conclude that the charge-charge interaction in atomic scale obey Coulomb law, i.e., $1/r$.

6.5.4 Identical Particles and Scattering

Collisions between identical particles are particularly interesting as a direct illustration of the fundamental differences between classical and quantum mechanics.

Classical case

The differential cross-section is

$$\sigma(\theta,\sigma) = |f(\theta,\phi)|^2 + |f(\pi-\theta,\phi+\pi)|^2$$

Scattering of two identical spinless bosons

The differential cross-section is

$$\sigma(\theta,\sigma) = |f(\theta,\phi) + f(\pi-\theta,\phi+\pi)|^2$$

Scattering of two identical spin-1/2 fermions

The differential cross-section is

$$\begin{aligned}\sigma(\theta,\sigma) &= \frac{1}{4}|f(\theta,\phi) + f(\pi-\theta,\phi+\pi)|^2 \\ &\quad + \frac{3}{4}|f(\theta,\phi) - f(\pi-\theta,\phi+\pi)|^2\end{aligned}$$

6.6 Landau-Zener Problem

This two level problem can be introduced in this course.

Chapter 7

Selected Topics

7.1 Quantum Statistics

Quantum statistical mechanics is the branch of physics dealing with systems in mixed states; it is the quantum analogue of classical statistical mechanics. It should be noted that statistics enters at two levels in quantum statistical mechanics: first, because of the statistical interpretation of the wave function and second, because of our incomplete knowledge of dynamical state of the system.

7.1.1 Density Operator and Ensembles

Question: How to describe quantum mechanically an ensemble of physical systems for which, say ω_α =60 are characterized by $|\alpha\rangle$ and the remaining ω_β =40 are characterized by some other ket $|\beta\rangle$.

Example: a general state for S=1/2 system

$$|\alpha\rangle = c_+ |+\rangle + c_- |-\rangle$$

which characterizes a state ket whose spin is pointing some definite direction. We should not confuse the probability weight of the states $|+\rangle$ and $|-\rangle$, $\omega_\pm$, and $|c_\pm|^2$.

Ensemble average and density operator.

Pure ensemble: $|\alpha\rangle$

Mixed ensembles:

$$\begin{array}{cc} \omega_1 & \left|\alpha^{(1)}\right\rangle \\ \omega_2 & \left|\alpha^{(2)}\right\rangle \\ \omega_3 & \left|\alpha^{(3)}\right\rangle \\ \vdots & \vdots \end{array}$$

with the normalization condition

$$\sum_i \omega_i = 1.$$

The ensemble average

$$\begin{aligned} \langle A\rangle &= \sum_i \omega_i \langle\alpha_i |A| \alpha_i\rangle \\ &= \sum_i \omega_i \sum_n \langle\alpha_i | n\rangle \langle n| A| \alpha_i\rangle \\ &= \sum_{i,n} \omega_i |\langle n|\alpha_i\rangle|^2 a_n \end{aligned}$$

Alternatively,

$$\begin{aligned} \langle A\rangle &= \sum_{i,n} \omega_i \langle n|\alpha_i\rangle \langle\alpha_i|n\rangle \langle n |A| n\rangle \\ &= \sum_n \langle n| \sum_i \{\omega_i |\alpha_i\rangle \langle\alpha_i| A\} |n\rangle \\ &= Tr(\rho A) \end{aligned}$$

where

$$\rho = \sum_i \omega_i \left|\alpha_i\right\rangle \left\langle\alpha_i\right| .$$

ρ is the density matrix operator and is independent of representation.

Two properties:

(a). ρ is Hermitian;

(b). ρ satisfies the normalization condition.

$$Tr(\rho) = 1.$$

A pure ensemble: $\omega_n = 1$ for some $|\alpha_n\rangle$

$$\rho = \left|\alpha_n\right\rangle \left\langle\alpha_n\right|$$

which is just a projection operator.

Several examples of density operator:

(1) A completely polarized beam with S_z+

$$\begin{aligned} \rho &= \left|+\right\rangle \left\langle+\right| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \end{aligned}$$

(2) A completely polarized beam with S_x+

$$\begin{aligned} \rho &= \left|S_x, +\right\rangle \left\langle S_x, +\right| \\ &= \frac{1}{2^{1/2}} \left(\left|+\right\rangle + \left|-\right\rangle\right) \frac{1}{2^{1/2}} \left(\left\langle+\right| + \left\langle-\right|\right) \\ &= \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \end{aligned}$$

(3) A partially polarized beam with 75 S_z+ and 25 S_x+

$$\begin{aligned}\rho &= 0.75\,|+\rangle\langle+| + 0.25\,|S_x,+\rangle\langle S_x,+| \\ &= \frac{1}{8}\begin{pmatrix} 7 & 1 \\ 1 & 1 \end{pmatrix}\end{aligned}$$

7.1.2 Quantum Statistical Mechanism

Order and Disorder

The density matrix of a pure ensemble

$$\rho = \begin{pmatrix} 0 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 0 \end{pmatrix}$$

The density matrix of a completely random ensemble

$$\rho = \begin{pmatrix} \frac{1}{N} & & & & \\ & \frac{1}{N} & & & \\ & & \ddots & & \\ & & & \frac{1}{N} & \end{pmatrix}$$

We define a quantity

$$\begin{aligned}\sigma &= -tr\,(\rho \ln \rho) \\ &= -\sum_n \rho_{nn} \ln \rho_{nn}\end{aligned}$$

For a pure ensemble

$$\sigma = 0$$

For a completely random ensemble

$$\sigma = \ln N$$

This quantity is related to the entropy in thermodynamics,

$$S = ktr\,(\rho \ln \rho)$$

where k is the Boltzmann constant.

Basic assumption: Nature tends to maximize σ subject to the constraint that the ensemble average of the Hamiltonian has a certain value.

To minimize σ:

$$\delta\sigma = 0$$

i.e.,

$$\delta\rho_{nn}(\ln \rho_{nn} + 1) = 0$$

with the conditions

$$\text{(a).}\ \langle H \rangle = u = tr(\rho H)$$

$$\text{(b).}\ tr\rho = 1$$

we obtain

$$\delta\rho_{nn}\left[(\ln \rho_{nn} + 1) + \beta E_n + \gamma\right] = 0$$

$$\rho_{nn} = e^{-\beta E_k - \gamma}$$

$$= \frac{1}{\sum_n e^{-\beta E_n}} e^{-\beta E_k}$$

The partition function:

$$Z = \sum_n e^{-\beta E_n}$$

$$= tr(e^{-\beta H})$$

Thus the density matrix operator is

$$\rho = \frac{1}{Z} e^{-\beta H}$$

The parameter β is related to the temperature T as follows

$$\beta = 1/kT$$

Example: Spin-1/2 particle in a magnetic field

Consider a spin-1/2 particle having a magnetic momentum

$$\mu = -g\mu_B S/\hbar$$

subjected to a constant magnetic field along the z-axis.

$$H = g\mu_B \sigma_z/2 = \omega\sigma_z$$

The density operator

$$\begin{aligned} \rho &= \frac{1}{Z} e^{-\beta H} \\ &= \begin{pmatrix} \frac{1}{Z} e^{-\beta\omega} & 0 \\ 0 & \frac{1}{Z} e^{+\beta\omega} \end{pmatrix} \end{aligned}$$

where

$$Z = e^{-\beta\omega} + e^{\beta\omega}$$

The average value of the z-component of spin at the temperature T is

$$\begin{aligned} \langle S_z \rangle &= \frac{\hbar}{2} \frac{e^{-\beta\omega} - e^{\beta\omega}}{e^{-\beta\omega} + e^{\beta\omega}} \\ &= -\frac{\hbar}{2} \tanh(\beta\omega) \end{aligned}$$

7.1.3 Quantum Statistics

Consider a system with two identical particles. Each particle has three non-degenerate states: $|1\rangle$, $|2\rangle$, $|3\rangle$ with E_1, E_2, E_3 . For classical identical particles: there 9 possible configurations

$$|1,1\rangle \quad |1,2\rangle \quad |1,3\rangle$$

$$|2,1\rangle \quad |2,2\rangle \quad |2,3\rangle$$

$$|3,1\rangle \quad |3,2\rangle \quad |3,3\rangle$$

The wave function is

$$\Phi = \Phi_{E_i}(1)\Phi_{E_j}(2)$$

For bosons: there are 6 possible configurations

$$|1,1\rangle, \quad |2,2\rangle, \quad |3,3\rangle$$

$$\left(|1,2\rangle + |2,1\rangle\right)/2^{1/2}$$

$$\left(|1,3\rangle + |3,1\rangle\right)/2^{1/2}$$

$$\left(|3,2\rangle + |2,3\rangle\right)/2^{1/2}$$

The wave function

$$\Phi = \Phi_{E_i}(1)\Phi_{E_j}(2) + \Phi_{Ej}(1)\Phi_{E_i}(2)$$

For fermions: there are 3 possible configurations

$$\left(|1,2\rangle - |2,1\rangle\right)/2^{1/2}$$

$$\left(|1,3\rangle - |3,1\rangle\right)/2^{1/2}$$

$$\left(|3,2\rangle - |2,3\rangle\right)/2^{1/2}$$

The wave function

$$\Phi = \Phi_{E_i}(1)\Phi_{E_j}(2) - \Phi_{Ej}(1)\Phi_{E_i}(2)$$

7.1.4 Systems of non-interaction particles

We shall now discuss the properties of systems of large numbers of non-interacting objects which are equivalent and possess the same energy levels.

Maxwell-Boltzmann Statistics

(Classical identical particles)

If E_j (j=1, 2, $\cdots$) denotes an energy level of one of the particles, the total energy of the system E can be written

$$E = \sum_j n_j E_j$$

where the sum runs over all the eigenenergies of a single particle, and where n_j is the number of particles with the energy E_j. The total number of particles is

$$N = \sum_i n_j.$$

In a Maxwell-Boltzmann system, any number of particles can be in each level, so that nj can either be zero or any positive integer. If all the energies Ej are different, each permutation of the particles results in a different wave function, thus each energy level of the total system is N!-fold degenerate. However if nj>1, the interchange between these particles do not alter the wave function. Thus the number of distinct states corresponding to a given value of the total energy of the system is

$$g_E^{MB} = \frac{N!}{\prod_i n_i!}$$

The partition function can be expressed as

$$\begin{aligned} Z &= \sum_{\{n_j\}} g_E^{MB} \exp(-\beta \sum_j n_j E_j) \\ &= \sum_{\{n_j\}} \frac{N!}{\prod_i n_i!} \exp(-\beta \sum_j n_j E_j) \\ &= \left[\sum_j \exp(-\beta n_j E_j) \right]^2 \end{aligned}$$

The average distribution is

$$\begin{aligned} \langle n_i \rangle &= \frac{1}{Z} \sum_{\{n_j\}} g_E^{MB} \exp(-\beta \sum_j n_j E_j) n_j \\ &= -\frac{\partial \ln Z}{\partial \beta E_i} \\ &= \frac{N}{Z} e^{-\beta E_i} = e^{-\beta E_i - \alpha} \end{aligned}$$

Bose-Einstein Statistics (for bosons)

The wave function of many bosons is symmetric and the energy level of the system is non-degenerate

$$g_E^{BE} = 1, \text{ for any } n_j$$

Here we use the grand canonical ensemble ($N \to +\infty$)

$$\langle n_i \rangle = \frac{1}{Z} \sum_{\{n_j\}} g_E^{BE} \exp(-\beta \sum_j n_j E_j - \alpha \sum_j n_j) n_j$$

where

$$\begin{aligned} Z &= \sum_{\{n_j\}} \exp(-\beta \sum_j n_j E_j - \alpha \sum_j n_j) \\ &= \prod_j \left(\sum_{\{n_j\}} \exp(-\beta n_j E_j - \alpha n_j) \right) \\ &= \prod_j (1 - \exp(-\beta E_j - \alpha))^{-1} \end{aligned}$$

In the case,

$$\begin{aligned} \langle n_j \rangle &= -\frac{\partial \ln Z}{\partial \beta E_i} \\ &= \frac{1}{\exp(\beta E_j + \alpha) - 1} \end{aligned}$$

Fermi-Dirac Statistics (for fermions)

The wave function of many bosons is antisymmetric, and the energy level of the system is non-degenerate

$$\begin{aligned} g_E^{FD} &= 1, \text{ for } n_j = 1 \text{ or } 0 \\ &= 0, \text{ otherwise.} \end{aligned}$$

Here we use the grand canonical ensemble ($N \to +\infty$)

$$\langle n_i \rangle = \frac{1}{Z} \sum_{\{n_j\}} g_E^{FD} \exp(-\beta \sum_j n_j E_j - \alpha \sum_j n_j) n_j$$

where

$$\begin{aligned} Z &= \sum_{\{n_j\}} g_E^{FD} \exp(-\beta \sum_j n_j E_j - \alpha \sum_j n_j) \\ &= \prod_j \left(\sum_{n_j=0}^{1} \exp(-\beta n_j E_j - \alpha n_j) \right) \\ &= \prod_j (1 + \exp(-\beta E_j - \alpha)) \end{aligned}$$

In the case,

$$\begin{aligned} \langle n_j \rangle &= -\frac{\partial \ln Z}{\partial \beta E_i} \\ &= \frac{1}{\exp(\beta E_j + \alpha) + 1} \end{aligned}$$

7.1.5 Bose-Einstein Condensation

One of the main features of boson system is that bosons tend to occupy the lowest energy state at low temperatures. At high temperatures, both distribution laws for bosons and for fermions become equal to that for the Maxwell-Boltzmann case approximately. The density of particles on a certain state always tends to be zero. For a boson system, as

$$\langle n_j \rangle = \frac{1}{\exp(\beta E_j + \alpha) - 1} \to +\infty$$

if both E and α are equal to zero, the density of the particle at E=0 can be nonzero in the high density limit at low temperatures.

Consider a non-interacting boson gas in a three-dimensional system. The spectrum of energy is

$$E = \frac{\hbar^2}{2m} k^2$$

The density of particle is

$$\rho = \rho_0 + \frac{1}{(2\pi)^3}\int dk^3 n(E)$$

where $\rho 0$ is the density of particles in the lowest energy state.

$$\frac{1}{(2\pi)^3}\int dk^3 n(E) = \int dE D(E) n(E)$$

where

$$D(E) = \frac{1}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}$$

This is the density of state at E.

$$\begin{aligned}\rho - \rho_0 &= \frac{1}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^{+\infty} dE \frac{E^{1/2}}{e^{\beta E+\alpha}-1} \\ &= \frac{1}{4\pi^2}\left(\frac{2mkT}{\hbar^2}\right)^{3/2} f_{1/2}(\alpha)\end{aligned}$$

where

$$f_{1/2}(\alpha) = \int_0^{+\infty} dx \frac{x^{1/2}}{e^{x+\alpha}-1}.$$

Since $\alpha \geq 0$, the largest possible values of $f_{1/2}(\alpha)$ occurs when $\alpha = 0$ and numerically

$$f_{1/2}(\alpha = 0) = 2.315.$$

It follows;; that at $T < T_0$ where

$$T_0 = \frac{\hbar^2}{2mk}\left(\frac{4\pi^2\rho}{2.315}\right)^{2/3}$$

the function $(\rho - \rho_0)/\rho$ becomes less than unit, and the system increasingly condensed into the lowest energy state.

Bose-Einstein condensation was predicted by Albert Einstein and Satyendra Nath Bose at 1924 to 25. It was first observed in Helium-4 liquid. Recent years it was observed in some systems with cooling atoms. It is one of the most active branches in condensed matter physics. If you are interested in the recent development in this field, please visit Web site:

http://www.aip.org/pt/webwatch/ww9703.html.

7.1.6 Free fermion gas

The free particle Schrodinger equation in three dimensions is

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial x^{z2}}\right)\Psi_k(r)=\epsilon_k\Psi_k(r)$$

If the particle are confined to a cube of edge L and we require the wave function to be periodic in x, y, z direction with L, i.e.,

$$\begin{aligned}\Psi_k(x+L,y,z) &= \Psi_k(x+L,y,z)\\ \Psi_k(x,y+L,z) &= \Psi_k(x,y+L,z)\\ \Psi_k(x,y,z+L) &= \Psi_k(x,y,z+L)\end{aligned}$$

the wave functions are

$$\Psi_k(r)=\frac{1}{(2\pi)^{3/2}}e^{ik\cdot r}$$

provided that the components of the wave vector k satisfies

$$k_{x,y,z}=0,\pm\frac{2\pi}{L},\pm\frac{4\pi}{L},\pm\frac{6\pi}{L},\cdots$$

Any component of k is of the form $2n\pi/L$, where n is a positive integer. The energy spectrum with n is

$$\epsilon_k=\frac{\hbar^2}{2m}\left(k_x^2+k_y^2+k_z^2\right)$$

As two indistinguishable fermions cannot have all their quantum numbers identical, each energy level (or state) can be occupied by at most one particle. Thus we start filling the energy level from that with the lowest energy (i.e., k=0 here) until all N particles are accommodated.

The occupied energy levels may be represented as points inside a sphere in the k-space. The energy at the surface of the sphere is the Fermi energy; the wave vectors at the Fermi surface have a magnitude k_F such that

$$\epsilon_F = \frac{\hbar^2}{2m} k_F^2.$$

The total number of energy levels inside the sphere is

$$N = \frac{1}{(2\pi/L)^3} \frac{4\pi}{3} k_F^3$$

Then

$$k_F = \left(6\pi^2 N/V\right)^{1/3}.$$

In short, a boson gas condensates into the lowest energy state, and a fermion gas forms a Fermi sphere in the k-space at absolute zero temperature.

7.2 Quantum Hall Effect

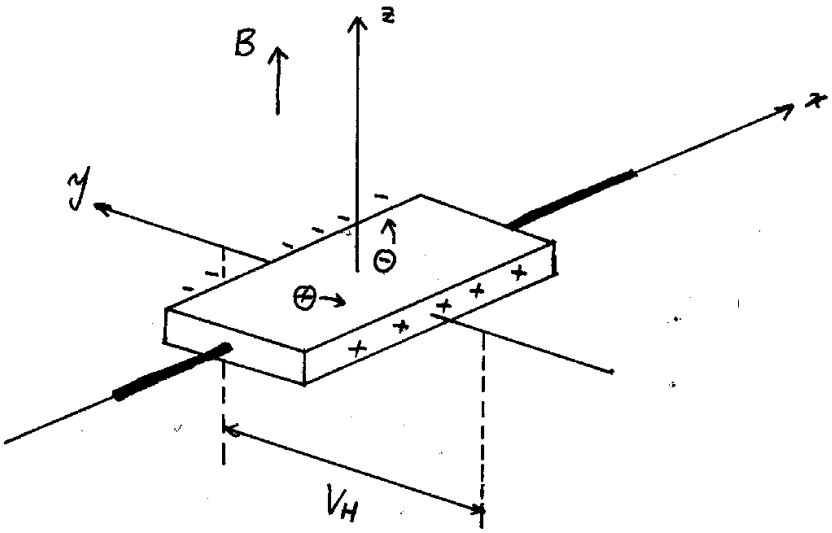
The quantum Hall effect is a remarkable phenomenon discovered experimentally in 1980s in which the Hall conductivity of a two-dimensional system of electrons is found to have plateaus as a function of variables which determine the number of electrons participating in the effect. The integer quantum Hall effect was observed by von Klitzing et al in 1980. Simple theory suggests that the Hall conductivity at he plateaus should be an integral multiple of $e^2/\hbar$ and the experiments agree with that prediction to within an accuracy of nearly 0.1 ppm. An application of great importance is to metrology, the quantum Hall effect promises a method of providing very precise resistance standards that are insensitive to the particular sample and the details of its fabrication. With a more powerful magnetic field and lower temperature, Daniel C. Tsui and Horst L. Stormer discovered that the plateaus

of the conductivity is a fractional multiples of the basic unit $e^2/\hbar$. Within a year of their discovery, Rovert B. Laughlin has succeeded in explaining their result. Through theoretical analysis he showed that the electrons in a powerful magnetic field can condense to form a kind of quantum fluid related to the quantum fluids that occur in superconductivity and in liquid helium.

What makes these fluids particularly important for researchers is that events in a drop of quantum fluid can afford more profound insights into the general inner structure and dynamics of matter. The Royal Swedish Academy of Sciences awarded The 1998 Nobel Prize in Physics jointly to Tsui, Stomer and Laughlin "for their discovery of a new form of quantum fluid with fractionally charged excitations."

7.2.1 Hall Effect

The Hall effect occurs when the charge carriers moving through a material experience a deflection because of an applied magnetic field. This deflection results in a measurable potential difference across the side of the material which is transverse to the magnetic field and current direction.



In Figure, a voltage V drives a current I in the positive X direction. Normal Ohmic resistance is V/I . A magnetic field tin the positive z direction shifts positive charge carriers in the negative y direction. This generates a Hall potential (V_H/I) in the y direction.

Quantitatively, Hall effect indicates that a transverse electric field will be produced. Charges will accumulate on the transverse edges until a strong enough electric field is developed to force remaining charges to continue undeflected. The condition is

$$E = \frac{V_d}{c} B.$$

The drift velocity is given by

$$V_d = J/n_e = \frac{i/A}{ne}$$

where n is the density of charge carrier. The electric field is

$$E = V_H/d$$

where l is the thickness of material and d the width. Hence we obtain an expression for the density of charge carriers in a substance

$$n = \frac{i}{eA} \cdot \frac{1}{v_d} = \frac{iB}{V_H lec}$$

Therefore this effect can be used to determine the density of charge carriers in conductors and semi-conductors, and has become a standard tool in physics laboratories over all the world. The Hall conductivity

$$\begin{aligned} \sigma &= i/E \\ &= \frac{Anec}{B} \propto \frac{n}{B} \end{aligned}$$

7.2.2 Quantum Hall Effect

In 1980 the German physicist Klaus von Klitzing discovered in a similar experiment that the Hall resistance does not vary in linear fashion, but "step-wise" with the strength of the magnetic field. The steps occur at resistance values that do not depend on the properties of the material but are given by a combination of fundamental physical constants divided by an integer. We say that the resistance is quantized. At quantized Hall resistance values, normal Ohmic resistance disappears and the material becomes in a sense superconducting. For his discovery of what is termed the integer quantum Hall effect von Klitzing was awarded the Nobel Prize in 1985.

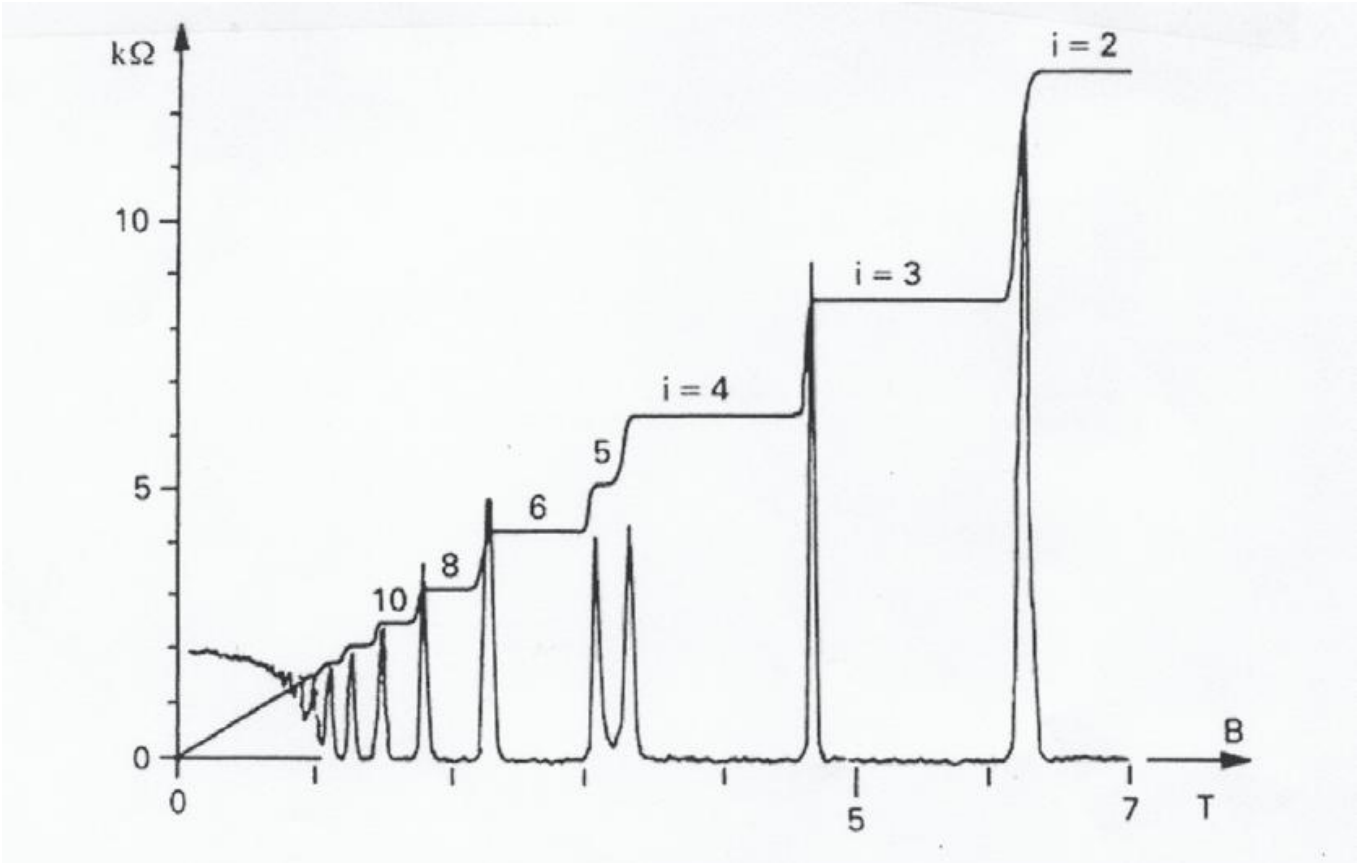


Fig. 2. The Hall resistance varies stepwise with changes in magnetic field B. Step height is given by the physical constant h/e^2 (value approximately 25 kilo-ohm) divided by an integer i. The figure shows steps for i =2,3,4,5,6,8 and 10. The effect has given rise to a new international standard for resistance. Since 1990 this has been represented by the unit 1 klitzing, defined as the Hall resistance at the fourth step ($h/4e^2$). The lower peaked curve represents the Ohmic resistance, which disappears at each step. (Kosmos 1986)

In their refined experimental studies of the quantum Hall effect, using among other things lower temperatures and more powerful magnetic field, Stomer, Tsui and their co-workers found to their great surprise a new step in the Hall resistance which was three times higher than von Klitzing's highest. They subsequently found more and more new steps, both above and between the integers. All the new step heights can be expressed with the same constant as earlier but now divided by different fractions. For this reason the new discovery is named the fractional quantum Hall effect..

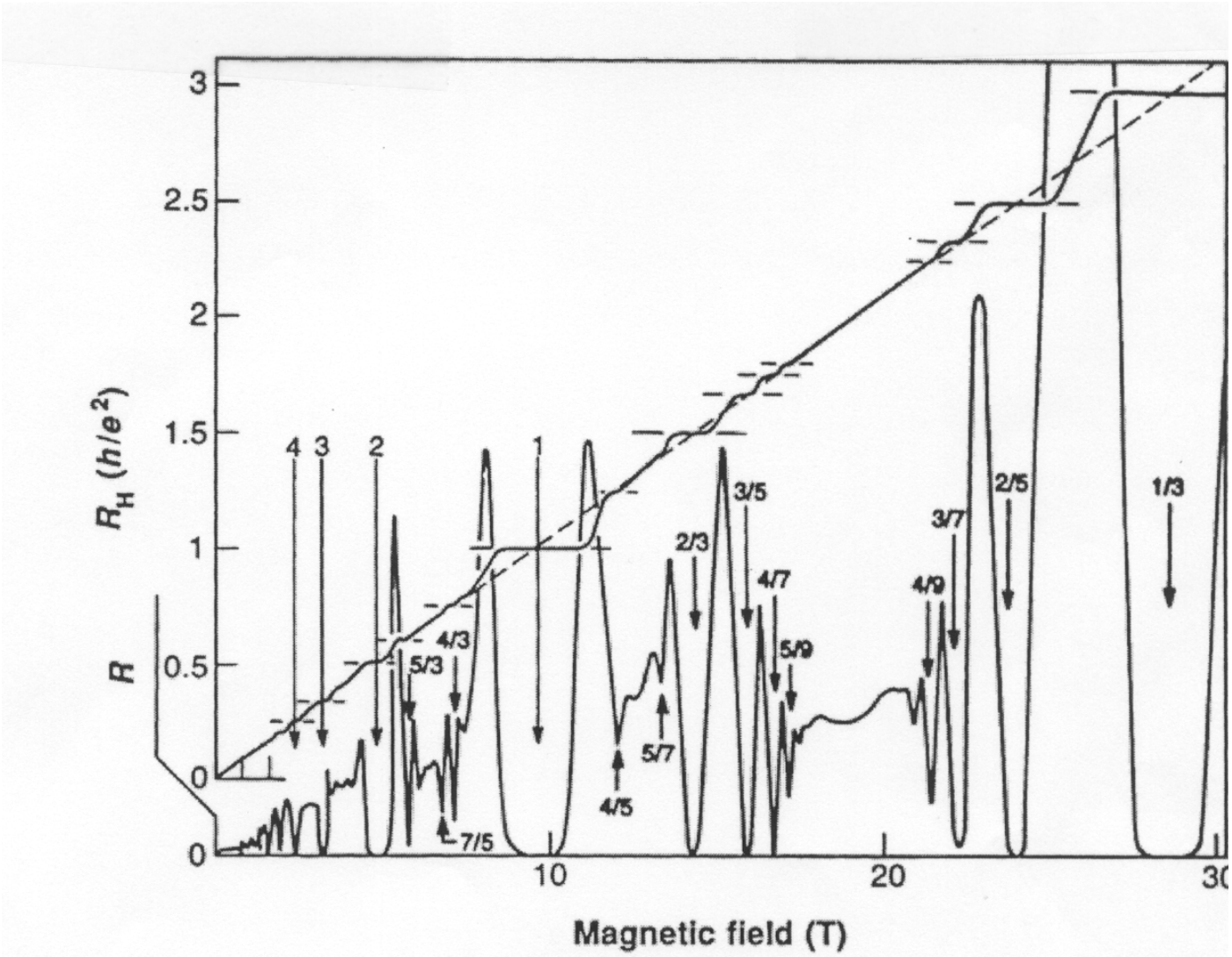


Fig. 3. The dashed diagonal line represents the classical Hall resistance and the full drawn diagonal stepped curve the experimental results. The magnetic fields causing the steps are marked with arrows. Note particularly the step first discovered by Störmer and Tsui (1/3) at highest value of the magnetic field and the steps earlier discovered by von Klitzing (integer with a weaker magnetic field. (Science 1990)

7.2.3 Laughlin's Theory

A year after the discovery of the fractional quantum Hall effect, Laughlin offered a theoretical explanation. According to his theory the low temperature and the powerful magnetic field compel the electron gas to condense to form a new type of quantum fluid. Since electrons are most reluctant to condense (They are what is termed fermions) they first, in a sense,

combine with the "flux quanta" of magnetic field. Particularly for the first step ($\gamma = 1/3$) discovered by Stomer and Tsui, each of electrons captures three flux quanta thus forming a kind of composite particle with no objection to condensing. (They become what is termed bosons). Quantum fluids have earlier occurred at very low temperatures in liquid helium and in superconductors. They have certain properties in common, e.g. superfluidity, but they also show important differences in behaviors. Apart from its superfluidity which explains the disappearance of Ohmic resistance at the Hall resistance steps„ the new quantum fluid proposed by Laughlin has many unusual properties. One of the most remarkable is that if one electron is added the fluid will be affected (excited) and a number of fractionally charged "quasiparticles" created. These quasiparticles are not particles in the normal sense but a result of the common dance of electrons in the quantum fluid. Laughlin was the first to demonstrate that the quasiparticles have precisely the correct fractional charge to explain the fractional quantum Hall effect. Subsequent measurements have demonstrated more and more fractional charged steps in the Hall effect, and Laughlin's quantum fluid has proved capable of explaining all the steps experimentally. The new quantum fluid strongly resists compression; it is said to be incompressible.

Further reading

1. B. Davis, *Splitting the electron*, New Scientist, 31 Jan, 1998, p36

2. G. P. Collins, *Fractionally charged quasiparticles signal their presence with noise*, Physics Today, Nov,1997, p17,

3. S. Kivelson, D. H. Lee and S. C. Zhang, *Electrons in flatband*, Scientific American, March,1996, p64.

7.2.4 Charged particle in the presence of a magnetic field

We consider a charged particle moving on a plane in the presence of a perpendicular uniform magnetic field B. The mass of the particle is M and charge e. The Hamiltonian is

$$\begin{aligned} H &= \frac{1}{2m}(P + \frac{e}{c}A)^2 \\ &= \frac{1}{2m}[(-i\hbar\frac{\partial}{\partial x} + \frac{e}{c}A_x)^2 + (-i\hbar\frac{\partial}{\partial y} + \frac{e}{c}A_y)^2] \end{aligned}$$

The vector potential **A**, is such that its curl is equal to B:

$$B_z = (\nabla \times \mathbf{A})_z$$

We will work in the isotropic gauge

$$\mathbf{A} = -\frac{1}{2}\mathbf{B} \times \mathbf{r}$$

i.e.

$$\begin{aligned} A_x &= -\frac{1}{2}By \\ A_y &= \frac{1}{2}Bx \end{aligned}$$

In the gauge

$$\begin{aligned} H &= \frac{1}{2m}(-i\hbar\frac{\partial}{\partial x} - \frac{e}{2c}By)^2 \\ &\quad + \frac{1}{2m}(-i\hbar\frac{\partial}{\partial y} + \frac{e}{2c}Bx)^2 \end{aligned}$$

Denote

$$\begin{aligned} \Pi_x &= -i\hbar\frac{\partial}{\partial x} - \frac{e}{2c}By \\ \Pi_y &= -i\hbar\frac{\partial}{\partial y} + \frac{e}{2c}Bx \end{aligned}$$

The commutator is constant,

$$[\Pi_x.\Pi_y] = -i\frac{\hbar eB}{c}.$$

The Hamiltonian is expressed as

$$\begin{aligned} H &= \frac{1}{2m}\{(\Pi_y - i\Pi_x)(\Pi_y + \Pi_x) + i[\Pi_x, \Pi_y]\} \\ &= \frac{1}{2m}[(\Pi_y - i\Pi_x)(\Pi_y + \Pi_x) + \frac{\hbar eB}{c} \\ &= \hbar\frac{eB}{Mc}[a^+a + \frac{1}{2}] \end{aligned}$$

where

$$\begin{aligned} a^+ &= \left(\frac{c}{2\hbar eB}\right)^{1/2}(\Pi_y - i\Pi_x) \\ &= \left(\frac{c}{2\hbar eB}\right)^{1/2}(-i\hbar\frac{\partial}{\partial x} + \frac{eB}{2c}iy - i\hbar\frac{\partial}{\partial y} + \frac{eB}{2c}x) \\ &= 2^{1/2}(-\frac{\partial}{\partial \bar{z}} + \frac{1}{4}z) \end{aligned}$$

$$a = 2^{1/2}(+\frac{\partial}{\partial z} + \frac{1}{4}\bar{z})$$

where $z = (x + iy)/l_0$ and $\vec{z} = (x - iy)/l_0$. The length unit $l_0 = (\hbar c/eB)^{1/2}$.

Hence the Hamiltonian is reduced to

$$H = \hbar\omega_c(a^+a + \frac{1}{2})$$

where

$$\omega_c = \frac{eB}{Mc}.$$

a and a^+satisfy $[a, a^+] = 1$.

Comparing to the simple harmonic oscillator„ the motion of a charged particle in a uniform magnetic field is equivalent to it. A set of the wave function has the form

$$f_n(z, \bar{z}) = z^n e^{-z\bar{z}/4}$$

The energy eigenvalue is

$$E_n = \hbar\omega_c(n + \frac{1}{2})$$

The wave functions are also eigenstates of angular momentum operator

$$\begin{aligned} L_z &= -i\hbar(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}) \\ &= \hbar(z\frac{\partial}{\partial z} - \bar{z}\frac{\partial}{\partial \bar{z}}). \end{aligned}$$

with the eigenvalue

$$L_z f_n(z, \vec{z}) = n\hbar f_n(z, \vec{z}).$$

The energy level E_n is called n^{th} Landau level

The Landau levels have a huge degeneracy which is determined by

$$N_\phi = \frac{\phi}{\phi_0} = \frac{BA}{2\pi\frac{\hbar c}{e}} = \frac{A}{2\pi l_0^2}$$

To make this degeneracy more apparent, we assume the system has the shape of a square with dimension L. We introduce another pair of operators

$$\begin{aligned} k^+ &= 2^{1/2}(\frac{\partial}{\partial z} - \frac{1}{4}\vec{z}) \\ k &= 2^{1/2}(-\frac{\partial}{\partial z} - \frac{1}{4}z) \\ ([k, k^+] &= 1) \end{aligned}$$

The two operators commute with H,

$$[k, H] = [k^+, H] = 0.$$

Also , the operator k annihilates the wave function $f_n(z, \vec{z})$, just like the operator a.

$$k f_n(z, \vec{z}) = 0$$

Define

$$\bar{T} = \exp[i2\pi l_0 k/L]$$

$$T = \exp[2\pi l_0 k^{\dagger}/L]$$

Thus, f_n is an engenstate of $\bar{T}$

$$\bar{T} f_n = f_n$$

A complete set of eigenstates of the nth Landau level $\{f_{n,m}\}$can be constructed ($m = 1, ...N_\phi$)

$$f_{n,m}(z,\bar{z}) = T^m f_n(z,\bar{z})$$

$$= \exp[i2m\pi l_0 k/L] f_n(z,\bar{z})$$

From the definitions of T and $\bar{T}$

$$\bar{T}T = T\bar{T}\exp[i2\pi l_0 k/L, 2\pi l_0 k^{\dagger}/L]$$

$$= \exp[i2\pi/N_\phi] T\bar{T}$$

Therefore the states $f_{n,m}(z,\bar{z})$ have

$$H f_{n,m^{(z,\bar{z})}} = \hbar\omega(n+\frac{1}{2}) f_{n,m}(z,\bar{z})$$

$$\bar{T} f_{n,m^{(z,\bar{z})}} = \exp[i2m\pi/N_\phi] f_{n,m}(z,\bar{z})$$

7.2.5 Landau Level and Quantum Hall Effect

The degeneracy of the Landau energy levels is $N_\phi-$fold. The ratio of the number of electrons to N_ϕ

$$\gamma = N_e/N_\phi$$

is called the filling number of Landau level. When $\gamma = 1$,it means that the first Landau level is fully filled and when $\gamma = 2$, the second landau level is also filled. There is a simple relation between the filling number and the quantized Hall conductivity. Suppose the total charge of the sample is

$$Q = \gamma N_\phi e$$

The current **J** is then equal to

$$\mathbf{J} = \gamma N_\phi e \vec{\nu}$$

$\vec{\nu}$ is determined by the magnetic field **B** and electric field **E**

$$\frac{\nu}{c} = \frac{E}{B}$$

So the current density $\mathbf{j} = \mathbf{J}/dL$

$$\begin{aligned} j &= \frac{\gamma N_\phi e}{dL}\nu = \frac{\nu N_\phi e}{BdL}Ec \\ &= \frac{\nu N_\phi e}{N_\phi \cdot \frac{\hbar c}{e}}Ec = \gamma\frac{e^2}{\hbar}E. \end{aligned}$$

The Hall conductance is

$$\sigma_{ny} = \gamma\frac{e^2}{\hbar}.$$

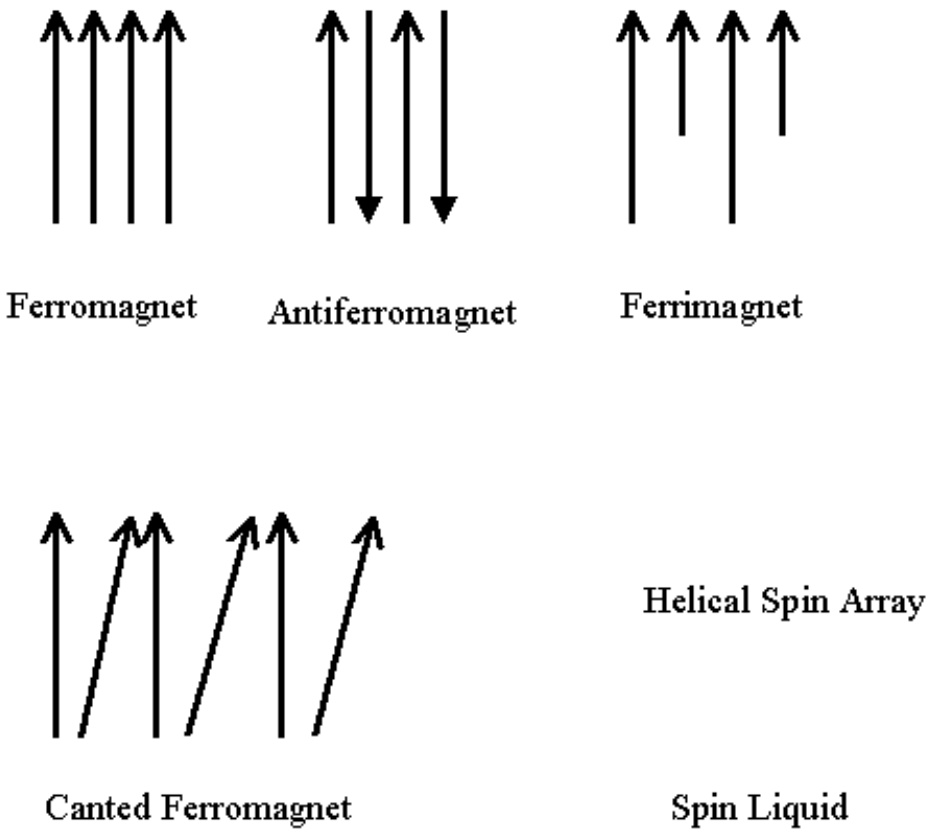
The integer quantum Hall effect occurs at $\gamma = integer$, (1,2,...) and the fractional Hall effect occurs at $\gamma = fractional$: 1/3, 1/5, 2/3, ...

7.3 Quantum Magnetism

Magnetism is inseparable from quantum mechanics, for a strictly classical system in thermal equilibrium can display no magnetic momentum, even in a magnetic field. The magnetic momentum of a free atom has three principal sources: the spin with which electrons are

endowed, their orbital angular momentum about the nucleus; and the change in the orbital moment induced by an applied magnetic field.

Ordered arrangements of electron spins



7.3.1 Spin Exchange

Ferromagnetism is obtained in solids when the magnetic moments of many electrons align. Antiferromagnetism and spin density waves describe oscillatory ordering of magnetic moments. The classical dipolar interaction between the electron moments (which is of order $10^5 eV$) is for too weak to explain the observed magnetic transition temperature (which are

of order $10^2 - 10^3\ ^0k$ in transition metal and rare earth compounds)

The coupling mechanism that gives rise to magnetism derives from the following fundamental properties of electrons:

- The electron's spin
- The electron's kinetic energy
- Pauli exclusion principle
- Coulomb repulsion

Before we introduce the physical origin of the magnetic coupling between electrons in solids, we simply review some standard definitions and basic relations of second quantization.

For an orthonormal single-particle basis, $\{|\phi_i\rangle\}$

$$\langle \phi_i | \phi_j \rangle = \delta_{ij}.$$

The creation operator of state i is $a_i^\dagger$ and its Hermitian conjugate is annihilation operator a_i. Both are defined with respect to the vacuum state $|0\rangle_i$such that

$$|\phi_i\rangle = a_i^\dagger |0\rangle_i$$

$$a_i |0\rangle_i = 0.$$

The number operator is defined as

$$n_i = a_i^\dagger a_i$$

For bosons,

$$\left[a_i, a_j^\dagger\right] = a_i a_j^\dagger - a_j^\dagger a_i = \delta_{ij}$$

$$\{a_i, a_j\} = 0$$

For electrons with spin $s = 1/2$, we have to introduce a pair of operators, $c^{\dagger}_{i,\sigma}$ where $\sigma = \uparrow, \downarrow$ such that

$$\{c_{i\sigma}, c^{\dagger}_{j\sigma}\} = \delta_{ij}\delta_{\sigma\sigma},$$

$$\{c_{i\sigma}, c_{j\sigma},\} = 0$$

The spin operator can be expressed as

$$S^{\dagger}_i = S_{ix} + iS_{iy} = \hbar c^{\dagger}_{i\uparrow} c_{i\downarrow}$$

$$S^{-}_i = S_{ix} - iS_{iy} = \hbar c^{\dagger}_{i\downarrow} c_{i\uparrow}$$

$$S^{z}_i = \frac{\hbar}{2}(c^{\dagger}_{i\uparrow} c_{i\uparrow} - c^{\dagger}_{i\downarrow} c_{i\downarrow})$$

The commutation relations:

$$[S^{\dagger}_i, S^{-}_i] = 2\hbar S^{z}_i$$

$$[S^{z}_i, S^{\pm}_i] = \pm\hbar S^{\pm}_i$$

7.3.2 Two-Site Problem

The Hersenberg spin exchange interaction is written as

$$H = J\mathbf{S}_1 \cdot \mathbf{S}_2$$

To obtain the eigenstates of H, we check the following relations,

(1) $[\mathbf{S}^2_1, H] = 0$,but $[\mathbf{S}_1, H] \neq 0$

(2) $[\mathbf{S}^2_2, H] = 0$,but $[\mathbf{S}_2, H] \neq 0$

(3) $[\mathbf{S}_1 + \mathbf{S}_2, H] = 0$

Therefore $\mathbf{S}_1^2$, $\mathbf{S}_2^2$,and $\mathbf{S}_{tot}^2 = (\mathbf{S}_1 + \mathbf{S}_2)^2$ and its z-component $\mathbf{S}_{tot}^z$ are good quantum numbers, but S_1^z, S_2^z are not. Hence we can denote the simultaneous eigenkets of $\mathbf{S}_{tot}^2$, $\mathbf{S}_{tot}^z$, $\mathbf{S}_1^2$ and $\mathbf{S}_2^2$ by

$$|S_{tot}, S_{tot}^z, S_1, S_2\rangle$$

such that

$$\begin{aligned}
&\mathbf{S}_1^2 \,|S_{tot}, S_{tot}^z, S_1, S_2\rangle \\
= \quad & S_1(S_1+1)\,|S_{tot}, S_{tot}^z, S_1, S_2\rangle \\
&\mathbf{S}_2^2 \,|S_{tot}, S_{tot}^z, S_1, S_2\rangle \\
= \quad & S_2(S_2+1)\,|S_{tot}, S_{tot}^z, S_1, S_2\rangle \\
&\mathbf{S}_{tot1}^z \,|S_{tot}, S_{tot}^z, S_1, S_2\rangle \\
= \quad & S_{tot}(S_{tot}+1)\,|S_{tot}, S_{tot}^z, S_1, S_2\rangle \\
&\mathbf{S}_{tot1}^z \,|S_{tot}, S_{tot}^z, S_1, S_2\rangle \\
= \quad & S_{tot}^z \,|S_{tot}, S_{tot}^z, S_1, S_2\rangle
\end{aligned}$$

Fortunately, the state kets are also the eigenkets of H:

$$H\,|S_{tot}, S_{tot}^z, S_1, S_2\rangle = E\,|S_{tot}, S_{tot}^z, S_1, S_2\rangle$$

where

$$E = \frac{J}{2}\left[S_{tot}(S_{tot}+1) - S_1(S_1+1) - S_2(S_2+1)\right]$$

and

$$S_{tot} = |S_1 - S_2|\,, |S_1 - S_2| + 1, ...S_1 + S_2$$

Since the energy eigenvalues are independent of S^z_{tot} can be $-S_{tot}, ...S_{tot}$ the energy eigenstates are $(2S_{tot}+1)-$fold degenerated. From the point of view of symmetry, the degeneracy of the eigenstates originates from the invariance of H under the $SU(2)$ symmetry rotation,

$$UHU^{\dagger} = H$$

where

$$U = \exp[-i\mathbf{S}_{tot} \cdot \mathbf{n}\phi/\hbar]$$

The ground state:

The lowest energy state is determined by the sign of J: when $J > 0$, S_{tot} should be taken to be minimum, otherwise S_{tot} should be taken to be maximal.

The case of $J > 0$:

$$S_{tot} = S_1 - S_2, \ (S_1 > S_2)$$

The two spins are antiparallel, which is called antiferromagnetic. The ground state energy

$$E_g = -J(S_1 + 1)S_2$$

The case of $J < 0$

$$S_{tot} = S_1 + S_2$$

The two spins are parallel, which is ferromagnetic

$$E_g = -\left|J\right| S_1 S_2$$

7.3.3 Ferromagnetic Exchange $(J < 0)$

Ferromagnetic exchange coupling originates from the direct Coulomb interaction and the Pauli exclusion principle. In the second quantized form, the two-body Coulomb interaction

is given by

$$V = \frac{1}{2}\int dxdy\tilde{v}(x,y)\Psi_s^\dagger(x)\Psi_{s'}^\dagger(y)\Psi_{s'}(y)\Psi_s(x).$$

The field operator

$$\Psi_s^\dagger(x) = \sum_i \phi_i^*(x)c_{is}^\dagger.$$

The interaction can be expressed as

$$\begin{aligned} V &= \frac{1}{2}\int dxdy\tilde{v}(x,y) \\ &\quad \times\phi_i^\dagger(x)\phi_j^\dagger(y)\phi_k(y)\phi_l(x)c_{is}^\dagger c_{js'}^\dagger c_{ks'}c_{ls} \\ &= \sum_i U_{ii}n_{is}n_{i-s} \\ &\quad + \sum_{i,i'} U_{ii'}(n_{i\uparrow}+n_{i\downarrow})(n_{i'\uparrow}+n_{i'\downarrow}) \\ &\quad + \sum_{i,i'} J_{ii'}^F c_{is}^\dagger c_{i's'}^\dagger c_{is'}c_{i's} \\ &\quad + \cdots \end{aligned}$$

where

$$\begin{aligned} U_{ii'} &= \frac{1}{2}\int dxdy\left|\phi_i(x)\right|^2\left|\phi_{i'}(y)\right|^2\tilde{v}(x,y) \\ J_{ii'}^F &= \frac{1}{2}\int dxdy\tilde{v}(x,y)\phi_{i'}^\dagger(x)\phi_i^\dagger(y)\phi_{i'}(y)\phi_i(x) \end{aligned}$$

The exchange interaction J^Facts as a Hersenberg interaction:

$$J_{ij'}^F\sum c_{is}^+c_{i's'}^+c_{is'}c_{i's} = -2J_{ij'}^F\sum(S_i\cdot S_{i'}+\frac{1}{4}n_i\cdot n_{i'})$$

The positivity of $J_{ij'}^F$ can be proved as follows:

(1) Complete screening:

$$v = \delta(x-y)$$

In the case,

$$J_{ii'}^F = \frac{1}{2}\int dx\,|\phi_i(x)|^2\,|\phi_{i'}(x)|^2 > 0$$

(2) Long-ranged Coulomb interaction

$$\tilde{v} = \frac{e^2}{|\vec{x}-\vec{y}|}$$

Assume ϕ_i is the plane wave

$$\begin{aligned} J_{ii'}^F &\propto \int dx \exp[ik\cdot x]\frac{e^2}{|x|} \\ &= 4\pi\frac{e^2}{k^2} > 0 \end{aligned}$$

This is ferromagnetic!

7.3.4 Antiferromagnetic Exchange

Two-site (or atom) problem with two electrons

Let's consider two orthogonal orbitals localized on two atoms labelled by $i = 1, 2$. Tunnelling between the two atoms (or states) is described by a hopping Hamiltonian

$$H^t = -t\sum_s (C_{1s}^+ C_{2s} + C_{2s}^+\, C_{1s})$$

For simplicity, we consider an on-site interaction

$$H_u = U\sum n_{i\uparrow}\cdot n_{i\downarrow}$$

To explore the physical origin of anti-ferromagnetic coupling, we consider a special case: $u >> t$. In the case, we choose H_u to be the zero-order(or unperturbed) Hamiltonian and H^+ to be the perturbation.

For $H_{u:}$ there are six possible configurations which are eigenstates of H $_u$

(1) E=0, $|1\uparrow, 2\uparrow\rangle$, $|1\uparrow, 2\downarrow\rangle$, $|1\downarrow, 2\uparrow\rangle$, $|1\downarrow, 2\downarrow\rangle$;

(2) E=U, $|1\uparrow, 1\downarrow\rangle$, $|2\downarrow, 2\uparrow\rangle$

Denote $|\alpha\rangle$ the unperturbed state with energy 0 and $|n\rangle$ denote the two state with E=U (n=1,2). In terms of the c-operators,

$$|\alpha\rangle = c_{1s}^{+} c_{2s'}^{+} |0\rangle$$

and

$$\begin{aligned} |1\rangle &= C_{1\uparrow}^{\dagger} C_{1\downarrow}^{\dagger} |0\rangle \\ |2\rangle &= C_{2\uparrow}^{\dagger} C_{2\downarrow}^{\dagger} |0\rangle \end{aligned}$$

In the first-order perturbation theory

$$\langle \alpha | H_t | \alpha' \rangle = 0$$

In the second-order perturbation theory

$$\begin{aligned} \left\langle \alpha \left| \Delta H^{(2)} \right| \alpha \right\rangle &= \sum_{n=1,2} \frac{\langle \alpha | H^t | n \rangle \langle n | H^t | \alpha \rangle}{\langle \alpha | H_u | \alpha \rangle - \langle n | H_u | n \rangle} \\ &= -\frac{1}{U} \sum \left\langle \alpha \left| H^t \right| n \right\rangle \left\langle n \left| H^t \right| \alpha \right\rangle \end{aligned}$$

$|n\rangle \langle n|$ is a projection operator

$$\begin{aligned} |1\rangle \langle 1| &= n_{1\uparrow} n_{1\downarrow} (1 - n_{2\uparrow})(1 - n_{2\downarrow})(\uparrow\downarrow -) \\ |2\rangle \langle 2| &= (1 - n_{1\uparrow})(1 - n_{1\downarrow}) n_{2\uparrow} n_{2\downarrow} (- \uparrow\downarrow) \end{aligned}$$

$$
\begin{aligned}
& \langle \alpha \left| H^t \right| 1 \rangle \langle 1 \left| H^t \right| \alpha' \rangle \\
= \; & \langle \alpha | \left(C^\dagger_{2\uparrow} C_{i\uparrow} + C^\dagger_{2\downarrow} C_{i\downarrow} + \hbar.c \right) \\
& \times n_{1\uparrow} n_{1\downarrow} (1 - n_{2\uparrow})(1 - n_{2\downarrow}) \\
& \left(C^\dagger_{2\uparrow} C_{i\uparrow} + C^\dagger_{2\downarrow} C_{i\downarrow} + \hbar.c \right) | \alpha' \rangle \\
= \; & \langle \alpha | \left(C^\dagger_{2\uparrow} C_{i\uparrow} + C^\dagger_{2\downarrow} C_{i\downarrow} \right) n_{1\uparrow} n_{1\downarrow} (1 - n_{2\uparrow})(1 - n_{2\downarrow}) \\
& \times \left(C^\dagger_{1\uparrow} C_{i\uparrow} + C^\dagger_{1\downarrow} C_{i\downarrow} \right) | \alpha' \rangle \\
= \; & \langle \alpha | \left(-C^\dagger_{1\downarrow} C_{i\uparrow} C^\dagger_{2\uparrow} C_{i\downarrow} - C^\dagger_{1\uparrow} C_{i\downarrow} C^\dagger_{2\downarrow} C_{i\uparrow} \right) + n_{1\uparrow} n_{2\downarrow} \\
& + n_{1\downarrow} n_{2\uparrow}) | \alpha' \rangle \\
= \; & \langle \alpha | - 2 S_1 \cdot S_2 + \frac{1}{2} (n_{1\uparrow} + n_{1\downarrow})(n_{2\uparrow} + n_{2\downarrow}) | \alpha' \rangle
\end{aligned}
$$

Therefore the effective Hamiltonian $\Delta H^{(2)}$ can be written as an isotropic antiferromagnetic Hersenberg spin exchange form.

$$\Delta H^{(2)} = + \frac{4t^2}{U} (\vec{S}_1 \cdot \vec{S}_2 - \frac{1}{4})$$

As $4t^2/U > 0$, the exchange coupling is antiferromagnetic! The ground state of this two-site problem is spin singlet, i.e. $S = 0$. Our discussion on the two-site problem can be easily generalized to a many-site system. The Hersenberg model is defined on a lattice

$$H = \sum J_{ij} S_i \cdot S_j$$

where i and j are the lattice sites and usually are of the nearest neighbour pair. S_i can be taken any value of half-integer, $S = 1/2, 1....$

One of the most important application of spin superexchange with current inter-

ests is the high temperature superconductivity. the so-called "$t - J$" model is extensively discussed over the last decade.

$$H = -t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + \frac{4t^2}{U} \sum_{i,j} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i \; n_j)$$

which is limited within the Hilbert space excluding double occupancy of electrons on the same site.