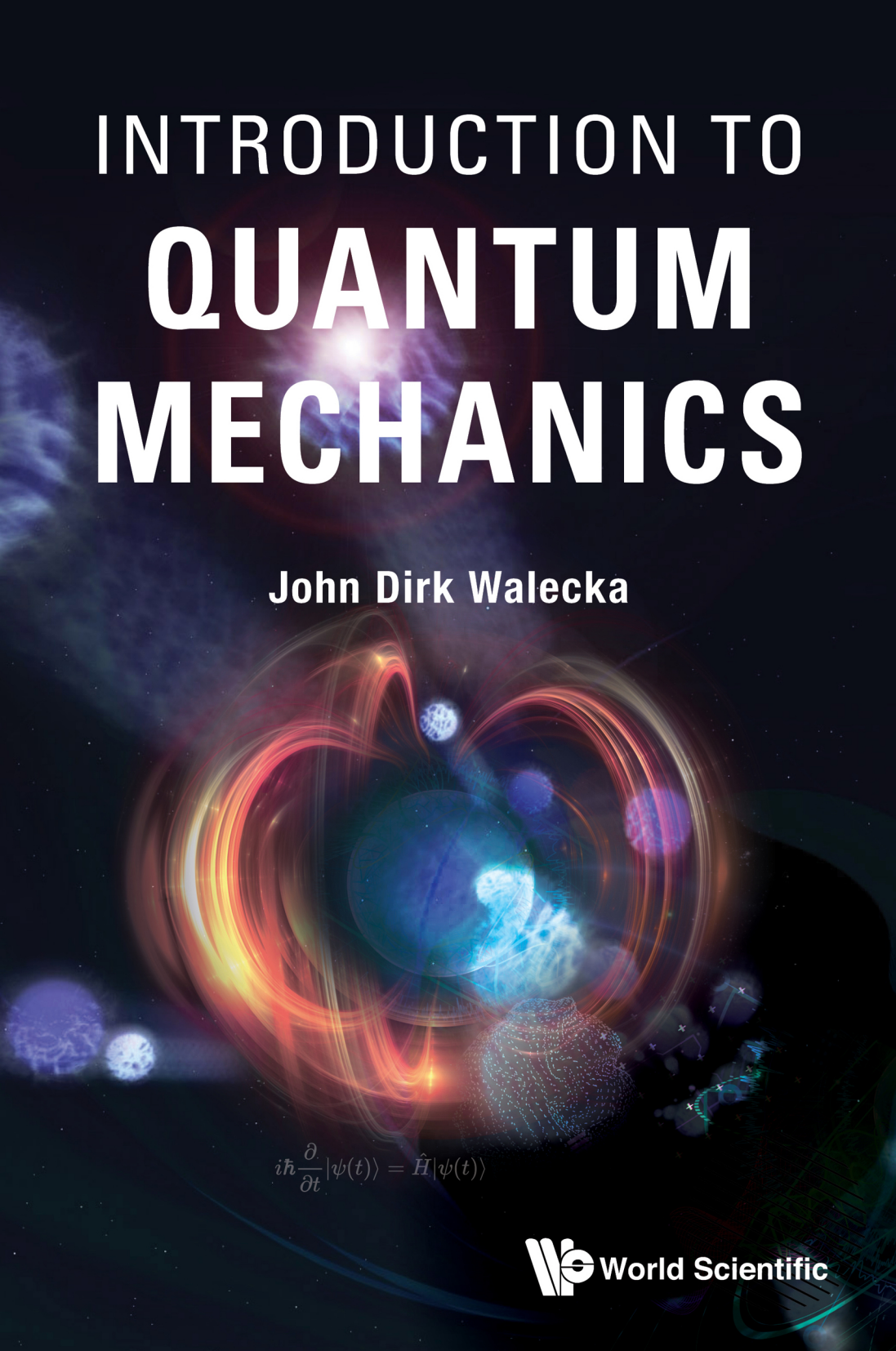
INTRODUCTION TO QUANTUM MECHANICS

John Dirk Walecka



$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$

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John Dirk Walecka
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For John and Ann

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Preface

The author recently published a book entitled *Introduction to Electricity and Magnetism* [Walecka-18]. It is based on an introductory course taught several years ago at Stanford, with over 400 students enrolled. The only requirements were an elementary knowledge of calculus and familiarity with vectors and Newton's laws; the development was otherwise self-contained. The lectures, although relatively concise, take one from Coulomb's law to Maxwell's equations and special relativity in a lucid and logical fashion.

Although never presented in an actual course, it occurred to the author that it would be fun to compose an equivalent set of lectures, aimed at the very best students, that would serve as a *prequel* to that *Electricity and Magnetism* text. This book has now also been published as *Introduction to Classical Mechanics* [Walecka-20]. The goal of this second text is to provide a clear and concise set of lectures that take one from the introduction and application of Newton's laws up to Hamilton's principle and the lagrangian mechanics of continuous systems.

Both of these texts on classical physics are meant for initial one-quarter physics courses. These lectures, aimed at the very best students, assume a good concurrent course in calculus; they are otherwise self-contained. Both texts contain an extensive set of accessible problems that enhances and extends the coverage. As an aid to teaching and learning, the solutions to these problems have now been published in additional texts [Walecka-19, Walecka-21].

The present text completes the first-year introduction to physics with a set of lectures on *Introduction to Quantum Mechanics*, the very successful theory of the microscopic world. The Schrödinger equation is motivated and presented. Several applications are explored, including scattering and transition rates. The applications are extended to include both quantum

electrodynamics and quantum statistics. There is a discussion of quantum measurements. The lectures then arrive at a formal presentation of quantum theory together with a summary of its postulates. A concluding chapter provides a brief introduction to relativistic quantum mechanics. An extensive set of accessible problems again enhances and extends the coverage.

The goal of these three texts is to provide a good, understandable, one-year introduction to the fundamentals of classical and quantum physics. It is my hope that students and teachers alike will find the use of these books rewarding and share some of the pleasure I took in writing them.

Quantum mechanics is a huge field, and no attempt has been made to provide a complete bibliography. The references given in the text are only directly relevant to the discussion at hand. It is important, however, to mention some of the good, existing books that the author has found particularly useful, such as [Wentzel (1949); Bjorken and Drell (1964); Bjorken and Drell (1965); Schiff (1968); Itzykson and Zuber (1980); Landau and Lifshitz (1981); Shankar (1994); Merzbacher (1997); Gottfried and Yan (2004); Feynman and Hibbs (2010)]. In addition, appendix B lists some significant names in quantum mechanics, both in its theory and in its applications.

I would like to once again thank my editor, Ms. Lakshmi Narayanan, for her help and support on this project. I am also grateful to Paolo Amore for his reading of the manuscript.

Williamsburg, Virginia
January 8, 2021

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Contents

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Chapter 1

Motivation

1.1 Classical Optics

Consider a non-dispersive wave which is the real part of

$$\Psi(x,t) = e^{i(kx-\omega t)} = e^{ik(x-ct)} \qquad ;\ \omega = kc \tag{1.1}$$

Here c is the velocity of the wave, and the frequency and wavelength are related by

$$\omega = 2\pi\nu = kc = 2\pi\frac{c}{\lambda} \tag{1.2}$$

As we have seen, this could be an electromagnetic wave in vacuum, a transverse wave on a string under tension, or the sound wave in a medium. This wave satisfies the wave equation

$$\frac{\partial^2\Psi(x,t)}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2\Psi(x,t)}{\partial t^2} \qquad ;\ \text{wave equation} \tag{1.3}$$

We have also seen that a linear combination of two such waves with slightly different wavenumbers k, produces an amplitude modulated signal. A more general linear combination can produce a localized wave packet, or pulse.

Huygen's principle states that each point on a wavefront acts as a source of an outgoing spherical wave. From this, and its generalizations, one derives single-slit diffraction, two-slit and multi-slit interference, and most of classical wave optics.[1]

[1] See Probs. 1.1–1.2. For a more detailed discussion here, see [Wiki (2021)].

1.2 Planck Distribution

Early in the twentieth century, Planck was studying the distribution of energy as a function of frequency for the electromagnetic radiation in a cavity. Normal modes are uncoupled simple harmonic oscillators. The classical equipartition theorem says that the energy of a simple harmonic oscillator at an absolute temperature T is

$$\langle \varepsilon(\nu) \rangle = k_B T \qquad ; \text{ equipartition for s.h.o.} \tag{1.4}$$

where k_B is Boltzmann's constant

$$k_B = 1.381 \times 10^{-23}\,\mathrm{J/^oK} \qquad ; \text{ Boltzmann's constant} \tag{1.5}$$

Since there is no limit to how small the wavelength can be, or how high the frequency, this classical result says there should be an ever-increasing energy as a function of frequency for the radiation in a cavity, the so-called *ultraviolet catastrophe*.[2]

To fit his data, Planck employed an *empirical* expression of the form

$$\langle \varepsilon(\nu) \rangle = \frac{h\nu}{e^{h\nu/k_B T} - 1} \qquad ; \text{ Planck distribution} \tag{1.6}$$

where h is a constant obtained from the fit, now known as Planck's constant

$$\frac{h}{2\pi} \equiv \hbar = 1.055 \times 10^{-34}\,\mathrm{Js} \qquad ; \text{ Planck's constant} \tag{1.7}$$

Note that at *low* frequency, the Planck distribution reproduces the equipartition result

$$\frac{h\nu}{e^{h\nu/k_B T} - 1} \;\rightarrow\; k_B T \qquad ; \; h\nu \ll k_B T \tag{1.8}$$

while at *high* frequency, it now disappears exponentially

$$\frac{h\nu}{e^{h\nu/k_B T} - 1} \;\rightarrow\; h\nu e^{-h\nu/k_B T} \qquad ; \; h\nu \gg k_B T \tag{1.9}$$

One can ask where this empirical Planck distribution might come from. Suppose that in each mode with frequency ν in the cavity it is possible to have any number n of *photons*, each with energy

$$\varepsilon = h\nu \qquad ; \text{ photon energy} \tag{1.10}$$

[2] See Prob. 1.3.

Then the mean energy in the mode at the temperature T follows from an elementary statistical calculation with the Boltzmann weighting factor $e^{-nh\nu/k_BT}$ as

$$\begin{aligned}\langle\varepsilon(\nu)\rangle &= \frac{\sum_{n=0}^{\infty}(nh\nu)e^{-nh\nu/k_BT}}{\sum_{n=0}^{\infty}e^{-nh\nu/k_BT}} \\ &= -\frac{d}{d(1/k_BT)}\ln\left(\sum_{n=0}^{\infty}e^{-nh\nu/k_BT}\right)\end{aligned} \tag{1.11}$$

The sum is just a geometric series[3]

$$\sum_{n=0}^{\infty}x^n = \frac{1}{1-x} \tag{1.12}$$

It follows that

$$\begin{aligned}\langle\varepsilon(\nu)\rangle &= \frac{d}{d(1/k_BT)}\ln\left(1-e^{-h\nu/k_BT}\right) \\ &= \frac{h\nu}{e^{h\nu/k_BT}-1}\end{aligned} \tag{1.13}$$

This reproduces Planck's distribution.

1.3 Photons

The fact that light waves actually consist of photons, which manifest particle properties, was demonstrated by Einstein in his examination of the photoelectric effect, where light shining on various solids ejects electrons. The photons of light each have an energy

$$\varepsilon = h\nu \qquad ;\ \text{photon} \tag{1.14}$$

We know the momentum flux in an electromagnetic wave is $1/c$ times the energy flux, and hence each photon in light also has a momentum

$$p = \frac{h\nu}{c} \qquad ;\ \text{photon} \tag{1.15}$$

Photons are now observed every day in the laboratory as single events in low-intensity radiation detectors.

[3]Note $e^{-nh\nu/k_BT} = \left(e^{-h\nu/k_BT}\right)^n$.

Sound waves in materials also regularly exhibit particle properties through *phonons*, which satisfy analogous relations to the above.[4]

1.4 Davisson–Germer Experiment

We have seen that waves exhibit particle properties. The Davisson–Germer experiment in 1927 showed that *particles also exhibit wave properties.* They took electrons from an oven, let them impinge on a crystal, and looked for Bragg diffraction maxima (Fig. 1.1).

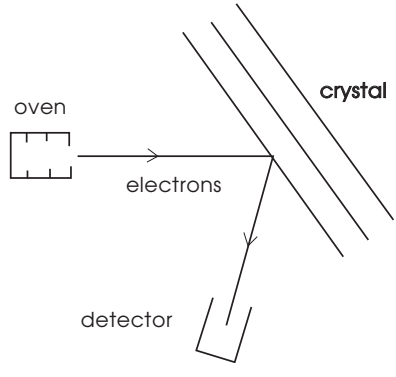

Fig. 1.1 Sketch of Davisson–Germer experiment.

They observed a diffraction pattern as in classical optics,[5] and quantum mechanics was on!

[4]Remember that c is the appropriate wave velocity.
[5]Again, see [Wiki (2021)] for more details.

Chapter 2

Wave Packet for Free Particle

2.1 de Broglie Relation

In attempting to write a wave relation for a non-relativistic particle of mass m, de Broglie appealed to the analogous photon relations from the above. He associated a wavelength with the momentum according to

$$p = mv = \hbar k = \frac{h}{\lambda} \qquad ; \text{ de Broglie wavelength} \tag{2.1}$$

As one immediate consequence, if one fits an integral number n of wavelengths around a circle of radius a, then

$$2\pi a = n\lambda = \frac{nh}{mv} \tag{2.2}$$

The angular momentum $|\vec{L}\,|$ of a particle moving around in the circle is then

$$|\vec{L}\,| = mva = n\hbar \qquad ; \text{ angular momentum} \tag{2.3}$$

As we have seen, this is precisely the quantization condition that leads to the Bohr theory of the one-electron atom![1]

2.2 Schrödinger Equation

With the de Broglie relation, and the angular frequency $\omega(k)$ given by

$$\varepsilon = \hbar\omega(k) = \frac{p^2}{2m} = \frac{(\hbar k)^2}{2m} \tag{2.4}$$

[1] See Prob. 1.5.

the wave in Eq. (1.1) now takes the dispersive form

$$\Psi(x,t) = e^{i[kx-\omega(k)t]} = e^{i[kx-(\hbar k^2/2m)t]} \tag{2.5}$$

Appropriate linear combinations of these waves can again describe a localized wave packet.[2]

Let us ask what wave equation this $\Psi(x,t)$ satisfies. Evidently

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} \tag{2.6}$$

The momentum of the particle is $p = \hbar k$. This quantity is obtained from the wave in Eq. (2.5) by taking a partial derivative with respect to x. Let us therefore define the momentum p to be the differential operator

$$p \equiv \frac{\hbar}{i}\frac{\partial}{\partial x} \qquad ;\text{ momentum} \tag{2.7}$$

and write the hamiltonian $H(p)$ for a free particle as

$$H = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \qquad ;\text{ hamiltonian} \tag{2.8}$$

Then this wave $\Psi(x,t)$ for a free particle satisfies the *Schrödinger equation*

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = H\Psi(x,t) \qquad ;\text{ Schrödinger equation} \tag{2.9}$$

We make a few comments on this result:

- This equation is inherently complex, so then is the wave function $\Psi(x,t)$. Hence, we will have to arrive at some new physical interpretation of $\Psi(x,t)$. We will proceed to investigate this below;
- The differential equation explicitly contains Planck's constant $\hbar$;
- The differential equation is linear in the time derivative, and thus it looks more like a complex diffusion equation than a wave equation;
- It involves the classical hamiltonian $H(p,x)$, where p now becomes a differential operator involving Planck's constant

$$p = \frac{\hbar}{i}\frac{\partial}{\partial x} \tag{2.10}$$

[2]See Prob. 2.7; see also [Walecka (2008)].

- The momentum p and the position x now satisfying the basic *commutation relation*

$$[p, x]\Psi(x,t) \equiv (px - xp)\Psi(x,t) = \frac{\hbar}{i}\Psi(x,t) \qquad (2.11)$$
$$; \text{ commutation relation}$$

- In fact, the argument can be turned around. One says that the system is quantized by *imposing* the canonical commutation relation in Eq. (2.11), which can be satisfied by writing the momentum as the differential operator in Eq. (2.10).

2.3 Interpretation

The complex Schrödinger wave function $\Psi(x,t)$, for which we write the underlying differential equation in quantum mechanics, is not a physical observable. As you might imagine, this leads to substantial complications. On the other hand, we do know intuitively that the wave function should be large where the particle is, and small where it is not. Born suggested that we interpret the square of the modulus of $\Psi(x,t)$ as the *probability density* of finding the particle at the position x at the time t

$$\rho(x,t) \equiv |\Psi(x,t)|^2 = \Psi^*(x,t)\Psi(x,t) \qquad ; \text{ probability density} \quad (2.12)$$

Here $\Psi^*(x,t)$ is the complex conjugate of $\Psi(x,t)$.

We should at least find a *continuity equation* for the probability density $\rho(x,t)$, and the consequent conservation of probability, in the theory. Let us try to establish that. Consider

$$\frac{\partial \rho}{\partial t} = \frac{\partial \Psi^*(x,t)}{\partial t}\Psi(x,t) + \Psi^*(x,t)\frac{\partial \Psi(x,t)}{\partial t} \qquad (2.13)$$

The complex conjugate of the Schrödinger equation gives

$$-i\hbar\frac{\partial \Psi^*(x,t)}{\partial t} = [H\Psi(x,t)]^* \qquad (2.14)$$

Hence

$$\frac{\partial \rho}{\partial t} = \frac{1}{i\hbar}\left\{\Psi^*(x,t)\,[H\Psi(x,t)] - [H\Psi(x,t)]^*\,\Psi(x,t)\right\} \qquad (2.15)$$

Insertion of the differential form of $H = -\hbar^2\partial^2/\partial x^2$ allows this to be written as

$$\frac{\partial \rho}{\partial t} = -\frac{\partial S(x,t)}{\partial x} \tag{2.16}$$

where

$$\begin{aligned} S(x,t) &= \frac{1}{2m}\left\{\Psi^\star(x,t)\frac{\hbar}{i}\frac{\partial \Psi(x,t)}{\partial x} + \left[\frac{\hbar}{i}\frac{\partial \Psi(x,t)}{\partial x}\right]^* \Psi(x,t)\right\} \\ &= \frac{1}{2m}\left\{\Psi^\star(x,t)p\Psi(x,t) + [p\Psi(x,t)]^* \Psi(x,t)\right\} \qquad (2.17) \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad ; \text{ probability flux} \end{aligned}$$

Thus we have achieved our continuity equation for the probability density. Note that the *probability flux* $S(x,t)$ is just a mean value of p/m for the particle, or its *mean velocity*. Note also that $S(x,t)$ is explicitly *real*.

2.4 Stationary States

Let us look for separated solutions to the partial differential Schrödinger equation

$$\Psi(x,t) = \Phi(t)\psi(x) \tag{2.18}$$

We will eventually build the general solution out of these. Substitution into the equation, and division by $\Psi = \Phi\psi$, gives

$$i\hbar\frac{1}{\Phi(t)}\frac{d\Phi(t)}{dt} = \frac{1}{\psi(x)}H\psi(x) \tag{2.19}$$

In order for this to hold for all (x,t), both expressions must simply be equal to some constant E.

For the first term, one then has

$$i\hbar\frac{d\Phi(t)}{dt} = E\Phi(t) \tag{2.20}$$

The solution to this equation is

$$\Phi(t) = e^{-iEt/\hbar} \tag{2.21}$$

For the second term, one has

$$H\psi(x) = E\psi(x) \tag{2.22}$$

This is a differential eigenvalue equation, where E is the *eigenvalue*, and $\psi(x)$ is the *eigenfunction*. Multiply this equation on the left by ψ^*, and integrate over the appropriate range in x. This gives

$$\frac{\int dx\, \psi^*(x) H \psi(x)}{\int dx\, |\psi(x)|^2} = E \tag{2.23}$$

Let us assume that the hamiltonian is *hermitian* and satisfies

$$\int dx\, \psi^*(x) H \psi(x) = \int dx\, \left[H\psi(x)\right]^* \psi(x) \qquad ;\ \text{hermitian} \tag{2.24}$$

We will discuss this property is some detail below. In this case, one has

$$E = E^* \qquad ;\ \text{real} \tag{2.25}$$

The eigenvalue E of the hermitian hamiltonian H is real, and since it is just the mean value of the hamiltonian by Eq. (2.23), we can identify it as the *energy* of the system.

The separated solution thus has the form

$$\Psi(x,t) = \psi(x) e^{-iEt/\hbar} \tag{2.26}$$

If this is substituted into Eqs. (2.12) and (2.17), one has

$$\begin{aligned} \rho(x) &= |\psi(x)|^2 \\ S(x) &= \frac{1}{2m} \left\{ \psi^\star(x) p \psi(x) + \left[p\psi(x)\right]^* \psi(x) \right\} \end{aligned} \tag{2.27}$$

The probability density and probability current are *independent of time*, and the separated solution in Eq. (2.26) is known as a *stationary state*.

2.5 Eigenfunctions and Eigenvalues

Let us start with the simplest case of the eigenfunctions and eigenvalues of the momentum operator

$$p\psi(x) = \frac{\hbar}{i} \frac{d\psi(x)}{dx} = \hbar k \psi(x) \tag{2.28}$$

Here we have denoted the eigenvalues by $\hbar k$. The solutions to this equation are

$$\psi(x) \propto e^{ikx} \tag{2.29}$$

Now it is crucial to supply some *boundary conditions* for the problem. Here we shall just consider the simplest case of *periodic boundary conditions* (p.b.c.). Imagine the particle is running around a large circle of length L, and let x denote the distance along the circle (see Fig. 2.1).

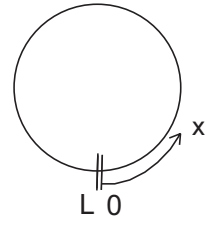

Fig. 2.1 Free particle going around a large circle of length L, with the distance x along the circle. Basis for periodic boundary conditions (p.b.c.).

The p.b.c. in this case is

$$\psi(x+L) = \psi(x) \qquad ;\ \text{p.b.c.} \tag{2.30}$$

The eigenvalues of the momentum then follow immediately through

$$k_n = \frac{2\pi n}{L} \qquad ;\ n = 0, \pm 1, \pm 2, \cdots \tag{2.31}$$

The normalized eigenfunctions are

$$\psi_n(x) = \frac{1}{\sqrt{L}} e^{2\pi i n x/L} \tag{2.32}$$

A simple calculation shows these solutions are *orthonormal*

$$\int_0^L dx\, \psi_n^*(x)\psi_m(x) = \delta_{m,n} \tag{2.33}$$

where $\delta_{m,n}$ is the Kronecker delta

$$\begin{aligned} \delta_{m,n} &= 1 \qquad ;\ \text{if } m = n \\ &= 0 \qquad ;\ \text{if } m \neq n \end{aligned} \tag{2.34}$$

Now consider the following expression

$$\int_0^L dx\, \psi_m^*(x) p \psi_n(x) = \frac{\hbar}{i} \int_0^L dx\, \psi_m^*(x) \frac{d\psi_n(x)}{dx} \tag{2.35}$$

A partial integration gives

$$\int_0^L dx\, \psi_m^*(x) \frac{d\psi_n(x)}{dx} = [\psi_m^*(x)\psi_n(x)]_0^L - \int_0^L dx \frac{d\psi_m^*(x)}{dx}\psi_n(x) \quad (2.36)$$

With our boundary conditions, the first term on the r.h.s. *vanishes*, and hence the momentum operator p is *hermitian*

$$\int_0^L dx\, \psi_m^*(x) p\psi_n(x) = \int_0^L dx\, [p\psi_m(x)]^*\, \psi_n(x) \qquad ;\text{ hermitian} \quad (2.37)$$

Note that the hermiticity of the operator depends crucially on the boundary conditions in the problem.

It is evident that the above momentum eigenfunctions are also eigenfunctions of the hamiltonian $H = p^2/2m$

$$\begin{aligned} H\psi_n(x) &= E_n\psi_n(x) \\ E_n &= \frac{(\hbar k_n)^2}{2m} \end{aligned} \quad (2.38)$$

A repetition of the previous calculation shows that the hamiltonian $H = p^2/2m$ is also hermitian [see Eq. (2.24)].

These stationary states for a particle going around in a circle are eigenstates of momentum, with a discrete quantum difference

$$\hbar\Delta k = \frac{2\pi\hbar}{L} \quad (2.39)$$

between the eigenvalues. The probability density in each stationary state is *constant*

$$\rho_n(x) = |\psi_n(x)|^2 = \frac{1}{L} \quad (2.40)$$

There is no preferred position on the circle.

2.6 General Solution

Let us try to construct the general solution to the Schrödinger equation for a free particle moving around the circle from these separated solutions

$$\Psi(x,t) = \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar} \qquad ;\text{ general solution} \quad (2.41)$$

Since the Schrödinger equation is linear, the principle of *superposition* holds, and any linear combination of solutions is again a solution.

The Schrödinger equation is first order in the time derivative, so one has to specify the wave function everywhere in space at the initial time (say $t = 0$) to specify the solution

$$\Psi(x, 0) \equiv g(x) = \sum_n c_n \, \psi_n(x) \tag{2.42}$$

Use the orthonormality of the eigenfunctions to determine the expansion coefficients

$$c_m = \int_0^L dx \, \psi_m^*(x) g(x) \tag{2.43}$$

The functions $\psi_n(x)$ form a *complete set*, and it is known that an arbitrary piecewise continuous function can be expanded in such a complex Fourier series.[3]

[3]See [Fetter and Walecka (2003)]; see also Prob. 9.1.

Chapter 3

Include Potential $V(x)$

3.1 Schrödinger Equation

Let us try and extend the Schrödinger equation to describe a non-relativistic particle of mass m moving in a real potential $V(x)$. An evident approach is to just appeal to our classical mechanics arguments and extend the hamiltonian by

$$\frac{p^2}{2m} \;\rightarrow\; \frac{p^2}{2m} + V(x) \tag{3.1}$$

Let us see what happens to our previous quantum mechanics arguments if we work with the following hamiltonian

$$H(p,x) = \frac{p^2}{2m} + V(x) \qquad ;\text{ hamiltonian} \tag{3.2}$$

We will continue to write the momentum in the Schrödinger equation as

$$p = \frac{\hbar}{i}\frac{\partial}{\partial x} \qquad ;\text{ momentum} \tag{3.3}$$

The hamiltonian is still *hermitian*, since a real potential is hermitian

$$\int dx\, \psi^*(x) V\psi(x) = \int dx\, \left[V\psi(x)\right]^* \psi(x) \qquad ;\text{ hermitian} \tag{3.4}$$

The separated solutions are then again stationary states

$$\Psi(x,t) = \psi(x) e^{-iEt/\hbar} \tag{3.5}$$

where E is the real energy

$$\frac{\int dx\, \psi^*(x) H\psi(x)}{\int dx\, |\psi(x)|^2} = E \tag{3.6}$$

The potential *cancels* on the r.h.s. of Eq. (2.15)

$$\frac{1}{i\hbar}\left\{\Psi^*(x,t)\left[V\Psi(x,t)\right]-\left[V\Psi(x,t)\right]^*\Psi(x,t)\right\}=0 \tag{3.7}$$

Thus the argument on the continuity equation for the probability density goes through unaltered

$$\frac{\partial\rho(x,t)}{\partial t}+\frac{\partial S(x,t)}{\partial x}=0 \qquad ;\text{ continuity equation} \tag{3.8}$$

where

$$\begin{aligned}\rho(x,t)&=|\Psi(x,t)|^2 && ;\text{ probability density}\\ S(x,t)&=\frac{1}{2m}\left\{\Psi^\star(x,t)p\Psi(x,t)+\left[p\Psi(x,t)\right]^*\Psi(x,t)\right\} && \\ & && ;\text{ probability flux}\end{aligned} \tag{3.9}$$

In particular, the probability density and flux are still time-independent in the stationary states

$$\begin{aligned}\rho(x)&=|\psi(x)|^2 && ;\text{ stationary states}\\ S(x)&=\frac{1}{2m}\left\{\psi^\star(x)p\psi(x)+\left[p\psi(x)\right]^*\psi(x)\right\} &&\end{aligned} \tag{3.10}$$

3.2 Particle in a Box

Before investigating the general boundary conditions, let us first consider another simple physical situation where the potential is repulsive and grows very large. The potential then effectively presents a *wall* to the particle where the wave function must *vanish*. If a particle moves in one dimension along the x-axis and is in a box of length L, the boundary conditions become (see Fig. 3.1)

$$\psi(0)=\psi(L)=0 \qquad ;\text{ particle in box} \tag{3.11}$$

The energy eigenstates in this case are

$$\begin{aligned}\psi_n(x)&=\sqrt{\frac{2}{L}}\,\sin k_n x &&\\ k_n&=\frac{n\pi}{L} && ;\ n=1,2,3,\cdots\end{aligned} \tag{3.12}$$

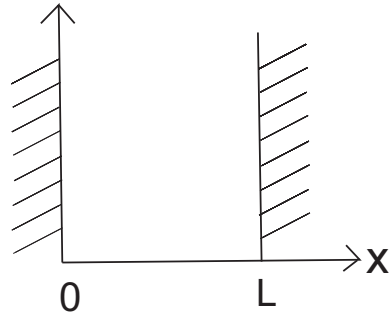

Fig. 3.1 Free particle moving in a one-dimensional box of length L, with the distance x along the axis. There is an infinite repulsive potential, or wall, on both sides.

The corresponding energy eigenvalues are

$$E_n = \frac{(\hbar k_n)^2}{2m} = \frac{(\hbar \pi n)^2}{2mL^2} \tag{3.13}$$

The energy eigenstates are no longer also eigenstates of momentum, since now the particle is bouncing off the walls; however, the momentum operator is still *hermitian* since the boundary term on the r.h.s. of Eq. (2.36) still vanishes

$$[\psi_m^*(x)\psi_n(x)]_0^L = 0 \tag{3.14}$$

We show the first four eigenfunctions and corresponding probability densities in Figs. 3.2 and 3.3. If one has some way of repeatedly observing the location of the particle in these stationary states, then one will indeed observe the spatial distribution in Fig. 3.3. *This is a real, quite amazing, consequence of quantum mechanics!*

The general solution to the problem of a non-relativistic particle in a one-dimensional box is constructed exactly as in the last chapter

$$\Psi(x,t) = \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar} \qquad ; \text{ general solution} \tag{3.15}$$

The eigenfunctions again satisfy the orthonormality condition

$$\int_0^L dx\, \psi_n^*(x)\psi_m(x) = \delta_{m,n} \tag{3.16}$$

The expansion coefficients are thus obtained from the initial condition just

as before

$$\Psi(x,0) \equiv g(x) = \sum_n c_n \, \psi_n(x)$$

$$c_m = \int_0^L dx \, \psi_m^*(x) g(x) \tag{3.17}$$

The functions $\psi_n(x)$ form a *complete set*, and it is known that an arbitrary piecewise continuous function can be expanded in such a Fourier sine series.[1]

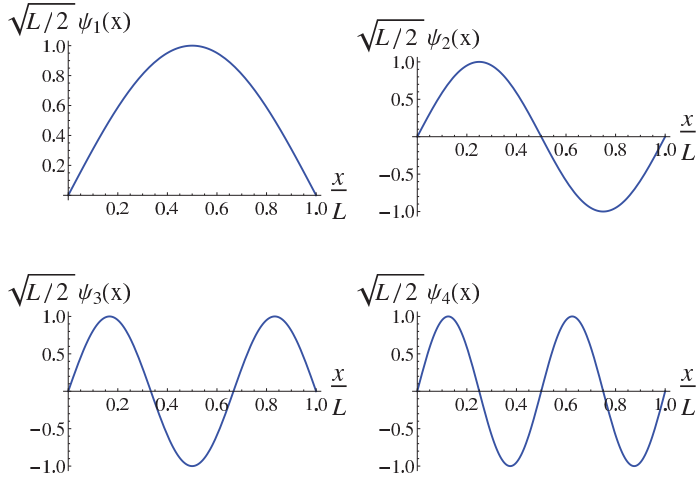

Fig. 3.2 First four wave functions of a particle in a one-dimensional box of length L. Taken from [Amore and Walecka (2013)].

3.3 Boundary Conditions

The separated Schrödinger equation is a second-order differential equation in space. With no additional input, the evident boundary condition is to ask that the physically acceptable solutions, and their first derivatives, be *continuous*

$$\psi(x),\ \psi'(x) \quad \text{continuous} \qquad ;\ \text{boundary conditions} \tag{3.18}$$

[1] Again, see [Fetter and Walecka (2003)].

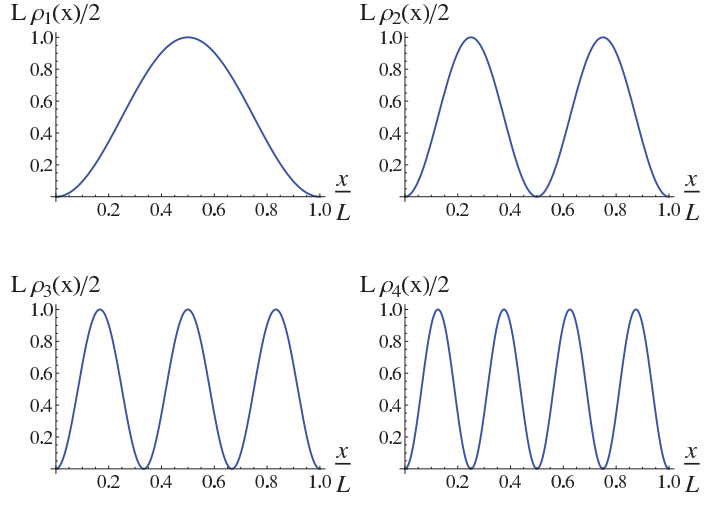

Fig. 3.3 Probability densities corresponding to the first four wave functions of a particle in a one-dimensional box of length L. Taken from [Amore and Walecka (2013)].

This sounds so obvious, but as we shall now see, this has essential, and quite unexpected, consequences.

3.4 Barrier Penetration

Consider a non-relativistic particle moving in one dimension against a barrier of height V_0 extending for all $x > 0$. Suppose its energy is less than the barrier height. Then classically it can never get into the barrier, since its kinetic energy is a positive definite quantity

$$\begin{aligned} E &= \frac{m}{2}\dot{x}^2 + V_0 \qquad ; \; x > 0 \\ E - V_0 &= \frac{m}{2}\dot{x}^2 \geq 0 \end{aligned} \tag{3.19}$$

Let us now ask what happens in quantum mechanics with the above boundary conditions. Consider a stationary state with an energy $E < V_0$ below the barrier. To the left of the barrier, we have both an incident and reflected wave (see Fig. 3.4)

$$\psi(x) = e^{ikx} + a\, e^{-ikx} \qquad ; \; x < 0 \tag{3.20}$$

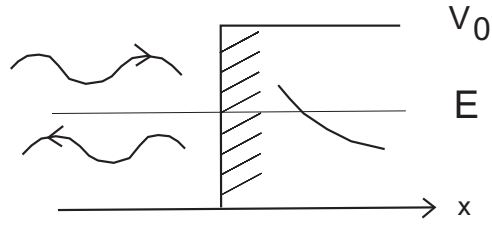

Fig. 3.4 Free particle moving in one dimension against a barrier of height V_0 with $E < V_0$. There is an incident and reflected wave, as well as a decaying wave inside the barrier.

Inside the barrier, the Schrödinger equation reads

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\right]\psi(x) = E\psi(x) \qquad ;\ x > 0 \tag{3.21}$$

This can be rearranged to read

$$\begin{aligned} \frac{d^2\psi(x)}{dx^2} &= \kappa^2\psi(x) \qquad ;\ x > 0 \\ \kappa^2 &\equiv \frac{2m(V_0 - E)}{\hbar^2} \end{aligned} \tag{3.22}$$

The acceptable solution inside the barrier, which extends out to infinity, is evidently

$$\psi(x) = b\, e^{-\kappa x} \qquad ;\ x > 0 \tag{3.23}$$

Let us now match the wave functions, and their first derivatives, at the origin $x = 0$

$$\begin{aligned} 1 + a &= b \\ ik(1 - a) &= -\kappa b \end{aligned} \tag{3.24}$$

The solution to these equations gives

$$b = \frac{2k}{k + i\kappa} \tag{3.25}$$

Several features of this result are of interest:

- In contrast to the classical result, there is now a finite probability of finding the particle *inside* the barrier;

- This comes from our choice of boundary conditions in Eq. (3.18). We might, instead, have just imposed the classical result $\psi(0) = 0$. This would have been *incorrect*;
- As the barrier height increases, that is as $\kappa \to \infty$, the amplitude $b \to 0$. The amplitude to find the particle inside the barrier vanishes, and in this limit we indeed have a *wall*;
- If the barrier were to be of finite spatial extent, there would be some amplitude for the wave to actually get through it.[2] This *barrier penetration is entirely a quantum effect!* It is now observed every day in the laboratory.

3.5 Bound States

As another application of the one-dimensional Schrödinger equation, consider the lowest-energy ground state in an attractive square-well potential

$$V(x) = -V_0 \qquad ; -L < x < L \tag{3.26}$$

Here $V_0 > 0$. We are looking for a *bound state* with (see Fig. 3.5)

$$E = -E_b < 0 \qquad ; \text{ bound state} \tag{3.27}$$

The ground state will be symmetric, and so we only have to consider $x > 0$.

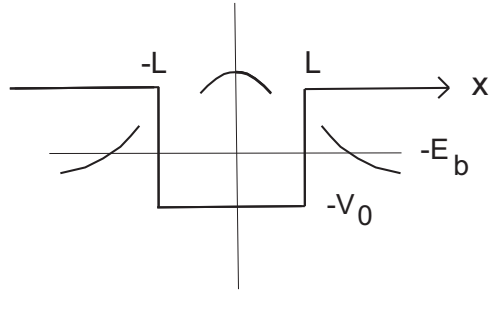

Fig. 3.5 Bound ground state in a square-well potential in one dimension. Here we make the minus signs explicit, with $V = -V_0 < 0$, and $E = -E_b < 0$. We are looking for the symmetric ground-state eigenfunction, with no nodes and minimum curvature.

[2] See, for example, [Walecka (2008)].

Inside the potential, we want the symmetric solution with minimum curvature, and so

$$\begin{aligned} \psi(x) &= a\,\cos(\kappa_i x) \qquad\qquad ;\ x < L \\ \kappa_i^2 &= \frac{2m}{\hbar^2}(V_0 - E_b) \end{aligned} \tag{3.28}$$

Outside the potential, since we seek the bound state confined by the potential, we keep just the decreasing exponential

$$\begin{aligned} \psi(x) &= b\,e^{-\kappa_o x} \qquad\qquad ;\ x > L \\ \kappa_o^2 &= \frac{2m}{\hbar^2}E_b \end{aligned} \tag{3.29}$$

Now match the wave functions and their derivatives at $x = L$. Better yet, match the *logarithmic derivative*, which is the ratio of the derivative to the function, since one then gets rid of the amplitudes. Thus, with a change in sign,

$$\kappa_i \tan(\kappa_i L) = \kappa_o \qquad ;\ \text{eigenvalue equation} \tag{3.30}$$

Given V_0, this transcendental eigenvalue equation must be solved numerically for E_b. Fortunately, we can readily extract two limiting cases:

(1) Suppose V_0 is very large, then E_b will also be very large, and so will the r.h.s. of Eq. (3.30). Now adjust V_0. Start with $V_0 = E_b$, in which case the l.h.s. vanishes. Move V_0 away from E_b. By the time one gets to $(\kappa_i L) = \pi/2$, one will have found a solution to Eq. (3.30) since the l.h.s. is infinite at that point. Hence, as $V_0 \to \infty$ one has

$$E_b = V_0 - \frac{\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2 \qquad ;\ V_0 \to \infty \tag{3.31}$$

When the well is very deep, the ground state looks just like the ground state of a particle in a one-dimensional box of length $2L$.

(2) Suppose V_0 goes to zero. E_b then also goes to zero, and the r.h.s. of Eq. (3.30) is very small.[3] Again, start with $V_0 = E_b$ in which case the l.h.s. vanishes. Move V_0 away from E_b a little. An expansion of the l.h.s. of Eq. (3.30) for small $(\kappa_i L)$ gives

$$\kappa_i(\kappa_i L) = \kappa_o \tag{3.32}$$

[3]The wave function now falls off only very slowly outside of the potential.

It is best to write this in dimensionless form. Introduce

$$v_0 \equiv \frac{2mL^2}{\hbar^2}V_0 \qquad ;\ \varepsilon_b \equiv \frac{2mL^2}{\hbar^2}E_b \tag{3.33}$$

The eigenvalue Eq. (3.32) then reads

$$v_0 - \varepsilon_b = \sqrt{\varepsilon_b} \qquad ;\ v_0 \to 0 \tag{3.34}$$

As $v_0 \to 0$, the solution to this equation is

$$\varepsilon_b = v_0^2 \qquad ;\ v_0 \to 0 \tag{3.35}$$

For the attractive square-well in one dimension with $v_0 \to 0$, there will always be a bound ground state with this binding energy ε_b. Furthermore, in this state, the normalized wave function exists almost entirely outside of the potential! Again, a quite amazing result of quantum mechanics.

3.6 Higher Dimensions

So far, for simplicity, we have worked in just one dimension where the Schrödinger equation reads

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t} \tag{3.36}$$

Here the partial derivatives imply that the other variable in the set (x,t) is to be kept constant. To increase the number of dimensions, we can simply follow our work on the wave equation and replace

$$\frac{\partial^2}{\partial x^2} \to \nabla^2 \tag{3.37}$$

where ∇^2 is the *laplacian*

$$\begin{aligned}
\nabla^2 &= \frac{\partial^2}{\partial x^2} && ;\ \text{one dimension} \\
&= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} && ;\ \text{two dimensions} \\
&= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} && ;\ \text{three dimensions}
\end{aligned} \tag{3.38}$$

This is equivalent to writing the Schrödinger equation as

$$H\Psi(\vec{x},t) = \left[\frac{\vec{p}^{\,2}}{2m} + V(\vec{x})\right]\Psi(\vec{x},t) = i\hbar\frac{\partial\Psi(\vec{x},t)}{\partial t} \tag{3.39}$$

and expanding the momentum to read

$$p_j = \frac{\hbar}{i}\frac{\partial}{\partial x_j} \qquad ;\ j = 1, 2, \cdots \tag{3.40}$$

where the index j now labels the cartesian axes.

As one example, consider a particle of mass m in a square two-dimensional box with sides L. Here the boundary conditions are those of walls, and the eigenfunctions and eigenvalues are evidently

$$\psi_{n_x,n_y}(x,y) = \left(\frac{2}{L}\right)\sin\left(\frac{n_x\pi x}{L}\right)\sin\left(\frac{n_y\pi y}{L}\right) \qquad ;\ (n_x, n_y) = 1, 2, 3, \cdots$$
$$E_{n_x,n_y} = \frac{\hbar^2\pi^2}{2mL^2}\left(n_x^2 + n_y^2\right) \tag{3.41}$$

The general solution to the Schrödinger equation is correspondingly

$$\Psi(x,y,t) = \sum_{n_x}\sum_{n_y} c_{n_x,n_y}\psi_{n_x,n_y}(x,y)\, e^{-iE_{n_x,n_y}\,t/\hbar} \tag{3.42}$$

3.7 Perturbation Theory

Suppose the hamiltonian has an additional small piece $\delta V(x)$, which makes the Schrödinger equation difficult to solve analytically

$$H \to H_0 + \delta V(x) \tag{3.43}$$

We return to Eq. (3.6)

$$E = \frac{\int dx\, \psi^*(x) H \psi(x)}{\int dx\, |\psi(x)|^2} = \frac{\int dx\, \psi^*(x)[H_0 + \delta V(x)]\psi(x)}{\int dx\, |\psi(x)|^2} \tag{3.44}$$

Let us use the eigenfunction $\psi_n(x)$ of H_0 in this expression to obtain

$$E_n = E_n^0 + \frac{\int dx\, \psi_n^*(x)[\delta V(x)]\psi_n(x)}{\int dx\, |\psi_n(x)|^2} \tag{3.45}$$

This provides the first-order *perturbation theory* expression for the shift in the eigenvalue

$$\delta E_n = \frac{\int dx\, \psi_n^*(x)[\delta V(x)]\psi_n(x)}{\int dx\, |\psi_n(x)|^2} \quad ;\ \text{perturbation theory} \tag{3.46}$$

The small shift in the eigenvalue is the integral of the perturbation over the eigenfunction.

As an example, suppose that with the particle in the box in Fig. 3.1 there is a small, narrow potential step at the midpoint

$$\delta V(x) = \nu_0 \qquad ; \left| x - \frac{L}{2} \right| < l \tag{3.47}$$

where $l \ll L$. The eigenfunctions are $\sqrt{2/L}\,\sin(n\pi x/L)$. For odd n, the magnitude of the sine is unity at the midpoint where $x = L/2$. For even n, it vanishes there.[4] Hence, for $l \ll L$, one has

$$\begin{aligned} \delta E_n &= 4\nu_0 \frac{l}{L} \qquad ; \; n = 1, 3, 5, \cdots \\ &= 0 \qquad\qquad ; \; n = 2, 4, 6, \cdots \end{aligned} \tag{3.48}$$

3.7.1 *Non-Degenerate Perturbation Theory*

Let us make the analysis more general. We want to solve for the eigenfunctions and eigenvalues in the Schrödinger equation

$$H\psi(x) = [H_0 + \delta V(x)]\psi(x) = E\psi(x) \tag{3.49}$$

Expand the wave function $\psi(x)$ in the complete set of eigenstates of H_0

$$\begin{aligned} \psi(x) &= \sum_m c_m\, \psi_m(x) \\ H_0\psi_m(x) &= E_m^0 \psi_m(x) \end{aligned} \tag{3.50}$$

Substitute this in the above equation

$$\sum_m \left(E - E_m^0\right) c_m \psi_m(x) = \delta V(x)\psi(x) \tag{3.51}$$

Now multiply by $\psi_n^*(x)$ on the left, integrate over x, and use the orthonormality of the eigenfunctions

$$c_n = \frac{1}{E - E_n^0} \int dx\, \psi_n^*(x)\delta V(x)\psi(x) \tag{3.52}$$

We now make a rather unusual choice of norm for $\psi(x)$

$$c_n = 1 \qquad ; \text{ choice of norm} \tag{3.53}$$

Let us discuss this:

- This choice is for a given n;

[4] See Figs. 3.2 and 3.3.

- The Schrödinger equation is a homogeneous differential equation, and any norm of $\psi(x)$ can be chosen, as long as physical results are calculated from expressions analogous to Eq. (2.23);
- This choice will yield ($\psi \to \psi_n$, $E \to E_n^0$) as $\delta V \to 0$, which allows us to focus on the evolution of a given eigenfunction and eigenvalue as the perturbation is turned on;
- As long as no denominators vanish, we then have the following *exact results*

$$\psi(x) = \psi_n(x) + \sum_{m \neq n} \frac{\psi_m(x)}{E - E_m^0} \int dy\, \psi_m^*(y) \delta V(y) \psi(y)$$

$$E = E_n^0 + \int dx\, \psi_n^*(x) \delta V(x) \psi(x) \tag{3.54}$$

This comprises a complicated *inhomogeneous integral equation* for $\psi(x)$ and E.

Although the above expression is complicated, we obtain very useful results by consistently expanding as a *power series in δV!*

$$\psi(x) = \psi_n(x) + \sum_{m \neq n} \frac{\psi_m(x)}{E_n^0 - E_m^0} \int dy\, \psi_m^*(y) \delta V(y) \psi_n(y) + \cdots$$

$$E = E_n^0 + \int dx\, \psi_n^*(x) \delta V(x) \psi_n(x) + \sum_{m \neq n} \frac{1}{E_n^0 - E_m^0} \left| \int dy\, \psi_m^*(y) \delta V(y) \psi_n(y) \right|^2 + \cdots \tag{3.55}$$

This is *non-degenerate perturbation theory*, where we have assumed that none of the denominators vanish. Note that a given order in δV in the wave function always yields the energy shift to one higher order.

Problems 3.5 and 3.6 contain some applications of these results. If there is degeneracy present, then one has to get fancier with the perturbation theory.[5]

[5] See, for example, [Walecka (2013)].

Chapter 4

Scattering

We turn to some elementary considerations on the scattering of a particle in three dimensions from a spherically symmetric potential $V(r)$.

4.1 Incident Plane Wave

Suppose we prepare a particle in a state of definite incident momentum

$$\psi_{\rm inc}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} \qquad ;\ \vec{p} = \hbar\,\vec{k} \tag{4.1}$$

This is also an eigenstate of energy, with

$$E = \frac{(\hbar\vec{k})^2}{2m} \tag{4.2}$$

It satisfies the free Schrödinger equation

$$\left(\nabla^2 + k^2\right)\psi_{\rm inc}(\vec{x}) = 0 \tag{4.3}$$

Since we are eventually going to compute ratios of fluxes, the choice of overall norm is immaterial.

Now use $\vec{k}\cdot\vec{x} = kr\cos\theta$ and expand the plane wave in a complete set of functions of $\cos\theta$

$$e^{ikr\cos\theta} = \sum_l (2l+1) i^l\, j_l(kr)\, P_l(\cos\theta) \tag{4.4}$$

Here $P_l(\cos\theta)$ is a *Legendre polynomial* satisfying

$$\int_{-1}^{1} d\cos\theta\; P_l(\cos\theta)P_{l'}(\cos\theta) = \frac{2}{2l+1}\delta_{l,l'}$$

$$P_0(\cos\theta) = 1 \qquad ;\; P_1(\cos\theta) = \cos\theta \qquad ;\; P_2(\cos\theta) = \frac{1}{2}(3\cos^2\theta - 1)$$
$$;\ \text{etc.} \tag{4.5}$$

We can then solve for the amplitude $j_l(kr)$ according to

$$j_l(kr) = \frac{1}{2i^l}\int_{-1}^{1} d\cos\theta\, P_l(\cos\theta)e^{ikr\cos\theta} \tag{4.6}$$

This defines the non-singular *spherical Bessel function* $j_l(kr)$. Let us compute the first two, with $\rho \equiv kr$ and $\mu \equiv \cos\theta$,

$$j_0(\rho) = \frac{1}{2}\int_{-1}^{1} d\mu\, e^{i\rho\mu} = \frac{1}{2i\rho}\left(e^{i\rho} - e^{-i\rho}\right) = \frac{\sin\rho}{\rho}$$
$$j_1(\rho) = \frac{1}{2i}\int_{-1}^{1} d\mu\,\mu e^{i\rho\mu} = -\frac{dj_0(\rho)}{d\rho} = \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho} \tag{4.7}$$

Note that through this order[1]

$$j_l(\rho) \to \frac{\rho^l}{(2l+1)!!} \qquad ;\; \rho \to 0$$
$$j_l(\rho) \to \frac{1}{\rho}\cos\left[\rho - (l+1)\pi/2\right] \qquad ;\; \rho \to \infty \tag{4.8}$$

where $(2l+1)!! = 1\cdot 3\cdot 5\cdots(2l+1)$.

4.2 *S*-Wave Scattering

The separated solutions in Eq. (4.4) satisfy the Schrödinger equation in spherical coordinates. Let us focus on the $l = 0$ term, which is the dominant term at low energy where $kr \to 0$,

$$\left(\nabla^2 + k^2\right) j_0(kr) = \left(\nabla^2 + k^2\right)\frac{\sin(kr)}{kr} = 0 \tag{4.9}$$

Evidently the radial part of the laplacian in spherical coordinates is

$$\nabla^2 \doteq \frac{1}{r}\left(\frac{\partial^2}{\partial r^2}\right) r \tag{4.10}$$

[1]These relations actually hold to all orders; see also Prob. 4.2.

for then the above becomes[2]

$$\left(-k^2 + k^2\right) \frac{\sin(kr)}{kr} = 0 \tag{4.11}$$

Let us now include a potential $V(r)$, and work at very low energy. The separated $l = 0$ Schrödinger equation, or *s-wave equation*, becomes

$$\left[\frac{1}{r}\frac{\partial^2}{\partial r^2} r - v(r) + k^2\right] \psi(r) = 0 \qquad ;\ v(r) \equiv \frac{2m}{\hbar^2} V(r) \tag{4.12}$$

Let us define

$$\psi(r) \equiv \frac{u(r)}{r} \qquad ;\ s\text{-wave} \tag{4.13}$$

The s-wave Schrödinger equation for $u(r)$ then becomes

$$\left[\frac{d^2}{dr^2} - v(r) + k^2\right] u(r) = 0 \qquad ;\ s\text{-wave eqn} \tag{4.14}$$

4.3 Spherical Square Well

Let us solve the s-wave Schrödinger equation for an attractive square-well potential of the form

$$v(r) = -v_0 \qquad ;\ r < d \tag{4.15}$$

Outside the potential we will have some linear combination of sine and cosine, which we can write

$$u_{\text{out}}(r) = A \sin(kr + \delta_0) \qquad ;\ r > d \tag{4.16}$$

where δ_0 is the s-wave *phase shift*. Inside the potential, if we assume there is no bound-state and keep just the solution that is non-singular at the origin, we have

$$\begin{aligned} u_{\text{in}}(r) &= B \sin(\kappa r) \qquad ;\ r < d \\ \kappa^2 &\equiv k^2 + v_0 \end{aligned} \tag{4.17}$$

[2]The laplacian in spherical coordinates is actually

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial \phi^2}$$

The first term is the same as in Eq. (4.10).

Upon equating the logarithmic derivative at the potential boundary, we obtain an equation for the phase shift $\delta_0(k)$

$$k \cot(kd + \delta_0) = \kappa \cot(\kappa d) \tag{4.18}$$

4.4 Scattering Boundary Condition

We first note that a spherical wave going out from the origin is a solution to the Schrödinger equation, just as in Eq. (4.11),

$$(\nabla^2 + k^2)\frac{e^{ikr}}{r} = 0 \qquad ; \text{ outgoing wave} \tag{4.19}$$

We now require, on physical grounds, that the solution to the scattering problem far away from the potential should consist of the incident wave plus an outgoing scattered wave

$$\psi = \psi_{\text{inc}} + \psi_{\text{scatt}} \qquad ; \ r \to \infty \tag{4.20}$$

This is known as the *scattering boundary condition.* In detail, this says that

$$\psi(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} + f(k,\theta)\frac{e^{ikr}}{r} \qquad ; \ r \to \infty$$
$$; \text{ scattering b.c.} \tag{4.21}$$

The amplitude of the outgoing scattered wave $f(k,\theta)$ is known as the *scattering amplitude.*

Let us see how this works for our s-wave scattering. In order to satisfy this boundary condition, we must choose a particular form for the amplitude A of the wave function outside of the potential in Eq. (4.16)

$$u_{\text{out}}(r) = \frac{e^{i\delta_0}}{k}\sin(kr + \delta_0) \qquad ; \ r > d$$
$$\psi(r) = \frac{u_{\text{out}}(r)}{r} \tag{4.22}$$

Now look at

$$\psi_{\text{scatt}}(r) = \psi(r) - \psi_{\text{inc}}(r) \qquad ; \ r > d \tag{4.23}$$

This gives

$$\begin{aligned}\psi_{\text{scatt}}(r) &= \frac{e^{i\delta_0}}{kr}\sin\left(kr+\delta_0\right) - \frac{\sin(kr)}{kr} \\ &= \frac{e^{i\delta_0}}{2ikr}\left[e^{i(kr+\delta_0)} - e^{-i(kr+\delta_0)}\right] - \frac{1}{2ikr}\left(e^{ikr} - e^{-ikr}\right) \\ &= \frac{1}{2ik}\left(e^{2i\delta_0} - 1\right)\frac{e^{ikr}}{r} \end{aligned} \tag{4.24}$$

Note that the incoming wave has *cancelled*, and we satisfy the scattering boundary condition. Furthermore, we can identify the s-wave scattering amplitude as

$$f_0(k) = \frac{1}{2ik}\left(e^{2i\delta_0} - 1\right) = \frac{e^{i\delta_0}}{k}\sin\delta_0 \qquad ;\ s\text{-wave} \tag{4.25}$$

The general expression for the scattering amplitude, including all partial waves, is

$$f(k,\theta) = \sum_l (2l+1) f_l(k) P_l(\cos\theta) \tag{4.26}$$

As $k \to 0$ it is only the s-wave that contributes to the scattering amplitude, since it is only the s-wave that gets into the potential.

4.5 Cross-Section

The classical concept of a scattering or reaction cross-section is as follows: One prepares a beam of particles, with a certain incident flux I_{inc}, where the incident flux is the number of particles crossing a unit transverse area per unit time. The *cross-section* is then a little element of transverse area such that if a particle goes through it, a certain event takes place. Hence the *rate* of such events taking place is

$$I_{\text{inc}}\, d\sigma_{fi} = \text{number of events } i \to f \text{ per unit time} \tag{4.27}$$

In quantum mechanics we deal with *probability*, and its rates and fluxes. The probability flux in three dimensions follows from Eq. (3.10) as

$$\vec{S}(\vec{x}\,) = \frac{\hbar}{2im}\left[\psi^\star\vec{\nabla}\psi - \left(\vec{\nabla}\psi\right)^*\psi\right] \tag{4.28}$$

This has the interpretation as the amount of probability flowing through a unit transverse area per unit time. The elastic scattering cross-section

$d\sigma$ for the scattering of a particle into a solid angle $d\Omega$ (and corresponding area $r^2 d\Omega$) in quantum mechanics is therefore[3]

$$\left(\hat{k} \cdot \vec{S}_{\rm inc}\right) d\sigma = \left(\hat{r} \cdot \vec{S}_{\rm scatt}\right) r^2 d\Omega \tag{4.29}$$

With the incident and scattered wave functions in Eq. (4.21), one has

$$\begin{aligned} \hat{k} \cdot \vec{S}_{\rm inc} &= \frac{\hbar k}{m} \\ \hat{r} \cdot \vec{S}_{\rm scatt} &= \frac{\hbar k}{m r^2} |f(k,\theta)|^2 \end{aligned} \tag{4.30}$$

Here, in the second line, we have only taken the radial derivatives of the exponential as $r \to \infty$. Hence, the differential cross-section for elastic scattering into the solid angle $d\Omega$ in quantum mechanics is the absolute square of the scattering amplitude

$$\frac{d\sigma}{d\Omega} = |f(k,\theta)|^2 \qquad ;\ \text{elastic scattering} \tag{4.31}$$

For s-waves, one has

$$\frac{d\sigma}{d\Omega} = \frac{\sin^2 \delta_0}{k^2} \qquad ;\ s\text{-waves} \tag{4.32}$$

Prepare a beam of particles with a definite momentum $\hbar\vec{k}$. Count how many particles go through a unit transverse area in front of the target over some period of time. Multiply this number by the cross-section $d\sigma$. This will give you the number of particles that you have observed being scattered into the solid angle $d\Omega$. And your particle distribution will look like $|f(k,\theta)|^2$. It works! It is amazing that all this information is contained in the single wave function $\psi(\vec{x}\,)$!

4.6 High Energy

Let us look at the other scattering limit of high energy where very many partial waves contribute to the scattering amplitude. Recall that in electrostatics if we have the electrostatic potential satisfying

$$\nabla^2 \Phi = -\frac{1}{\varepsilon_0} \rho \tag{4.33}$$

[3]In this chapter, $(\hat{k}, \hat{r})$ are unit vectors.

where ρ is the charge density, then the potential is obtained by summing over the Coulomb interaction with each small charge element

$$\Phi(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\int \frac{1}{|\vec{r}-\vec{r}'|}\rho(\vec{r}')d^3r' \tag{4.34}$$

Here, we want to solve the equation

$$\left(\nabla^2 + k^2\right)\psi = v\psi \qquad ;\ v = \frac{2m}{\hbar^2}V(r) \tag{4.35}$$

In direct analogy, we can obtain the scattered wave by summing over the *outgoing wave* from each little source element[4]

$$\psi_{\text{scatt}}(\vec{r}) = -\frac{1}{4\pi}\int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}v(r')\psi(\vec{r}')d^3r' \tag{4.36}$$

With the inclusion of ψ_{inc}, which satisfies the homogeneous differential equation, the whole wave function then looks like

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi}\int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}v(r')\psi(\vec{r}')d^3r' \tag{4.37}$$

This produces an (exact) *inhomogeneous integral equation* for ψ.

Let us look at the asymptotic behavior of ψ_{scatt} for large r.[5] The distance $|\vec{r}-\vec{r}'|$ can be expanded as

$$|\vec{r}-\vec{r}'| = r - \hat{r}\cdot\vec{r}' + O(r'/r) \tag{4.38}$$

With the identification of the final scattering momentum $\vec{p}'$ through

$$\vec{p}' = \hbar\vec{k}' \equiv \hbar k\hat{r} \qquad ;\ \text{final momentum} \tag{4.39}$$

and the simple replacement of the denominator by r for large r, one has

$$\psi_{\text{scatt}}(r) = \frac{e^{ikr}}{r}\left[-\frac{1}{4\pi}\int e^{-i\vec{k}'\cdot\vec{r}'}v(r')\psi(\vec{r}')d^3r'\right] \tag{4.40}$$

This both demonstrates that ψ satisfies the correct scattering *boundary condition*, and it also allows us to identify the scattering *amplitude* as

$$f(k,\theta) = -\frac{1}{4\pi}\int e^{-i\vec{k}'\cdot\vec{r}'}v(r')\psi(\vec{r}')d^3r' \tag{4.41}$$

[4] We are actually employing the *Green's functions* for the differential equations.

[5] We assume sufficient convergence of the integral.

Now, just as with perturbation theory, we can start iterating the expressions to obtain a power series in v. The first iteration simply replaces ψ in the scattering amplitude by $\psi_{\rm inc}$, where

$$\psi_{inc}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \tag{4.42}$$

This produces first *Born approximation* for the scattering amplitude

$$f_{BA}(k,\theta) = -\frac{1}{4\pi}\int e^{i\vec{q}\cdot\vec{r}\,'} v(r')d^3r' \qquad ; \text{ Born approximation} \tag{4.43}$$

Here the *momentum transfer* $\hbar\vec{q}$ is defined through

$$\begin{aligned} \vec{q} &\equiv \vec{k} - \vec{k}\,' \\ q^2 &= 4k^2 \sin^2\frac{\theta}{2} \end{aligned} \tag{4.44}$$

The Born approximation for the scattering amplitude is simply the three-dimensional Fourier transform of the potential with respect to the momentum transfer! We give two applications in Probs. 4.5 and 4.6.

Chapter 5

Transition Rate

So far, we have focused on very simple physical systems in order to concentrate on the quantum mechanics (although we did get more realistic with s-wave scattering and the Born approximation). Let us continue in that vein as we turn to a study of *transition rates* in quantum theory.

5.1 Model Problem

Consider *two* particles moving in one dimension along the x-axis. Particle one is free to move in a large circle as in Fig. 2.1, so it satisfies periodic boundary conditions. It has the eigenfunctions and eigenvalues of Eqs. (2.31) and (2.32)

$$\begin{aligned} \psi_n(x) &= \frac{1}{\sqrt{L}} e^{2\pi i n x/L} \qquad ;\ n = 0, \pm 1, \pm 2, \cdots \\ E_n &= \frac{(2\pi\hbar)^2}{2mL^2} n^2 \qquad ;\ \text{particle one} \end{aligned} \tag{5.1}$$

The eigenfunctions satisfy the orthonormality condition in Eq. (2.33).

The second particle is confined to a box of a much shorter length as in Fig. 3.1, and it has the eigenfunctions and eigenvalues of Eqs. (3.12) and (3.13)[1]

$$\begin{aligned} \psi_n(x) &= \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \qquad ;\ n = 1, 2, 3, \cdots \\ E_n &= \frac{(\pi\hbar)^2}{2mL^2} n^2 \qquad ;\ \text{particle two} \end{aligned} \tag{5.2}$$

These eigenfunctions are illustrated in Figs. 3.2 and 3.3. They are also

[1] We will subsequently use the lengths L_1 for the big circle and L_2 for the box.

orthonormal. It is assumed here that the box is completely *transparent* to the first particle, which passes right through it.[2]

The starting hamiltonian and general solution for this two-particle system are then

$$\begin{aligned} H_0 &= \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V_{\rm box}(x_2) \\ \Psi_0(x_1, x_2, t) &= \sum_{n_1,n_2} c^0_{n_1,n_2}(t)\, \psi_{n_1}(x_1) e^{-iE_{n_1}t/\hbar}\, \psi_{n_2}(x_2) e^{-iE_{n_2}t/\hbar} \end{aligned} \tag{5.3}$$

This wave function satisfies the Schrödinger equation

$$i\hbar \frac{\partial \Psi_0(x_1, x_2, t)}{\partial t} = H_0 \Psi_0(x_1, x_2, t) \tag{5.4}$$

We have left a time-dependence in the coefficients $c^0_{n_1,n_2}(t)$ for generality, but let us see what happens when we substitute this solution in the Schrödinger equation

$$\begin{aligned} &\sum_{n_1,n_2} \left[i\hbar \frac{dc^0_{n_1,n_2}(t)}{dt} + (E_{n_1} + E_{n_2})\, c^0_{n_1,n_2}(t) \right] \psi_{n_1}(x_1) e^{-iE_{n_1}t/\hbar}\, \psi_{n_2}(x_2) e^{-iE_{n_2}t/\hbar} \\ &= \sum_{n_1,n_2} (E_{n_1} + E_{n_2})\, c^0_{n_1,n_2}(t)\, \psi_{n_1}(x_1) e^{-iE_{n_1}t/\hbar}\, \psi_{n_2}(x_2) e^{-iE_{n_2}t/\hbar} \end{aligned} \tag{5.5}$$

Upon cancellation of the common terms, and the use of the orthonormality of the eigenfunctions to extract a given coefficient, one obtains

$$\frac{dc^0_{n_1,n_2}(t)}{dt} = 0 \tag{5.6}$$

Hence, the expansion coefficients are independent of the time (which we already knew!), and we can simply evaluate them at the initial time, say $t = 0$

$$c^0_{n_1,n_2}(t) = c^0_{n_1,n_2}(0) \qquad ;\ \text{time-independent} \tag{5.7}$$

If we were to start in a given state $\psi_{n_1^0}(x_1)\psi_{n_2^0}(x_2)$, then all but one coefficient would vanish

$$c^0_{n_1,n_2} = \delta_{n_1,n_1^0}\, \delta_{n_2,n_2^0} \qquad ;\ \text{given initial state} \tag{5.8}$$

[2]The second particle might be bound to the target by a strong force that the projectile does not feel, for example.

Now let us make the problem a little more complicated and assume that the two particles *interact* through some short-range potential, so that the hamiltonian becomes

$$\begin{aligned} H &= H_0 + H' \\ H' &= V(x_1, x_2) \qquad ; \text{ interaction} \end{aligned} \tag{5.9}$$

The Schrödinger equation then reads

$$\begin{aligned} i\hbar \frac{\partial \Psi(x_1, x_2, t)}{\partial t} &= H\Psi(x_1, x_2, t) \\ &= (H_0 + H')\Psi(x_1, x_2, t) \end{aligned} \tag{5.10}$$

Let us again expand

$$\Psi(x_1, x_2, t) = \sum_{n_1, n_2} c_{n_1, n_2}(t)\, \psi_{n_1}(x_1) e^{-iE_{n_1}t/\hbar}\, \psi_{n_2}(x_2) e^{-iE_{n_2}t/\hbar} \tag{5.11}$$

A repetition of the above argument then gives

$$i\hbar \frac{dc_{n_1, n_2}(t)}{dt} = \sum_{n_1', n_2'} \langle n_1, n_2 | H' | n_1', n_2' \rangle\, c_{n_1', n_2'}(t) e^{i(E_{n_1} + E_{n_2} - E_{n_1'} - E_{n_2'})t/\hbar} \tag{5.12}$$

where

$$\begin{aligned} \langle n_1, n_2 | H' | n_1', n_2' \rangle \equiv \int_0^{L_1} dx_1 \int_0^{L_2} dx_2 \times \\ \psi_{n_1}^*(x_1) \psi_{n_2}^*(x_2)\, H'(x_1, x_2)\, \psi_{n_1'}(x_1) \psi_{n_2'}(x_2) \end{aligned} \tag{5.13}$$

The above provides an exact set of coupled, linear, first-order differential equations in the time for the expansion coefficients $c_{n_1, n_2}(t)$ in the presence of the interaction H'.

5.2 Golden Rule

Now, as previously, we are in a position to *iterate* these equations and obtain a power series in H'. Since the r.h.s. of Eqs. (5.12) is already linear in H', we can just make use of our previous coefficients $c^0_{n_1', n_2'}(t) = c^0_{n_1', n_2'}$

on the r.h.s.! This gives

$$i\hbar\frac{dc_{n_1,n_2}(t)}{dt} = \sum_{n_1',n_2'} \langle n_1,n_2|H'|n_1',n_2'\rangle\, c^0_{n_1',n_2'} e^{i(E_{n_1}+E_{n_2}-E_{n_1'}-E_{n_2'})/\hbar} + \cdots \tag{5.14}$$

Suppose it is the state $\psi_{n_1^0}(x_1)\psi_{n_2^0}(x_2)$ that is occupied at the initial time $t = 0$, so that

$$c^0_{n_1',n_2'} = \delta_{n_1',n_1^0}\,\delta_{n_2',n_2^0} \qquad ;\ \text{given initial state} \tag{5.15}$$

Then, at a later time, the amplitude for finding the system in a *different two-particle state* satisfies

$$i\hbar\frac{dc_{n_1,n_2}(t)}{dt} = \langle n_1,n_2|H'|n_1^0,n_2^0\rangle e^{i(E_{n_1}+E_{n_2}-E_{n_1^0}-E_{n_2^0})t/\hbar} \qquad ;\ (n_1,n_2)\neq(n_1^0,n_2^0) \tag{5.16}$$

Integration of this relation between the initial time $t = 0$, and the total elapsed time $t = T$, gives

$$c_{n_1,n_2}(T) = -\frac{1}{\hbar}\langle n_1,n_2|H'|n_1^0,n_2^0\rangle\,\frac{1}{\omega}\left(e^{i\omega T}-1\right) \tag{5.17}$$

where the initial and final energies of the pair, and energy *differences*, are defined by

$$\begin{aligned} E_0 &\equiv E_{n_1^0} + E_{n_2^0} \\ E &\equiv E_{n_1} + E_{n_2} \\ \hbar\omega &\equiv E - E_0 \end{aligned} \tag{5.18}$$

Now, by our general interpretation of quantum mechanics, the *probability* of finding the system in the state with (n_1, n_2) after time T, if it initially started in the state with (n_1^0, n_2^0), is given to leading order H' by

$$\begin{aligned} P_{fi}(T) &= |c_{n_1,n_2}(T)|^2 \qquad ;\ \text{transition probability} \\ &= \frac{1}{\hbar^2}\left|\langle n_1,n_2|H'|n_1^0,n_2^0\rangle\right|^2 \frac{4}{\omega^2}\sin^2\left(\frac{\omega T}{2}\right) \end{aligned} \tag{5.19}$$

The transition *rate* is the transition probability divided by the time

$$R_{fi}(T) \equiv \frac{P_{fi}(T)}{T} \qquad ;\ \text{transition rate} \tag{5.20}$$

Hence

$$R_{fi}(T) = \frac{1}{\hbar^2} \left| \langle n_1, n_2 | H' | n_1^0, n_2^0 \rangle \right|^2 f_T(\omega)$$
$$f_T(\omega) \equiv \left[T \frac{\sin^2 (\omega T/2)}{(\omega T/2)^2} \right] \tag{5.21}$$

Let us examine the function $f_T(\omega)$, which we plot in Fig. 5.1.

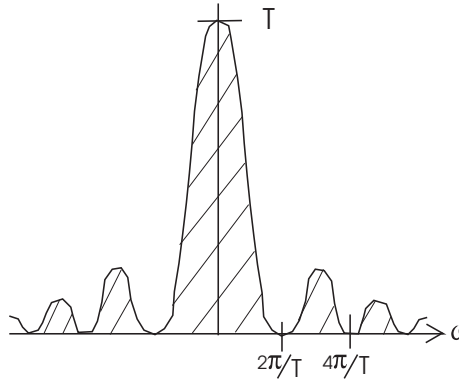

Fig. 5.1 Sketch of the function $f_T(\omega)$.

The function $f_T(\omega)$ has the following properties:

(1) For large T, at the origin ($\omega = 0$), it grows as T

$$f_T(0) \to T \qquad ; \; T \to \infty \tag{5.22}$$

(2) For large T, away from the origin ($\omega \neq 0$), it goes to zero

$$f_T(\omega) \to 0 \qquad ; \; T \to \infty \quad \omega \neq 0 \tag{5.23}$$

(3) When integrated over all ω, a simple change of variables $x \equiv \omega T/2$ gives

$$\int_{-\infty}^{\infty} f_T(\omega)\, d\omega = 2 \int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2}\, dx = 2\pi \qquad ; \text{ all } T \tag{5.24}$$

The last result is obtained from any good table of integrals;

(4) When multiplied by a well-behaved $F(\omega)$ and integrated over ω, then for large T one simply gets that function evaluated at the origin

$$\int_{-\infty}^{\infty} F(\omega) f_T(\omega)\, d\omega = 2\pi F(0) \qquad ;\ T \to \infty \tag{5.25}$$

Now we can either continue to work with the well-defined function $f_T(\omega)$ in the very large T limit, or we can introduce a *shorthand* for the above results. We introduce the *Dirac delta function*

$$\mathrm{Lim}_{T\to\infty}\, f_T(\omega) = 2\pi\delta(\omega) = 2\pi\hbar\,\delta(E - E_0) \tag{5.26}$$

It has the following properties:

$$\begin{aligned} \delta(E - E_0) &= 0 \qquad &;\ \text{if } E \neq E_0 \\ \delta(E - E_0) &= \infty \qquad &;\ \text{if } E = E_0 \\ \int F(E)\delta(E - E_0)\, dE &= F(E_0) \end{aligned} \tag{5.27}$$

For large T, the transition rate in Eq. (5.21) then becomes[3]

$$R_{fi} = \frac{P_{fi}(T)}{T} = \frac{2\pi}{\hbar}\left|\langle n_1, n_2|H'|n_1^0, n_2^0\rangle\right|^2 \delta(E - E_0) \qquad ;\text{transition rate} \tag{5.28}$$

We make several comments on this result:

- This expression is *exact* to $O(H')$;
- It is independent of T;
- It gives the transition rate to *any other* two-particle state in the space;
- One only recovers *energy conservation* for the transitions as $T \to \infty$;
- Fermi called Eq. (5.28) the "Golden Rule";
- It is one of the most useful results in quantum mechanics!

Although we will be content here to work to leading order in H', it is important for our understanding of quantum mechanics to realize that the full wave function $\Psi(x_1, x_2, t)$ in Eq. (5.11) simultaneously carries information on *all* the exact probability amplitudes $c_{n_1,n_2}(t)$.

[3]If you are uncomfortable working with the Dirac delta function, just continue to work with $f_T(\omega)$ for large T.

5.3 Density of Final States

Suppose we are doing a scattering experiment in our simple model. We can prepare the target in a given state with energy $E_{n_2^0}$, and we can prepare an incident beam with a well-defined energy $E_{n_1^0} = \hbar^2 k_0^2/2m_1$, where $k_0 = 2\pi n_1^0/L_1$. We certainly can achieve the energy resolution to determine that the target ends up in another state with discrete energy E_{n_2}; however, with the scattered particle, the situation is more complicated. Let us, for simplicity, call the size of the big region in which the first particle moves $L_1 \equiv L$. The final particle energy is $E_{n_1} = \hbar^2 k^2/2m_1$ with $k = 2\pi n_1/L$, and as L becomes very large, these energies are very closely spaced. Thus no matter how small our resolution dk is on the final particle, *many final states will lie within this resolution!* For large L, the *number* of these states dn_f is

$$dn_f = \frac{L}{2\pi} dk \qquad ;\ L \to \infty \tag{5.29}$$

Thus *all* of these states will get into our final detector, and the transition rate that we actually measure is of necessity

$$R_{fi}\, dn_f = R_{fi} \left(\frac{L}{2\pi} dk \right) \qquad ;\ \text{measured rate} \tag{5.30}$$

Equation (5.28) then reads

$$R_{fi}\, dn_f = \frac{2\pi}{\hbar} \left| \langle n_1, n_2 | H' | n_1^0, n_2^0 \rangle \right|^2 \delta(E - E_0) \left(\frac{L}{2\pi} dk \right) \tag{5.31}$$

Multiply and divide this expression by dE. It is then possible to immediately do the integral over E using Eq. (5.27), where we have summed over all of the energy-conserving events that get into our detector. Hence[4]

$$R_{fi}\, dn_f = \frac{2\pi}{\hbar} \left| \langle n_1, n_2 | H' | n_1^0, n_2^0 \rangle \right|^2 \rho_E \tag{5.32}$$

where ρ_E is known as the *density of final states*

$$\rho_E = \frac{L}{2\pi} \left(\frac{dk}{dE} \right) \qquad ;\ \text{density of final states} \tag{5.33}$$

[4]We suppress the integral symbol on the l.h.s., although we have now used $\int \delta(E - E_0) dE = 1$; we leave it this way because there are usually some variables left in dn_f [see, for example, Eq. (5.43)].

It follows that with a projectile energy of $E = \hbar^2 k^2/2m_1$, this density of final states is given by

$$\rho_E = \frac{L}{2\pi}\left(\frac{m_1}{\hbar^2 k}\right) \qquad ;\ E = \frac{(\hbar k)^2}{2m_1} \tag{5.34}$$

5.4 Incident Flux

The incident probability flux of the first particle in our model problem with an incident wave of the form

$$\psi_{n_1^0}(x_1) = \frac{1}{\sqrt{L}}\, e^{ik_0 x_1} \qquad ;\ \text{incident wave} \tag{5.35}$$

is given by Eq. (2.27) as

$$I_{\text{inc}} = \frac{1}{L}\left(\frac{\hbar k_0}{m_1}\right) \qquad ;\ \text{incident flux} \tag{5.36}$$

This is the probability flow of the incident particle past a given point per unit time. It is the *ratio* of the transition rate to the incident flux that is the physical observable here.

5.5 Summary

In *summary*, in our model problem the ratio of the transition rate to incident flux that we measure in our final particle detector is

$$\frac{1}{I_{\text{inc}}} R_{fi}\, dn_f = \left(\frac{k}{k_0}\right)\left(\frac{m_1}{\hbar^2 k}\right)^2 |\langle k, n_2|H'|k_0, n_2^0\rangle|^2 \tag{5.37}$$

$$\langle k, n_2|H'|k_0, n_2^0\rangle = \int_0^L dx_1\, e^{i(k_0-k)x_1} \int_0^{L_2} dx_2\, \psi^*_{n_2}(x_2) H'(x_2, x_1) \psi_{n_2^0}(x_2)$$

Note that the two factors of L coming from the density of final states and incident flux just cancel the factors of $(1/L)^2$ coming from the normalization of the projectile wave functions. If the integral over x_1 is convergent, its upper limit can be extended to infinity, and the size of the big region L in which the projectile moves has then *disappeared from the problem!* The above expression is analyzed in more detail in Prob. 5.1.[5]

[5] It is useful to note that the p.b.c. allows the integral over the coordinate x_1 of the first particle in the matrix element in Eq. (5.13) to be rewritten as $\int_{-L_1/2}^{L_1/2} dx_1$.

The extension to *higher dimensions* follows immediately from

$$\begin{aligned} dn_f &= \left(\frac{L}{2\pi}\right)^2 d^2k \qquad ; \text{ two-dimensions} \\ &= \left(\frac{L}{2\pi}\right)^3 d^3k \qquad ; \text{ three-dimensions} \end{aligned} \tag{5.38}$$

5.6 Born Approximation

Let us return to our three-dimensional problem of the scattering of a particle from a potential $V(r)$, and we calculate to lowest order in $V(r)$. This is now a one-body problem. We work in a large box of volume L^3 and apply p.b.c. The initial and final particle wave functions and energies are

$$\begin{aligned} \psi_i(\vec{x}\,) &= \frac{1}{\sqrt{L^3}} e^{i\vec{k}\cdot\vec{x}} \qquad ; \; E = \frac{(\hbar k)^2}{2m} \\ \psi_f(\vec{x}\,) &= \frac{1}{\sqrt{L^3}} e^{i\vec{k}'\cdot\vec{x}} \qquad ; \; E' = \frac{(\hbar k')^2}{2m} \end{aligned} \tag{5.39}$$

The initial probability flux is

$$I_{\text{inc}} = \hat{k}\cdot\vec{S}(\vec{x}\,) = \frac{1}{L^3}\frac{\hbar k}{m} \tag{5.40}$$

The transition rate multiplied by the number of final states is

$$R_{fi}\, dn_f = \frac{2\pi}{\hbar}|\langle f|V|i\rangle|^2 \delta(E'-E)\left[\frac{L^3}{(2\pi)^3} d^3k'\right] \tag{5.41}$$

Here the matrix element of the potential is given by

$$\langle f|V|i\rangle = \frac{1}{L^3}\int d^3x\, e^{i\vec{q}\cdot\vec{x}}\, V(r) \qquad ; \; \vec{q} \equiv \vec{k} - \vec{k}' \tag{5.42}$$

Multiply and divide the transition rate by dE', do the integral over the Dirac delta function, and invoke the resulting energy conservation to obtain

$$R_{fi}\, dn_f = \frac{2\pi}{\hbar}|\langle f|V|i\rangle|^2 \left[\frac{L^3}{(2\pi)^3} k^2 \left(\frac{dk}{dE}\right) d\Omega\right] \tag{5.43}$$

where $d\Omega$ is the solid angle into which the particle is scattered. Now use

$$\frac{dE}{dk} = \frac{\hbar^2 k}{m} \tag{5.44}$$

The differential scattering cross-section is then given by

$$\begin{aligned} d\sigma &= \frac{1}{I_{\rm inc}} R_{fi}\, dn_f \\ &= \left(\frac{m}{\hbar k}\right) \frac{1}{(2\pi)^2 \hbar} \left| \int d^3x\, e^{i\vec{q}\cdot\vec{x}}\, V(r) \right|^2 k^2 \left(\frac{m}{\hbar^2 k}\right) d\Omega \end{aligned} \tag{5.45}$$

Note that the factors of L have cancelled from this expression, which can be rewritten as

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= |f_{BA}(k,\theta)|^2 \\ f_{BA}(k,\theta) &= -\frac{1}{4\pi} \int d^3x\, e^{i\vec{q}\cdot\vec{x}}\, v(r) \qquad ;\ v(r) \equiv \frac{2m}{\hbar^2} V(r) \end{aligned} \tag{5.46}$$

This is precisely the Born approximation result in Eq. (4.43)!

It is quite amazing that with so many different factors coming from so many different places, we obtain the same result from our transition-rate analysis as we did from the time-independent scattering study. In the end, the transition-rate approach is more powerful and useful.

5.7 Two-State Mixing

So far in looking at transition rates we have worked to leading order in H'. We now simplify the problem enough so that we can treat H' *exactly*. We still seek separated solutions to the Schrödinger equation as in Eqs. (2.18)–(2.22), so that we have

$$\begin{aligned} \Psi(x,t) &= \psi(x) e^{-iEt/\hbar} \\ H\psi(x) &= E\psi(x) \qquad ;\ H = H_0 + H' \end{aligned} \tag{5.47}$$

The eigenfunction $\psi(x)$ can be expanded in the complete set of solutions to the unperturbed problem

$$\begin{aligned} \psi(x) &= \sum_n a_n \psi_n(x) \\ H_0 \psi_n(x) &= E_n^0 \psi_n(x) \end{aligned} \tag{5.48}$$

Substitution into the eigenvalue equation, and the use of the orthonormality of the eigenfunctions $\psi_n(x)$, gives

$$\sum_{n'} \left[\left(E_n^0 - E\right) \delta_{n,n'} + \langle n|H'|n'\rangle \right] a_{n'} = 0 \tag{5.49}$$

This relation is still exact, and there is one equation for each n. We are thus faced with an infinite set of coupled algebraic equations for the amplitudes $(a_1, a_2, a_3, \cdots)$; however, we now make some simplifying assumptions:

- We assume that it is only the mixing of a *pair* of states (ψ_1, ψ_2) that is important for us;
- We assume that the pair is degenerate, with energy E_0;[6]
- We assume that the diagonal elements of H' vanish.
- We assume the off-diagonal elements of H' are real, with $H'_{12} = H'_{21}$.

The above equations then reduce to the following simple *pair* of equations

$$\begin{aligned} (E_0 - E)a_1 + H'_{12}\, a_2 &= 0 \\ H'_{12}\, a_1 + (E_0 - E)a_2 &= 0 \end{aligned} \tag{5.50}$$

This is a pair of linear, homogeneous, algebraic equations for the amplitudes (a_1, a_2). These equations will only have a non-trivial solution if the determinant of the coefficients of (a_1, a_2) vanishes. Hence

$$(E_0 - E)^2 - (H'_{12})^2 = 0 \tag{5.51}$$

It follows that the eigenvalues and corresponding (normalized) eigenfunctions are

$$\begin{aligned} E_+ &= E_0 + H'_{12} \qquad ;\ \psi_+(x) = \frac{1}{\sqrt{2}}\left[\psi_1(x) + \psi_2(x)\right] \\ E_- &= E_0 - H'_{12} \qquad ;\ \psi_-(x) = \frac{1}{\sqrt{2}}\left[\psi_1(x) - \psi_2(x)\right] \end{aligned} \tag{5.52}$$

The general solution to the two-level problem is then obtained as the linear combination of the separated solutions

$$\Psi(x,t) = c_+\, \psi_+(x)\, e^{-iE_+ t/\hbar} + c_-\, \psi_-(x)\, e^{-iE_- t/\hbar} \tag{5.53}$$

Suppose that at the initial time $t = 0$ we start in the state $\psi_1(x)$, so that

$$\begin{aligned} \Psi(x,0) &= \psi_1(x) \qquad ;\ \text{initial condition} \\ c_+ &= c_- = \frac{1}{\sqrt{2}} \end{aligned} \tag{5.54}$$

[6]These could be the pair of first excited states of a particle in the square two-dimensional box, for example. [See Eqs. (3.41).]

Then at a later time

$$\begin{aligned}\Psi(x,t) &= a_1(t)\psi_1(x) + a_2(t)\psi_2(x)\\ a_1(t) &= \frac{1}{2}\left(e^{-iE_+t/\hbar} + e^{-iE_-t/\hbar}\right)\\ a_2(t) &= \frac{1}{2}\left(e^{-iE_+t/\hbar} - e^{-iE_-t/\hbar}\right)\end{aligned} \tag{5.55}$$

The probability of finding the particle in the state $\psi_1(x)$ after time t is then

$$P_1(t) = |a_1(t)|^2 = \cos^2\left(H'_{12}\,t/\hbar\right) \tag{5.56}$$

while the probability of finding it in the state $\psi_2(x)$ is

$$P_2(t) = |a_2(t)|^2 = \sin^2\left(H'_{12}\,t/\hbar\right) \tag{5.57}$$

Evidently the particle *oscillates back and forth* between the states (ψ_1, ψ_2) with an angular frequency $H'_{12}/\hbar$, and

$$P_1(t) + P_2(t) = 1 \tag{5.58}$$

This is essentially the analysis that applies to neutrino mixing, or that of the neutral kaon, in particle physics.[7]

[7] See, for example, [Walecka (2008)].

Chapter 6

Quantum Electrodynamics

In order to do more physics, we need to get more realistic. An essential part of modern physics is the interaction of a charged particle with an electromagnetic field. We certainly cannot do all of quantum electrodynamics here, and we will be content to include the electromagnetic field through vector and scalar potentials $(\vec{A}, \Phi)$. This will allow us to describe

(1) A static Coulomb field, as in an atom,

$$\Phi(\vec{x}, t) = \Phi_{\text{Coulomb}}(r) \qquad ; \ \vec{A} = 0 \tag{6.1}$$

(2) A static magnetic field[1]

$$\vec{B}(\vec{x}) = \vec{\nabla} \times \vec{A}(\vec{x}) \qquad ; \ \Phi = 0 \tag{6.2}$$

(3) A transverse radiation field[2] with

$$\begin{aligned} \vec{B}(\vec{x}, t) &= \vec{\nabla} \times \vec{A}(\vec{x}, t) && ; \ \Phi = 0 \\ \vec{E}(\vec{x}, t) &= -\frac{\partial \vec{A}(\vec{x}, t)}{\partial t} \\ \vec{A}(\vec{x}, t) &= \text{Re}\left[\vec{e}_{\vec{k}s}\, e^{i(\vec{k}\cdot\vec{x} - \omega t)}\right] && ; \ \omega = kc \end{aligned} \tag{6.3}$$

where $\vec{e}_{\vec{k}s}$ with $s = (1, 2)$ are transverse unit vectors.

To proceed, we need to construct the hamiltonian for a charged particle in such an electromagnetic field.

[1] With $\vec{\nabla} \cdot \vec{B} = 0$.

[2] See [Walecka (2018)].

6.1 Hamiltonian

The classical hamiltonian for a charged particle in an electromagnetic field with vector and scalar potentials $(\vec{A}, \Phi)$ is given by

$$H = \frac{1}{2m}\left[\vec{p} - e\vec{A}(\vec{x},t)\right]^2 + e\Phi(\vec{x},t) \tag{6.4}$$

We shall justify this by showing that the classical Hamilton's equations produce the Lorentz force on the particle

$$\vec{F} = e\left(\vec{E} + \vec{v}\times\vec{B}\right) \qquad ;\ \text{Lorentz force} \tag{6.5}$$

Hamilton's equations read

$$\begin{aligned} \frac{\partial H}{\partial p_i} &= \frac{dx_i}{dt} \qquad ;\ i = 1,2,3 \\ \frac{\partial H}{\partial x_i} &= -\frac{dp_i}{dt} \end{aligned} \tag{6.6}$$

The first of Hamilton's equations expresses the particle velocity as

$$v_i = \frac{dx_i}{dt} = \frac{1}{m}\left[\vec{p} - e\vec{A}(\vec{x},t)\right]_i \tag{6.7}$$

Differentiation of this relation gives

$$\frac{dp_i}{dt} = m\frac{d^2x_i}{dt^2} + e\frac{dA_i(\vec{x},t)}{dt} \tag{6.8}$$

The second of Hamilton's equations then yields the force on the particle through[3]

$$\begin{aligned} m\frac{d^2x_i}{dt^2} &= -e\frac{dA_i(\vec{x},t)}{dt} - \frac{\partial H}{\partial x_i} \\ &= -e\left[\frac{\partial A_i}{\partial x_j}v_j + \frac{\partial A_i}{\partial t}\right] + e\left[v_j\frac{\partial A_j}{\partial x_i}\right] - e\frac{\partial\Phi}{\partial x_i} \\ &= eE_i + ev_j\left[\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j}\right] \end{aligned} \tag{6.9}$$

where the electric field $\vec{E}$ receives a contribution from both potentials

$$\vec{E} = -\vec{\nabla}\Phi - \frac{\partial\vec{A}}{\partial t} \tag{6.10}$$

[3]We use our convention that repeated Latin indices are summed from one to three.

Now use the vector manipulations

$$\begin{aligned}\left[\vec{v}\times\left(\vec{\nabla}\times\vec{A}\right)\right]_i &= \varepsilon_{ijk}v_j\left(\vec{\nabla}\times\vec{A}\right)_k = \varepsilon_{ijk}\,\varepsilon_{klm}v_j\frac{\partial A_m}{\partial x_l}\\ &= \left[\delta_{il}\,\delta_{jm}-\delta_{im}\,\delta_{jl}\right]v_j\frac{\partial A_m}{\partial x_l}\\ &= v_j\left[\frac{\partial A_j}{\partial x_i}-\frac{\partial A_i}{\partial x_j}\right]\end{aligned} \tag{6.11}$$

The magnetic field $\vec{B}$ is obtained from the vector potential through

$$\vec{B}=\vec{\nabla}\times\vec{A} \tag{6.12}$$

Hamilton's equations then reproduce the Lorentz force equation

$$\vec{F}=e\left(\vec{E}+\vec{v}\times\vec{B}\right) \qquad ;\ \text{Lorentz force} \tag{6.13}$$

6.2 Schrödinger Equation

Thus, for our purposes, the Schrödinger equation for a non-realtivistic particle in a potential $V(r)$, in the presence of additional electromagnetic fields with vector and scalar potentials $(\vec{A},\Phi)$, is given by

$$\begin{aligned}i\hbar\frac{\partial\Psi(\vec{x},t)}{\partial t} &= H\Psi(\vec{x},t) \qquad ;\ \text{Schrödinger eqn}\\ H &= \frac{1}{2m}\left[\vec{p}-e\vec{A}(\vec{x},t)\right]^2+e\Phi(\vec{x},t)+V(r)\end{aligned} \tag{6.14}$$

Upon quantization, in order to satisfy the basic commutation relation

$$[p_i,x_j]=\frac{\hbar}{i}\delta_{ij} \tag{6.15}$$

we continue to employ

$$\vec{p}=\frac{\hbar}{i}\vec{\nabla} \qquad ;\ \text{canonical momentum} \tag{6.16}$$

6.3 Ionization in Oscillating Electric Field

We start the discussion of electromagnetic interactions with a *very* simple example, where we explicitly have all the wave functions. Suppose a charged particle is moving in the ground-state of the one-dimensional box, and it is

boosted into the continuum by an electric field that is oscillating along the x-axis according to

$$\mathcal{E}_x = \mathcal{E}_0 \cos\omega_0 t = \mathcal{E}_0 \frac{1}{2}\left(e^{i\omega_0 t} + e^{-i\omega_0 t}\right) \tag{6.17}$$

The interaction hamiltonian is then

$$H' = -e\mathcal{E}_0 x \cos(\omega_0 t) \doteq -\left(\frac{e\mathcal{E}_0}{2}\right) x\, e^{-i\omega_0 t} \tag{6.18}$$

where it is only the final term that will *increase* the energy of the bound particle in Eqs. (5.17) and (5.18).

The initial and final wave functions and energies are[4]

$$\begin{aligned} \psi_i(x) &= \psi_{n_0}(x) \qquad ;\ E_i = \frac{\hbar^2\pi^2}{2md^2} n_0^2 \\ \psi_f(x) &= \frac{1}{\sqrt{L}} e^{ik_f x} \qquad ;\ E_f = \frac{(\hbar k_f)^2}{2m} \qquad ;\ \text{p.b.c.} \end{aligned} \tag{6.19}$$

The transition rate times the number of final states is then

$$R_{fi} dn_f = \left(\frac{e\mathcal{E}_0}{2}\right)^2 \frac{2\pi}{\hbar} |\langle f|x|i\rangle|^2 \delta(E_f - E_i - \hbar\omega_0) \left[\frac{L}{(2\pi)} dk_f\right] \tag{6.20}$$

We can now carry out some familiar manipulations and use

$$\frac{dE_f}{dk_f} = \frac{\hbar^2 k_f}{m} \tag{6.21}$$

The maximum energy density of the electric field is

$$U_0 = \frac{\varepsilon_0}{2}\mathcal{E}_0^2 \qquad ;\ \text{field energy density} \tag{6.22}$$

The transition rate per unit field energy density follows as

$$\frac{1}{U_0} R_{fi}\, dn_{fi} = \pi\alpha \left(\frac{ck_f}{E_f}\right) \left| \int_0^L dx\, e^{-ik_f x}\, x\, \psi_{n_0}(x) \right|^2 \qquad ;\ E_f = E_i + \hbar\omega_0 \tag{6.23}$$

were α is the dimensionless fine-structure constant

$$\alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c} = \frac{1}{137.0} \tag{6.24}$$

[4]Here d is the size of the confining box.

The transition rate is proportional to the absolute square of the transition dipole moment. If the integral converges, then the expression in Eq. (6.23) is again independent of the length L of the region of the final continuum particle. It is also easy to check that the expression in Eq. (6.23) has the correct dimensions.

6.4 Interaction With the Radiation Field

To lowest order, the interaction with the radiation field in the hamiltonian in Eq. (6.14) is

$$H' = -\frac{e}{2m}\left[\vec{p}\cdot\vec{A}(\vec{x},t) + \vec{A}(\vec{x},t)\cdot\vec{p}\right] \qquad ;\ \vec{p} = \frac{\hbar}{i}\vec{\nabla}$$
$$\vec{A}(\vec{x},t) = A(\vec{k},s)\,\vec{e}_{\vec{k}s}\,\frac{1}{2}\left[e^{i(\vec{k}\cdot\vec{x}-\omega t)} + e^{-i(\vec{k}\cdot\vec{x}-\omega t)}\right] \tag{6.25}$$

Here $A(\vec{k},s)$ is the amplitude of the vector potential in the classical wave. Since the fields are transverse with $\vec{k}\cdot\vec{e}_{\vec{k}s} = 0$, we can move $\vec{p}$ through to the right in the first term, and rewrite

$$H' = -e\vec{A}(\vec{x},t)\cdot\frac{\vec{p}}{m} \tag{6.26}$$

To leading order in $\vec{A}$, this looks like the classical expression $-e\vec{A}(\vec{x},t)\cdot\vec{v}$. If we are looking at transitions that put energy *into* the system, then, as before, we can simply use[5]

$$\vec{A}(\vec{x},t) \doteq \frac{1}{2}A(\vec{k},s)\,\vec{e}_{\vec{k}s}\,e^{i(\vec{k}\cdot\vec{x}-\omega t)} \qquad ;\ E_f = E_i + \hbar\omega \tag{6.27}$$

We also know that the time-average energy flux in the classical wave is[6]

$$S_{\text{inc}} = \left[\frac{\varepsilon_0\omega^2}{2}A^2(\vec{k},s)\right]c \qquad ;\ \text{energy flux} \tag{6.28}$$

6.5 Photoionization

We are now in a position to make a more realistic calculation of photoionization by the radiation field. We work in three dimensions with initial and

[5] See Prob. 6.3.

[6] See [Walecka (2018)]; remember that now $\vec{E} = -\partial\vec{A}/\partial t$, and the magnitude of the time-average Poynting vector for the electromagnetic field is $S_{\text{inc}} = \langle\varepsilon_0\vec{E}^{\,2}\rangle c$.

final particle wave functions and energies

$$\begin{aligned} \psi_i(\vec{x}) &= \psi_0(\vec{x}) \qquad\qquad ;\ E_i = E_0 \\ \psi_f(\vec{x}) &= \frac{1}{\sqrt{L^3}} e^{i\vec{k}_f\cdot\vec{x}} \qquad ;E_f = \frac{(\hbar k_f)^2}{2m} \end{aligned} \tag{6.29}$$

The transition rate multiplied by the number of final states, and divided by the incident flux, is then

$$\begin{aligned} \frac{1}{S_{\rm inc}} R_{fi}\, dn_f =& \left(\frac{e^2}{2\varepsilon_0\omega^2 c}\right)\left(\frac{1}{m^2L^3}\right)\times\left(\frac{2\pi}{\hbar}\right)\left|\vec{e}_{\vec{k}s}\cdot\int d^3x\, e^{i(\vec{k}-\vec{k}_f)\cdot\vec{x}}\,\vec{p}\,\psi_0(\vec{x})\right|^2 \\ &\times\delta(E_f - E_0 - \hbar\omega)\left[\frac{L^3}{(2\pi)^3}d^3k_f\right] \end{aligned} \tag{6.30}$$

Write $d^3k_f = k_f^2\, d\Omega_f\, dk_f$, and use

$$\frac{dE_f}{dk_f} = \frac{\hbar^2 k_f}{m} \tag{6.31}$$

This yields

$$\begin{aligned} \omega_{fi} &\equiv \frac{1}{S_{\rm inc}} R_{fi}\, dn_f \qquad\qquad ;\ \text{photoionization} \\ &= \frac{\alpha}{2\pi c^2}\left(\frac{k_f}{2E}\right)\left|\vec{e}_{\vec{k}s}\cdot\int d^3x\, e^{i(\vec{k}-\vec{k}_f)\cdot\vec{x}}\left(\frac{\vec{p}}{m}\right)\psi_0(\vec{x})\right|^2 d\Omega_f \end{aligned} \tag{6.32}$$

where the energy E is defined by

$$E \equiv \frac{(\hbar k)^2}{2m} \tag{6.33}$$

This is a nice result. It is the general expression for photoionization by the classical radiation field to lowest order in α. Note that the factors of L^3 have again cancelled. One can again check that this has the correct dimensions.

6.6 Normal Mode Expansion of the Electromagnetic Field

The next challenge is to express the free electromagnetic field in *normal modes*, that is, as a set of uncoupled simple harmonic oscillators. We work in a big cubical box of volume $\Omega = L^3$, and apply periodic boundary conditions.

The total energy in the free electromagnetic field in the box is obtained through the sum of the squares of the electric and magnetic fields. In SI units it is given by

$$E = \frac{1}{2}\int_\Omega d^3x \left(\varepsilon_0 \vec{E}^{\,2} + \frac{1}{\mu_0}\vec{B}^{\,2}\right) \qquad ;\ \text{field energy} \tag{6.34}$$

One has the freedom of choosing a gauge for the electromagnetic potentials,[7] and here we work in the *Coulomb gauge*. This gauge has the great advantage that, when quantized, there is a one-to-one correspondence of the resulting quanta with physical photons. For free fields, the Coulomb gauge is defined by

$$\vec{\nabla}\cdot\vec{A} = 0 \qquad ;\ \Phi = 0 \qquad ;\ \text{Coulomb gauge} \tag{6.35}$$

The electric and magnetic fields are then given by

$$\vec{E} = -\frac{\partial \vec{A}}{\partial t} \qquad ;\ \vec{B} = \vec{\nabla}\times\vec{A} \tag{6.36}$$

With periodic boundary conditions, the normal modes are given by plane waves

$$\begin{aligned} q_{\vec{k}}(\vec{x},t) &= \frac{1}{\sqrt{\Omega}} e^{i(\vec{k}\cdot\vec{x}-\omega_k t)} \qquad ;\ \vec{k} = \frac{2\pi}{L}(n_x,n_y,n_z) \\ \omega_k &= |\vec{k}|c \qquad\qquad ;\ n_i = 0,\pm1,\pm2,\cdots\ ;\ i = x,y,z \end{aligned} \tag{6.37}$$

Once again, we have an infinite, discrete set of wavenumbers, and the normal modes are orthonormal

$$\int_\Omega d^3x\, q^\star_{\vec{k}}(\vec{x},t)\, q_{\vec{k}'}(\vec{x},t) = \delta_{\vec{k},\vec{k}'} \tag{6.38}$$

Now introduce a set of orthogonal, transverse unit vectors $\vec{e}_{\vec{k}s}$ for each $\vec{k}$ as shown in Fig. 6.1. They satisfy

$$\begin{aligned} \vec{e}_{\vec{k}s}\cdot\vec{k} &= 0 \qquad ;\ s = 1,2 \\ \vec{e}_{\vec{k}s}\cdot\vec{e}_{\vec{k}s'} &= \delta_{s,s'} \end{aligned} \tag{6.39}$$

[7] See Probs. 6.1 and 6.2.

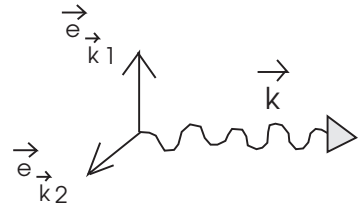

Fig. 6.1 Orthogonal, transverse unit vectors $\vec{e}_{\vec{k}s}$ for each $\vec{k}$.

The vector potential can now be expanded in normal modes as follows

$$\vec{A}(\vec{x},t) = \sum_{\vec{k}} \sum_{s=1}^{2} \left(\frac{\hbar}{2\omega_k \varepsilon_0 \Omega} \right)^{1/2} \left[a_{\vec{k}s} \vec{e}_{\vec{k}s} e^{i(\vec{k}\cdot\vec{x}-\omega_k t)} + a^{\star}_{\vec{k}s} \vec{e}_{\vec{k}s} e^{-i(\vec{k}\cdot\vec{x}-\omega_k t)} \right] \tag{6.40}$$

where we have chosen particular amplitudes for the normal modes which will make the energy come out nicely. This expansion has the following features to recommend it:

- This expression is *real*, giving rise to real $(\vec{E}, \vec{B})$;
- Since only the transverse polarization vectors are used in the expansion, one has ensured that

$$\vec{\nabla} \cdot \vec{A} = 0 \tag{6.41}$$

- $\vec{A}(\vec{x},t)$ satisfies the wave equation, and, since the order of partial derivatives can always be interchanged, so do the fields $(\vec{E}, \vec{B})$

$$\Box \vec{A}(\vec{x},t) = 0 \tag{6.42}$$

$$\Rightarrow \qquad \Box \vec{E}(\vec{x},t) = \Box \vec{B}(\vec{x},t) = 0 \tag{6.43}$$

- The periodic boundary conditions are obeyed;
- There is enough freedom to match the initial conditions.

The normal-mode expansion in Eq. (6.40) can now be substituted in the expression for the energy in Eq. (6.34), making use of the definition of the fields in Eqs. (6.36). This is classical E&M. The calculation is

straightforward, and the details are given in appendix A. The result is[8]

$$E = \sum_{\vec{k}} \sum_{s=1}^{2} \hbar\omega_k \frac{1}{2} \left(a^\star_{\vec{k}s} a_{\vec{k}s} + a_{\vec{k}s} a^\star_{\vec{k}s} \right) \qquad ; \text{ normal modes} \tag{6.44}$$

The problem has been reduced to normal modes. One has an infinite, uncoupled set of simple harmonic oscillators, one for each value of the wavenumber $\vec{k}$ and polarization s.

6.7 Quantization of the Oscillator

We will spend some time with the quantization of the simple harmonic oscillator, since that will be central to what we do in quantum mechanics. The hamiltonian for the one-dimensional oscillator is

$$H = \frac{p^2}{2m} + \frac{\kappa q^2}{2} \qquad ; \text{ oscillator} \tag{6.45}$$

Introduce the *destruction* and *creation* operators by

$$\begin{aligned} a &= \frac{p}{(2m\hbar\omega)^{1/2}} - iq \left(\frac{m\omega}{2\hbar} \right)^{1/2} \qquad ; \ \omega^2 = \frac{\kappa}{m} \\ a^\dagger &= \frac{p}{(2m\hbar\omega)^{1/2}} + iq \left(\frac{m\omega}{2\hbar} \right)^{1/2} \end{aligned} \tag{6.46}$$

From our discussion of the hermiticity of operators, it is clear that $a^\dagger$ is the hermitian adjoint of a.[9] The canonical commutation relation between the momentum and coordinate is

$$[p, q] = \frac{\hbar}{i} \tag{6.47}$$

It follows that the creation and destruction operators satisfy

$$[a, a^\dagger] = 1 \qquad ; \text{ commutation relation} \tag{6.48}$$

Written in terms of these new operators, the hamiltonian takes the form

$$H = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) \equiv \hbar\omega \left(N + \frac{1}{2} \right) \tag{6.49}$$

[8] Recall $c^2 = 1/\varepsilon_0\mu_0$.

[9] See Prob. 6.4. Here we label the coordinate more generally as q.

Here we have defined the *number* operator by

$$N \equiv a^\dagger a \qquad ; \text{ number operator} \tag{6.50}$$

It further follows from our discussion of hermiticity that the number operator N is hermitian; consequently, it has *real* eigenvalues.[10]

Now we could write and solve the simple harmonic oscillator as a one-dimensional differential Schrödinger equation in coordinate space.[11] It is of great interest, however, to see how far we can get on the spectrum of the number operator, and on the application of the creation and and destruction operators to those eigenstates, using only the general principles of quantum mechanics, in particular, the commutation relations of the creation and destructions operators.

We shall therefore proceed to work in an *abstract occupation number space*, where we write the eigenvalue equation for the number operator in abstract form as[12]

$$N|n\rangle = n|n\rangle \qquad ; \text{ abstract eigenvalue equation} \tag{6.51}$$

The abstract eigenstates are *orthonormal*, with an *inner product* satisfying

$$\langle n'|n\rangle = \delta_{n,n'} \qquad ; \text{ orthonormal} \tag{6.52}$$

This relation actually follows by taking a matrix element of Eq. (6.51) and using the hermiticity of N

$$\langle n'|N|n\rangle = n\langle n'|n\rangle = n'\langle n'|n\rangle \tag{6.53}$$

Hence

$$(n' - n)\,\langle n'|n\rangle = 0 \tag{6.54}$$

The abstract states are also *complete*, satisfying the relation

$$\sum_n |n\rangle\langle n| = 1 \qquad ; \text{ complete} \tag{6.55}$$

[10] Again, see Prob. 6.4. The hermitian adjoint of a product of operators is the product of hermitian adjoints in reverse order.

[11] As done, for example, in [Walecka (2013)].

[12] The coordinate-space wave function is the component form of this abstract state vector; in the language of Chapter 9, one has $\langle x|n\rangle = \psi_n(x)$, where $\psi_n(x)$ is the coordinate-space wave function.

To justify this, take an arbitrary matrix element $\langle n_2|\cdots|n_1\rangle$ of this relation

$$\sum_n \langle n_2|n\rangle\langle n|n_1\rangle = \sum_n \delta_{n_2,n}\delta_{n,n_1} = \delta_{n_2,n_1} = \langle n_2|n_1\rangle \tag{6.56}$$

which is the correct answer.

Let us now see how far we can get in this abstract occupation number space using just the general principles of quantum mechanics. Consider

$$[N, a^\dagger] = a^\dagger a a^\dagger - a^\dagger a^\dagger a = a^\dagger [a, a^\dagger] = a^\dagger \tag{6.57}$$

It follows that

$$N a^\dagger |n\rangle = a^\dagger \left(N + 1\right) |n\rangle = (n+1) a^\dagger |n\rangle \tag{6.58}$$

Hence $a^\dagger$ *raises* the eigenvalue by 1

$$a^\dagger |n\rangle = C(n)|n+1\rangle \tag{6.59}$$

In the same vein, consider

$$[N, a] = a^\dagger a a - a a^\dagger a = -[a, a^\dagger] a = -a \tag{6.60}$$

As before

$$N a|n\rangle = a\left(N - 1\right)|n\rangle = (n-1) a|n\rangle \tag{6.61}$$

It follows that a *lowers* the eigenvalue by 1

$$a|n\rangle = \bar{C}(n)|n-1\rangle \tag{6.62}$$

Let us demonstrate that this lowering property must *terminate*, since the eigenvalues of n must be non-negative. Consider the matrix element

$$n = \langle n|N|n\rangle = \langle n|a^\dagger a|n\rangle = |\bar{C}(n)|^2 \geq 0 \tag{6.63}$$

In order that the lowering process not actually produce a state with negative eigenvalue, one must have

$$a|n_{\min}\rangle = 0 \tag{6.64}$$

Hence, the lowest eigenvalue of the number operator is zero

$$N|n_{\min}\rangle = N|0\rangle = 0 \tag{6.65}$$

The states with integer n are then obtained from this by repeatedly applying $a^\dagger$ to it using Eq. (6.59).[13] The norm of the raised state is given by

$$\begin{aligned}\langle n|aa^\dagger|n\rangle &= \langle n|N+1|n\rangle = n+1 \\ &= |C(n)|^2\end{aligned} \tag{6.66}$$

Let us choose the relative phase of all the basis states so that

$$C(n) = \sqrt{n+1} \tag{6.67}$$

It follows that

$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{6.68}$$

Similarly

$$a^\dagger|n-1\rangle = \sqrt{n}\,|n\rangle \tag{6.69}$$

Operate on this state with a

$$aa^\dagger|n-1\rangle = (N+1)|n-1\rangle = n|n-1\rangle = \sqrt{n}\,a|n\rangle \tag{6.70}$$

Hence, with our phase convention

$$a|n\rangle = \sqrt{n}\,|n-1\rangle \tag{6.71}$$

In *summary*, we have found the eigenstates and eigenvalues of the simple harmonic oscillator hamiltonian in Eq. (6.49)

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) \equiv \hbar\omega\left(N + \frac{1}{2}\right) \tag{6.72}$$

using the commutation relation

$$[a, a^\dagger] = 1 \tag{6.73}$$

and the general principles of quantum mechanics. We have also found the effect of the creation and destruction operators on these abstract eigenstates

$$\begin{aligned} H|n\rangle &= \hbar\omega\left(n+\frac{1}{2}\right)|n\rangle \qquad ;\ n = 0,1,2,3,\cdots \\ a|n\rangle &= \sqrt{n}\,|n-1\rangle \\ a^\dagger|n\rangle &= \sqrt{n+1}\,|n+1\rangle \end{aligned} \tag{6.74}$$

[13] See Prob. 6.5.

It is really quite remarkable that we are able to obtain all of these results using only the general principles of quantum mechanics and the commutation relations of the creation and destruction operators!

6.8 Quantization of the Electromagnetic Field

We are now in a position to *quantize* the electromagnetic field. We treat the normal-mode amplitudes as creation and destruction operators, and write the uncoupled energy in Eq. (6.44) and commutation relations as

$$H = \sum_{\vec{k}} \sum_{s=1}^{2} \hbar\omega_k \left(N_{\vec{k}s} + \frac{1}{2} \right) = \sum_{\vec{k}} \sum_{s=1}^{2} \hbar\omega_k \left(a^\dagger_{\vec{k}s} a_{\vec{k}s} + \frac{1}{2} \right)$$

$$[a_{\vec{k}s},\, a^\dagger_{\vec{k}'s'}] = \delta_{\vec{k},\vec{k}'}\, \delta_{s,s'} \tag{6.75}$$

We then have an infinite set of uncoupled simple harmonic oscillators, one for each mode. The state vector is the direct product of abstract state vectors, one for each mode, that satisfy

$$a^\dagger_{\vec{k}s} a_{\vec{k}s} |n_{\vec{k}s}\rangle = n_{\vec{k}s} |n_{\vec{k}s}\rangle \qquad ;\ n_{\vec{k}s} = 0, 1, 2, \cdots \tag{6.76}$$

The quanta are called *photons*, and we are back to where we started the course!

The vector potential in Eq. (6.40) now becomes a *quantum field* operator that creates and destroys photons

$$\vec{A}(\vec{x}, t) = \sum_{\vec{k}} \sum_{s=1}^{2} \left(\frac{\hbar}{2\omega_k \varepsilon_0 \Omega} \right)^{1/2} \left[a_{\vec{k}s} \vec{e}_{\vec{k}s} e^{i(\vec{k}\cdot\vec{x} - \omega_k t)} + a^\dagger_{\vec{k}s} \vec{e}_{\vec{k}s} e^{-i(\vec{k}\cdot\vec{x} - \omega_k t)} \right] \tag{6.77}$$

As does the interaction with a non-relativistic charged particle in Eq. (6.26)

$$H' = -e\vec{A}(\vec{x}, t) \cdot \frac{\vec{p}}{m} \tag{6.78}$$

6.9 Radiative Decay

We now have enough information to compute the rate for the radiative decay $\psi_i \to \psi_f + \gamma$. With the interaction in Eqs. (6.77) and (6.78), it is the appropriate creation operator in the vector potential that makes the

transition to the final photon state of $|1_{\vec{k}s}\rangle$. The decay rate then follows as in Eq. (6.30)

$$R_{fi}\, dn_f = \left(\frac{\hbar e^2}{2\omega_k \varepsilon_0 \Omega}\right)\left(\frac{2\pi}{\hbar}\right)\left|\vec{e}_{\vec{k}s}\cdot\int d^3x\, e^{-i\vec{k}\cdot\vec{x}}\,\psi_f^*(\vec{x})\,\frac{\vec{p}}{m}\,\psi_i(\vec{x})\right|^2 \times$$
$$\delta(E_f - E_i + \hbar\omega_k)\left[\frac{L^3}{(2\pi)^3}d^3k\right] \tag{6.79}$$

The volume element $\Omega = L^3$ cancels. Now use $d^3k = k^2\, dk\, d\Omega_k$, and

$$\frac{dk}{d(\hbar\omega_k)} = \frac{1}{\hbar c} \tag{6.80}$$

This gives the photon emission rate

$$\begin{aligned}\omega_{fi} &= R_{fi}\, dn_f \\ &= \frac{\alpha}{2\pi c^2}\omega_k\left|\vec{e}_{\vec{k}s}\cdot\int d^3x\, e^{-i\vec{k}\cdot\vec{x}}\,\psi_f^*(\vec{x})\,\frac{\vec{p}}{m}\,\psi_i(\vec{x})\right|^2 d\Omega_k\end{aligned} \tag{6.81}$$

This is a powerful result. We have calculated the rate for photon emission by a charged particle making a transition in *any quantum system*!

6.10 Schrödinger Picture

In the *Schrödinger picture*, the operators are time-independent, and all the time dependence is put into the wave function. Thus the Schrödinger equation for a non-relativistic particle in a potential $V(r)$, in the presence of additional electromagnetic fields with vector and scalar potentials $(\vec{A}, \Phi)$, in the Schrödinger picture is given by

$$\begin{aligned} i\hbar\frac{\partial\Psi(\vec{x},t)}{\partial t} &= H\Psi(\vec{x},t) \qquad ;\ \text{Schrödinger picture} \\ H &= \frac{1}{2m}\left[\vec{p} - e\vec{A}(\vec{x})\right]^2 + e\Phi(\vec{x}) + V(r)\end{aligned} \tag{6.82}$$

Upon quantization, in order to satisfy the basic commutation relation

$$[p_i, x_j] = \frac{\hbar}{i}\delta_{ij} \tag{6.83}$$

we continue to employ

$$\vec{p} = \frac{\hbar}{i}\vec{\nabla} \qquad ; \text{ canonical momentum} \tag{6.84}$$

The vector potential $\vec{A}(\vec{x})$ is quantized in Eq. (6.77), where it is $\vec{A}(\vec{x}, 0)$. Note that one then has a full interacting quantum field theory.

Other pictures, in particular the *interaction picture* where the free-field time dependence is put into the quantum field operators [see Eqs. (6.14)] are discussed in Sec. 9.7. [14]

6.11 Lasers

Suppose we have a whole array of excited systems in the same state prepared to make a radiative transition down to another state. When making the radiative transition, the creation operator in the vector potential acts on the state $|n_{\vec{k}s}\rangle$ in which there are already photons present. It gives

$$a^\dagger_{\vec{k}s}|n_{\vec{k}s}\rangle = \sqrt{n_{\vec{k}s}+1}\,|n_{\vec{k}s}+1\rangle \tag{6.85}$$

The larger the value of $n_{\vec{k}s}$, the larger the amplitude $\sqrt{n_{\vec{k}s}+1}$. Hence, as $n_{\vec{k}s}$ grows, the emitted photons are more and more likely to go into the same single mode with a given value of $\vec{k}s$. The result will be an intense electromagnetic wave with a single value of $\vec{k}s$. This is the *laser*.

[14] Quantum electrodynamics (QED) is examined in detail in [Walecka (2010); Walecka (2013)].

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Chapter 7

Quantum Statistics

If we have a system of many identical particles, we have to be concerned with the *quantum statistics* of these particles. Let us start by considering a collection of *bosons*.

7.1 Bosons

Let us order the available single-particle states as $0, 1, 2, \cdots, i, j, k, \cdots$. The state vector for the many-particle system in the abstract occupation number space is then just the direct product over all the single-particle states with the number of particles in each mode

$$|n_0\, n_1\, n_2\, \cdots\rangle = |n_0\rangle|n_1\rangle|n_2\rangle\cdots \qquad ;\ \text{abstract state vector} \tag{7.1}$$

The operators in this space are just our previous simple harmonic oscillator operators for each mode, and for bosons, we will now denote these operators by b and $b^\dagger$. They satisfy the commutation relations

$$[b_i, b_j^\dagger] = \delta_{ij} \qquad ;\ \text{commutation relations} \tag{7.2}$$

All of the properties of these operators follow exactly as in Sec. 6.7. As we have seen, this analysis holds for photons. It also holds for non-relativistic spin-zero systems such as ^{4}He atoms, which are also bosons. Let us here focus on this latter case.

Suppose we have a single-particle operator such as the kinetic energy for this many-body system. We write this operator as

$$\hat{T} = \sum_i \sum_j b_j^\dagger \langle j|T|i\rangle\, b_i \qquad ;\ \text{one-body operator} \tag{7.3}$$

Some comments:

- From now on we use a hat over a quantity to indicate an operator in the abstract space, except for the creation and destruction operators where this is obvious;
- Here $\langle j|T|i\rangle$ is the appropriate single-particle matrix element for the problem at hand

$$\langle j|T|i\rangle = \int d^3x\, \psi_j^*(\vec{x}) T \psi_i(\vec{x}) \tag{7.4}$$

- If T is diagonal, then

$$\hat{T} = \sum_j \langle j|T|j\rangle b_j^\dagger b_j = \sum_j \langle j|T|j\rangle \hat{n}_j \tag{7.5}$$

- In this last case, the many-body matrix element of the kinetic energy operator is

$$\langle n_1\, n_2\, \cdots |\hat{T}| n_1\, n_2\, \cdots\rangle = \sum_j \langle j|T|j\rangle n_j \tag{7.6}$$

  This just adds up the kinetic energy of all the filled states, and it is clearly the correct answer.

We can rewrite this one-body operator $\hat{T}$ by introducing the non-relativistic *quantum field*

$$\begin{aligned} \hat{\psi}(\vec{x}) &\equiv \sum_j \psi_j(\vec{x})\, b_j \qquad\quad ;\ \text{quantum field} \\ \hat{\psi}^\dagger(\vec{x}) &\equiv \sum_j \psi_j^*(\vec{x})\, b_j^\dagger \end{aligned} \tag{7.7}$$

The one-body operator is then

$$\hat{T} = \int d^3x\ \hat{\psi}^\dagger(\vec{x}) T \hat{\psi}(\vec{x}) \tag{7.8}$$

Suppose one has a *two-body* operator, such as the potential between all the pairs

$$V = \frac{1}{2} \sum_i \sum_j V\left(|\vec{x}_i - \vec{x}_j|\right) \tag{7.9}$$

The extension of the above is simply[1]

$$\hat{V} = \frac{1}{2}\int d^3x \int d^3y\ \hat{\psi}^\dagger(\vec{y})\hat{\psi}^\dagger(\vec{x})V(|\vec{x}-\vec{y}\,|)\,\hat{\psi}(\vec{x})\hat{\psi}(\vec{y}) \tag{7.10}$$

One can then construct a hamiltonian and write the *many-body Schrödinger equation* in this abstract occupation number space as

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle &= \hat{H}|\Psi(t)\rangle \qquad ;\ \text{Schrödinger eqn} \\ \hat{H} &= \hat{T}+\hat{V} \end{aligned} \tag{7.11}$$

This is often referred to as *second quantization.*[2]

If the number of bosons is conserved, as in the case of ^{4}He atoms, then there will be one Schrödinger equation in each subspace of given N.

7.1.1 *Bose Condensation*

Suppose we have a non-interacting collection of bosons at very low temperature. They will all occupy the same lowest-energy single-particle state, and the ground state of the many-body system becomes

$$|N,0,0,\cdots\rangle = |N\rangle|0\rangle|0\rangle\cdots \tag{7.12}$$

This is known as *Bose condensation.*

Consider the creation and destruction operators $(b_0^\dagger, b_0)$ for the zero-mode. Redefine these operators as

$$\xi_0 \equiv \frac{b_0}{\sqrt{N}} \qquad ;\ \xi_0^\dagger = \frac{b_0^\dagger}{\sqrt{N}} \tag{7.13}$$

Consider the commutator of these new operators

$$[\xi_0,\,\xi_0^\dagger] = \frac{[b_0,\,b_0^\dagger]}{N} = \frac{1}{N} \approx 0 \tag{7.14}$$

This vanishes for large N. We can therefore forget about the fact that these new quantities are *operators* and just treat them as classical quantities ("*c*-numbers"). What is their value? Take the matrix element of

$$\frac{1}{N}\langle N|b_0^\dagger b_0|N\rangle = |\xi_0|^2 = 1 \tag{7.15}$$

[1]There is no self-interaction, and we can always subtract it off as a one-body operator to eliminate it, if need be.

[2]See [Fetter and Walecka (2003a)].

Hence the c-number ξ_0 is a pure phase.

Consider the first term in the quantum field operator

$$\begin{aligned} \psi_0(\vec{x})b_0 &= \xi_0\sqrt{N}\,\psi_0(\vec{x}) \\ &\equiv \phi_0(\vec{x}) \end{aligned} \tag{7.16}$$

For Bose condensation with large N, the quantum field operator can thus be separated into two parts

$$\hat{\psi}(\vec{x}) = \phi_0(\vec{x}) + \sum_{j\geq 1} \psi_j(\vec{x})\, b_j \tag{7.17}$$

We observe the following:

- The first term is a c-number;
- It has the spatial dependence of the lowest-energy single-particle state $\psi_0(\vec{x})$;
- It serves as a wave function for the condensed many-body system;
- Since the Bose condensate is described with a single-particle wave function, it is not surprising that it exhibits many of the unusual features of a *quantum fluid*, such as quantized vortices; [3]
- The remainder of the above quantum field is an operator acting on the states above the condensate.

7.2 Fermions

There is another class of particles, for example, electrons and nucleons, that show a very different behavior. These are the *fermions* that obey the *Pauli exclusion principle*, which states that

One cannot put two identical fermions into the same state.

We have to go back and build this principle into the fermion operators in the abstract occupation number space. Consider the operators in one mode $(a, a^\dagger)$. Instead of imposing commutation relations, we impose *anti-commutation* relations

$$\begin{aligned} \{a,\, a^\dagger\} &\equiv aa^\dagger + a^\dagger a = 1 \\ \{a,\, a\} &= aa + aa = 0 \\ \{a^\dagger,\, a^\dagger\} &= a^\dagger a^\dagger + a^\dagger a^\dagger = 0 \end{aligned} \tag{7.18}$$

[3] See [Walecka (2008)]; see also Prob. 7.5.

Consider the action of these operators on the two states $|0\rangle$ and $|1\rangle$, where

$$\begin{aligned} |1\rangle &= a^\dagger|0\rangle \\ a|1\rangle &= |0\rangle \end{aligned} \tag{7.19}$$

- The number operator then gives the correct values

$$\begin{aligned} a^\dagger a|1\rangle &= \left(1 - aa^\dagger\right) a^\dagger|0\rangle = |1\rangle \\ a^\dagger a|0\rangle &= \left(a^\dagger a\right)\, a|1\rangle = 0 \end{aligned} \tag{7.20}$$

- And further application of $a^\dagger$ and a takes one out of this subspace

$$\begin{aligned} a^\dagger|1\rangle &= a^\dagger a^\dagger|0\rangle = 0 \\ a|0\rangle &= aa|1\rangle = 0 \end{aligned} \tag{7.21}$$

- Thus these operators fulfill the condition that one can have either $|0\rangle$ or $|1\rangle$ particles in a given state, but no more.

The anti-commutation relations we then impose in the abstract occupation number space for fermions are

$$\begin{aligned} \{a_i,\, a_j^\dagger\} &= \delta_{i,j} \qquad\qquad\qquad ;\ \text{fermions} \\ \{a_i,\, a_j\} &= \{a_i^\dagger,\, a_j^\dagger\} = 0 \end{aligned} \tag{7.22}$$

The only challenge now is keeping track of signs, since the operators for different modes *anti-commute*. One has

$$\begin{aligned} a_s|n_0 \cdots n_{s-1}\, 1_s\, n_{s+1} \cdots\rangle &= (-1)^{S_s}|n_0 \cdots n_{s-1}\, 0_s\, n_{s+1} \cdots\rangle \\ a_s^\dagger|n_0 \cdots n_{s-1}\, 0_s\, n_{s+1} \cdots\rangle &= (-1)^{S_s}|n_0 \cdots n_{s-1}\, 1_s\, n_{s+1} \cdots\rangle \\ S_s &= n_0 + n_1 + \cdots + n_{s-1} \end{aligned} \tag{7.23}$$

The trick is to keep the operators paired until they reach the state on which they operate. For example

$$a_s^\dagger a_s|n_0 \cdots n_s \cdots\rangle = n_s|n_0 \cdots n_s \cdots\rangle \tag{7.24}$$

For fermions, the field operators now become[4]

$$\begin{aligned} \hat{\psi}(\vec{x}) &\equiv \sum_j \psi_j(\vec{x})\, a_j \qquad\qquad ;\ \text{quantum field} \\ \hat{\psi}^\dagger(\vec{x}) &\equiv \sum_j \psi_j^*(\vec{x})\, a_j^\dagger \end{aligned} \tag{7.25}$$

[4]For the spin-1/2 electrons and nucleons the single-particle wave functions become a little more complicated — see below.

The kinetic and potential energies in this abstract occupation number space again take the form[5]

$$\hat{T} = \int d^3x\ \hat{\psi}^\dagger(\vec{x})T\hat{\psi}(\vec{x})$$
$$\hat{V} = \frac{1}{2}\int d^3x \int d^3y\ \hat{\psi}^\dagger(\vec{y})\hat{\psi}^\dagger(\vec{x})V(|\vec{x}-\vec{y}|)\,\hat{\psi}(\vec{x})\hat{\psi}(\vec{y}) \qquad (7.26)$$

and the many-body Schrödinger equation is again

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle \qquad ;\ \text{Schrödinger eqn}$$
$$\hat{H} = \hat{T} + \hat{V} \qquad (7.27)$$

The quantum many-body problem is discussed in detail in [Fetter and Walecka (2003a)].

7.3 Connection Between Spin and Statistics

It follows from some of the more esoteric aspects of relativistic quantum field theory that there is a connection between spin and statistics

> *Half-integral spin particles obey Fermi statistics, while integer spin particles obey Bose statistics.*

Electrons and nucleons have spin-1/2, and they obey Fermi statistics. ^{4}He atoms have spin zero and photons have unit helicity (the component of spin along the direction of motion); they obey Bose statistics.

We can keep track of the helicity of the photons with the polarization vectors

$$\vec{e}_{\vec{k},\pm1} = \mp\frac{1}{\sqrt{2}}\left(\vec{e}_{\vec{k}1} \pm i\vec{e}_{\vec{k}2}\right) \qquad (7.28)$$

For the spin-1/2 particles, we keep track of the spin projection along the z-axis with a set of two-component column vectors[6]

$$\phi_\uparrow = \begin{pmatrix}1\\0\end{pmatrix} \qquad ;\ \phi_\downarrow = \begin{pmatrix}0\\1\end{pmatrix} \qquad (7.29)$$

[5]Note that the two-body potential now vanishes if the initial or final pair of single-particle states are identical since $a_j^2 = (a_j^\dagger)^2 = 0$.

[6]One then uses the complex conjugate transpose $\psi_j^\dagger(\vec{x})$, or *adjoint*, of the single-particle wave function in the field [note Eq. (11.41)].

Chapter 8

Quantum Measurements

In discussing measurements in quantum mechanics, it is always good to have a specific experiment in hand. We start our discussion with the Stern–Gerlach experiment — one of the pioneering measurements in quantum mechanics that led Pauli to the concept of spin.

8.1 Stern–Gerlach Experiment

In this experiment a beam of neutral particles with internal angular momentum $\hbar\vec{\mathcal{S}}$, here assumed to be spin-1/2 with $\mathcal{S}_z = \pm 1/2$, and a magnetic moment $\vec{\mu} = 2\mu\vec{\mathcal{S}}$ in the direction of the spin, is passed through an inhomogeneous magnetic field (see Fig. 8.1).

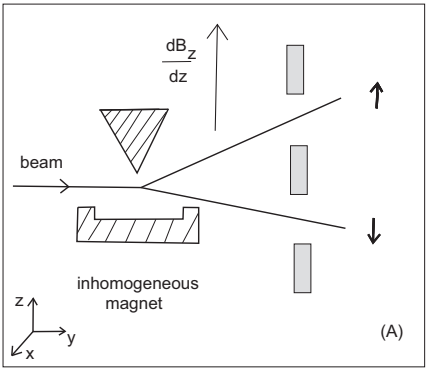

Fig. 8.1 Stern–Gerlach experiment on a spin-1/2 system with a magnetic moment $\vec{\mu} = 2\mu\vec{\mathcal{S}}$, and $\mathcal{S}_z = \pm 1/2$. The z-axis is in the plane and vertical.

The particles feel a force in the z-direction of

$$F_z = \mu_z \frac{dB_z}{dz} \tag{8.1}$$

Instead of seeing a continuous distribution of particles coming out of the detector in the z-direction, one observes only *two* beams, corresponding to $\mathcal{S}_z = \pm 1/2$. This illustrates the *discrete quantization* of the angular momentum. One observes just the eigenvalues of $\mathcal{S}_z$.

In quantum mechanics we understand what is happening by saying the initial internal state of each particle is a linear combination of the two spin states[1]

$$|\psi_{\text{int}}(t)\rangle = c_\uparrow(t)\,|\uparrow\rangle + c_\downarrow(t)\,|\downarrow\rangle \tag{8.2}$$

The *probability* that we will measure spin up is then $|c_\uparrow(t)|^2$, and the probability that we will measure spin down is $|c_\downarrow(t)|^2$, where

$$|c_\uparrow(t)|^2 + |c_\downarrow(t)|^2 = 1 \tag{8.3}$$

The internal Schrödinger equation tracks the behavior of *both* components as time progresses.

Suppose one now passes the top beam through a second detector identical to the first one as illustrated in Fig. 8.2.

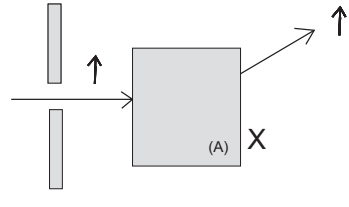

Fig. 8.2 Repeat of Stern–Gerlach experiment on upper beam using detector (A).

One will now observe that all of the particles coming out again have their spin up, and there are none coming out with their spin down.[2] We conclude from this that measurements are *reproducible*, and if we measure that the particle has spin up, then another measurement immediately afterwards will again say that it has spin up.

[1] Here the states $|\uparrow\rangle$ and $|\downarrow\rangle$ are one-particle states in the abstract occupation number space.

[2] We assume pure pass measurements here.

But in quantum mechanics, we actually have something more profound. The act of the first measurement has *changed the system.* It is no longer in the state in Eq. (8.2). The act of measurement has *reduced the basis.* The act of measurement has placed it entirely in the new state

$$|\psi_{\rm int}(t)\rangle = c(t)\,|\uparrow\rangle \qquad ;\ |c(t)|^2 = 1 \tag{8.4}$$

It is even more interesting than this. Suppose that instead of being oriented in the same z-direction as the first detector, the second detector in Fig. 8.2 is rotated by $90^{\rm o}$ about the y-axis and oriented in the x-direction, which is normal to the plane in Fig. 8.1. What we will now observe coming out of the second detector is *two beams*, one corresponding to spin up along the x-direction $|\rightarrow\rangle$, and one corresponding to spin down along the x-direction $|\leftarrow\rangle$. How do we understand this? In quantum mechanics these two states form a complete basis in which the state $|\uparrow\rangle$ can be expanded

$$|\uparrow\rangle = \frac{1}{\sqrt{2}}\,(\,|\rightarrow\rangle + |\leftarrow\rangle\,) \tag{8.5}$$

Hence, the above state can be rewritten as

$$|\psi_{\rm int}(t)\rangle = \frac{c(t)}{\sqrt{2}}\,(\,|\rightarrow\rangle + |\leftarrow\rangle\,) \tag{8.6}$$

The *probability* that we will now find the system in the state $|\rightarrow\rangle$ is then $|c(t)|^2/2$, and the probability that we will find $|\leftarrow\rangle$ is also $|c(t)|^2/2$. The act of measurement again *prepares the system in a new state.* The internal Schrödinger equation again tracks the behavior of *both* components as time progresses.

Suppose we now select a system coming out in the $|\rightarrow\rangle$ state with its spin pointed up along the x-axis. We have then prepared a known linear combination of the original states[3]

$$|\rightarrow\rangle = \tilde{c}_\uparrow(t)\,|\uparrow\rangle + \tilde{c}_\downarrow(t)\,|\downarrow\rangle \tag{8.7}$$

and the process starts all over again!

Whenever you get confused by abstract discussions of measurements in quantum mechanics, it is always worthwhile coming back to this example, where the concepts are quite intuitive.

[3]You can now figure out what happens if we put detector (A) after either one of these beams (see Prob. 8.2).

8.2 Reduction of the Basis

Let us try to formalize this measurement theory. Suppose we are looking at a single particle, and we have a complete set of the eigenfunctions of some hermitian operator with real eigenvalues at our disposal

$$F\psi_f(x) = f\psi_f(x) \qquad ; \text{ eigenfunctions} \tag{8.8}$$

Order the eigenvalues $f_0 \leq f_1 \leq f_2 \cdots$, and expand the wave function $\Psi(x,t)$ in this complete set of eigenfuctions

$$\Psi(x,t) = \sum_f c_f(t)\psi_f(x) \qquad ; \text{ complete set} \tag{8.9}$$

The state is normalized, so that

$$\sum_f |c_f(t)|^2 = 1 \tag{8.10}$$

Measurement theory then assumes the following:

(1) If we make a precise measurement of the quantity F, we will observe one of the eigenvalues f;
(2) If we perform a pure pass measurement at a time t_0 that lets the eigenvalue f through, then the wave function is reduced to[4]

$$\begin{aligned} &\Psi(x,t) = c_f(t)\psi_f(x) \qquad ; \ t \geq t_0 \\ &|c_f(t)|^2 = 1 \end{aligned} \tag{8.11}$$

The measurement is *reproducible* and the *basis is reduced*.
(3) If the measurement simply lets the eigenvalues in the set $f_1 \leq f \leq f_2$ through, then the basis is reduced to

$$\begin{aligned} &\Psi(x,t) = \sum_f{}' c_f(t)\psi_f(x) \qquad ; \ t \geq t_0 \\ &\sum_f{}' |c_f(t)|^2 = 1 \end{aligned} \tag{8.12}$$

where the sum $\sum_f'$ goes over $f_1 \leq f \leq f_2$.

[4]Note that the coefficient $c_f(t)$ must be *rescaled* to achieve this norm (see Prob. 10.2).

8.3 A Second Experiment — π^0 Decay

As a second, more complex, experiment, consider observations of the decay into two photons of the neutral, spin-zero, π^0 meson. We work in an abstract occupation number space where there are three states (see Fig. 8.3)

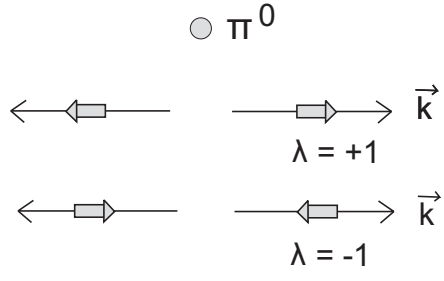

Fig. 8.3 The three states used in the discussion of the π^0-decay experiment.

(1) There is a single π^0 at rest in the state $|\pi^0\rangle$;
(2) There is one two-photon state with equal and opposite wave vectors $\vec{k}$ and unit positive helicities $\lambda = +1$, where the helicity is the component of the angular momentum along the direction of motion. With the use of the photon operators $b^\dagger_{\vec{k}\lambda}$ this state is

$$|\vec{k}, +1\rangle \,|\, -\vec{k}, +1\rangle = b^\dagger_{\vec{k},+1} b^\dagger{}_{-\vec{k},+1}|0\rangle \tag{8.13}$$

(3) There is a similar two-photon state with equal and opposite wave vectors $\vec{k}$ and unit negative helicities $\lambda = -1$

$$|\vec{k}, -1\rangle \,|\, -\vec{k}, -1\rangle = b^\dagger_{\vec{k},-1} b^\dagger{}_{-\vec{k},-1}|0\rangle \tag{8.14}$$

Since the pion at rest has no angular momentum, and angular momentum is conserved, there can be no net angular momentum along the direction of motion of the photons, and therefore it is only two-photon states with the *same helicity* that can be accessed during the decay. The state we are describing in the abstract occupation number space is a linear combination

of these three states [5]

$$|\Psi(t)\rangle = \int \frac{d\Omega_k}{2\pi} \left\{ c_+(t)\,|\vec{k},+1\rangle\,|-\vec{k},+1\rangle + c_-(t)\,|\vec{k},-1\rangle\,|-\vec{k},-1\rangle \right\} + c_0(t)|\pi^0\rangle \tag{8.15}$$

The Schrödinger equation then tracks all three coefficients in this state vector as a function of time.

- At the initial time $t = 0$ we prepare a π^0 at rest so that

$$c_0(0) = 1 \qquad ;\ c_+(0) = c_-(0) = 0 \qquad ;\ t = 0 \tag{8.16}$$

- There is a piece of the hamiltonian H that converts the π_0 to two photons; we do not need to know just what this is, only that it is there. As the time progresses, the π^0 will disappear and the two photons will appear. The decrease in $|c_0(t)|^2$ with time gives the *decay rate*;
- After some time, the π_0 is gone, and the state is

$$|\Psi(t)\rangle = \int \frac{d\Omega_k}{2\pi} \left\{ c_+(t)\,|\vec{k},+1\rangle\,|-\vec{k},+1\rangle + c_-(t)\,|\vec{k},-1\rangle\,|-\vec{k},-1\rangle \right\} \qquad ;\ t \gg 0 \tag{8.17}$$

With no further information, we expect these coefficients to be equal

$$|c_+(t)|^2 = |c_-(t)|^2 \tag{8.18}$$

Now suppose we do an experiment where we set up a detector to look at the photon with a given momentum $\hbar\vec{k}$ coming from the decay of a pion, and we measure the *helicity* of that photon. We do that experiment over and over again. The *probability* that we will measure a given helicity is obtained from Eq. (8.18). It is equally likely that we will measure $\lambda = +1$ as $\lambda = -1$. If we do measure $\lambda = +1$ in a pure pass measurement, for example, then the state vector becomes

$$|\Psi(t)\rangle = c(t)\,|\vec{k},+1\rangle\,|-\vec{k},+1\rangle \qquad ;\ |c(t)|^2 = 1 \tag{8.19}$$

We have *reduced the basis*, and the measurement is now *reproducible*.

Let us do another experiment. We have a collaborator who sets up a second detector to measure the helicity of the second photon with opposite momentum $-\hbar\vec{k}$. If there is no coordination in our measurements, he or

[5] For illustration, we keep only the asymptotic energy-conserving states with $2\hbar kc = m_\pi c^2$.

she will find the same probability distribution as obtained from Eq. (8.18)– equal numbers of $\lambda = \pm 1$.

But suppose we arrange the timing to make sure we are doing a *coincidence* experiment where we measure the two photons coming from the decay of the same π^0. Now if I find a helicity λ, my collaborator will find *the same helicity* λ*!* It is only those states that are contained in the state vector, which supposedly describes the system for all time. Equation (8.18) implies that the probability that we will both measure a pair with $\lambda = +1$ is the same as the probability that we will measure a pair with $\lambda = -1$. We will never measure a pair with opposite helicities, which would imply a breakdown in the conservation of angular momentum, since there are no such pairs in the state vector.

We can go further. If I do a pure pass experiment for helicity $\lambda = +1$, for example, the state vector is reduced by my measurement to the state vector in Eq. (8.19), and the subsequent measurement of the second helicity, whenever it would occur, would also then give $\lambda = +1$ with *unit probability.* My measurement has determined what the second observer will subsequently see. And it does not matter how far we are apart when we make these measurements; the results are now *correlated.* When we get together later offline and compare our results for the same π^0 decay, we will find we have measured the same helicities. It is only those states that are contained in the state vector.[6]

It is important to note that the Schrödinger equation *simultaneously* tracks the time development of the states of *both* helicities $\lambda = \pm 1$. It is only a measurement that selects one or the other of the possibilities.

It is the observations that the Schrödinger equation simultaneously tracks *all* the components of the state vector, and that a measurement of one component *reduces* the basis and can determine what a second observer will see, which form the foundation of *quantum computing.*[7]

[6]There is a principle in relativistic quantum field theory known as *microscopic causality*, which states that information cannot be transmitted faster than the speed of light. That principle cannot be violated, and this experiment does not do so.

[7]See, for example, [Bernhardt (2019)].

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Chapter 9

Formal Structure of Quantum Mechanics

In mechanics and electricity and magnetism we write the fundamental equations, Newton's laws and Maxwell's equations, in abstract form in the sense that we write them as relations between *vectors*. The component form of these relations is just a calculational tool. The underlying relationships are between the vectors themselves. Our goal here is to achieve a similar abstract form for the Schrödinger equation. We have actually seen good examples of this in our use of the abstract occupation number space for electrodynamics and for the quantum statistics of many-body Bose and Fermi systems. Our first step is to generalize the notions of vectors and the scalar dot product of vectors to infinite dimensional complex linear vector spaces with an inner-product norm.

9.1 Hilbert Space

Ordinary three-dimensional vectors have cartesian components, and a dot product defined by

$$\begin{aligned} \vec{v} &= (v_1, v_2, v_3) \\ \vec{a} \cdot \vec{b} &= \sum_{i=1}^{3} a_i b_i \end{aligned} \tag{9.1}$$

Let us generalize this in two ways:

- Extend the space to have an infinite number of dimensions;
- Let the components of the vector become complex.

One then has

$$\vec{v} = (v_1, v_2, v_3, \cdots)$$
$$\vec{a}^{\,*} \cdot \vec{b} = \sum_{i=1}^{\infty} a_i^* b_i \tag{9.2}$$

The square of the length of the vector is then given by

$$|\vec{v}\,|^2 = \vec{v}^{\,*} \cdot \vec{v} = \sum_{i=1}^{\infty} |v_i|^2 \tag{9.3}$$

An infinite dimensional linear vector space with an inner-product norm is known as a *Hilbert space*. Our goal is to write the Schrödinger equation as an operator relation in an abstract Hilbert space.

9.2 Component Form

Let us start with the component form of our relations. In order to do this we need to introduce the concept of a continuous component, and we also need to make use of the Dirac delta function that was introduced when discussing transition rates. In fact, the concepts and notation for what we are doing here were originally introduced by Dirac in his fundamental work.[1]

We first label the components of the abstract state vectors that we are studying with a subscript x, and calculate the inner product of two of those vectors as[2]

$$\langle \psi_m | \psi_n \rangle = \sum_x (\psi_m)_x^* \, (\psi_n)_x \tag{9.4}$$

We now have to define the continuous sum, as well as the components in the x-direction. We do this by writing the sum as an *integral* and using our coordinate-space *wave functions* for the components

$$\langle \psi_m | \psi_n \rangle = \sum_x (\psi_m)_x^* \, (\psi_n)_x \equiv \int dx \, \psi_m^*(x) \psi_n(x) \tag{9.5}$$

This defines the continuous sum. It is just the integral over the appropriate interval of two of our previous wave functions.

[1] See [Dirac (1930)].

[2] We go back to one dimension for simplicity.

Let us further introduce the eigenstates of the hermitian position operator $\hat{x}$ [3]

$$\hat{x}\,|x\rangle = x\,|x\rangle \tag{9.6}$$

We can then rewrite the above as

$$\langle\psi_m|\psi_n\rangle = \sum_x (\psi_m)^*_x\,(\psi_n)_x = \sum_x \langle\psi_m|x\rangle\langle x|\psi_n\rangle \tag{9.7}$$

where we have identified the wave functions as

$$\begin{aligned}\langle x|\psi_n\rangle &= \psi_n(x)\\ \langle\psi_m|x\rangle &= \psi^*_m(x)\end{aligned} \tag{9.8}$$

We now have the consistent physical interpretation that the probability for finding the particle in the interval dx at the position x if it is in the state $|\psi_n\rangle$ is the absolute square of the probability amplitude obtained from the inner product $\langle x|\psi_n\rangle$

$$|\langle x|\psi_n\rangle|^2\,dx = |\psi_n(x)|^2\,dx \qquad ;\ \text{probability} \tag{9.9}$$

Equation (9.7) allows us to identify the *completeness* relation for the eigenstates of position

$$\sum_x |x\rangle\langle x| = \hat{1} \tag{9.10}$$

What about the inner product of these states? Here we are forced to deal with the fact that the eigenvalues of position are truly continuous, and we write[4]

$$\langle x|x'\rangle = \delta(x - x')\,) \tag{9.11}$$

The relation in Eq. (9.10) then gives us, consistently,

$$\begin{aligned}\langle x'\,|x''\,\rangle &= \sum_x \langle x'\,|x\rangle\langle x|x''\,\rangle = \int dx\,\delta(x' - x)\,\delta(x - x''\,)\\ &= \delta(x' - x''\,)\end{aligned} \tag{9.12}$$

[3] We here and henceforth again use a hat over a symbol to indicate an operator in the abstract Hilbert space (except for the creation and destruction operators, where it is obvious).

[4] Note the Dirac delta function is symmetric, with $\delta(x - x') = \delta(x' - x)$.

The matrix element of the potential energy in this coordinate representation is given by

$$\langle x'|V(\hat{x})|x\rangle = V(x)\langle x'|x\rangle = V(x)\delta(x-x') \tag{9.13}$$

The matrix element of the kinetic energy is a little more complicated, but still straightforward

$$\begin{aligned}\langle x'|\hat{T}|x\rangle &= -\frac{\hbar^2}{2m}\left\langle x'\left|\frac{d^2}{dx^2}\right|x\right\rangle = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\langle x'|x\rangle \\ &= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\delta(x-x')\end{aligned} \tag{9.14}$$

9.3 The Schrödinger Equation

Let $|\Psi(t)\rangle$ be a time-dependent vector in this abstract Hilbert space. The Schrödinger equation then reads

$$\begin{aligned}i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle &= \hat{H}|\Psi(t)\rangle \\ \hat{H} &= \hat{T}+\hat{V}\end{aligned} \tag{9.15}$$

Take a matrix element with $\langle x|$, and use completeness of the eigenstates of position[5]

$$i\hbar\frac{\partial}{\partial t}\langle x|\Psi(t)\rangle = \sum_{x'}\langle x|\hat{H}|x'\rangle\langle x'|\Psi(t)\rangle \tag{9.16}$$

Identify $\langle x|\Psi(t)\rangle$ as the wave function $\Psi(x,t)$, and use the expressions for the matrix elements of the kinetic and potential energies from above.[6] This gives

$$\begin{aligned}i\hbar\frac{\partial}{\partial t}\Psi(x,t) &= \int dx'\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\delta(x-x')\Psi(x',t) \\ &= \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\Psi(x,t)\end{aligned} \tag{9.17}$$

Low and behold, we recover our previous Schrödinger equation in coordinate space from the component form of the Schrödinger equation written in this abstract Hilbert space in Eq. (9.15)!

[5] Eigenstates of momentum are investigated in Probs. 9.1–9.3.

[6] Note that if the matrix element is real, and if the operator is hermitian (see the next section), then the matrix element is symmetric $\langle x'|\hat{H}|x\rangle^* = \langle x'|\hat{H}|x\rangle = \langle x|\hat{H}|x'\rangle$.

9.4 Hermitian Operators

Let $\hat{F}$ be an operator in the abstract Hilbert space. The *adjoint* operator $\hat{F}^\dagger$ is defined by

$$\langle\psi_n|\hat{F}|\psi_m\rangle^* = \langle\psi_m|\hat{F}^\dagger|\psi_n\rangle \qquad ; \text{ adjoint} \tag{9.18}$$

where $|\psi_m\rangle$ and $|\psi_n\rangle$ are any two acceptable states in the space. An operator is *hermitian* if it is self-adjoint

$$\hat{F} = \hat{F}^\dagger \qquad ; \text{ hermitian} \tag{9.19}$$

The *eigenstates* of a hermitian operator are defined by

$$\hat{F}|\psi_f\rangle = f\,|\psi_f\rangle \qquad ; \text{ eigenstates} \tag{9.20}$$

Here f is the *eigenvalue*, and it follows from Eqs. (9.18) and (9.19) that these eigenvalues are real. The projection of these eigenstates on the eigenstates of position yield the corresponding coordinate-space wave functions

$$\langle x|\psi_f\rangle = \psi_f(x) \qquad ; \text{ wave function} \tag{9.21}$$

It can be shown for certain classes of operators that the wave functions form a complete set, in which any other acceptable wave function can be expanded[7]

$$\Psi(x) = \sum_f c_f\,\psi_f(x) \qquad ; \text{ completeness} \tag{9.22}$$

The corresponding statement of completeness in abstract Hilbert space is

$$|\Psi\rangle = \sum_f c_f\,|\psi_f\rangle \qquad ; \text{ completeness} \tag{9.23}$$

9.5 Commutation Relations

The theory of quantum mechanics for a particle moving in one dimension in a potential $V(x)$ is constructed by imposing the following canonical *commutation relation* on the hermitian operators $\hat{p}$ and $\hat{x}$ representing the momentum and position of the particle in abstract Hilbert space

$$[\hat{p},\,\hat{x}] = \frac{\hbar}{i} \qquad ; \text{ commutation relation} \tag{9.24}$$

[7] See [Fetter and Walecka (2003)]; see also Prob. 9.1.

As in Eq. (9.17), this is satisfied in the coordinate representation with

$$\langle x|\hat{p}|x'\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\delta(x-x') \qquad ;\text{ coordinate rep} \tag{9.25}$$

9.6 Ehrenfest's Theorem

The formal solution to the Schrödinger equation in abstract Hilbert space can be written as

$$|\Psi(t)\rangle = e^{-i\hat{H}t/\hbar}\,|\Psi(0)\rangle \qquad ;\text{ formal solution} \tag{9.26}$$

where the exponential of the operator has a well-defined meaning in terms of its power-series expansion. If we consider the hermitian operator $\hat{F}$ then what we would measure for the time development of this quantity if the system is in the state $|\Psi(t)\rangle$ is the *expectation value*[8]

$$F(t) = \langle\Psi(t)|\hat{F}\,|\Psi(t)\rangle = \langle\Psi(0)|e^{i\hat{H}t/\hbar}\,\hat{F}\,e^{-i\hat{H}t/\hbar}\,|\Psi(0)\rangle \tag{9.27}$$

Differentiate this with respect to time

$$\frac{dF(t)}{dt} = \langle\Psi(t)|\,\frac{i}{\hbar}[\hat{H},\,\hat{F}]\,|\Psi(t)\rangle \tag{9.28}$$

The operator whose expectation value then yields the time development of $F(t)$ is given by the commutator with the hamiltonian

$$\left(\frac{dF}{dt}\right)_{\text{op}} = \frac{i}{\hbar}[\hat{H},\,\hat{F}] \tag{9.29}$$

If $\hat{F}$ should have an additional *explicit* time dependence, this relation becomes

$$\left(\frac{dF}{dt}\right)_{\text{op}} = \frac{\partial\hat{F}}{\partial t} + \frac{i}{\hbar}[\hat{H},\,\hat{F}] \qquad ;\text{ Ehrenfest's theorem} \tag{9.30}$$

This is known as *Ehrenfest's theorem*. We give three consequences:

(1) If the operator $\hat{F} = \hat{1}$, then we are simply investigating the time development of the *norm* of the state. It is evident that

$$\frac{i}{\hbar}[\hat{H},\hat{1}\,] = 0 \tag{9.31}$$

[8]The state is normalized (see below); see also Prob. 9.5.

Thus if the state is originally normalized, it will continue to be normalized as time progresses;

(2) Suppose we have a time-independent operator $\hat{O}$ that commutes with the hamiltonian. Then

$$\left(\frac{dO}{dt}\right)_{\text{op}} = \frac{i}{\hbar}[\hat{H},\, \hat{O}] = 0 \tag{9.32}$$

The expectation value of this operator does not change with time; hence, the operator $\hat{O}$ represents a *constant of the motion*;

(3) With a hamiltonian of the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \tag{9.33}$$

one has

$$\begin{aligned} \frac{i}{\hbar}[\hat{H}, \hat{x}] &= \frac{\hat{p}}{m} \\ \frac{i}{\hbar}[\hat{H}, \hat{p}] &= \frac{i}{\hbar}[V(\hat{x}), \hat{p}] \end{aligned} \tag{9.34}$$

In the coordinate representation, the last expression becomes

$$\frac{i}{\hbar}\langle x'|\,[V(\hat{x}), \hat{p}]\,|x\rangle = -\frac{\partial V(x)}{\partial x}\delta(x - x') \tag{9.35}$$

Equations (9.28)–(9.35) then become the quantum analogs of *Hamilton's equations* in classical mechanics.

9.7 Other Pictures

All of the above results hold in what is known as the *Schrödinger picture* where Eqs. (9.15) and (9.26) govern the time development of the abstract state vector. As we have seen, in many cases where

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \tag{9.36}$$

it is convenient to take out the free time dependence and have the time evolution be explicitly proportional to $\hat{H}_1$. We do this by going to the *interaction picture*. The Schrödinger equation is

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \left(\hat{H}_0 + \hat{H}_1\right)|\Psi(t)\rangle \tag{9.37}$$

Define

$$|\Psi(t)\rangle \equiv e^{-i\hat{H}_0 t/\hbar}\,|\Psi_0(t)\rangle \qquad ;\ \text{interaction picture} \tag{9.38}$$

Substitute this in the Schrödinger equation

$$\left(\hat{H}_0 + i\hbar\frac{\partial}{\partial t}\right)|\Psi_0(t)\rangle = e^{i\hat{H}_0 t/\hbar}\left(\hat{H}_0 + \hat{H}_1\right)e^{-i\hat{H}_0 t/\hbar}\,|\Psi_0(t)\rangle \tag{9.39}$$

The terms in $\hat{H}_0$ cancel, and one is left with a Schrödinger equation of the form

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\Psi_0(t)\rangle &= \hat{H}_1(t)|\Psi_0(t)\rangle \qquad ;\ \text{interaction picture} \\ \hat{H}_1(t) &= e^{i\hat{H}_0 t/\hbar}\,\hat{H}_1 e^{-i\hat{H}_0 t/\hbar} \end{aligned} \tag{9.40}$$

Here

$$|\Psi_0(t)\rangle \equiv e^{i\hat{H}_0 t/\hbar}\,|\Psi(t)\rangle \tag{9.41}$$

This is still an exact formulation of the problem, and always remember that physics lies in the *matrix elements*.

We can rewrite the time development of $|\Psi_0(t)\rangle$ as

$$|\Psi_0(t)\rangle = \hat{U}(t,t_0)|\Psi_0(t_0)\rangle \tag{9.42}$$

Then from Eq. (9.40), the time-development operator $\hat{U}(t,t_0)$ satisfies the following differential equation and initial condition

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0) &= \hat{H}_1(t)\hat{U}(t,t_0) \\ \hat{U}(t_0,t_0) &= 1 \end{aligned} \tag{9.43}$$

This can then be rewritten as an *integral equation*

$$\hat{U}(t,t_0) = \hat{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,\hat{H}_1(t')\hat{U}(t',t_0) \tag{9.44}$$

This integral equation can be iterated to obtain an explicit power series in $\hat{H}_1$ for the time-development operator

$$\hat{U}(t,t_0) = \hat{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,\hat{H}_1(t') + \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,\hat{H}_1(t')\hat{H}_1(t'') + \cdots \tag{9.45}$$

The Schrödinger state vector then develops in time according to Eq. (9.38)

$$|\Psi(t)\rangle = e^{-i\hat{H}_0 t/\hbar}\,\hat{U}(t,t_0)|\Psi_0(t_0)\rangle \tag{9.46}$$

Suppose we confine the discussion to operators $\hat{O}$ that have no explicit time dependence. Their expectation value in the Schrödinger picture, with a normalized state vector $|\Psi(t)\rangle$, is

$$\langle\hat{O}\rangle = \langle\Psi(t)|\hat{O}|\Psi(t)\rangle \tag{9.47}$$

The formal solution to the Schrödinger equation in abstract Hilbert space is given in Eq. (9.26)

$$|\Psi(t)\rangle = e^{-i\hat{H}t/\hbar}\,|\Psi(0)\rangle \tag{9.48}$$

The *Heisenberg picture*, which has exactly the same physical content as the Schrödinger picture, is defined by putting all of the time dependence into the operators

$$\hat{O}_H(t) \equiv e^{i\hat{H}t/\hbar}\,\hat{O}\,e^{-i\hat{H}t/\hbar} \qquad ;\ \text{Heisenberg picture} \tag{9.49}$$

The state vector is then independent of time, and

$$\langle\hat{O}\rangle = \langle\Psi(0)|\hat{O}_H(t)|\Psi(0)\rangle \tag{9.50}$$

The equation of motion of the Heisenberg operator is given by

$$\frac{d\hat{O}_H(t)}{dt} = \frac{i}{\hbar}[\hat{H},\,\hat{O}_H(t)\,] \tag{9.51}$$

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Chapter 10

Quantum Mechanics Postulates

Here we *summarize* the quantum mechanics postulates arrived at in the previous discussion. They are formulated in the abstract Hilbert space.

(1) There is a state vector $|\Psi(t)\rangle$ that provides a complete dynamical description of a system;
(2) An observable F is represented by a linear hermitian operator $\hat{F}$;
(3) The operators obey canonical commutation relations, in particular

$$[\hat{p}, \hat{x}] = \frac{\hbar}{i} \tag{10.1}$$

(4) The dynamics is given by the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle \tag{10.2}$$

(5) The eigenstates of a linear hermitian operator form a complete set[1]

$$\begin{aligned} \hat{F}|f_n\rangle &= f_n |f_n\rangle \qquad ;\ n = 1, 2, \cdots, \infty \\ \sum_n |f_n\rangle\langle f_n| &= \hat{1} \end{aligned} \tag{10.3}$$

(6) Measurement postulate:
   (a) A precise measurement of F must yield one of the eigenvalues f_n;
   (b) If the state vector is normalized, then the probability of observing an eigenvalue f_n at the time t is $|\langle f_n|\Psi(t)\rangle|^2$;
   (c) A measurement $f' \le f \le f''$ at time t_0 reduces the state vector to

$$|\Psi(t_0)\rangle' = \frac{\sum'_n a_{f_n}(t_0)|f_n\rangle}{\left(\sum'_n |a_{f_n}(t_0)|^2\right)^{1/2}} \qquad ;\ \text{where } f' \le f_n \le f'' \tag{10.4}$$

[1] See Prob. 10.1.

Through his many years in physics, the author has found this to be a complete and essential set of postulates for the implementation of quantum mechanics.

Chapter 11

Relativity

11.1 Special Relativity

The final chapter in the text *Introduction to Electricity and Magnetism* [Walecka (2018)] discusses special relativity. The speed of light is observed to be the same in all inertial frames. Lorentz came up with a coordinate transformation involving the position and the time that leaves the wave operator unaltered by the transformation

$$\frac{\partial^2}{\partial x'^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t'^2} = \frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} \tag{11.1}$$

Einstein took this transformation seriously in his special theory of relativity and said this is how the spatial and time coordinates are actually related between frames. The amazing implications of Lorentz contraction and time dilation are repeatedly exhibited in the laboratory today.

An elegant way of summarizing the Lorentz transformation is to say we live in a complex *Minkowski space*. Suppose the origins of the frames coincide at the initial times. With the use of the coordinate along the direction of relative motion of the frames, and the subsequent time, one can form a *two-vector* $x_\mu = (x, ict)$ in the first frame. The square of the length of this two-vector is the *interval*

$$\sum_{\mu=1}^{2} x_\mu x_\mu = x^2 - c^2 t^2 \qquad ; \text{ interval} \tag{11.2}$$

A Lorentz transformation to the second frame is then an orthogonal transformation (a *rotation*) $a_{\mu\nu}$ in this space that leaves the interval invariant

$$\sum_{\mu=1}^{2} x'_\mu x'_\mu = x'^2 - c^2 t'^2 = \sum_{\mu=1}^{2} x_\mu x_\mu = x^2 - c^2 t^2 \tag{11.3}$$

The calculation proceeds in a familiar fashion

$$\sum_{\mu=1}^{2} x'_\mu x'_\mu = \sum_{\mu=1}^{2}\sum_{\nu=1}^{2}\sum_{\nu'=1}^{2} a_{\mu\nu} a_{\mu\nu'} x_\nu x_{\nu'} = \sum_{\nu=1}^{2}\sum_{\nu'=1}^{2} \delta_{\nu,\nu'} x_\nu x_{\nu'} = \sum_{\nu=1}^{2} x_\nu x_\nu \tag{11.4}$$

With the inclusion of the two (unaffected) transverse spatial coordinates, the analysis is extended to four-vectors $x_\mu = (\vec{x}, ict)$, and the Lorentz-invariant scalar product of four-vectors. The theory of special relativity is then readily developed in this complex, four-dimensional, Minkowski space in which we live. A detailed discussion can be found in the text [Walecka (2008)].

Relativistic quantum mechanics is a huge field, and it forms the basis for everything that goes on in today's nuclear and particle physics. We certainly cannot give a comprehensive introduction to relativistic quantum mechanics here. We can, however, cover two topics that provide a good, firm foundation for future study. We discuss the quantum field theory of a massive, neutral scalar field, and we introduce the Dirac equation for relativistic spin-1/2 systems.

11.2 Massive Scalar Field

The relativistic relation between energy and momentum for a particle with rest mass m_0 is

$$E = \sqrt{\vec{p}^2 c^2 + m_0^2 c^4} \tag{11.5}$$

If we identify this with the hamiltonian H, and attempt to quantize with $\vec{p} = (\hbar/i)\vec{\nabla}$, the Schrödinger equation becomes

$$i\hbar \frac{\partial \phi(\vec{x}, t)}{\partial t} = \left[-(\hbar c)^2 \vec{\nabla}^2 + (m_0 c^2)^2 \right]^{1/2} \phi(\vec{x}, t) \tag{11.6}$$

The square-root causes difficulties.[1] A repeated application of this expression, however, leads to a much simpler expression

$$\left(\Box - m^2\right)\phi(\vec{x},t) = 0 \qquad ;\; m \equiv \frac{m_0 c}{\hbar} \tag{11.7}$$

This is the relativistic wave equation for a particle with inverse Compton wavelength $m = m_0 c/\hbar$.

We know from the previous text *Introduction to Classical Mechanics* [Walecka (2020)] how to do classical continuum mechanics with the wave equation.[2] There the analysis is applied to the string, where the wave equation holds. Introduce the two-vector $x_\mu = (x_1, x_2) = (x, ict)$, with $c^2 = \tau/\sigma$ and i the imaginary number $\sqrt{-1}$. Also, introduce the convention that repeated Greek indices are summed from 1 to 2. The basic equation of motion is then obtained from Hamilton's principle of stationary action

$$\delta \int d^2x\, \mathcal{L}\left(q, \frac{\partial q}{\partial x_\mu}\right) = 0 \qquad ;\; d^2x \equiv dx\, cdt \tag{11.8}$$

The lagrangian density for the string is

$$\mathcal{L} = \frac{\sigma}{2}\left[\frac{\partial q(x,t)}{\partial t}\right]^2 - \frac{\tau}{2}\left[\frac{\partial q(x,t)}{\partial x}\right]^2 \tag{11.9}$$

This can be rewritten as

$$\mathcal{L} = -\frac{\tau}{2}\left(\frac{\partial q}{\partial x_\mu}\right)\left(\frac{\partial q}{\partial x_\mu}\right) = -\frac{\tau}{2}\left(\frac{\partial q}{\partial x_\mu}\right)^2 \qquad ;\; \text{string} \tag{11.10}$$

Lagrange's equation for the string then follows as

$$\frac{\partial}{\partial t}\left[\frac{\partial \mathcal{L}}{\partial(\partial q/\partial t)}\right] + \frac{\partial}{\partial x}\left[\frac{\partial \mathcal{L}}{\partial(\partial q/\partial x)}\right] - \frac{\partial \mathcal{L}}{\partial q} = 0 \tag{11.11}$$

With the above conventions, this can be written as

$$\frac{\partial}{\partial x_\mu}\left[\frac{\partial \mathcal{L}}{\partial(\partial q/\partial x_\mu)}\right] - \frac{\partial \mathcal{L}}{\partial q} = 0 \qquad ;\; \text{Lagrange's eqn} \tag{11.12}$$

Now just extend the definition of x_μ to include two additional spatial coordinates $x_\mu = (x_1, x_2, x_3, x_4) = (\vec{x}, ict)$, and take the above analysis over

[1] One can always start expanding it (see Prob. 11.1).

[2] See also the book *Introduction to Classical Mechanics: Solutions to Problems* [Walecka (2020)]; in particular, see the solution to Prob. 15.10.

to the scalar field $\phi(\vec{x},t)$.[3] Hamilton's principle reads

$$\delta \int d^4x\, \mathcal{L}\left(\phi, \frac{\partial\phi}{\partial x_\mu}\right) = 0 \qquad ;\ d^4x \equiv dx^3\, cdt \quad (11.13)$$

Lagrange's equation reads

$$\frac{\partial}{\partial x_\mu}\left[\frac{\partial\mathcal{L}}{\partial(\partial\phi/\partial x_\mu)}\right] - \frac{\partial\mathcal{L}}{\partial\phi} = 0 \qquad ;\ \text{Lagrange's eqn} \quad (11.14)$$

To get the proper scalar field equation we employ

$$\mathcal{L} = -\frac{c^2}{2}\left(\frac{\partial\phi}{\partial x_\mu}\right)^2 - \frac{1}{2}m^2c^2\phi^2 \qquad ;\ \text{scalar field} \quad (11.15)$$

Lagrange's equation then reproduces Eq. (11.7)

$$\left(\Box - m^2\right)\phi(\vec{x},t) = 0 \quad (11.16)$$

The field ϕ and the lagrangian density $\mathcal{L}$ are both Lorentz scalars. Thus Hamilton's principle and Lagrange's equation are here both *Lorentz invariant*.

The canonical momentum density is given by

$$\Pi(\vec{x},t) = \frac{\partial\mathcal{L}}{\partial(\partial\phi/\partial t)} = \frac{\partial\phi(\vec{x},t)}{\partial t} \quad (11.17)$$

The hamiltonian density then follows as

$$\mathcal{H} = \Pi\frac{\partial\phi}{\partial t} - \mathcal{L} \quad (11.18)$$

This gives[4]

$$\mathcal{H}(\vec{x},t) = \frac{1}{2}\left[\frac{\partial\phi(\vec{x},t)}{\partial t}\right]^2 + \frac{c^2}{2}\left[\vec{\nabla}\phi(\vec{x},t)\right]^2 + \frac{1}{2}m^2c^2\phi^2(\vec{x},t) \quad (11.19)$$

With periodic boundary conditions, the normal modes for the scalar meson field are given by plane waves

$$q_{\vec{k}}(\vec{x},t) = \frac{1}{\sqrt{\Omega}}e^{i(\vec{k}\cdot\vec{x}-\omega_k t)} \qquad ;\ \vec{k} = \frac{2\pi}{L}(n_x,n_y,n_z)$$
$$\omega_k = c\sqrt{\vec{k}^{\,2}+m^2} \qquad ;\ n_i = 0,\pm1,\pm2,\cdots\ ;\ i = x,y,z \quad (11.20)$$

[3] Now, of course, c is the speed of light.

[4] Note that this hamiltonian density is positive definite.

They satisfy the wave equation

$$\left(\Box - m^2\right) q_{\vec{k}}(\vec{x}, t) = 0 \tag{11.21}$$

We have an infinite, discrete set of wavenumbers, and the normal modes are orthonormal

$$\int_\Omega d^3x \, q^\star_{\vec{k}}(\vec{x}, t) \, q_{\vec{k}'}(\vec{x}, t) = \delta_{\vec{k},\vec{k}'} \tag{11.22}$$

The scalar field can be expanded in normal modes according to

$$\phi(\vec{x}, t) = \sum_{\vec{k}} \left(\frac{\hbar}{2\omega_k \Omega}\right)^{1/2} \left[c_{\vec{k}} \, e^{i(\vec{k}\cdot\vec{x} - \omega_k t)} + c^\star_{\vec{k}} \, e^{-i(\vec{k}\cdot\vec{x} - \omega_k t)}\right] \tag{11.23}$$

The total energy follows by substituting this expansion in the hamiltonian density and doing the spatial integration. The calculation proceeds just as in appendix A, only here it is simpler. We leave the details as a problem, and the result is[5]

$$E = \frac{1}{2} \sum_{\vec{k}} \hbar\omega_k \left(c^\star_{\vec{k}} \, c_{\vec{k}} + c_{\vec{k}} \, c^\star_{\vec{k}}\right) \tag{11.24}$$

Since the analysis has been reduced to a set of uncoupled simple harmonic oscillators, we can immediately quantize the massive scalar field. We impose the oscillator commutation relations of Sec. 6.7

$$[c_{\vec{k}}, \, c^\dagger_{\vec{k}'}] = \delta_{\vec{k},\vec{k}'} \tag{11.25}$$

The total energy, which is the hamiltonian, then simply becomes the sum over the number of quanta in each mode

$$\hat{H} = \sum_{\vec{k}} \hbar\omega_k \left(\hat{N}_{\vec{k}} + \frac{1}{2}\right) \tag{11.26}$$

The energy of each quantum is just the correct relativistic expression for the energy of a particle with momentum $\vec{p} = \hbar\vec{k}$

$$\hbar\omega_k = E_k = \sqrt{(\hbar\vec{k}c)^2 + (m_0 c^2)^2} \tag{11.27}$$

Let us summarize what we can take away from our discussion of the massive neutral scalar field:

- This provides the simplest example of *relativistic quantum field theory*;

[5]See Prob. 11.2.

- The lagrangian density is Lorentz invariant, and hence so is Lagrange's equation here;
- Lagrange's equation produces the relativistic wave equation for a massive scalar field;
- The hamiltonian is obtained from the lagrangian through the canonical procedure;[6]
- The normal-mode expansion of the massive scalar field reduces the hamiltonian to a set of uncoupled simple harmonic oscillators;
- The field is then quantized using the oscillator results;
- The quanta of the field are massive scalar particles, with the correct relativistic relation between energy and momentum;
- The quantum scalar field $\hat{\phi}(\vec{x}, t)$ now creates and destroys these quanta, which are bosons;
- Interactions can now be included in the lagrangian density. For example, an acceptable self-coupling of the field here is obtained by incrementing the lagrangian density with

$$\mathcal{L}_1(\phi) = -\frac{\lambda}{4!}\phi^4 \tag{11.28}$$

Relativistic quantum field theory of a massive scalar field plays a central role in the standard model of electroweak interactions in particle physics, as well as in model field theories of the nuclear interaction in nuclear physics.[7]

11.3 The Dirac Equation

The first successful union of quantum mechanics and special relativity for a single-particle was achieved by Dirac, and here we give the lovely historical argument [Dirac (1926)].

One wants the theory to possess the following features:

(1) A positive-definite probability density

$$\rho = \Psi^\star \Psi \geq 0 \qquad ; \text{ probability density} \tag{11.29}$$

[6]We also know from the *Introduction to Classical Mechanics* text how to obtain the energy-momentum tensor $T_{\mu\nu}$ and the energy flux [Walecka (2020)].

[7]See [Walecka (2004)]. Relativistic quantum field theory is developed in detail in [Walecka (2010)].

(2) A Schrödinger equation that is first-order in the time derivative

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi \qquad ;\ \text{Schrödinger equation} \tag{11.30}$$

(3) A continuity equation

$$\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot\vec{S} = 0 \qquad ;\ \text{continuity equation} \tag{11.31}$$

As before, this will provide a basis for the interpretation of the theory and ensure that, for a localized particle,

$$\frac{d}{dt}\int \rho(\vec{x},t)\, d^3x = 0 \tag{11.32}$$

(4) The correct relativistic relation between energy and momentum

$$E^2 = \vec{p}^{\,2}c^2 + m_0^2c^4 \qquad ;\ \text{relativistic relation} \tag{11.33}$$

Now we do know of a theory that is Lorentz covariant and involves only first-order time derivatives, and that is the set of Maxwell's equations in electrodynamics.[8] Here one has a set of eight *coupled* equations for the components of the electric and magnetic fields $(\vec{E},\vec{B}\,)$. Dirac argued by analogy. He introduced a wave function Ψ that had a set of n components

$$\psi_\sigma \qquad ;\ \sigma = 1,2,\cdots,n \quad \text{components of } \Psi \tag{11.34}$$

with a corresponding positive-definite probability density defined by

$$\rho \equiv \sum_{\sigma=1}^{n} \psi_\sigma^\star\psi_\sigma \tag{11.35}$$

To satisfy Lorentz covariance, one expects to have to treat space and time on an equal footing, and to satisfy the second requirement above, they must then occur linearly. Thus Dirac assumed an equation of motion of the form

$$i\hbar\frac{\partial\psi_\sigma}{\partial(ct)} = \frac{\hbar}{i}\sum_{k=1}^{3}\sum_{\rho=1}^{n}\alpha^k_{\sigma\rho}\frac{\partial\psi_\rho}{\partial x_k} + m_0c\sum_{\rho=1}^{n}\beta_{\sigma\rho}\psi_\rho \quad ;\ \text{Dirac eqn} \quad \sigma = 1,\cdots,n \tag{11.36}$$

Here $(\alpha^k_{\sigma\rho},\beta_{\sigma\rho})$ are simply constants that couple the various components of the wave function. One now has a set of n coupled, linear, partial

[8] See *Introduction to Electricity amd Magnetism* [Walecka (2018)].

differential equations. In order to satisfy the third requirement above, we need to investigate $\partial\rho/\partial t$. To this end, consider

$$i\hbar\frac{\partial}{\partial(ct)}\sum_\sigma \psi^\star_\sigma\psi_\sigma = \sum_\sigma \psi^\star_\sigma\left[\frac{\hbar}{i}\sum_{k=1}^{3}\sum_\rho \alpha^k_{\sigma\rho}\frac{\partial\psi_\rho}{\partial x_k} + m_0c\sum_\rho \beta_{\sigma\rho}\psi_\rho\right] + \sum_\sigma \psi_\sigma\left[\frac{\hbar}{i}\sum_{k=1}^{3}\sum_\rho \alpha^{k\star}_{\sigma\rho}\frac{\partial\psi^\star_\rho}{\partial x_k} - m_0c\sum_\rho \beta^\star_{\sigma\rho}\psi^\star_\rho\right] \quad (11.37)$$

where the second line is obtained from the complex conjugate of Eq. (11.36). Now interchange dummy summation indices $\sigma \rightleftharpoons \rho$ in the second term on the r.h.s., and add it to the first term. The result can be written as

$$\begin{aligned} i\hbar\frac{\partial}{\partial(ct)}\sum_\sigma \psi^\star_\sigma\psi_\sigma = {} & \frac{\hbar}{i}\sum_{k=1}^{3}\frac{\partial}{\partial x_k}\left(\sum_\sigma\sum_\rho \psi^\star_\sigma\alpha^k_{\sigma\rho}\psi_\rho\right) \\ & - \frac{\hbar}{i}\sum_{k=1}^{3}\sum_\sigma\sum_\rho\left(\frac{\partial\psi^\star_\sigma}{\partial x_k}\right)\left(\alpha^k_{\sigma\rho} - \alpha^{k\star}_{\rho\sigma}\right)\psi_\rho \\ & + m_0c\sum_\sigma\sum_\rho \psi^\star_\sigma\left(\beta_{\sigma\rho} - \beta^\star_{\rho\sigma}\right)\psi_\rho \end{aligned} \quad (11.38)$$

To have a continuity equation, the r.h.s. should be the divergence of some quantity. It will be a divergence if the last two terms are absent. They will disappear if the numerical coefficients in Eq. (11.36) are required to satisfy the relations

$$\begin{aligned} \beta_{\sigma\rho} &= \beta^\star_{\rho\sigma} \\ \alpha^k_{\sigma\rho} &= \alpha^{k\star}_{\rho\sigma} \end{aligned} \quad (11.39)$$

These requirements can be rewritten in *matrix notation* as [9]

$$\begin{aligned} \beta &= \beta^\dagger \\ \alpha^k &= \alpha^{k\,\dagger} \qquad ;\ k = 1,2,3 \end{aligned} \quad (11.40)$$

Here we have used the fact that the complex conjugate transpose of a matrix is the *adjoint*

$$\left[\underline{m}^\dagger\right]_{\sigma\rho} \equiv m^\star_{\rho\sigma} \qquad ;\ \text{adjoint} \quad (11.41)$$

[9] It is assumed that the reader has an elementary knowledge of matrix manipulations (see Prob. 11.5). Here we forgo the underlining of $(\vec{\alpha}, \beta)$, and later, of Ψ; furthermore $\alpha^k \equiv \alpha_k$.

If one defines the "vector" $\vec{\alpha} \equiv (\alpha_1, \alpha_2, \alpha_3)$, then Eqs. (11.40) take the form

$$\begin{aligned} \beta &= \beta^\dagger && ;\ \text{hermitian} \\ \vec{\alpha} &= \vec{\alpha}^\dagger && \vec{\alpha} = (\alpha_1, \alpha_2, \alpha_3) \end{aligned} \tag{11.42}$$

Such matrices are said to be *hermitian*.

The previous results can also be rewritten in matrix notation as follows. Introduce the column vector

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix} \qquad ;\ \text{Dirac wave function} \tag{11.43}$$

Then the probability density in Eq. (11.35) takes the form

$$\rho = \Psi^\dagger \Psi \qquad ;\ \text{probability density} \tag{11.44}$$

The Dirac Eq. (11.36) becomes

$$\begin{aligned} i\hbar \frac{\partial \Psi}{\partial t} &= H\Psi && ;\ \text{Dirac equation} \\ H &\equiv c\vec{\alpha} \cdot \vec{p} + \beta m_0 c^2 && ;\ \vec{p} = \frac{\hbar}{i}\vec{\nabla} \end{aligned} \tag{11.45}$$

It follows from Eqs. (11.38) and (11.39) that the continuity equation can be written in matrix notation as

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{S} &= 0 && ;\ \text{continuity equation} \\ \rho &= \Psi^\dagger \Psi && ;\ \text{probability density} \\ \vec{S} &= c\, \Psi^\dagger \vec{\alpha}\, \Psi && ;\ \text{probability flux} \end{aligned} \tag{11.46}$$

It remains to satisfy point (4) and obtain the correct relativistic relation between energy and momentum. As with the Schrödinger equation, one looks for stationary-state solutions to the Dirac equation and converts it to time-independent form

$$\begin{aligned} \Psi &= \psi(\vec{x})\, e^{-iEt/\hbar} \\ H\psi &= (c\vec{\alpha} \cdot \vec{p} + \beta m_0 c^2)\psi = E\psi \end{aligned} \tag{11.47}$$

If H is applied to both sides once again, one obtains

$$H^2\psi = E^2\psi = (c^2\vec{p}^{\,2} + m_0^2 c^4)\psi \tag{11.48}$$

The r.h.s. is the required result. The quantity H^2 on the l.h.s. is now obtained through matrix multiplication[10]

$$H^2 = \left(c\vec{\alpha}\cdot\vec{p}+\beta m_0c^2\right)\left(c\vec{\alpha}\cdot\vec{p}+\beta m_0c^2\right) \tag{11.49}$$

Since matrices do not commute, one must keep careful track of the order of the factors in this expression. Thus

$$H^2 = c^2\sum_{k=1}^{3}\sum_{l=1}^{3}\alpha^k\alpha^l p_k p_l + m_0c^3\sum_{k=1}^{3}\left(\alpha^k\beta+\beta\alpha^k\right)p_k + m_0^2c^4\beta^2 \tag{11.50}$$

Since the components of p_k do commute with each other, a change of dummy summation variables allows the first term on the r.h.s. to be rewritten as

$$c^2\sum_k\sum_l\alpha^k\alpha^l p_k p_l = c^2\sum_k\sum_l\frac{1}{2}\left(\alpha^k\alpha^l+\alpha^l\alpha^k\right)p_k p_l \tag{11.51}$$

The required expression for H^2 in Eq. (11.48) is then reproduced, provided the following relations are imposed on the Dirac matrices $(\vec{\alpha},\beta)$

$$\begin{aligned}\beta\alpha^k+\alpha^k\beta &= 0 \qquad &&;\ \text{anti-commute}\\ \alpha^k\alpha^l+\alpha^l\alpha^k &= 2\delta_{kl} \qquad &&(\vec{\alpha},\beta)\ \ n\times n\ \text{matrices}\\ \beta^2 &= 1 \qquad &&\end{aligned} \tag{11.52}$$

Thus (α^k,β) must be hermitian, *anti-commuting*, $n\times n$ matrices that satisfy the last two conditions.[11]

The smallest dimension with which one can satisfy the relations in Eqs. (11.52) is $n = 4$. The *standard representation* of the Dirac matrices can then be exhibited in 2×2 form as

$$\vec{\alpha} = \begin{pmatrix}0 & \vec{\sigma}\\ \vec{\sigma} & 0\end{pmatrix} \qquad ;\ \beta = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \qquad ;\ \text{standard representation}\ 2\times 2\ \text{form} \tag{11.53}$$

Here $\vec{\sigma} = (\sigma_x,\sigma_y,\sigma_z)$ are the *Pauli matrices* given by[12]

$$\sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \ ;\ \sigma_y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} \ ;\ \sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \qquad ;\ \text{Pauli matrices} \tag{11.54}$$

[10]Note that one has effectively taken $\sqrt{c^2\vec{p}^2+m_0^2c^4}$ through the clever use of matrices!

[11]The unit matrix is again suppressed on the r.h.s. of the last two relations.

[12]Note that in this discussion, $k = (1,2,3)$ is the same as $k = (x,y,z)$.

For a free particle in a cubical box of volume Ω with periodic boundary conditions, one can again look for solutions to the Dirac equation of the form

$$\begin{aligned} \psi &= \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\cdot\vec{x}} u(\vec{k}\,) \\ \vec{p} &= \hbar\vec{k} \qquad\qquad ;\ \text{eigenvalue} \end{aligned} \tag{11.55}$$

Equation (11.48) then becomes

$$E_k^2 = (\hbar\vec{k}c)^2 + m_0^2 c^4 \qquad ;\ \text{eigenvalue} \tag{11.56}$$

11.3.1 *Non-Relativistic Reduction*

In order to relate this discussion to that of the one-particle Schrödinger equation, consider a non-relativistic reduction of the Dirac equation. Write the Dirac wave function in the following two-component form

$$\psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \qquad ;\ \text{two-component form} \tag{11.57}$$

Now use the standard representation of the Dirac matrices in Eqs. (11.53), and substitute Eq. (11.57) into the last of Eqs. (11.47). The stationary-state Dirac equation then takes the form

$$\left[\begin{pmatrix} 0 & c\vec{\sigma}\cdot\vec{p} \\ c\vec{\sigma}\cdot\vec{p} & 0 \end{pmatrix} + m_0 c^2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] \begin{pmatrix} \phi \\ \chi \end{pmatrix} = E \begin{pmatrix} \phi \\ \chi \end{pmatrix} \tag{11.58}$$

The upper and lower components of this matrix relation are

$$\begin{aligned} c\vec{\sigma}\cdot\vec{p}\,\chi + m_0 c^2 \phi &= E\phi \\ c\vec{\sigma}\cdot\vec{p}\,\phi - m_0 c^2 \chi &= E\chi \end{aligned} \tag{11.59}$$

We remind the reader that each of these equations is itself a two-component relation, the $\vec{\sigma}$ are the Pauli matrices, $\vec{p} = (\hbar/i)\vec{\nabla}$, and E is the eigenvalue. Equations (11.59) are still exact.

Consider the positive energy eigenvalue with [compare Eq. (11.56)]

$$E = +\sqrt{(m_0 c^2)^2 + \cdots} \qquad ;\ \text{positive-energy solution} \tag{11.60}$$

The second of Eqs. (11.59) can be written as

$$\chi = \frac{c\vec{\sigma}\cdot\vec{p}}{E + m_0 c^2}\,\phi \tag{11.61}$$

This term is now of $O(\vec{p}/m_0c)$, and hence it is small in the NRL. Substitution of Eq. (11.61) into the first of Eqs. (11.59) gives

$$\frac{(c\vec{\sigma}\cdot\vec{p})^2}{E+m_0c^2}\,\phi = (E-m_0c^2)\phi \tag{11.62}$$

Write out the numerator on the l.h.s.

$$(\vec{\sigma}\cdot\vec{p})^2 = \sum_{i=1}^{3}\sum_{j=1}^{3}\sigma_i\sigma_j p_i p_j = \sum_{i=1}^{3}\sum_{j=1}^{3}\frac{1}{2}\left(\sigma_i\sigma_j+\sigma_j\sigma_i\right)p_i p_j \tag{11.63}$$

The last equality comes from a change of dummy indices $i \rightleftharpoons j$ and the fact that the p_i commute. The properties of the Pauli matrices in Prob. 11.6 reduce this expression to

$$(\vec{\sigma}\cdot\vec{p})^2 = \vec{p}^{\,2} \tag{11.64}$$

Now in the NRL

$$\begin{aligned} E-m_0c^2 &\equiv \varepsilon \qquad\qquad ;\ \text{NRL-eigenvalue} \\ E+m_0c^2 &= 2m_0c^2+\varepsilon \approx 2m_0c^2 \end{aligned} \tag{11.65}$$

Thus in the NRL, the positive-energy, stationary-state Dirac Eq. (11.59) for the upper components ϕ of the Dirac wave function reduces to the free-particle Schrödinger equation[13]

$$\frac{\vec{p}^{\,2}}{2m_0}\,\phi = -\frac{\hbar^2\nabla^2}{2m_0}\,\phi = \varepsilon\phi \qquad ;\ \text{Schrödinger equation} \tag{11.66}$$

11.3.2 *Dirac Hole Theory*

We have to face the problem of the *negative-energy* solutions to the Dirac equation, for example, those with eigenvalue $-\sqrt{(\hbar\vec{k}c)^2+(m_0c^2)^2}$ in Eq. (11.56). Within the principles of quantum mechanics, under some perturbation, an isolated particle can simply keep falling down into these levels without end. There is no ground state for a free particle!

Dirac came up with an extremely clever solution to this problem by invoking the Pauli exclusion principle. We shall see below that the Dirac equation describes a particle of spin-1/2, which is then a fermion. Dirac assumed that *all the negative-energy states are already filled with identical fermions.* Thus they are unavailable to the particle in a positive-energy

[13]The lower components are then given in the NRL by $\chi = (\vec{\sigma}\cdot\vec{p}/2m_0c)\phi$.

state. Everything is then measured with respect to this filled negative-energy sea, the new vacuum.

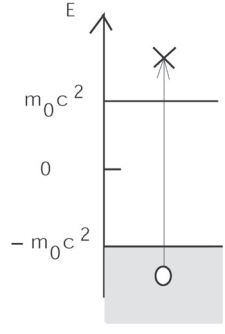

Fig. 11.1 Particle promoted to a positive-energy state, leaving a hole in the filled negative-energy Dirac sea.

This picture has some immediate consequences, for example:

- Within this picture, one of the negative-energy fermions can be promoted to a positive-energy state leaving a *hole* in the negative-energy sea (Fig. 11.1). The hole must have just the opposite properties of the particle, since if it is filled with a particle, one returns to the vacuum. The hole is thus just an *antiparticle*. Based on this picture, Dirac *predicted* the existence of antiparticles before they were discovered!
- Within this picture, the vacuum has dynamics. For example, the charge in the vacuum can be rearranged by the presence of another charge, and the vacuum is *polarizable*.

Both of these observations imply that, from the outset, one is faced with a *many-body problem* in relativistic quantum mechanics.

11.3.3 *Electromagnetic Interactions*

Consider a Dirac particle in an electromagnetic field. Such fields can be described in terms of potentials $(\vec{A}, \Phi)$ according to

$$\begin{aligned} \vec{B} &= \vec{\nabla} \times \vec{A} \qquad\qquad ; \text{ electromagnetic potentials} \\ \vec{E} &= -\vec{\nabla}\Phi - \frac{\partial \vec{A}}{\partial t} \end{aligned} \tag{11.67}$$

In quantum mechanics, as well as in classical mechanics, these fields can be incorporated by making the following replacements

$$\begin{aligned} \vec{p} &\to \vec{p} - e\vec{A} \qquad ; \text{ incorporate E-M field} \\ H &\to H + e\Phi \end{aligned} \tag{11.68}$$

Thus the Dirac equation in the presence of an electromagnetic field becomes

$$\left[c\vec{\alpha}\cdot(\vec{p} - e\vec{A}) + \beta m_0 c^2 + e\Phi\right]\Psi = i\hbar\frac{\partial\Psi}{\partial t} \qquad ; \text{ Dirac eqn} \tag{11.69}$$

This Dirac equation leads to the following remarkable results:[14]

(1) When applied to an electron in a static magnetic field described by $\vec{A}(\vec{x})$, one finds a magnetic moment of

$$\vec{\mu}_{\text{el}} = \frac{e\hbar}{2m_e}\,2\vec{\mathcal{S}} \qquad ; \vec{\mathcal{S}} = \frac{1}{2}\vec{\sigma} \tag{11.70}$$

Thus

- Since $\hbar\vec{\mathcal{S}}$ is a spin angular momentum, one concludes that the Dirac equation describes a *particle of spin-1/2*;
- The electron is predicted to have a *g-factor of* $g_s = 2$, in accord with observation;

(2) In a static, central, electric field described by $\Phi(r)$, the electrons experience a *spin-orbit interaction*

$$V_{\text{SO}} = e\left(\frac{\hbar}{2m_e c}\right)^2 \frac{1}{r}\left(\frac{d\Phi}{dr}\right) 2\vec{\mathcal{S}}\cdot\vec{l} \tag{11.71}$$

where the orbital angular momentum is $\hbar\vec{l}$. This is again in accord with the experimental observation.

In *summary*, Dirac's rather simple arguments on incorporating relativity and quantum mechanics lead to an absolutely remarkable, and far-reaching, theory of spin-1/2 fermions!

11.4 Path Integrals

Let us go back to the starting point in this chapter. There is another approach to quantum mechanics that makes use of *path integrals*.[15] In the

[14] See Probs. 11.9–11.10; see also [Walecka (2008)].

[15] See [Feynman and Hibbs (2010); Shankar (1994); Walecka (2010)].

theory of quantum mechanics, the transition probability amplitude for a particle to go from a point (q_1, t_1) to a point (q_2, t_2) can be written[16]

$$\langle q_2 t_2 | q_1 t_1 \rangle = \int \mathcal{D}(q) \exp\left\{ \frac{i}{\hbar} S(2,1) \right\} \qquad ; \text{ path integral} \quad (11.72)$$

where $S(2,1)$ is the action

$$S(2,1) = \int_1^2 dt\, L\,(q, \dot{q}) \quad (11.73)$$

Here the integral goes over all possible *paths* between the two points (it is a *path integral*). In the *classical limit* where Planck's constant $\hbar \to 0$, the phase oscillates very rapidly. The method of *stationary phase* for evaluating such an integral (see [Fetter and Walecka (2003)]) implies that if one can find a path that leaves the phase *stationary*, then the integral receives all of its contribution along that path. The condition for finding a stationary path is precisely Hamilton's principle

$$\delta S(2,1) = 0 \qquad ; \ \hbar \to 0 \quad (11.74)$$

The present text is an *introduction* to quantum mechanics, and going into the path-integral approach takes us too far from our stated goals; however, as a guide to future study, we do want to at least make the reader aware of some of the features of functional methods and path integrals as applied to relativistic quantum mechanics:[17]

- This approach unites quantum mechanics, field theory, and statistical mechanics;
- It provides an alternative to doing quantum mechanics with canonical quantization;
- Exact expressions are obtained for quantum mechanical transition amplitudes;
- Everything is written in terms of *classical quantities*, in particular, the classical lagrangian and classical action;
- The price for this is that one has to consider *other dynamical paths* than the classical one given by Hamilton's principle of stationary action;
- With this approach, one can readily study the implications of various symmetries of the lagrangian, even with highly nonlinear interactions

[16] See [Walecka (2010)].

[17] Two basic references here are [Feynman and Hibbs (2010); Abers and Lee (1973)]—see also [Itzykson and Zuber (1980)].

with derivative couplings, where canonical quantization becomes prohibitively difficult;

- Reduction to multiple convergent integrals lends itself to numerical methods.

Chapter 12

Problems

1.1 The discussion started with a classical wave that is the real part of

$$\Psi(x,t) = e^{i(kx-\omega t)} \tag{12.1}$$

Suppose we have two oscillating functions with the same frequency

$$\begin{aligned} \mathrm{Re}\left(\alpha e^{-i\omega t}\right) &= \frac{1}{2}\left(\alpha e^{-i\omega t} + \alpha^* e^{i\omega t}\right) \\ \mathrm{Re}\left(\beta e^{-i\omega t}\right) &= \frac{1}{2}\left(\beta e^{-i\omega t} + \beta^* e^{i\omega t}\right) \end{aligned} \tag{12.2}$$

and suppose we are interested in the *product* of these functions, as in the energy, energy flux, etc. Furthermore, suppose we want the *time average* of such products, which we denote by $\langle \cdots \rangle$.

(a) Show

$$\langle \mathrm{Re}\left(\alpha e^{-i\omega t}\right)\ \mathrm{Re}\left(\beta e^{-i\omega t}\right)\rangle = \frac{1}{4}\left(\alpha\beta^* + \alpha^*\beta\right) = \frac{1}{2}\mathrm{Re}\left(\alpha\beta^*\right) \tag{12.3}$$

(b) Suppose the wave function is a superposition of two such terms

$$\Psi(x,t) = \mathrm{Re}\left(\alpha e^{-i\omega t}\right) + \mathrm{Re}\left(\beta e^{-i\omega t}\right) \tag{12.4}$$

Show

$$\langle \Psi^2(x,t)\rangle = \frac{1}{2}\left|\alpha+\beta\right|^2 \tag{12.5}$$

These are extremely useful relations when using complex solutions to the classical wave equation while describing real situations.[1]

1.2 Consider a classical plane wave incident on two slits separated by a distance d. If we seek the amplitude of the wave on the other side of the

[1] See [Fetter and Walecka (2003)].

slits, we can just add the waves $\mathrm{Re}[Ae^{i(kx-\omega t)}]$ coming from each slit, where x is the distance to the observing screen. For small angles, the difference in optical pathlength Δ from the second slit is

$$\Delta \approx \theta d \tag{12.6}$$

where d is the slit separation (see Fig. 12.1).

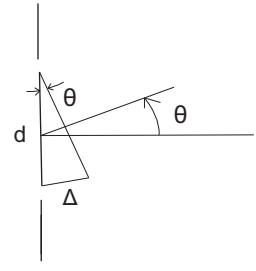

Fig. 12.1 Difference in optical pathlength Δ for two-slit interference pattern measured at an angle θ. A plane wave is incident from the left, and the interference pattern shows up on a screen to the right. The transmitted wave is uniform in the direction normal to this plane.

(a) Use the result in the previous problem to show that the time-average intensity pattern on the observing screen is proportional to

$$\langle \Psi^2(x,y)\rangle = 2|A|^2 \cos^2\left(\frac{k\Delta}{2}\right) \qquad ;\ \text{interference pattern} \tag{12.7}$$

(b) Show the condition for the first interference minimum is then

$$\theta \approx \frac{\lambda}{2d} \qquad ;\ \text{first minimum} \tag{12.8}$$

Note that no matter how small the slit separation d, if the incident wavelength λ is comparable to it, then this interference pattern will show up at a *finite angle* on the screen.

1.3 (a) Suppose we have a physical system satisfying the classical wave equation and obeying periodic boundary conditions (p.b.c.) in one dimension

$$k = \frac{2\pi n}{L} \qquad ;\ n = 0, \pm 1, \pm 2, \cdots \tag{12.9}$$

Write the differential form of this relation as

$$dk = \frac{2\pi}{L} dn \tag{12.10}$$

Use $\omega = kc$ to conclude that the number of normal modes per unit length is given by

$$\frac{1}{L} dn = \frac{1}{c} d\nu \tag{12.11}$$

(b) Extend this result to two dimensions, and show

$$\frac{1}{L^2} d^2 n = \frac{1}{L^2} dn_x dn_y = \frac{1}{c^2} d\nu_x d\nu_y \tag{12.12}$$

If this is summed over all modes with a given length ν, then show the number of modes per unit area is

$$\frac{1}{L^2} d^2 n = \frac{2\pi}{c^2} \nu \, d\nu \tag{12.13}$$

(c) Show that in three dimensions, the number of modes per unit volume of frequency ν is given by

$$\frac{1}{L^3} d^3 n = \frac{4\pi}{c^3} \nu^2 \, d\nu \tag{12.14}$$

If there is a degeneracy of g for the types of normal modes at a given frequency, then

$$\frac{1}{L^3} d^3 n = \frac{4\pi g}{c^3} \nu^2 \, d\nu \tag{12.15}$$

(d) With the use of $g = 2$ for the two transverse polarizations of a free electromagnetic wave, and with the equipartition result for the energy of a normal mode in Eq. (1.4), show that one obtains the following classical expression for the electromagnetic energy density in a cavity

$$U(\nu, T) = \frac{8\pi k_B T \nu^2}{c^3} \qquad ; \text{ classical energy density} \tag{12.16}$$

1.4 A photon has a frequency just into the ultraviolet

$$\nu = 10^{15} \text{ Hz} \tag{12.17}$$

What is its wavelength? What is its energy? What is its momentum?

1.5 (a) In the books on *Introduction to Classical Mechanics* it is shown that the energy E and radius a of a particle of mass μ and charge e performing circular orbits about a point charge $-Ze$ are

$$\begin{aligned} E &= -\frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{2a} && ;\ \text{energy} \\ a &= \frac{4\pi\varepsilon_0}{Ze^2}\frac{\vec{L}^{\,2}}{\mu} && ;\ \text{radius} \end{aligned} \tag{12.18}$$

where $|\vec{L}\,| = \mu a v$ is the angular momentum. Verify these results;

(b) We shall show at the beginning of the next chapter that de Broglie's relation for the wavelength of a particle implies that the angular momentum of the above system is *quantized* as $|\vec{L}\,| = n\hbar$ with $\hbar = h/2\pi$ where h is Planck's constant, and n is an integer $n = 1, 2, \cdots$. Show this immediately yields Bohr's quantum theory of the spectrum of one-electron atoms.[2]

1.6 (a) Suppose we analyze a photon-electron collision through the conservation of momentum and energy

$$\begin{aligned} \vec{p}_e &= \vec{p}_0 - \vec{p}_1 && ;\ \text{momentum conservation} \\ h\nu_0 &= h\nu_1 + \frac{\vec{p}_e^{\,2}}{2m} && ;\ \text{energy conservation} \end{aligned} \tag{12.19}$$

Show the substitution of the first relation in the second leads to

$$\begin{aligned} h(\nu_0 - \nu_1) &= \frac{1}{2m}(\vec{p}_0 - \vec{p}_1)^2 = \frac{1}{2m}\left(\frac{h}{c}\right)^2 (\nu_0^2 + \nu_1^2 - 2\nu_0\nu_1\cos\theta) \\ \nu_0 - \nu_1 &= \frac{h}{mc^2}\nu_0\nu_1\left[(1-\cos\theta) + \frac{(\nu_0-\nu_1)^2}{2\nu_0\nu_1}\right] \end{aligned} \tag{12.20}$$

(b) Show that if the energy shift is small, the last term can be neglected for all θ of interest

$$\frac{(\nu_0-\nu_1)^2}{2\nu_0\nu_1} \ll 1 \tag{12.21}$$

(c) The frequency of the light is related to its wavelength by $\nu_0 = c/\lambda_0$ and $\nu_1 = c/\lambda_1$. Hence show that one arrives at the lovely, simple Compton formula for the shift in wavelength[3]

$$\lambda_1 - \lambda_0 = \frac{h}{mc}(1-\cos\theta) \qquad ;\ \text{Compton formula} \tag{12.22}$$

[2] See [Walecka (2008)].

[3] With the use of proper relativistic kinematics for the particle, this result holds without approximation.

This is in complete agreement with the experimental results. The results on Compton scattering confirmed the particle nature of the photon introduced by Einstein in his explanation of the photoelectric effect.

2.1 Suppose one repeatedly prepares a non-relativistic particle in the plane-wave state of definite momentum in Eq. (2.5) and sends it against the two-slit opening in Fig. 12.1. Show the measured particle density on the screen will exhibit an interference pattern *identical* to that in Prob. 1.2.

2.2 (a) Consider a particle of mass m_0 constrained to move in a circle of radius a in the (x, y)-plane. Show the classical hamiltonian is

$$H = \frac{1}{2I} L_z^2 \qquad ; \; I = m_0 a^2 \tag{12.23}$$

where L_z is the angular momentum in the z-direction, and I is the moment of inertia;

(b) In quantum mechanics, L_z is given by

$$L_z = x p_y - y p_x = \frac{\hbar}{i} \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \tag{12.24}$$

It is convenient to measure angular momentum in units of $\hbar$, and to define $L_z \equiv \hbar l_z$. It follows that

$$l_z = \frac{1}{i} \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \qquad ; \; L_z \equiv \hbar l_z \tag{12.25}$$

Consider an eigenfunction of l_z with eigenvalue m

$$l_z f(x, y) = m f(x, y) \qquad ; \text{ eigenvalue } m \tag{12.26}$$

Make this an implicit function of the rotation angle ϕ by defining

$$\begin{aligned} \psi(\phi) \equiv f(x(\phi), y(\phi)) \qquad & ; \; x = a \cos\phi \\ & ; \; y = a \sin\phi \end{aligned} \tag{12.27}$$

Show

$$\frac{1}{i} \frac{d\psi(\phi)}{d\phi} = \frac{1}{i} \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) f(x, y) = l_z f(x, y) \tag{12.28}$$

Hence conclude that the eigenvalue equation for the z-component of the angular momentum can be *rewritten* as

$$l_z \psi(\phi) \equiv \frac{1}{i} \frac{d\psi(\phi)}{d\phi} = m \psi(\phi) \tag{12.29}$$

(c) Show the eigenfunctions of l_z obeying p.b.c. are

$$\psi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \qquad ;\ m = 0, \pm 1, \pm 2, \cdots \quad (12.30)$$

(d) Show these are simultaneous eigenstates of the hamiltonian, with energy eigenvalues

$$E_m = \frac{\hbar^2}{2I}\, m^2 \quad (12.31)$$

2.3 The results in the previous problem can be used to write the Schrödinger equation in polar coordinates in two dimensions. Introduce the coordinates (r, ϕ), and let a partial derivative in these coordinates indicate that the other variable in this pair is to be held fixed.

(a) Show from the previous problem that

$$\frac{\partial \psi(r,\phi)}{\partial \phi} = \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) f(x,y) \qquad ;\ x = r\cos\phi$$
$$;\ y = r\sin\phi \quad (12.32)$$

(b) In exactly the same manner, show

$$\left(r \frac{\partial}{\partial r} \right) \psi(r,\phi) = \left(x \frac{\partial}{\partial x} + y \frac{\partial}{\partial y} \right) f(x,y) \quad (12.33)$$

(c) Apply these relations twice, add, and divide by r^2 to obtain the laplacian in polar coordinates

$$\left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} \right] \psi(r,\phi) = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) f(x,y) \quad (12.34)$$

2.4 The eigenfunctions and eigenvalues for a particle of mass m_0 constrained to move in a circle of radius a in the (x, y)-plane are given in Prob. 2.2 as

$$\psi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \qquad ;\ m = 0, \pm 1, \pm 2, \cdots$$
$$E_m = \frac{\hbar^2}{2I}\, m^2 \quad (12.35)$$

(a) Show the corresponding probability density is a uniform constant;

(b) Show the general solution is

$$\Psi(\phi, t) = \sum_m c_m \psi_m(\phi) e^{-iE_m t/\hbar} \quad (12.36)$$

(c) Suppose one creates an initial state

$$\Psi(\phi,0)=\frac{1}{\sqrt{2}}\left[\psi_{m_1}(\phi)+\psi_{m_2}(\phi)\right] \tag{12.37}$$

Construct the corresponding general solution, and show the probability density now oscillates as a function of time.

(d) What is the frequency of this oscillation?

2.5 (a) Show the corresponding probability current in Prob. 2.4 is[4]

$$S(\phi,t)=\frac{1}{2m_0a}\left\{\Psi^{\star}(\phi,t)\frac{\hbar}{i}\frac{\partial\Psi(\phi,t)}{\partial\phi}+\left[\frac{\hbar}{i}\frac{\partial\Psi(\phi,t)}{\partial\phi}\right]^{*}\Psi(\phi,t)\right\} \tag{12.38}$$

(b) Interpret this quantity;

(c) Calculate $S(\phi,t)$ for the solution $\Psi(\phi,t)=\psi_m(\phi)\,e^{-iE_mt/\hbar}$.

2.6 The mean value of a hermitian operator O with a normalized wave function $\psi(x)$ is

$$\langle O\rangle=\int dx\,\psi^{*}(x)O\psi(x) \tag{12.39}$$

In quantum mechanics we are dealing with probability distributions, and the *mean-square-deviation* from this mean value is given by

$$(\Delta O)^2\equiv\left\langle\left(O-\langle O\rangle\right)^2\right\rangle=\langle O^2\rangle-\langle O\rangle^2 \tag{12.40}$$

Make use of the normalized ground-state wave function for a particle in a one-dimensional box of length L in Eq. (3.12) [recall Figs. 3.2 and 3.3], and demonstrate the following:

(a) Show that for the momentum

$$\langle p\rangle=0 \qquad ;\ \langle p^2\rangle=\hbar^2\left(\frac{\pi}{L}\right)^2 \tag{12.41}$$

(b) Show that for the spatial coordinate[5]

$$\langle x\rangle=\frac{L}{2} \qquad ;\ \langle x^2\rangle=\frac{L^2}{3}\left(1-\frac{3}{2\pi^2}\right) \tag{12.42}$$

[4]Recall Eq. (4.28); here m_0 is the rest mass, and ϕ is the polar angle.

[5]Note the following definite integrals

$$\int_0^{\pi}du\,u\sin^2(u)=\frac{\pi^2}{4} \qquad ;\ \int_0^{\pi}du\,u^2\sin^2(u)=\frac{\pi^3}{6}-\frac{\pi}{4}$$

(c) Combine these results to obtain

$$(\Delta p)^2 (\Delta x)^2 = \frac{\hbar^2 \pi^2}{12}\left(1 - \frac{6}{\pi^2}\right)$$
$$\Delta p\, \Delta x = 0.568\, \hbar \tag{12.43}$$

This is an example of the Heisenberg uncertainty principle. The momentum and position (p, q) of a particle *cannot both be specified precisely.* Given the commutation relation $[p, q] = \hbar/i$, it is possible to give a rigorous proof that for a normalized wave function[6]

$$\Delta p\, \Delta q \geq \frac{1}{2}\hbar \qquad ;\ \text{uncertainty principle} \tag{12.44}$$

The uncertainty principle represents a significant break from classical mechanics where one initializes a mechanical system at a given point (p, q) in phase space, and then follows it in a deterministic fashion from there.

2.7 Although the solutions to the Schrödinger equation and corresponding probability densities for a particle in a box in Figs. 3.2 and 3.3 are so simple and clear, the solution for a free particle is more subtle.[7] For example, the probability density obtained from our motivating wave in Eq. (2.5) is *independent of position and time!* In order to construct a probability density that moves with the particle, we need to construct a *wave packet.*

(a) Take a *superposition* of the waves in Eq. (2.5) with an amplitude sharply peaked about a wavenumber corresponding to the classical momentum $p_0 = \hbar k_0$.[8] Construct

$$\Psi(x, t) = \int dk\ A(k - k_0) e^{i[kx - \omega(k)t]} \qquad ;\ \omega(k) = \hbar k^2/2m \tag{12.45}$$

Show this satisfies the Schrödinger equation for a free particle;

(b) Show that at the initial time $t = 0$, the wave function and probability density are

$$\Psi(x, 0) = e^{ik_0 x} F(x) \qquad ;\ |\Psi(x, 0)|^2 = |F(x)|^2$$
$$F(x) = \int dl\ A(l)\, e^{ilx} \tag{12.46}$$

where the amplitude $A(l) = A(k - k_0)$ is sharply peaked about $l = 0$;

(c) As an example, take $A(l) = 1$ for $|l| < l_0$; calculate and plot $|F(x)|^2$;

[6] See, for example, [Walecka (2008)].

[7] This is why we have left it as a problem—so as not to interrupt the flow of the text.

[8] Recall the previous problem on the uncertainty principle.

(d) Since $A(l)$ is sharply peaked about $l = 0$, we can make a Taylor series expansion of $\omega(k)$ about k_0 and keep just the first term

$$\omega(k) \approx \omega(k_0) + (k - k_0) \left[\frac{d\omega(k)}{dk} \right]_{k_0} \tag{12.47}$$

Show that for finite time, the probability density then becomes

$$|\Psi(x,t)|^2 = |F(x - v_{\rm gp}t)|^2 \tag{12.48}$$

Here $v_{\rm gp}$ is the *group velocity*[9]

$$v_{\rm gp} = \left[\frac{d\omega(k)}{dk} \right]_{k_0} = \frac{\hbar k_0}{m} = \frac{p_0}{m} \tag{12.49}$$

Thus the probability density for the localized wave packet moves with the classical particle velocity!

3.1 Suppose the potential in Fig. 3.4 has the opposite sign and is an *attractive half-space*, with $V(x) = -V_0 < 0$ for all positive x. Write the transmitted wave as

$$\psi(x) = t\, e^{i\kappa x} \qquad ;\ \kappa^2 = \frac{2m}{\hbar^2}(E + V_0) \tag{12.50}$$

Match the boundary conditions at $x = 0$, and show the transmitted amplitude is

$$t = \frac{2k}{k + \kappa} \tag{12.51}$$

Discuss.

3.2 Show that the expansion coefficients in the general solution for a particle in a square box in Eq. (3.42) are obtained from the initial condition

$$\Psi(x, y, 0) = g(x, y) \tag{12.52}$$

according to

$$c_{n_x,n_y} = \int_0^L dx \int_0^L dy\, \psi^*_{n_x,n_y}(x, y)\, g(x, y) \tag{12.53}$$

[9]The *phase velocity* of a wave is $v_{\rm ph} = \omega(k)/k$. Note that for this free-particle wave packet, the group velocity is twice the phase velocity.

3.3 (a) Suppose one prepares the following initial state for the particle in the one-dimensional box[10]

$$\Psi(x,0) = \frac{1}{\sqrt{2}}\left[\psi_1(x) + \psi_2(x)\right] \tag{12.54}$$

Plot the initial wave function and probability distribution.

(b) Construct the solution $\Psi(x,t)$ and probability distribution $|\Psi(x,t)|^2$ for later times;

(c) Show that probability distribution oscillates back and forth in the box;

(d) What is the frequency of that oscillation?

3.4 Suppose one prepares an initial state for the particle in a box that is simply constant over the box

$$\Psi(x,0) = \frac{1}{\sqrt{L}} \qquad ;\ 0 \le x \le L \tag{12.55}$$

Show the solution to the Schrödinger equation for all subsequent time is

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}$$
$$c_n = \frac{\sqrt{2}}{\pi}\left[\frac{1-(-1)^n}{n}\right] \tag{12.56}$$

It is interesting that this simplest of initial conditions gives rise to such a complicated wave function.

3.5 Suppose there is a small circular potential at the center of the two-dimensional square box of the form

$$\delta V(\vec{r}) = \nu_0 \qquad ;\ |\vec{r} - \vec{r}_0| < a \tag{12.57}$$

where $\vec{r}_0$ is located at the center of the box. Assume $a \ll L$. Use perturbation theory to show that the shift in the ground-state eigenvalue is then

$$\delta E_{1,1} = 4\nu_0 \frac{\pi a^2}{L^2} \tag{12.58}$$

3.6 Consider the non-degenerate perturbation theory in Eqs. (3.55).

(a) Show that this analysis holds for a particle in a one-dimensional box with an additional potential $\delta V(x)$;

[10] See Figs. 3.2 and 3.3.

(b) Suppose the perturbation $\delta V(x)$ is *odd* about the midpoint of the box. Show that all the first-order energy shifts then vanish;

(c) Show that the second-order energy shift always *lowers* the energy of the ground state.

4.1 Suppose the spherical square-well potential in Chapter 4 is just deep enough to have one bound state at $k^2 = 0$.

(a) Show the depth of the potential is $2mV_0/\hbar^2 = \pi^2/4d^2$;

(b) What is the s-wave wave function inside the potential?

(c) What is it outside?

4.2 In the separated radial Schrödinger equation for a free particle in spherical coordinates there are two types of solutions that form a fundamental system in which any radial solution can be expanded. These are the spherical Bessel functions $j_l(\rho)$ and *spherical Neumann functions* $n_l(\rho)$.

(a) For $l = 0$ the spherical Neumann function is

$$n_0(\rho) = -\frac{\cos\rho}{\rho} \tag{12.59}$$

Show this satisfies the same radial equations as $j_0(\rho)$;

(b) For $l = 1$ the spherical Neumann function is

$$n_1(\rho) = -\frac{\cos\rho}{\rho^2} - \frac{\sin\rho}{\rho} \tag{12.60}$$

Show this satisfies the same radial equation as $j_1(\rho)$;

(c) Show that through this order, the Neumann functions satisfy the general relations

$$\begin{aligned} n_l(\rho) &\to -\frac{1\cdot 1\cdot 3\cdots(2l-1)}{\rho^{l+1}} \qquad ;\ \rho \to 0 \\ n_l(\rho) &\to \frac{1}{\rho}\sin\left[\rho - (l+1)\pi/2\right] \qquad ;\ \rho \to \infty \end{aligned} \tag{12.61}$$

Note that the spherical Neumann functions are singular at the origin.

4.3 The spherical harmonics are the non-singular solutions to the angular part of the Schrödinger equation in spherical coordinates. For $l = 1$ one has

$$Y_{1,0}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta \qquad ;\ Y_{1,\pm1}(\theta,\phi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi} \tag{12.62}$$

Show these satisfy the angular equation

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]Y_{l,m}(\theta,\phi)=-l(l+1)Y_{l,m}(\theta,\phi) \tag{12.63}$$

4.4 This problem involves the explicit verification of some results on the probability flux quoted in the text:

(a) Verify Eqs. (4.30);

(b) Verify Eq. (5.36).

4.5 Suppose one has a Yukawa potential of the form

$$v(r)=\lambda\frac{e^{-\mu r}}{r} \qquad ;\ \text{Yukawa potential} \tag{12.64}$$

Show that Born approximation for the scattering amplitude is given by

$$f_{BA}(k,\theta)=-\frac{\lambda}{q^2+\mu^2} \tag{12.65}$$

Sketch and discuss.

4.6 Suppose one has a spherical potential of the form

$$v(r)=v_0 \qquad ;\ r<d \qquad ;\ \text{spherical potential} \tag{12.66}$$

Show that Born approximation for the scattering amplitude is given by

$$f_{BA}(k,\theta)=-(v_0d^3)\,\frac{j_1(qd)}{qd} \tag{12.67}$$

Sketch and discuss.

5.1 Suppose the interaction in our model problem is an integrable short-range potential of the form

$$H'(x_2,x_1)=V(|x_2-x_1|) \qquad ;\ \text{integrable potential} \tag{12.68}$$

(a) Define the momentum transfer by

$$q\equiv k_0-k \qquad ;\ \text{momentum transfer} \tag{12.69}$$

Show the matrix element of the interaction in Eqs. (5.37) takes the form

$$\begin{aligned}\langle k, n_2|H'|k_0, n_2^0\rangle &= \tilde{V}(q)\,\tilde{\rho}_{fi}(q)\\ \tilde{V}(q) &= \int_{-\infty}^{\infty} dx\; e^{iqx}\, V(|x|)\\ \tilde{\rho}_{fi}(q) &= \int_0^{L_2} dx\; e^{iqx}\,\psi^*_{n_2}(x)\psi_{n_2^0}(x)\end{aligned} \tag{12.70}$$

(b) Show the rate in Eqs. (5.37) becomes

$$\frac{1}{I_{\rm inc}} R_{fi}\, dn_f = \left(\frac{k}{k_0}\right)\left|\left(\frac{m_1}{\hbar^2 k}\right)\tilde{V}(q)\right|^2 |\tilde{\rho}_{fi}(q)|^2 \tag{12.71}$$

(c) Show this has the correct dimensions.

5.2 The previous problem provides an expression for the ratio of the transition rate to the incident flux in our model problem of the scattering of one particle from another trapped inside a box in one dimension. It remains to evaluate the target transition matrix element $\tilde{\rho}_{fi}(q)$. Since everything now concerns the particle in the box, we can drop the superfluous subscript 2. For the transition from the ground state with $n = 1$ to an excited state with n, one needs the integral

$$\tilde{\rho}_{n,1}(q) = \frac{2}{L}\int_0^L dx\, e^{iqx} \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{\pi x}{L}\right) \tag{12.72}$$

where the quantum number n and the size L now refer to the box.[11]

(a) Evaluate this integral and show

$$\tilde{\rho}_{n,1}(q) = \frac{1}{i}\frac{4n\pi^2(qL)}{[(qL)^2 - (n^2+1)\pi^2]^2 - (2n\pi^2)^2}\left[1 + (-1)^n\, e^{iqL}\right] \tag{12.73}$$

(b) Make a plot $|\tilde{\rho}_{n,1}(q)|^2$ as a function of qL (see Fig. 12.2). Discuss.[12]

5.3 Consider the *back scattering* of the projectile in our model problem.

(a) Show that the only modification of the results in Probs. 5.1 and 5.2 is that the momentum transfer now becomes

$$q = k_0 + k \qquad ;\ \text{back scattering} \tag{12.74}$$

(b) Show that this can be made arbitrarily large for a given energy transfer, and hence one can experimentally map out the results in Prob. 5.2(b).

[11] Recall Fig. 3.2.

[12] It is of interest to make at least one log plot to see the diffraction structure.

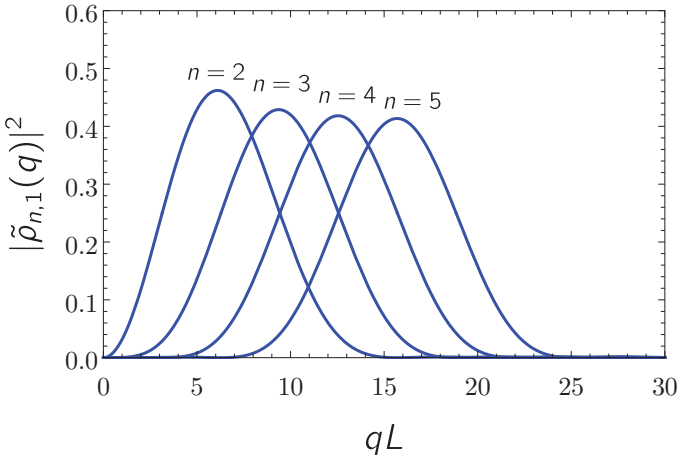

Fig. 12.2 Plot of $|\tilde{\rho}_{n,1}(q)|^2$ as a function of (qL) for four values of n. Here $L \equiv L_2$ is the size of the box. (The author would like to thank Paolo Amore for preparing this figure.)

5.4 The goal of the two-state mixing example is to treat the interaction H' to all orders. The system starts in the state ψ_1 at $t = 0$. Expand the expression for the probability of finding the system in the state ψ_2 after time T in Eq. (5.57), and divide by T, to get the transition rate as $H' \to 0$. Show

$$R_{fi}(T) = \frac{1}{T} P_{fi}(T) = \frac{1}{\hbar^2} |\langle \psi_2 | H' | \psi_1 \rangle|^2 \, T \qquad ; \; H' \to 0 \tag{12.75}$$

Show this reproduces the *lowest-order* expression for the transition rate in Eq. (5.21) at energy conservation $\hbar\omega = 0$.

6.1 The electromagnetic fields $(\vec{E}, \vec{B})$ are related to the potentials by

$$\begin{aligned} \vec{B}(\vec{x}, t) &= \vec{\nabla} \times \vec{A}(\vec{x}, t) \\ \vec{E}(\vec{x}, t) &= -\frac{\partial \vec{A}(\vec{x}, t)}{\partial t} - \vec{\nabla} \Phi(\vec{x}, t) \end{aligned} \tag{12.76}$$

Let $\Lambda(\vec{x}, t)$ be a well-defined function of position and time.

(a) Show the electromagnetic fields are unchanged under a *gauge*

transformation

$$\vec{A}(\vec{x},t) \to \vec{A}(\vec{x},t) + \vec{\nabla}\Lambda(\vec{x},t) \qquad ;\ \text{gauge transformation}$$
$$\Phi(\vec{x},t) \to \Phi(\vec{x},t) - \frac{\partial\Lambda(\vec{x},t)}{\partial t} \tag{12.77}$$

Since the fields are unchanged, the physics should be unchanged.

(b) Show that the terms in Λ can be eliminated from the Schrödinger equation by making a *local phase transformation* on the wave function

$$\Psi(\vec{x},t) \to e^{ie\Lambda(\vec{x},t)/\hbar}\,\Psi(\vec{x},t) \tag{12.78}$$

Remember that the wave function is *not* a physical observable.

6.2 Suppose one has chosen a vector potential $\vec{A}'(\vec{x},t)$ which reproduces the $(\vec{E},\vec{B})$ fields, and suppose the *divergence* of this field is non-zero

$$\vec{\nabla}\cdot\vec{A}'(\vec{x},t) = \rho'(\vec{x},t) \tag{12.79}$$

(a) Make a gauge transformation as in Prob. 6.1, and show that with the new vector potential $\vec{A}(\vec{x},t)$

$$\vec{\nabla}\cdot\vec{A}(\vec{x},t) = \rho'(\vec{x},t) + \nabla^2\Lambda(\vec{x},t) \tag{12.80}$$

(b) Conclude that one can always work in the *Coulomb gauge*, where

$$\vec{\nabla}\cdot\vec{A}(\vec{x},t) = 0 \qquad ;\ \text{Coulomb gauge} \tag{12.81}$$

6.3 Show that if one were to retain just the first term in the time-dependent interaction in Eq. (6.17), so that

$$H' = -e\mathcal{E}_0 x\cos(\omega_0 t) \doteq -\left(\frac{e\mathcal{E}_0}{2}\right) x\, e^{i\omega_0 t} \tag{12.82}$$

then the rate R_{fi} in Eq. (6.20) would become

$$R_{fi} = \left(\frac{e\mathcal{E}_0}{2}\right)^2 \frac{2\pi}{\hbar}|\langle f|x|i\rangle|^2\delta(E_f - E_i + \hbar\omega_0) \qquad ;\ \text{de-excitation} \tag{12.83}$$

Compare this with the rate R_{fi} in Eq. (6.20)

$$R_{fi} = \left(\frac{e\mathcal{E}_0}{2}\right)^2 \frac{2\pi}{\hbar}|\langle f|x|i\rangle|^2\delta(E_f - E_i - \hbar\omega_0) \qquad ;\ \text{excitation} \tag{12.84}$$

Now fix E_i and $\hbar\omega_0$, and conclude the following:

- As a function of E_f there are two non-overlapping rate expressions, one for $E_f = E_i - \hbar\omega_0$, and one for $E_f = E_i + \hbar\omega_0$;
- Since there is no overlap of the two expressions, one can ignore any *interference term* between them in the calculation of the rates;
- In leading order, the real time-dependent perturbation H' in Eq. (6.17) therefore describes both *de-excitation* and *excitation* of the system;
- Correspondingly, the perturbation H' in Eq. (6.26) describes both *emission* and *absorption* of radiation.

6.4 This problem reviews the main aspects of *adjoints* and *hermiticity*. For simplicity, we go back to one dimension and express the matrix element of an operator N between two acceptable wave functions as

$$\langle\psi_f|N|\psi_i\rangle = \int dx\ \psi_f^*(x) N\psi_i(x) \tag{12.85}$$

The *adjoint* operator $N^\dagger$ is then defined through the relation

$$\int dx\ \left[N^\dagger\psi_f(x)\right]^*\psi_i(x) = \int dx\ \psi_f^*(x) N\psi_i(x) \qquad ;\ \text{adjoint} \tag{12.86}$$

An operator is *hermitian* if it is identical to its adjoint

$$N^\dagger = N \qquad ;\ \text{hermitian} \tag{12.87}$$

(a) The eigenstates of N satisfy

$$N\psi_n(x) = n\,\psi_n(x) \tag{12.88}$$

Take the matrix element of this relation with $\psi_n^*(x)$, and prove that the eigenvalues of a hermitian operator are *real*;

(b) Suppose one has a *pair* of operators MN. Show

$$(MN)^\dagger = N^\dagger M^\dagger \tag{12.89}$$

(c) Reverify that the operators $p = (\hbar/i)d/dx$ and $H = p^2/2m + V(x)$ with a real $V(x)$ are hermitian;

(d) Show that in two-dimensions, the angular momentum operator L_z is hermitian.

6.5 (a) Show that the number of eigenstate $|n\rangle$ in Sec. 6.7 can actually be constructed as

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle \tag{12.90}$$

(b) Make use of the commutation relations to show this state is normalized

$$\langle n|n\rangle = 1 \tag{12.91}$$

6.6 Repeat the calculation of photoionization starting from the quantized radiation field and a single photon in the state $|1_{\vec{k}s}\rangle$. Use an incident photon flux of

$$I_{\rm inc} = \frac{c}{\Omega} \qquad ;\ \text{photon flux} \tag{12.92}$$

Show the *photoionization cross-section* becomes

$$\begin{aligned}\sigma_{fi} &\equiv \frac{1}{I_{\rm inc}} R_{fi}\, dn_f \qquad ;\ \text{photoionization} \\ &= \frac{\alpha}{2\pi c^2}\left(\frac{mc}{\hbar}\right)\left(\frac{k_f}{k}\right)\left|\hat{e}_{\vec{k}s}\cdot\int d^3x\, e^{i(\vec{k}-\vec{k}_f)\cdot\vec{x}}\left(\frac{\vec{p}}{m}\right)\psi_0(\vec{x})\right|^2 d\Omega_f\end{aligned} \tag{12.93}$$

6.7 The required transition matrix element for the quantum system in the general expression for the photon emission rate in Eq. (6.81) is

$$\vec{M}_{fi} = \int d^3x\, e^{-i\vec{k}\cdot\vec{x}}\,\psi_f^*(\vec{x})\,\frac{\vec{p}}{m}\,\psi_i(\vec{x}) \tag{12.94}$$

(a) Suppose the hamiltonian for that quantum system has the form

$$H = \frac{\vec{p}^{\,2}}{2m} + V(\vec{x}) \tag{12.95}$$

Show

$$[H,\vec{x}\,] = \frac{\hbar}{i}\frac{\vec{p}}{m} \tag{12.96}$$

Hence, show

$$\vec{M}_{fi} = \frac{i}{\hbar}\int d^3x\, e^{-i\vec{k}\cdot\vec{x}}\,\psi_f^*(\vec{x})\,[H,\vec{x}\,]\,\psi_i(\vec{x}) \tag{12.97}$$

(b) Now assume the wavelength of the light is such that $kR \ll 1$ where R is a measure of the size of the system. Then

$$e^{-i\vec{k}\cdot\vec{x}} \approx 1 \qquad ;\ kR \ll 1 \tag{12.98}$$

Show that in this limit the required matrix element becomes

$$\vec{M}_{fi} = \frac{i}{\hbar}(E_f - E_i)\int d^3x\ \psi_f^*(\vec{x})\,\vec{x}\,\psi_i(\vec{x}) \qquad ;\ \text{dipole approx.} \tag{12.99}$$

This is known as the *dipole approximation*.

7.1 Consider a non-interacting spin-1/2 Fermi gas inside a big box of volume $V = L^3$ with p.b.c. in all three directions. In its ground state, the levels are filled up to a wavenumber $|\vec{k}| = k_F$.

(a) Count the number of filled levels. Show the number of particles per unit volume is

$$n_0 \equiv \frac{N}{V} = \frac{1}{V}\left[\frac{2L^3}{(2\pi)^3}\int_0^{k_F} d^3k\right] = \frac{k_F^3}{3\pi^2} \tag{12.100}$$

(b) Show the energy per particle is

$$\frac{E}{N} = \frac{3}{5}\varepsilon_F \qquad ;\ \varepsilon_F = \frac{(\hbar k_F)^2}{2m} \tag{12.101}$$

where ε_F is the *Fermi energy*.

(c) Compute the pressure from the first law of thermodynamics $P = -(dE/dV)$.[13] Show

$$P = \frac{2}{5}\frac{\hbar^2}{2m}(3\pi^2)^{2/3}\, n_0^{5/3} \qquad ;\ \text{Fermi gas} \tag{12.102}$$

7.2 Consider a non-interacting spin-0 Bose gas of massive particles inside a big box of volume $V = L^3$ with p.b.c. in all three directions. In its ground state, the particles all occupy the $\vec{k} = 0$ level.

(a) Compute the pressure from the first law of thermodynamics $P = -(dE/dV)$. Show

$$P = 0 \qquad ;\ \text{Bose gas} \tag{12.103}$$

(b) Suppose instead, that the particles are confined to a large cubical box of volume $V = L^3$, where the ground-state single-particle energy is $\varepsilon_0 = (\hbar^2/2m)(3\pi^2/L^2)$. Show the pressure is

$$P = \frac{2}{3}\varepsilon_0 n_0 \qquad ;\ n_0 = \frac{N}{V} \tag{12.104}$$

Compare with the result in part (a). Discuss.

7.3 While the full quantum many-body problem is complicated, the Hartree self-consistent field approximation provides a surprisingly good first approximation for many finite systems such as the electron cloud in the

[13] Here the many-body system is in its ground state at a temperature $T = 0$.

atom or the atomic nucleus. Suppose there is a two-body interaction $V(|\vec{x}-\vec{y}\,|)$. The Hartree single-particle potential is defined by

$$U_H(\vec{x}) = \int d^3y\, V(|\vec{x}-\vec{y}\,|)n(\vec{y}) \tag{12.105}$$

where the particle density is given by the sum over all the occupied states of the absolute square of the single-particle wave functions

$$n(\vec{y}) = \sum_i |\psi_i(\vec{y})|^2 \qquad ;\text{ over occupied states} \tag{12.106}$$

These wave functions, in turn, are given by the solutions in the self-consistent potential

$$\left[-\frac{\hbar^2\nabla^2}{2m} + U_H(\vec{x}\,)\right]\psi_i(\vec{x}\,) = \varepsilon_i\psi_i(\vec{x}) \tag{12.107}$$

Provide a physical motivation for the Hartree equations, and give some indication as to how you would go about solving them.

7.4 Consider a Bose gas where essentially all the particles remain in the condensate. Suppose the two-particle interaction is a contact interaction.

(a) Show that the Hartree potential takes the form

$$U_H(\vec{x}\,) = \lambda|\phi_0(\vec{x}\,)|^2 \tag{12.108}$$

where ϕ_0 is the condensate wave function in Eqs. (7.16)–(7.17), and λ is a constant independent of N.

(b) Show that the Hartree equation for that condensate wave function then becomes

$$\left[-\frac{\hbar^2\nabla^2}{2m} + \lambda|\phi_0(\vec{x}\,)|^2\right]\phi_0(\vec{x}\,) = \varepsilon_0\phi_0(\vec{x}) \tag{12.109}$$

Note that this is now simply a local, nonlinear, differential equation.

7.5 Consider the non-interacting Bose condensate wave function $\phi_0 = \sqrt{N}\psi_0$ in Eq. (7.16), where ψ_0 is the ground-state single-particle level.[14] Suppose the particles are in a big box with p.b.c in all directions.

(a) Show the square of the modulus is

$$|\phi_0|^2 = n_0 \qquad ;\text{ particle density} \tag{12.110}$$

where n_0 is the particle density;

[14] We choose $\xi = 1$.

(b) Compute the probability flux $\vec{S}$ from Eq. (4.28) using this wave function, and show the medium is at rest

$$\vec{S}(\phi_0) = 0 \tag{12.111}$$

(c) The medium can be given a velocity by including a spatially-dependent phase in the single-particle wave function $\psi_0 \to \psi_0\, e^{i\chi(\vec{x})}$. Show the expression for the particle density is unchanged

$$|\phi_0 e^{i\chi}|^2 = n_0 \tag{12.112}$$

(d) The velocity of the medium can now be identified from the probability flux calculated with this new wave function. Give an argument that

$$n_0 \vec{v} = \vec{S}\left(\phi_0 e^{i\chi}\right) \tag{12.113}$$

Hence obtain

$$\vec{v} = \frac{\hbar}{m}\vec{\nabla}\chi \qquad ;\ \text{fluid velocity} \tag{12.114}$$

The fluid velocity of the Bose condensate is obtained from the gradient of the phase of the single-particle wave function.

(e) Show the fluid motion is irrotational

$$\vec{\nabla} \times \vec{v} = 0 \qquad ;\ \text{irrotational} \tag{12.115}$$

7.6 Repeat Prob. 7.1 for non-interacting spin-1/2 particles in a one-dimensional box.

(a) Show the particle density is given by

$$n_0 \equiv \frac{N}{L} = \frac{1}{L}\left[\frac{2L}{\pi}\int_0^{k_F} dk\right] = \frac{2k_F}{\pi} \tag{12.116}$$

(b) Show the energy per particle is

$$\frac{E}{N} = \frac{1}{3}\varepsilon_F \qquad ;\ \varepsilon_F = \frac{(\hbar k_F)^2}{2m} \tag{12.117}$$

(c) Show these are the *same results* one gets for particles moving on the large circle with p.b.c. (Remember to include both directions!)

7.7 One can go from plane-polarized photons to photons with a given helicity through a *canonical transformation*. Define

$$\vec{e}_{\vec{k},\pm 1} \equiv \mp\frac{1}{\sqrt{2}}\left(\vec{e}_{\vec{k}1} \pm i\vec{e}_{\vec{k}2}\right) \qquad ;\ b_{\vec{k},\pm 1} \equiv \mp\frac{1}{\sqrt{2}}\left(b_{\vec{k}1} \mp i b_{\vec{k}2}\right) \tag{12.118}$$

(a) Show

$$\sum_{s=1,2} \vec{e}_{\vec{k}s} b_{\vec{k}s} = \sum_{\lambda=\pm 1} \vec{e}_{\vec{k},\lambda} b_{\vec{k},\lambda} \qquad ; \sum_{s=1,2} \vec{e}_{\vec{k}s} b^\dagger_{\vec{k}s} = \sum_{\lambda=\pm 1} \vec{e}^{\,\dagger}_{\vec{k},\lambda} b^\dagger_{\vec{k},\lambda} \quad (12.119)$$

(b) Show

$$[b_{\vec{k},\lambda},\, b^\dagger_{\vec{k},\lambda'}] = \delta_{\lambda,\lambda'} \qquad ; [b_{\vec{k},\lambda},\, b_{\vec{k},\lambda'}] = [b^\dagger_{\vec{k},\lambda},\, b^\dagger_{\vec{k},\lambda'}] = 0 \quad (12.120)$$

The properties of the operators follow from these commutation relations.

8.1 This problem discusses the *spin* of spin-1/2 fermions.[15] The main thing to keep in mind here is that the spin operators and wave functions are very *simple*. The spin operator is

$$\hbar \vec{\mathcal{S}} = \frac{\hbar}{2} \vec{\sigma} \qquad ; \text{ spin operator} \quad (12.121)$$

where $\vec{\sigma}$ are the 2×2 Pauli matrices $(\sigma_x, \sigma_y, \sigma_z)$ defined in Eqs. (11.54). The spin wave functions ("spinors") for spin up and down along the z-axis are

$$\phi_\uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad ; \phi_\downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (12.122)$$

(a) Show these are eigenstates of σ_z

$$\sigma_z \phi_\uparrow = \phi_\uparrow \qquad ; \sigma_z \phi_\downarrow = -\phi_\downarrow \quad (12.123)$$

(b) The eigenstates of spin up and down along the x-axis can be constructed as

$$\phi_\rightarrow = \frac{1}{\sqrt{2}} (\phi_\uparrow + \phi_\downarrow) \qquad ; \phi_\leftarrow = \frac{1}{\sqrt{2}} (\phi_\uparrow - \phi_\downarrow) \quad (12.124)$$

Show

$$\sigma_x \phi_\rightarrow = \phi_\rightarrow \qquad ; \sigma_x \phi_\leftarrow = -\phi_\leftarrow \quad (12.125)$$

(c) Hence, show

$$\phi_\uparrow = \frac{1}{\sqrt{2}} (\phi_\rightarrow + \phi_\leftarrow) \qquad ; \phi_\downarrow = \frac{1}{\sqrt{2}} (\phi_\rightarrow - \phi_\leftarrow) \quad (12.126)$$

8.2 The Stern–Gerlach detector in Fig. 8.1 is rotated by 90° about the y-axis, and the beam with spin-up along the x-axis is separated. The

[15] This problem involves simple matrix manipulations. If these are unfamiliar to you, please do Probs. 11.5 and 11.6 first.

detector is now returned to its initial configuration in Fig. 8.1 and that beam is inserted into it. Express the state $|\rightarrow\rangle$ with spin-up along the x-axis as a linear combination of the states $|\uparrow\rangle$ and $|\downarrow\rangle$ with spin-up and spin-down along the z-axis, and describe what is now observed coming out of that detector returning to its initial configuration.

8.3 (a) Consider a particle of mass m_0 moving in a circle of radius a in the (x, y)-plane, as discussed in Probs. 2.2, 2.4 and 2.5. Suppose the particle has a charge e. We know from E&M that the little current loop has a magnetic moment $\mu_z = (\pi a^2) i_e$, where i_e is the current. Show

$$i_e = e\nu = e\frac{\omega}{2\pi} = e\frac{L_z}{2\pi I} \tag{12.127}$$

Hence, show the magnetic moment is

$$\mu_z = \frac{e}{2m_0} L_z \tag{12.128}$$

(b) When the angular momentum is quantized with $L_z = \hbar m$, show

$$\mu_z = \mu m \qquad ;\ \mu = \frac{e\hbar}{2m_0} \qquad ;\ m = 0, \pm 1, \pm 2, \cdots \tag{12.129}$$

(c) Discuss how the Stern–Gerlach apparatus can be used to prepare a state $\psi_m(\phi) = e^{im\phi}/\sqrt{2\pi}$;

(d) Discuss how photoabsorption on the ground state can be used to prepare a state $\psi = a\psi_m(\phi) + b\psi_{-m}(\phi)$.

9.1 Consider a particle moving in one dimension in a large circle of length L and satisfying periodic boundary conditions. The wave functions are[16]

$$\langle x|k\rangle = \psi_k(x) = \frac{1}{\sqrt{L}} e^{ikx}$$
$$k = \frac{2\pi n}{L} \qquad ;\ n = 0, \pm 1, \cdots \tag{12.130}$$

[16] Any piecewise continuous function $\psi(x)$ can actually be expanded in this set, and the basis functions are *complete* in the sense that

$$\text{Lim}_{N\to\infty} \int_0^L dx \left| \psi(x) - \sum_{n=-N}^{N} c_k \psi_k(x) \right|^2 = 0 \qquad ;\ \text{completeness}$$

This is all the completeness we will need for the physics in this volume.

(a) Use completeness of the eigenstates of position to show that

$$\langle k|k'\rangle = \delta_{k,k'} \tag{12.131}$$

(b) Show that the matrix elements of the kinetic energy operator are

$$\langle k|\hat{T}|k'\rangle = \frac{(\hbar k)^2}{2m}\delta_{k,k'} \tag{12.132}$$

(c) Show that the matrix elements of the potential $V(\hat{x})$ are

$$\begin{aligned}\langle k|\hat{V}|k'\rangle &= \frac{1}{L}\tilde{V}(k-k') \\ \tilde{V}(k-k') &= \int_0^L dx\, V(x)\, e^{-i(k-k')x}\end{aligned} \tag{12.133}$$

9.2 Look for stationary states in the abstract Hilbert space

$$\begin{aligned}|\Psi(t)\rangle &= e^{-iEt/\hbar}\,|\Psi\rangle \\ \hat{H}|\Psi\rangle &= E|\Psi\rangle\end{aligned} \tag{12.134}$$

Define the amplitude in the momentum representation as

$$\langle k|\Psi\rangle \equiv A(k) \tag{12.135}$$

(a) Use the results of Prob. 9.1 to show that the Schrödinger equation in the momentum representation is

$$\sum_{k'}\left\{\left[E - \frac{(\hbar k)^2}{2m}\right]\delta_{k,k'} - \frac{1}{L}\tilde{V}(k-k')\right\}A(k') = 0 \tag{12.136}$$

(b) Use the density of final states in one dimension to convert this to the *integral equation*

$$\left[E - \frac{(\hbar k)^2}{2m}\right]A(k) - \frac{1}{2\pi}\int_{-\infty}^{\infty} dk'\; \tilde{V}(k-k')A(k') = 0 \tag{12.137}$$

Note that the differential equation for the amplitude $\langle x|\Psi\rangle$ in the coordinate representation, and the integral equation for the amplitude $\langle k|\Psi\rangle$ in the momentum representation, both follow from the *same* Schrödinger equation in the abstract Hilbert space!

9.3 The abstract states in Probs. 9.1 and 9.2 are eigenstates of the hermitian momentum operator $\hat{p}$

$$\hat{p}|k\rangle = \hbar k|k\rangle \tag{12.138}$$

where the basic commutation relation in the abstract Hilbert space is

$$[\hat{p}, \hat{x}] = \frac{\hbar}{i} \tag{12.139}$$

(a) Verify that the eigenvalues $\hbar k$ are real;

(b) Show the projection of the first relation on the eigenstate of position is

$$\langle x|\hat{p}|k\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|k\rangle = \hbar k\langle x|k\rangle \tag{12.140}$$

(c) Show that in the momentum representation, the canonical commutation relation is satisfied with

$$\langle k|\hat{x}|k'\rangle = i\frac{\partial}{\partial k}\delta_{k,k'} \qquad ;\ \text{momentum rep} \tag{12.141}$$

9.4 The completeness relation in the abstract Hilbert space for the eigenstates of momentum for the particle moving on the large circle of length L with p.b.c. reads

$$\sum_k |k\rangle\langle k| = \hat{1} \qquad ;\ \text{completeness}$$

$$k = \frac{2\pi n}{L} \qquad ;\ n = 0, \pm 1, \cdots \tag{12.142}$$

(a) Use this to show

$$\langle x|x'\rangle = \sum_k \langle x|k\rangle\langle k|x'\rangle = \frac{1}{L}\sum_k e^{ik(x-x')} = \delta(x - x') \tag{12.143}$$

This is the completeness relation for the complex Fourier series;

(b) Similarly, use Eq. (12.132) to show that

$$\begin{aligned}\langle x|\hat{T}|x'\rangle &= \sum_k \sum_{k'} \langle x|k\rangle\langle k|\hat{T}|k'\rangle\langle k'|x'\rangle = \sum_k \frac{(\hbar k)^2}{2m}\langle x|k\rangle\langle k|x'\rangle \\ &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\langle x|x'\rangle \end{aligned} \tag{12.144}$$

(c) Show

$$\begin{aligned}\langle x|\hat{p}|x'\rangle &= \sum_k \sum_{k'} \langle x|k\rangle\langle k|\hat{p}|k'\rangle\langle k'|x'\rangle = \sum_k \hbar k\langle x|k\rangle\langle k|x'\rangle \\ &= \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|x'\rangle \end{aligned} \tag{12.145}$$

9.5 These are two problems on the *adjoint*.
(a) Show from Eq. (9.18) that

$$(i\hat{F})^\dagger = -i\hat{F}^\dagger \tag{12.146}$$

(b) Define $|\Psi_m(t)\rangle \equiv e^{i\hat{H}t/\hbar}\,|\psi_m\rangle$. Use the fact that $\hat{H}$ is hermitian to show that

$$\langle\Psi_m(t)|\psi_n\rangle = \langle\psi_m|^{-i\hat{H}t/\hbar}|\psi_n\rangle \tag{12.147}$$

9.6 The hamiltonian and number operator for the simple harmonic oscillator are given by

$$\hat{H}_0 = \hbar\omega\left(\hat{N} + \frac{1}{2}\right) \qquad ;\ \hat{N} = a^\dagger a \tag{12.148}$$

(a) Expand the exponential, rearrange the terms, and show that

$$e^{i\hat{H}_0 t/\hbar}\, a\, e^{-i\hat{H}_0 t/\hbar} = 1 + \frac{it}{\hbar}[\hat{H}_0, a] + \frac{1}{2!}\left(\frac{it}{\hbar}\right)^2 [\hat{H}_0,\, [\hat{H}_0,\, a]\,] + \cdots \tag{12.149}$$

(b) Use the commutation relations for the harmonic oscillator, and show that through this order

$$e^{i\hat{H}_0 t/\hbar}\, a\, e^{-i\hat{H}_0 t/\hbar} = a\, e^{-i\omega t} \tag{12.150}$$

(c) Similarly, show

$$e^{i\hat{H}_0 t/\hbar}\, a^\dagger\, e^{-i\hat{H}_0 t/\hbar} = a^\dagger\, e^{i\omega t} \tag{12.151}$$

9.7 Consider the time development operator in the interaction picture in Eq. (9.45)

$$\hat{U}(t, t_0) = \hat{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, \hat{H}_1(t') + \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, \hat{H}_1(t')\hat{H}_1(t'') + \cdots \tag{12.152}$$

Show that the double integral in the third term can be rewritten as

$$\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, \hat{H}_1(t')\hat{H}_1(t'') = \frac{1}{2!}\int_{t_0}^{t} dt' \int_{t_0}^{t} dt''\, T[\hat{H}_1(t')\hat{H}_1(t'')] \tag{12.153}$$

where the *time-ordering* operation $T[\hat{H}_1(t')\hat{H}_1(t'')]$ places the operator with the latest time to the left.

10.1 The statement of completeness for the eigenstates of the hermitian operator $\hat{F}$ in abstract Hilbert space is given in Eq. (9.23)[17]

$$|\Psi\rangle = \sum_f c_f \, |\psi_f\rangle \qquad ; \text{ completeness} \tag{12.154}$$

(a) Obtain the expansion coefficient as

$$c_f = \langle \psi_f | \Psi \rangle \tag{12.155}$$

(b) Substitute this back in to get

$$|\Psi\rangle = \sum_f |\psi_f\rangle \langle \psi_f | \Psi \rangle \tag{12.156}$$

(c) Conclude that the statement of completeness for the eigenstates of the hermitian operator $\hat{F}$ in abstract Hilbert space can be written as

$$\sum_f |\psi_f\rangle \langle \psi_f| = \hat{1} \qquad ; \text{ completeness} \tag{12.157}$$

10.2 (a) If one performs a pure pass measurement at a time t_0 that lets the eigenvalue f through, show that the rescaled reduced wave function at t_0 is[18]

$$\Psi(x, t_0) = \frac{c_f(t_0)}{|c_f(t_0)|} \psi_f(x) \qquad ; \; t = t_0 \tag{12.158}$$

(b) Give an argument that the reduced wave function at subsequent times is then

$$\Psi(x, t) = \frac{c_f(t_0)}{|c_f(t_0)|} \psi_f(x) \, e^{-iE_f(t-t_0)/\hbar} \qquad ; \; t \geq t_0 \tag{12.159}$$

11.1 (a) Expand the square-root in Eq. (11.6) to first order, and show that, apart from a constant term $m_0 c^2$ in the energy, one obtains the non-relativistic Schrödinger equation;

(b) What is the first relativistic correction to this Schrödinger equation?

11.2 As in appendix A, substitute the normal-mode expansion of the scalar field in Eq. (11.23) into the hamiltonian density in Eq. (11.19), do the spatial integrals, and derive the uncoupled oscillator expansion of the energy in Eq. (11.24).

[17] The corresponding statement for the wave functions is obtained by taking the inner product with $|x\rangle$.

[18] Recall Eq. (8.11).

11.3 (a) The canonical momentum density for the neutral massive scalar field is given by

$$\Pi(\vec{x},t) = \frac{\partial \mathcal{L}}{\partial(\partial\phi/\partial t)} = \frac{\partial \phi(\vec{x},t)}{\partial t} \tag{12.160}$$

The expansion of the scalar field in normal modes is

$$\phi(\vec{x},t) = \sum_{\vec{k}} \left(\frac{\hbar}{2\omega_k \Omega}\right)^{1/2} \left[c_{\vec{k}}\, e^{i(\vec{k}\cdot\vec{x}-\omega_k t)} + c^{\dagger}_{\vec{k}}\, e^{-i(\vec{k}\cdot\vec{x}-\omega_k t)}\right] \tag{12.161}$$

Hence, show that the canonical momentum density is

$$\Pi(\vec{x},t) = \frac{1}{i}\sum_{\vec{k}} \left(\frac{\hbar\omega_k}{2\Omega}\right)^{1/2} \left[c_{\vec{k}}\, e^{i(\vec{k}\cdot\vec{x}-\omega_k t)} - c^{\dagger}_{\vec{k}}\, e^{-i(\vec{k}\cdot\vec{x}-\omega_k t)}\right] \tag{12.162}$$

(b) Use the commutation relations of the creation and destruction operators to show that the equal-time commutation relation of the field and canonical momentum density is

$$[\Phi(\vec{x},t),\, \Pi(\vec{x}\,',t)] = \frac{i\hbar}{2}\sum_{\vec{k}} \frac{1}{\Omega}\left[e^{i\vec{k}\cdot(\vec{x}-\vec{x}')} + e^{-i\vec{k}\cdot(\vec{x}-\vec{x}')}\right] \tag{12.163}$$

(c) Each sum provides an integral representation of the three-dimensional Dirac delta function. Hence show that the canonical commutation relation in continuum mechanics between the field and canonical momentum density is

$$[\Phi(\vec{x},t),\, \Pi(\vec{x}\,',t)] = i\hbar\, \delta^{(3)}(\vec{x}-\vec{x}\,') \tag{12.164}$$

11.4 Suppose we include the additional nonlinear self-coupling of the neutral, massive scalar meson field of Eq. (11.28) in the lagrangian density

$$\mathcal{L}_1(\phi) = -\frac{\lambda}{4!}\phi^4 \tag{12.165}$$

(a) Show that since there are no additional derivative terms, the canonical momentum density, and canonical quantization procedure follow exactly as in the previous Prob. 11.3;

(b) Show the additional term in the hamiltonian density is simply

$$\mathcal{H}_1(\phi) = \frac{\lambda}{4!}\phi^4 \tag{12.166}$$

(c) Substitute the normal-mode expansion of Eq. (12.161), and enumerate the processes described by this hamiltonian density;

(d) What picture are we in?

11.5 Let $\underline{m}$ denote an $n \times n$ matrix

$$\underline{m} = \begin{bmatrix} m_{11} & m_{12} & \cdots & m_{1n} \\ m_{21} & m_{22} & \cdots & m_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ m_{n1} & m_{n2} & \cdots & m_{nn} \end{bmatrix} \tag{12.167}$$

Label an element of $\underline{m}$ by m_{jk} where j indicates the column and k indicates the row. Introduce the convention that repeated Latin indices are summed from 1 to n. The element of the matrix product of two such matrices $\underline{a}$ and $\underline{b}$ is then given by

$$[\underline{a}\,\underline{b}\,]_{jk} = a_{jl} b_{lk} \tag{12.168}$$

Pick the row for a_{jl} and the column for b_{lk}; then multiply the elements together and add them up.

(a) Evaluate the following matrix products

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad ; \quad \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad ; \quad \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{12.169}$$

(b) Let $\underline{\psi}$ denote an n-component column vector

$$\underline{\psi} = \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_n \end{bmatrix} \tag{12.170}$$

The matrix product $\underline{m}\,\underline{\psi}$ is given by

$$\left[\underline{m}\,\underline{\psi}\,\right]_j = m_{jk} \psi_k \tag{12.171}$$

Evaluate the following matrix products

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad ; \quad \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad ; \quad \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{12.172}$$

11.6 The Pauli matrices are defined in Eqs. (11.54).

(a) Show the matrix product of Pauli matrices satisfies

$$\sigma_i \, \sigma_j = i \varepsilon_{ijk} \sigma_k \qquad ; \; i \neq j \tag{12.173}$$

where ε_{ijk} is the completely antisymmetric Levi–Civita tensor;

(b) Show that the Pauli matrices satisfy the following anticommutation relation

$$\sigma_i\,\sigma_j + \sigma_j\,\sigma_i = 2\delta_{ij} \tag{12.174}$$

11.7 The *standard representation* of the Dirac matrices in 2×2 form is

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \qquad ;\ \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{12.175}$$

where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices defined in Eqs. (11.54).

(a) Show that the rules for matrix multiplication of the 4×4 matrices are satisfied by using matrix multiplication rules for the 2×2 submatrices;

(b) Show that the following relations are satisfied by the Dirac matrices[19]

$$\begin{aligned} \beta\alpha^k + \alpha^k\beta &= 0 \\ \alpha^k\alpha^l + \alpha^l\alpha^k &= 2\delta_{kl} \\ \beta^2 &= 1 \end{aligned} \tag{12.176}$$

11.8 Use the analysis in Sec. 11.3.1 to show that the non-relativistic limit of the positive-energy Dirac spinor for a free particle takes the form

$$u_\lambda(\vec{k}\,) = \begin{bmatrix} \phi_\lambda \\ (\vec{\sigma}\cdot\vec{p}/2m_0c)\phi_\lambda \end{bmatrix} \qquad ;\ \phi_\uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad ;\ \phi_\downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{12.177}$$

11.9 If the vector potential $\vec{A}$ in Eq. (11.69) is included in the non-relativistic reduction in Eq. (11.66), one has

$$\frac{1}{2m_0}\vec{\sigma}\cdot(\vec{p} - e\vec{A})\,\vec{\sigma}\cdot(\vec{p} - e\vec{A})\,\phi = \varepsilon\phi \tag{12.178}$$

With our convention that repeated Latin indices are summed from 1 to 3, and the results in Prob. 11.6, one has

$$\begin{aligned} \vec{\sigma}\cdot(\vec{p} - e\vec{A})\,\vec{\sigma}\cdot(\vec{p} - e\vec{A}) &= \sigma_i\sigma_j(p - eA)_i(p - eA)_j \\ &= (\delta_{ij} + i\varepsilon_{ijk}\sigma_k)(p - eA)_i(p - eA)_j \end{aligned} \tag{12.179}$$

[19] Once again, we do not underline the Pauli or Dirac matrices, and there is a suppressed unit matrix on the r.h.s. of Eqs. (12.174) and (12.176); also, $\alpha^k \equiv \alpha_k$.

(a) Show

$$\begin{aligned} i\sigma_k\varepsilon_{kij}(p-eA)_i(p-eA)_j &= -e\hbar\,\sigma_k\varepsilon_{kij}(\nabla_i A_j) \\ &= -e\hbar\,\vec{\sigma}\cdot(\vec{\nabla}\times\vec{A}) \\ &= -e\hbar\,\vec{\sigma}\cdot\vec{B} \end{aligned} \tag{12.180}$$

(b) Hence, conclude that the above non-relativistic reduction takes the form

$$\left[\frac{1}{2m_0}(\vec{p}-e\vec{A})^2 - \frac{e\hbar}{2m_0}\vec{\sigma}\cdot\vec{B}\right]\phi = \varepsilon\phi \tag{12.181}$$

(c) From this, conclude that a Dirac particle has the magnetic moment in Eq. (11.70).

11.10 (a) Consider the Dirac equation for a particle in a static, central, electric field given by $\vec{E} = -\vec{\nabla}\Phi(r)$. Show that in this case the Dirac equation can be reduced to

$$\left[c\vec{\sigma}\cdot\vec{p}\,\frac{1}{2m_0c^2+\varepsilon-e\Phi(r)}\,c\vec{\sigma}\cdot\vec{p}+e\Phi(r)\right]\phi = \varepsilon\phi \qquad ;\ \varepsilon \equiv E - m_0c^2 \tag{12.182}$$

(b) Show that[20]

$$\vec{\sigma}\cdot\vec{p}\,\Phi(r)\,\vec{\sigma}\cdot\vec{p} = \Phi\vec{p}^{\,2} + (\vec{p}\Phi)\cdot\vec{p} + \frac{\hbar}{r}\left(\frac{d\Phi}{dr}\right)\vec{\sigma}\cdot(\vec{r}\times\vec{p}) \tag{12.183}$$

(c) Hence conclude that if $|\varepsilon|/2m_0c^2 \ll 1$, and $e\Phi\left\{1+O[(p/m_0c)^2]\right\} \approx e\Phi$, then the Dirac equation reduces to the following Schrödinger equation for the upper components ϕ

$$\begin{aligned} H\phi &= \varepsilon\phi \\ H &= \frac{\vec{p}^{\,2}}{2m_0} + e\Phi(r) + \frac{e\hbar^2}{(2m_0c)^2}\frac{1}{r}\left(\frac{d\Phi}{dr}\right)\vec{\sigma}\cdot\vec{l} \end{aligned} \tag{12.184}$$

Here the spin-dependent contribution has been retained, and the angular momentum identified as $\vec{r}\times\vec{p} = \hbar\,\vec{l}$.

(d) Use this result to obtain Eq. (11.71).

[20] Note that $\vec{\nabla}\Phi(r) = (\vec{r}/r)(d\Phi/dr)$.

Appendix A

Electromagnetic Field in Normal Modes

One has the freedom of choosing a gauge for the electromagnetic potentials,[1] and here we work in the *Coulomb gauge*. This gauge has the great advantage that, when quantized, there is a one-to-one correspondence of the resulting quanta with physical photons. For free fields, the Coulomb gauge is defined by

$$\vec{\nabla} \cdot \vec{A} = 0 \qquad ; \ \Phi = 0 \qquad ; \text{ Coulomb gauge} \tag{A.1}$$

The electric and magnetic fields are then given in terms of the vector potential by

$$\vec{E} = -\frac{\partial \vec{A}}{\partial t} \qquad ; \ \vec{B} = \vec{\nabla} \times \vec{A} \tag{A.2}$$

With periodic boundary conditions, the normal modes are given by plane waves

$$\begin{aligned} q_{\vec{k}}(\vec{x}, t) &= \frac{1}{\sqrt{\Omega}} e^{i(\vec{k}\cdot\vec{x} - \omega_k t)} \qquad ; \ \vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z) \\ \omega_k &= |\vec{k}|c \qquad\qquad ; \ n_i = 0, \pm 1, \pm 2, \cdots \ ; \ i = x, y, z \end{aligned} \tag{A.3}$$

They satisfy the wave equation

$$\Box \, q_{\vec{k}}(\vec{x}, t) = 0 \tag{A.4}$$

We have an infinite, discrete set of wavenumbers, and the normal modes are orthonormal

$$\int_\Omega d^3x \, q^\star_{\vec{k}}(\vec{x}, t) \, q_{\vec{k}'}(\vec{x}, t) = \delta_{\vec{k},\vec{k}'} \tag{A.5}$$

[1] See Probs. 6.1 and 6.2.

Now introduce a set of orthogonal, transverse unit vectors $\vec{e}_{\vec{k}s}$ for each $\vec{k}$ (see Fig. 6.1). They satisfy

$$\begin{aligned} \vec{e}_{\vec{k}s} \cdot \vec{k} &= 0 \qquad ; \; s = 1, 2 \\ \vec{e}_{\vec{k}s} \cdot \vec{e}_{\vec{k}s'} &= \delta_{s,s'} \end{aligned} \tag{A.6}$$

The vector potential can then be expanded in normal modes as in Eq. (6.40)

$$\vec{A}(\vec{x}, t) = \sum_{\vec{k}} \sum_{s=1}^{2} \left(\frac{\hbar}{2\omega_k \varepsilon_0 \Omega} \right)^{1/2} \left[a_{\vec{k}s} \vec{e}_{\vec{k}s} e^{i(\vec{k}\cdot\vec{x} - \omega_k t)} + a^{\star}_{\vec{k}s} \vec{e}_{\vec{k}s} e^{-i(\vec{k}\cdot\vec{x} - \omega_k t)} \right] \tag{A.7}$$

where we have chosen particular amplitudes for the normal modes which will make the energy come out nicely.

With the use of Eqs. (A.2), the fields $(\vec{E}, \vec{B})$ are expressed in terms of the normal-mode expansion of the vector potential $\vec{A}(\vec{x}, t)$ as

$$\begin{aligned} \vec{E}(\vec{x}, t) &= i \sum_{\vec{k}} \sum_{s=1}^{2} \left(\frac{\hbar \omega_k}{2\varepsilon_0 \Omega} \right)^{1/2} \vec{e}_{\vec{k}s} \left[a_{\vec{k}s} e^{i(\vec{k}\cdot\mathbf{x} - \omega_k t)} - a^{*}_{\vec{k}s} e^{-i(\vec{k}\cdot\mathbf{x} - \omega_k t)} \right] \\ \vec{B}(\vec{x}, t) &= i \sum_{\vec{k}} \sum_{s=1}^{2} \left(\frac{\hbar}{2\omega_k \varepsilon_0 \Omega} \right)^{1/2} (\vec{k} \times \vec{e}_{\vec{k}s}) \; \times \\ &\qquad \left[a_{\vec{k}s} e^{i(\vec{k}\cdot\mathbf{x} - \omega_k t)} - a^{*}_{\vec{k}s} e^{-i(\vec{k}\cdot\mathbf{x} - \omega_k t)} \right] \end{aligned} \tag{A.8}$$

We will now substitute these expressions in the relation for the field energy in Eq. (6.34)

$$E = \frac{1}{2} \int_{\Omega} d^3x \left(\varepsilon_0 \vec{E}^{\,2} + \frac{1}{\mu_0} \vec{B}^{\,2} \right) \tag{A.9}$$

and use the orthonormality of the plane waves

$$\frac{1}{\Omega} \int_{\Omega} d^3x \, e^{i(\vec{k} - \vec{k}')\cdot\vec{x}} = \delta_{\vec{k},\vec{k}'} \tag{A.10}$$

Consider first the term containing the contribution of the electric field

$$\frac{\varepsilon_0}{2}\int_\Omega d^3x\,\vec{E}^{\,2} = \frac{1}{4}\sum_{\vec{k},s}\sum_{\vec{k}',s'}\hbar\omega_k\Big[\delta_{\vec{k},\vec{k}'}\delta_{s,s'}(a^*_{\vec{k}s}a_{\vec{k}s}+a_{\vec{k}s}a^*_{\vec{k}s}) \\ -\delta_{\vec{k},-\vec{k}'}\,(\vec{e}_{\vec{k}s}\cdot\vec{e}_{-\vec{k},s'})\left(a_{\vec{k}s}a_{-\vec{k},s'}\,e^{-2i\omega_k t}+a^*_{\vec{k}s}a^*_{-\vec{k},s'}\,e^{2i\omega_k t}\right)\Big] \tag{A.11}$$

Now consider the term containing the contribution of the magnetic field

$$\frac{1}{2\mu_0}\int_\Omega d^3x\;\vec{B}^{\,2} = \frac{1}{2\mu_0}\sum_{\vec{k},s}\sum_{\vec{k}',s'}\frac{\hbar}{2\omega_k\varepsilon_0}\Big[\delta_{\vec{k},\vec{k}'}\vec{k}^{\,2}\delta_{s,s'}(a^*_{\vec{k}s}a_{\vec{k}s}+a_{\vec{k}s}a^*_{\vec{k}s}) \\ -\delta_{\vec{k},-\vec{k}'}\;(\vec{k}\times\vec{e}_{\vec{k}s})\cdot(\vec{k}'\times\vec{e}_{\vec{k}'s'})\left(a_{\vec{k}s}a_{-\vec{k},s'}\,e^{-2i\omega_k t}+a^*_{\vec{k}s}a^*_{-\vec{k},s'}\,e^{2i\omega_k t}\right)\Big] \tag{A.12}$$

Use the vector identity[2]

$$(\vec{k}\times\vec{e}_{\vec{k}s})\cdot(\vec{k}\times\vec{e}_{-\vec{k},s'}) = \vec{k}^{\,2}(\vec{e}_{\vec{k}s}\cdot\vec{e}_{-\vec{k},s'}) \tag{A.13}$$

Recall $1/\mu_0\varepsilon_0 = c^2$ and $\omega_k^2 = \vec{k}^{\,2}c^2$, so that

$$\frac{\vec{k}^{\,2}}{\mu_0\varepsilon_0\omega_k} = \frac{\vec{k}^{\,2}c^2}{\omega_k} = \omega_k \tag{A.14}$$

The magnetic contribution then takes the form

$$\frac{1}{2\mu_0}\int_\Omega d^3x\;\vec{B}^{\,2} = \frac{1}{4}\sum_{\vec{k},s}\sum_{\vec{k}',s'}\hbar\omega_k\Big[\delta_{\vec{k},\vec{k}'}\delta_{s,s'}(a^*_{\vec{k}s}a_{\vec{k}s}+a_{\vec{k}s}a^*_{\vec{k}s}) \\ +\delta_{\vec{k},-\vec{k}'}\,(\vec{e}_{\vec{k}s}\cdot\vec{e}_{-\vec{k},s'})\left(a_{\vec{k}s}a_{-\vec{k},s'}\,e^{-2i\omega_k t}+a^*_{\vec{k}s}a^*_{-\vec{k},s'}\,e^{2i\omega_k t}\right)\Big] \tag{A.15}$$

When the electric and magnetic contributions are combined, the final time-dependent terms cancel identically, and the energy in the field is then indeed given by the normal-mode expansion in Eq. (6.44)

$$E = \frac{1}{2}\sum_{\vec{k}}\sum_{s=1}^{2}\hbar\omega_k\left(a^*_{\vec{k}s}a_{\vec{k}s}+a_{\vec{k}s}a^*_{\vec{k}s}\right) \tag{A.16}$$

[2]Note that $(\vec{k}'\times\vec{e}_{\vec{k}'s'})\to-(\vec{k}\times\vec{e}_{-\vec{k},s'})$; note also that $(\vec{k}\cdot\vec{e}_{-\vec{k}s'})=0$ for $s'=(1,2)$.

The electric and magnetic contributions to the energy of the free electromagnetic field oscillate back and forth with time, but the total energy is a constant of the motion.

Appendix B

Significant Names in Quantum Mechanics—Theory and Applications

Hendrik Antoon Lorentz (1853–1927)
Max Karl Ernst Ludwig Planck (1858–1947)
Albert Einstein (1879–1955)
Max Born (1882–1970)
Niels Henrik David Bohr (1885–1962)
Erwin Rudolf Josef Alexander Schrödinger (1885–1962)
Louis Victor Pierre Raymond duc de Broglie (1892–1987)
Satyendra Nath Bose (1894–1974)
Douglas Rayner Hartree (1897–1958)
Wolfgang Ernst Pauli (1900–1958)
Enrico Fermi (1901–1954)
Werner Karl Heisenberg (1901–1976)
Paul Adrien Maurice Dirac (1902–1984)
Eugene Paul Wigner (1902–1995)
Felix Bloch (1905–1983)
Hans Albrecht Bethe (1906–2005)
John Bardeen (1908–1991)
Lev Davidovich Landau (1908–1968)
Victor Frederick Weisskopf (1908–2002)
Julian Seymour Schwinger (1918–1994)
Richard Phillips Feynman (1919–1988)
Francis Eugene Low (1921–2007)
Marvin L. Goldberger (1922–2014)
Chen Ning Yang (1922–)
Freeman John Dyson (1923–2020)
John Clive Ward (1924–2000)
Mohammad Abdus Salam (1926–1996)

Murray Gell-Mann (1929–2019)
Leon Nathan Cooper (1930–)
John Robert Schrieffer (1931–2019)
Sheldon Lee Glashow (1932–)
Steven Weinberg (1933–)
Jeffrey Goldstone (1933–)
James Daniel Bjorken (1934–)
Kenneth Geddes Wilson (1936–2013)
David Jonathan Gross (1941–)
Hugh David Politzer (1949–)
Frank Wilczek (1951–)

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Index