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PREFACE

This book is intended as a first course on quantum mechanics and its applications. It is designed to be a first course rather than a complete one, and it is based on lectures given to mathematics and physics students in Cambridge. The book should be suitable also for engineering students.

The first five chapters deal with basic quantum mechanics, and are followed by a revision quiz with which the reader may test his understanding of them. Perhaps the most noticeable omission from these chapters is a detailed discussion of the mathematics of intrinsic spin (Pauli matrices, etc.). Our experience is that students initially find this more difficult than the other material, and since it is not needed for the applications described in the second part of the book, we have omitted it.

In most courses on quantum mechanics, the first application is to scattering problems. While recognising the importance of scattering theory, we have chosen rather to describe the application of quantum mechanics to physical phenomena that are of more everyday interest. These include molecular binding, the physics of masers and lasers, simple properties of crystalline solids arising from their electronic band structure, and the operation of junction transistors.

A few problems are included at the end of each chapter. We urge the student to work through all of these, as they form an integral part of the course. Some hints on their solution may be found at the end of the book.

We express our thanks to Sandra Evans, who typed the manuscript, and to David Branson, Ian Drummond, Sir James Lighthill, Michael Pepper and Ian Smith, who have very kindly read various parts of it and made valuable suggestions.

Christ's College, Cambridge Peter Landshoff
May 1978 Allen Metherell

CONSTANTS OF QUANTUM PHYSICS

Dirac's constant $\hbar = h/2\pi = 1.05 \times 10^{-34}$ J s

Charge of electron $-e = -1.60 \times 10^{-19}$ C

Fine-structure constant $e^2/4\pi\varepsilon_0\hbar c = 1/137$

Speed of light $c = 3.00 \times 10^8$ m s^{-1}

Mass of electron $m_e = 9.11 \times 10^{-31}$ kg

Mass of proton $m_p = 1.67 \times 10^{-27}$ kg

Electron volt 1 eV $= 1.60 \times 10^{-19}$ J

Boltzmann's constant $k_B = 1.38 \times 10^{-23}$ J K^{-1}

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1

Preliminaries

Atoms

An atom consists of a positively charged nucleus, together with a number of negatively charged electrons. Inside the nucleus there are protons, each of which carries positive charge e, and neutrons, which have no charge. So the charge on the nucleus is Ze, where Z, the atomic number, is the number of protons. The charge on each electron is $-e$, so that when the atom has Z electrons it is electrically neutral. If some of the electrons are stripped off, the atom then has net positive charge; it has been *ionised.*

The electrons are held in the atom by the electrostatic attraction between each electron and the nucleus. There is also an attraction because of the gravitational force, but this is about 10^{-40} times less strong, and so may be neglected. The protons and neutrons are held together in the nucleus by a different type of force, the nuclear force. The nuclear force is much stronger than the electrical force, and its attraction more than counteracts the electrostatic repulsion between pairs of protons. The nuclear force does not affect electrons. It is a very short-range force, so that it keeps the neutrons and protons very close together; the diameter of a nucleus is of the order of 10^{-15} m. By contrast, the diameter of the whole atom is about 10^{-10} m, so that for many purposes one can think of the nucleus as a point charge. The mass of the proton or neutron is some 2000 times that of the electron, so nearly all the mass of the atom is in the nucleus.

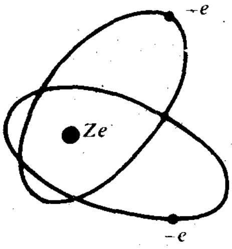
It is natural to think of the electrons as being in orbit round the nucleus, figure 1.1, just as the planets are in orbit round the sun. The electrostatic force that keeps the electrons in their orbits is an inverse-square-law force, just as is the gravitational force that keeps the planets in orbit, so that the two systems would seem to obey precisely similar equations. However, there is a serious difficulty. When a particle moves in a curved orbit its velocity vector is continuously changing: the particle is being accelerated towards the centre of its orbit. According to classical electrodynamics, when a charged particle is accelerated it inevitably radiates energy (this is the basic principle of radio transmission). So according to classical physics the electron would continuously lose energy and its orbit would form a spiral which would gradually collapse into the nucleus.

The reason that this does not happen is that very small systems, such as atoms, do not obey classical mechanics. To describe an atom one has to use quantum mechanics. In quantum mechanics, as opposed to classical mechanics, one cannot arbitrarily choose a value for the energy of the orbiting particle and then find an orbit corresponding to that energy; only certain discrete values of the energy are allowed. When the electron is in its lowest allowed energy level, it cannot radiate any more energy, and so the total collapse of the atom is not possible.

One can also use quantum mechanics to describe the solar system. Just as for the electrons, the allowed energy levels of the planets are discrete. If a planet in orbit is given an impulse, its energy is allowed to change only to that of one of the other allowed discrete levels. However, the separation between these levels is so small that this is not a very real restriction, and classical mechanics is perfectly adequate to describe the system. The effects of quantum mechanics are generally only important for submicroscopic systems.

The chemistry of an atom is determined by the charge on its nucleus. Thus atoms whose nuclei differ only in the number of neutrons that

Figure 1.1. Classical picture of negatively charged electrons in orbit round the positively charged nucleus of an atom.



they contain have similar chemical properties; they are said to be *isotopes* of the same element. For example, the atom of the common form of hydrogen contains just a single proton, that is, $Z = 1$; but hydrogen has a stable isotope, called deuterium, whose nucleus consists of one proton and one neutron. Atoms can be bound together to form molecules (see chapter 6), and different isotopes of the same element do this in the same way. Ordinary water consists of molecules containing two hydrogen nuclei and one oxygen nucleus, H_2O, while 'heavy' water has deuterium nuclei instead of the ordinary hydrogen, D_2O. The chemical properties of heavy water are exactly the same as those of ordinary water, but there are some differences in its physical properties. In particular, it is denser because of the extra neutrons.

Photons

In a metal, the atoms are effectively anchored to fixed sites by the electrostatic forces due to all the other atoms. The outermost orbital electrons of the atoms are almost free, and move through the metal when an electric field is applied. (See chapter 11.) If the metal is bombarded with light, some of the electrons can actually escape from the surface of the metal and can be detected as an electric current. This is the *photoelectric effect.* The number of electrons that escape in a given time rises with the intensity of the beam of light, but the energy with which they escape does not depend on the beam intensity. Rather it depends on the colour or frequency ν of the light. The kinetic energy T with which the electrons escape is found to obey the equation

$$h\nu = T + W. \tag{1.1}$$

Here h is Planck's constant,

$$h = 6.626 \times 10^{-34} \text{ J s},$$

and W is the energy that must be given to the electron to enable it to overcome the electrostatic attraction of the metal. (The value of W varies, according to the state within the metal from which the electron is ejected. For a given metal, there is a definite minimum value W_0, called the *work function* of the metal.)

These results are explained by the hypothesis that a beam of light can be thought of as a collection of particles, called *photons.* The number of photons is proportional to the intensity of the light, and the energy E of each photon is proportional to the frequency,

$$E = h\nu. \tag{1.2}$$

The electron is ejected from the metal when one of the photons collides with it and is absorbed by it, so giving up all its energy to the electron. The number of electrons ejected rises as the intensity of the light is increased because there are then more incident photons, and so there is a greater chance of a photon being absorbed.

Photons move with the speed of light, so their kinematics must be described by the laws of special relativity. The energy of a particle whose speed is v and whose rest mass is m is

$$E = mc^2/(1 - v^2/c^2)^{1/2}, \tag{1.3a}$$

so that when $v = c$ the energy can be finite only if $m = 0$; that is, photons have zero mass. In terms of the momentum p of the particle, (1.3a) reads

$$E = c(m^2c^2 + p^2)^{1/2}, \tag{1.3b}$$

so that for a photon

$$E = cp. \tag{1.4}$$

If a beam of light is shone normally on a perfect conductor it is reflected, that is, the momentum of each photon is reversed. This must occur by some sort of force being exerted on the photons, and the conductor must experience an equal and opposite force. This is a realisation of the classical idea of *radiation pressure*.

The equations (1.2) and (1.4) are tested in the *Compton effect*. When photons collide with free electrons or protons, not bound into a solid, they cannot be absorbed because it can be shown (see problem 1.2) that this would violate conservation of energy and momentum. (In the photoelectric effect some of the energy, W, is absorbed by the other particles in the metal). However, a free particle can scatter the photon, so changing its energy and therefore its frequency; at the same time the particle recoils. The kinematics of the process can be worked out using (1.2), (1.4) and the relativistic energy–momentum conservation laws (see problem 1.4), and the results are found to agree with experiment.

The equation (1.2) also helps to explain atomic spectra. We have said that, according to the results of quantum mechanics, the allowed energy levels of the electrons in atoms are discrete. If a beam of light is shone on a collection of atoms, the photons can be absorbed by the atoms if, and only if, their energy is equal to the difference between the energies of two electron levels. The absorption of the photon then excites the atom, sending the electron from the lower to the higher level. (The number of photons that can be absorbed in this way of course depends on how many atoms happen to be in the lower of the two states to start with.) Thus only photons with certain discrete frequencies are absorbed. Conversely, an atom in an excited state can decay by emitting a photon; the frequency of the photon depends on the difference between the initial and final energies:

$$h\nu = E_2 - E_1.$$

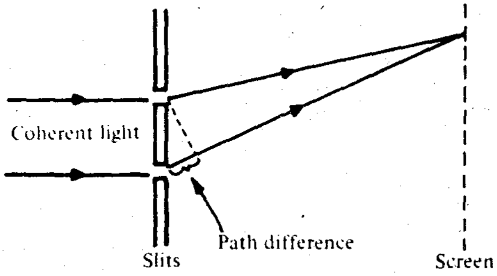
The energy levels of an atom (or molecule) depend on what element it is, so that the spectrum of frequencies absorbed and emitted provides a useful way of identifying substances.

Wave nature of matter

Although light can be thought of as a collection of photons, it also has wave-like properties. For example, a coherent beam of light is diffracted when it is shone through a pair of closely separated slits: if a screen is placed at large distance behind the slits, a pattern of light and dark fringes appears on it. The spacing of these fringes is calculated from the wavelength λ of the light. See figure 1.2. Dark fringes appear at points on the screen such that their distances from the two slits differ by $(n+\frac{1}{2})\lambda$, where n is an integer. Then the light received from the two slits is exactly out of phase; the two components cancel.

So quantum mechanics gives light a dual nature. In some respects it behaves like a collection of particles, in others like a wave. The same is

Figure 1.2. The double-slit experiment. There is darkness at points on the screen such that the path difference between rays that pass through the two slits is $(n+\frac{1}{2})\lambda$.



true for electrons and other particles; quantum mechanics associates waves with every kind of particle.

The necessity for this is illustrated by the phenomenon of electron diffraction. If a beam of electrons is passed through a crystal, it is diffracted. If a fluorescent screen is set up behind the crystal, a diffraction pattern appears on the screen. The regularly spaced atoms in the crystal cause the diffraction. The pattern can be explained by associating with the electrons a wave of wavelength λ, which changes with the momentum of the electrons according to de Broglie's relation

$$\lambda = h/p. \tag{1.5}$$

The waves may be assigned a characteristic frequency ν, which may be chosen so as to be related to the electron energy E by the relation $E = h\nu$ as for photons (see (1.2)). However, in the case of electrons, the frequency ν is not directly measurable and there is some arbitrariness in its definition; for example, E may or may not include the rest-mass energy of the electron. The part played in the theory by the electron frequency will become apparent in the next chapter.

The de Broglie relation (1.5) applies also to photons. This follows if we make the assumption that the quantum-mechanical waves that describe photons have the same frequency ν and wavelength λ as the corresponding classical electromagnetic waves. Because the classical waves have speed c, this implies that

$$\lambda\nu = c \tag{1.6}$$

and combining this relation with (1.2) and (1.4) gives (1.5).

Classical electromagnetic waves are associated with a very large number of photons (see problem 1.1). The waves of quantum mechanics may describe either a collection of particles or a single particle. It is important to understand that quantum-mechanical waves are more abstract than classical waves. Consider an experiment where light is diffracted through a pair of slits, or where electrons are diffracted through a crystal. Suppose that only one photon or electron is allowed to come into the experiment. In this case we cannot predict with certainty what will be the angle θ through which the photon or electron is diffracted. But if the experiment is repeated many times, we find a *probability distribution* for the angle θ that has the same shape as the variation of intensity with θ in an experiment where there is a continuous beam of photons or electrons.

This suggests that the association of a quantum-mechanical wave with a photon, or with any other kind of particle, is somehow statistical. We explore this in the following chapters. As will become clear, according to quantum theory one can never predict with certainty what will be the result of a particular experiment: the best that can be done is to calculate the *probability* that the experiment will have a given result, or one can calculate the *average value* of an observable quantity if the experiment that measures it is repeated many times.

Problems

1.1 A radio transmitter operates on a wavelength of 100 m at a power of 1 kW. How many photons does it emit per second?

1.2 Using energy–momentum conservation, show that an electron that is not in a bound state cannot absorb a photon.

1.3 A particle has mass 1 kg. How long does it take to move through a distance of 1 m if its de Broglie wavelength, (1.5), is comparable with the wavelength of visible light? What is the corresponding answer if the particle is an electron?

1.4 A photon of momentum p, and therefore of wavelength h/p, scatters on an electron that is initially at rest. Using relativistic kinematics, deduce from the conservation of energy and momentum that as the result of the scattering the wavelength of the photon changes by $(h/mc)(1-\cos\theta)$, where θ is the angle through which it scatters and m is its rest mass. (This scattering process is known as *Compton scattering,* and the quantity h/mc is the *Compton wavelength* of the electron.)

1.5 Associated with the electron there is an *antiparticle*, the positron, which has equal mass and equal, but opposite, charge.

A positron impinges on an electron which is at rest. They annihilate into two photons. Show that the sum of the wavelengths of the two photons is $\lambda_0(1-\cos\theta)$, where θ is the angle between their directions of motion and λ_0 is the Compton wavelength of the electron.

2

The Schrödinger equation

The basic equation of quantum mechanics is known as the Schrödinger equation. It is not possible to prove that the equation must be true, just as we cannot prove that Newton's laws, the basis of classical mechanics, must be true. All that can be done is to work out the consequences of the equation in different physical contexts, and to compare them as exhaustively as possible with experiment. In this chapter we begin by showing how the experimental facts that we have already described make the truth of the equation *plausible.*

The Schrödinger equation describes non-relativistic particles, whose energy E and momentum p are related by

$$E = p^2/2m. \tag{2.1}$$

Non-relativistic kinematics can be used so long as the energy E is not comparable with, or larger than, the rest-mass energy mc^2. Relativistic quantum mechanics is much more difficult than the non-relativistic theory, and will not concern us in this book. In particular, we shall not describe the quantum mechanics of the photon; for this particle $m = 0$, and so relativistic mechanics must always be used.

Wave functions and operators

We explained in chapter 1 that with a particle of energy E and momentum p we somehow associate a wave of frequency $\nu = E/h$ and wavelength $\lambda = h/p$. Instead of using ν and λ, it is convenient to introduce the angular frequency

$$\omega = 2\pi\nu$$

and the wave vector $\boldsymbol{k}$, whose direction is in the direction of wave propagation and whose magnitude is

$$k = 2\pi/\lambda.$$

We also work with

$$\hbar = h/2\pi$$

(pronounced '$\hbar$-cross') instead of h. Then we have

$$\begin{aligned} \boldsymbol{p} &= \hbar \boldsymbol{k} \\ E &= \hbar\omega. \end{aligned} \tag{2.2}$$

For a free particle, which is not interacting with any other particle or with a potential, $\boldsymbol{p}$ and E are constant. Hence we expect such a particle to be described by a wave for which $\boldsymbol{k}$ and ω are constant:

$$\Psi(\boldsymbol{r}, t) = N\,\mathrm{e}^{\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)}. \tag{2.3}$$

Here $\boldsymbol{r}$ denotes the position vector and N is a constant. In many physical applications, we write a wave in the form of a complex exponential, as is done here, and understand that only the real part is physically meaningful. In quantum mechanics, however, it will turn out that both the real and the imaginary parts of Ψ are needed. The plane wave (2.3) is the simplest example of a *wave function*: it describes a free particle. Instead of (2.3), we could use $N\,\mathrm{e}^{-\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)}$; the choice of sign is a matter of convention.

In order to guess how to arrive at wave functions that describe particles that are not free, we perform a simple manipulation on (2.3). Differentiation with respect to a component x_j ($j = 1$, 2 or 3) of $\boldsymbol{r}$ simply multiplies Ψ by i times the corresponding component k_j of $\boldsymbol{k}$. So, with (2.2), we have

$$(-\mathrm{i}\hbar\,\partial/\partial x_j)\Psi = p_j\Psi \qquad (j = 1, 2, 3) \tag{2.4a}$$

or, in more concise vector notation,

$$(-\mathrm{i}\hbar\nabla)\Psi = \boldsymbol{p}\Psi. \tag{2.4b}$$

The equation (2.4a) says that if we apply the differential operator $-\mathrm{i}\hbar\,\partial/\partial x_j$ to Ψ, the result is to multiply Ψ by the number p_j. We say that Ψ is an *eigenfunction* of the operator $(-\mathrm{i}\hbar\,\partial/\partial x_j)$ with *eigenvalue* p_j. (More properly, since the differential equations (2.4) do not determine Ψ until we have imposed suitable boundary and continuity conditions on Ψ, we should at this stage specify these conditions. However, we defer the discussion of this until the end of this chapter.) In this way, an experimentally observable quantity, the momentum $\boldsymbol{p}$ of a particle, is associated with a differential operator $-i\hbar\boldsymbol{\nabla}$. We generalise this to other experimentally observable quantities by introducing three *basic assumptions*:

(*a*) States of a system are described by wave functions Ψ.
(*b*) Observable quantities are associated with operators.
(*c*) When the value of an observable Q is known to be q, the system is in a state whose wave function is an eigenfunction of the operator $\hat{Q}$ corresponding to Q, with eigenvalue q. That is,

$$\hat{Q}\Psi = q\Psi. \tag{2.5}$$

We shall elaborate on these assumptions in chapter 4.

Consider the particular example of the observable that is the energy of a particle. If it is a free particle, this is just $\boldsymbol{p}^2/2m$. So one would expect the corresponding differential operator to be obtained by replacing $\boldsymbol{p}$ in this expression by its corresponding operator $-i\hbar\boldsymbol{\nabla}$, and so we have $(-i\hbar\boldsymbol{\nabla})^2/2m$, that is, $-\hbar^2\nabla^2/2m$. If the particle moves in a potential $V(\boldsymbol{r})$, this operator becomes†

$$H = (-\hbar^2/2m)\nabla^2 + V(\boldsymbol{r}) \tag{2.6}$$

corresponding to the classical expression $p^2/2m + V(\boldsymbol{r})$. H is called the Hamiltonian operator. To find the possible energy levels E of the particle, we must find the eigenvalues E of H, that is, we must solve the equation

$$H\Psi = E\Psi \tag{2.7a}$$

(subject to appropriate boundary conditions). This equation

$$[(-\hbar^2/2m)\nabla^2 + V(\boldsymbol{r})]\Psi(\boldsymbol{r}, t) = E\Psi(\boldsymbol{r}, t) \tag{2.7b}$$

is the *time-independent Schrödinger equation.*

Notice that if the particle is not a free particle, so that $V \neq 0$, the plane wave (2.3) is not a solution of the Schrödinger equation; the wave function Ψ will be more complicated.

The time-independent Schrödinger equation applies when the particle is in a state such that its energy takes a definite value E. In a general situation this may not be the case, for example when V depends explicitly on the time t as well as on the position $\boldsymbol{r}$ of the particle. In order to guess what is the generalisation of the Schrödinger

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† Although H is an operator, we shall follow the usual convention and not write the operator symbol $\hat{\ }$ over it.