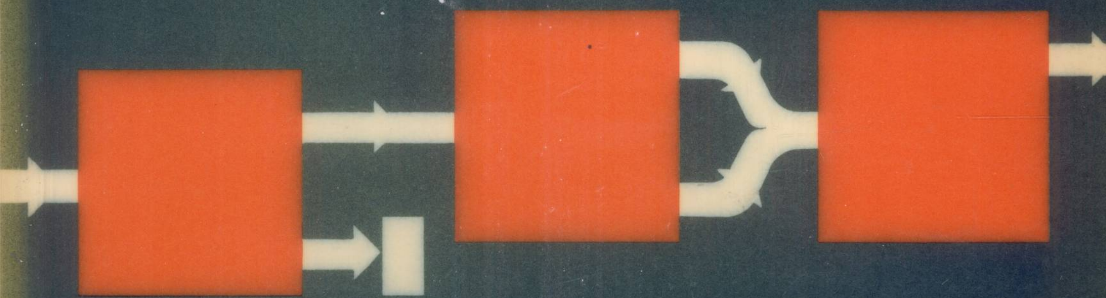
Quantum Mechanics

Alastair I. M. Rae



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PREFACE

Over the years the emphasis of undergraduate physics courses has moved away from the study of classical macroscopic phenomena towards the discussion of the microscopic properties of atomic and subatomic systems. As a result, students now have to study quantum mechanics at an earlier stage in their course without the benefit of a detailed knowledge of much of classical physics and, in particular, with little or no acquaintance with the formal aspects of classical mechanics. This book has been written with the needs of such students in mind. It is based on a course of about thirty lectures given to physics students at the University of Birmingham towards the beginning of their second year—although, perhaps inevitably, the coverage of the book is a little greater than I was able to achieve in the lecture course. I have tried to develop the subject in a reasonably rigorous way, covering the topics needed for further study in atomic, nuclear, and solid state physics, but relying only on the physical and mathematical concepts usually taught in the first year of an undergraduate course. On the other hand, by the end of their first undergraduate year most students have heard about the basic ideas of atomic physics, including the experimental evidence pointing to the need for a quantum theory, so I have confined my treatment of these topics to a brief introductory chapter.

While discussing those aspects of quantum mechanics required for further study, I have laid considerable emphasis on the understanding of the basic ideas and concepts behind the subject, culminating in the last chapter which contains an introduction to quantum measurement theory. Recent research, particularly the theoretical and experimental work inspired by Bell's theorem, has greatly clarified many of the conceptual problems in this area. However, most of the existing literature is at a research level and concentrates more on a rigorous presentation of results to other workers in the field than on making them accessible to a wider audience. I have found that many physics undergraduates are particularly interested in this aspect of the subject and there is therefore a need for a treatment suitable for this level. The last chapter of this book is an attempt to meet this need.

I should like to acknowledge the help I have received from my friends and colleagues while writing this book. I am particularly grateful to Robert Whitworth, who read an early draft of the complete book, and to Goronwy Jones and George Morrison, who read parts of it. They all offered many valuable and penetrating criticisms, most of which have been incorporated in this final version. I should also like to thank Ann Aylott who typed the manuscript and was always patient and helpful throughout many changes and revisions, as well as Martin Dowe who assisted with the proofreading. Naturally, none of this help in any way lessens my responsibility for whatever errors and omissions remain.

Alastair I. M. Rae

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ONE
INTRODUCTION

Quantum mechanics was developed as a response to the inability of the classical theories of mechanics and electromagnetism to provide a satisfactory explanation of some of the properties of electromagnetic radiation and of atomic structure. As a result a theory has emerged, whose basic principles can be used to explain not only the structure and properties of atoms, including the way they interact with each other in molecules and solids, but also those of nuclei and of 'elementary' particles such as the proton and neutron. Although there are still many features of the physics of such systems that are not fully understood, there are presently no indications that the fundamental ideas of quantum mechanics are incorrect. In order to achieve this success, quantum mechanics has been built on a foundation that contains a number of concepts that are fundamentally very different from those of classical physics and which have completely altered our view of the way the natural universe operates. This book will attempt to elucidate and discuss the conceptual basis of the subject as well as explaining its successes in describing the behaviour of atomic and subatomic systems.

Quantum mechanics is often thought to be a difficult subject, not only in its conceptual foundation, but also in the complexity of its mathematics. However, although a rather abstract formulation is required for a proper treatment of the subject, much of the apparent complication arises in the course of the solution of essentially simple mathematical equations applied to particular physical situations. We shall discuss a number of such applications in this book, because it is important to appreciate the success of quantum mechanics in explaining the results of real physical measurements. However, the reader should try not to allow the ensuing algebraic complication to hide the essential simplicity of the basic equations.

In this first chapter we shall discuss some of the key experiments that illustrate the failure of classical physics. However, although the experiments described were performed in the first quarter of this century and played an important role in the development of the subject, we shall not be giving a historically based account. Neither will our account be a complete description of the early experimental work; for example, we shall not describe the experiments on the properties of thermal radiation and the heat capacity of solids that provided early indications of the need for the quantization of the energy of electromagnetic radiation and of mechanical systems. The topics to be discussed have been chosen as those that point most clearly towards the basic ideas needed in the further development of the subject. As so often happens in physics, the way in which the theory actually developed was by a process of trial and error, often relying on flashes of inspiration, rather than the more logical approach suggested by hindsight.

1.1 THE PHOTOELECTRIC EFFECT

When light strikes a clean metal surface in a vacuum, it causes electrons to be emitted with a range of energies. For light of a given frequency ν the maximum electron energy E_x is found to be equal to the difference between two terms, one of which is proportional to the frequency of the incident light with a constant of proportionality h that is the same whatever the metal used, while the other is independent of frequency but varies from metal to metal. Moreover, neither term depends on the intensity of the incident light which affects only the rate of electron emission. Thus

$$E_x = h\nu - \phi \tag{1.1}$$

It is very difficult, if not impossible, to explain this result on the basis of the classical theory of light as an electromagnetic wave. This is because the energy contained in such a wave would arrive at the metal at a uniform rate and there is no apparent reason why this energy should be divided up in such a way that the maximum electron energy is proportional to the frequency and independent of the intensity of the light. Another important feature of the photoelectric effect is the dependence of the rate of electron emission on the light intensity. Although the average emission rate is proportional to the intensity, individual electrons are emitted at random, and when experiments are performed using very weak light, electrons are sometimes emitted well before sufficient electromagnetic energy should have arrived at the metal.

Such considerations led Einstein to postulate that the classical electromagnetic theory does not provide a complete explanation of the properties of light, but that we must also assume that the energy in an electromagnetic wave is 'quantized' in the form of small packets, known as *photons*, each of which carries an amount of energy equal to $h\nu$. Given this postulate, we can see that when light is incident on a metal, the maximum energy an electron can gain is that carried by one of the photons. Part of this energy will be given up by the electron as it escapes from the metal surface—so accounting for the quantity ϕ in (1.1), which is accordingly known as the *work function*—but the rest will be converted into the kinetic energy of the freed electron, in agreement with the experimental results summarized in Eq. (1.1). The photon postulate also explains the emission of photoelectrons at random times. Thus, although the average rate of photon arrival is proportional to the light intensity, individual photons arrive at random and, as each carries with it a quantum of energy, there will be occasions when an electron is emitted well before this would be classically expected.

The constant h connecting the energy of a photon with the frequency of the electromagnetic wave is known as *Planck's constant*, because it was originally postulated by Planck in order to explain some of the properties of thermal radiation. It is a fundamental constant that frequently occurs in the equations of quantum mechanics. We shall find it convenient to change this notation slightly and define another constant $\hbar$ as being equal to h divided by 2π; also, when referring to waves, we shall normally use the angular frequency ω $(=2\pi\nu)$, in preference to the frequency ν. Using this notation, the photon energy E can be expressed as

$$E = \hbar\omega \tag{1.2}$$

Throughout this book we shall write our equations in terms of $\hbar$ and avoid ever again referring to h. We note that $\hbar$ has the dimensions of action (energy $\times$ time) and its currently best accepted value is $(1.054\,589 \pm 0.000\,006) \times 10^{-34}$ J s.

1.2 THE COMPTON EFFECT

The existence of photons is also demonstrated by experiments first carried out by A. H. Compton that involve the scattering of X-rays by electrons. To understand these we must make the further postulate that a photon, as well as carrying a quantum of energy, also has a definite momentum and can therefore be treated in many ways just like a classical particle. An expression for the photon momentum is suggested by the classical theory of radiation pressure: it is known that if energy is transported by an electromagnetic wave at a rate W per unit area per second, then the wave exerts a pressure of magnitude W/c (where c is the velocity of light), whose direction is parallel to that of the wave vector $\mathbf{k}$ of the wave; if we now treat the wave as composed of photons of energy $\hbar\omega$ it follows that the photon momentum $\mathbf{p}$ should have a magnitude $\hbar\omega/c = \hbar k$ and that its direction should be parallel to $\mathbf{k}$. Thus

$$\mathbf{p} = \hbar\mathbf{k} \tag{1.3}$$

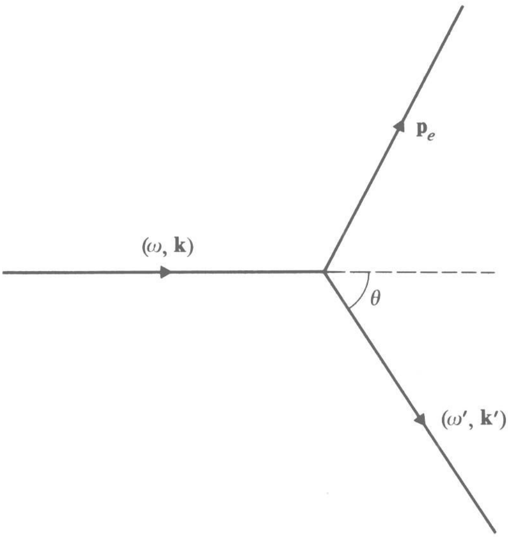

Figure 1.1 In Compton scattering an X-ray photon of angular frequency ω and wave vector $\mathbf{k}$ collides with an electron initially at rest. After the collision the photon frequency and wave vector are changed to ω' and $\mathbf{k}'$ respectively and the electron recoils with momentum $\mathbf{p}_e$.

We now consider a collision between such a photon and an electron of mass m that is initially at rest. After the collision we assume that the frequency and wave vector of the photon are changed to ω' and $\mathbf{k}'$ and that the electron moves off with momentum p_e as shown in Fig. 1.1. Assuming that energy and momentum are conserved we have

$$\hbar\omega - \hbar\omega' = p_e^2/2m \tag{1.4}$$

$$\hbar\mathbf{k} - \hbar\mathbf{k}' = \mathbf{p}_e \tag{1.5}$$

Squaring (1.5) and substituting into (1.4) we get

$$\begin{aligned}\hbar(\omega - \omega') &= \frac{\hbar^2}{2m}(\mathbf{k} - \mathbf{k}')^2 \\ &= \frac{\hbar^2}{2m}[(k-k')^2 + 2kk'(1-\cos\phi)]\end{aligned} \tag{1.6}$$

where ϕ is the angle between $\mathbf{k}$ and $\mathbf{k}'$ (cf. Fig. 1.1). Now the change in the magnitude of the wave vector $(k-k')$ always turns out to be very much smaller than either k or k' so we can neglect the first term in square brackets on the right-hand side of (1.6). Remembering that $\omega = ck$ and $\omega' = ck'$ we then get

$$\frac{1}{\omega'} - \frac{1}{\omega} = \frac{\hbar}{mc^2}(1-\cos\phi)$$

that is

$$\lambda' - \lambda = \frac{2\pi\hbar}{mc}(1-\cos\phi) \tag{1.7}$$

where λ and λ' are the X-ray wavelengths before and after the collision, respectively. It turns out that if we allow for relativistic effects when carrying out the above calculation, we obtain the same result as (1.7) without having to make any approximations.

Experimental studies of the scattering of X-rays by electrons in solids produce results in good general agreement with the above predictions. In particular, if the intensity of the radiation scattered through a given angle is measured as a function of the wavelength of the scattered X-rays, a peak is observed whose maximum lies just at the point predicted by (1.7). In fact such a peak has a small, but finite, width implying that some of the photons have been scattered in a manner slightly different from that described above, but this can be explained by taking into account the fact that the electrons in a solid are not necessarily at rest, but generally have a finite momentum before the collision. Compton scattering can therefore be used as a tool to measure the electron momentum, and we shall discuss this in more detail in Chapter 4.

Both the photoelectric effect and the Compton effect are connected with the interactions between electromagnetic radiation and electrons, and both provide conclusive evidence for the photon nature of electromagnetic waves. However, we might ask why there are two effects and why the X-ray photon is scattered by the electron with a change of wavelength, while the optical photon transfers all its energy to the photoelectron. The principal reason is that in the X-ray case the photon energy is much larger than the binding energy between the electron and the solid; the electron is therefore knocked cleanly out of the solid in the collision and we can treat the problem by considering energy and momentum conservation. In the photoelectric effect, on the other hand, the photon energy is only a little larger than the binding energy and, although the details of this process are rather complex, it turns out that the momentum is shared between the electron and the atoms in the metal and that the whole of the photon energy is used to free the electron and give it kinetic energy. However, none of these detailed considerations affects the conclusion that in both cases the incident electromagnetic radiation exhibits properties consistent with it being composed of photons whose energy and momentum are given by the expressions (1.2) and (1.3).

1.3 LINE SPECTRA AND ATOMIC STRUCTURE

When an electric discharge is passed through a gas, light is emitted which, when examined spectroscopically, is typically found to consist of a series of lines, each of which has a sharply defined frequency. A particularly simple example of such a line spectrum is that of hydrogen, in which case the observed frequencies are given by the formula

$$\omega_{mn} = 2\pi R_0 c\left(\frac{1}{n^2} - \frac{1}{m^2}\right) \tag{1.8}$$

where n and m are integers, c is the speed of light and R_0 is a constant known as the *Rydberg constant* (after J. R. Rydberg who first showed that the experimental results fitted this formula) whose currently accepted value is $(1.096\,775\,9 \pm 0.000\,000\,1) \times 10^7\,\mathrm{m}^{-1}$.

Following our earlier discussion, we can assume that the light emitted from the atom consists of photons whose energies are $\hbar\omega_{mn}$. It follows from this and the conservation of energy, that the energy of the atom emitting the photon must have been changed by the same amount, and the obvious conclusion to draw is that the energy of the hydrogen atom is itself quantized so that it can adopt only one of the values E_n where

$$E_n = -\frac{2\pi R_0 \hbar c}{n^2} \tag{1.9}$$

the negative sign corresponding to the negative binding energy of the electron in the atom. Similar constraints govern the values of the energies of atoms other than hydrogen although these cannot usually be expressed in such a simple form. We refer to allowed energies such as E_n as *energy levels*. Further confirmation of the existence of energy levels is obtained from the ionization energies and absorption spectra of atoms, which both display features consistent with the energy of an atom being quantized in this way. It will be one of the main aims of this book to develop a theory of quantum mechanics that will successfully explain the existence of energy levels and provide a theoretical procedure for calculating their values.

One feature of the structure of atoms that can be at least partly explained on the basis of energy quantization is the simple fact that atoms exist at all! According to classical electromagnetic theory, an accelerated charge always loses energy in the form of radiation, so a negative electron in motion about a positive nucleus should radiate, lose energy, and quickly coalesce with the nucleus. The fact that the radiation is quantized should not affect this argument, but if the energy of the atom is quantized, there will be a minimum energy level (that with $n = 1$ in the case of hydrogen) below which the atom cannot go and in which it will remain indefinitely.

1.4 DE BROGLIE WAVES

Following on from the fact that the photons associated with electromagnetic waves behave like particles, L. de Broglie suggested that particles such as electrons might also have wave properties. He further proposed that the frequencies and wave vectors of these 'matter waves' would be related to the energy and momentum of the associated particle in the same way as in the photon case. That is

$$\left.\begin{aligned} E &= \hbar\omega \\ \mathbf{p} &= \hbar\mathbf{k} \end{aligned}\right\} \tag{1.10}$$

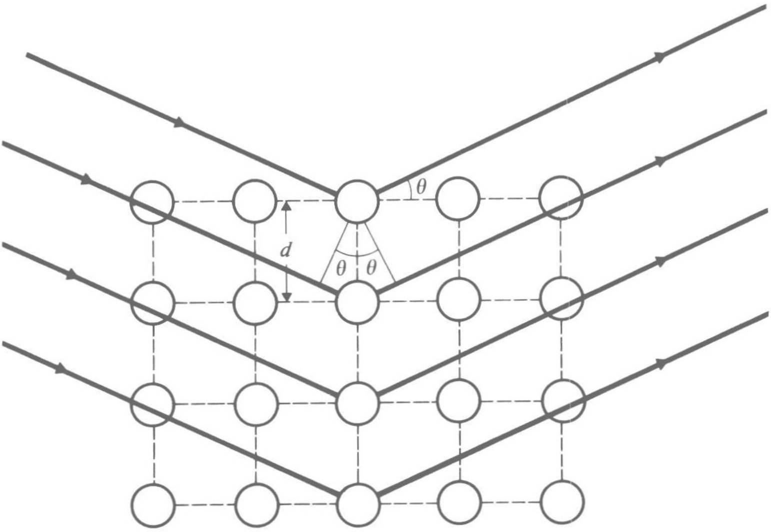

Figure 1.2 Electrons incident at an angle θ to planes of atoms in a crystal are diffracted so that the path difference between the de Broglie waves scattered by successive planes is a whole number of wavelengths.

In the case of matter waves, Eqs (1.10) are referred to as the de Broglie relations. We shall develop this idea in subsequent chapters when we shall find that it can be used to account for atomic energy levels. In the meantime we shall describe a simple experiment that provides direct confirmation of the existence of matter waves.

This experiment was performed by C. Davisson and L. H. Germer who studied the scattering of beams of electrons by single crystals of nickel. Particularly strong scattering was observed when, as shown in Fig. 1.2, the momenta of the incident and scattered electrons make the same angle θ with planes of atoms in the crystal, and when the wavelength λ of the de Broglie wave is related to the separation d of the atomic planes and to θ by

$$n\lambda = 2d \sin \theta \tag{1.11}$$

where n is an integer. Now Eq. (1.11) is identical to the well-known Bragg equation governing the diffraction of X-rays by crystals, where it follows directly from the requirement that waves scattered by successive planes in the crystal must be in phase (cf. Fig. 1.2). The Davisson–Germer experiment is therefore a direct demonstration that beams of electrons are similarly diffracted by crystals and must have wave properties. Moreover, from measurements of the scattering angles θ and knowledge of the interplanar spacing d, the wavelength λ can be calculated, and when this value is compared with that obtained from the electron momentum the de Broglie relations (1.10) are confirmed.

Nowadays the wave properties of electron beams are commonly observed experimentally and electron microscopes, for example, are often used to display the diffraction patterns of the objects under observation. Moreover, not only electrons behave in this way; neutrons of the appropriate energy can also be diffracted by crystals, this technique being commonly used to investigate structural and other properties of solids. Indeed all the evidence points to de Broglie waves being a universal property of matter so that all objects commonly thought of as particles exhibit wave properties under appropriate circumstances.

1.5 WAVE-PARTICLE DUALITY

Although we have just described the experimental evidence for the wave nature of electrons and similar bodies, it must not be thought that this description is complete or that these are any-the-less particles. Although in a diffraction experiment wave properties are manifested during the diffraction process and the intensity of the wave determines the average number of particles scattered through various angles, when the diffracted electrons are detected they are always found to behave just like point particles with the expected mass and charge and to have a particular energy. Conversely, although we need to postulate photons in order to explain phenomena such as the photoelectric and Compton effects, phenomena such as the diffraction of light by a grating or of X-rays by a crystal can be explained only if electromagnetic radiation has wave properties.

In many circumstances it is perfectly clear which model should be used in a particular physical situation. Thus, although electrons with a kinetic energy of 100 eV (1.6×10^{-17} J) have a de Broglie wavelength of about 10^{-10} m and are therefore diffracted by crystals according to the wave model, if their energy is very much higher (say 100 MeV) the wavelength is then so short (c. 10^{-14} m) that diffraction effects are not normally observed and such electrons nearly always behave like classical particles. A similar argument shows why the wave properties of everyday macroscopic particles are not apparent: even a small grain of sand of mass about 10^{-6} g moving at a speed of 10^{-3} m s^{-1} has a de Broglie wavelength of the order of 10^{-21} m and its wave properties are therefore quite undetectable; clearly this is even more true for heavier or faster moving objects. There are some experimental situations, however, which cannot be understood without involving both the wave and the particle properties and we shall now consider an example of such wave-particle 'duality'.

Figure 1.3 shows an experiment in which a parallel beam of light passes through a pair of slits and is detected some distance away by a row of detectors that are sensitive to the arrival of individual photons—possibly by making use of the photoelectric effect. Initially photons appear to arrive at the detectors at random, but after a large number have been detected, the total recorded by a given detector is found to be proportional to the intensity of the classical

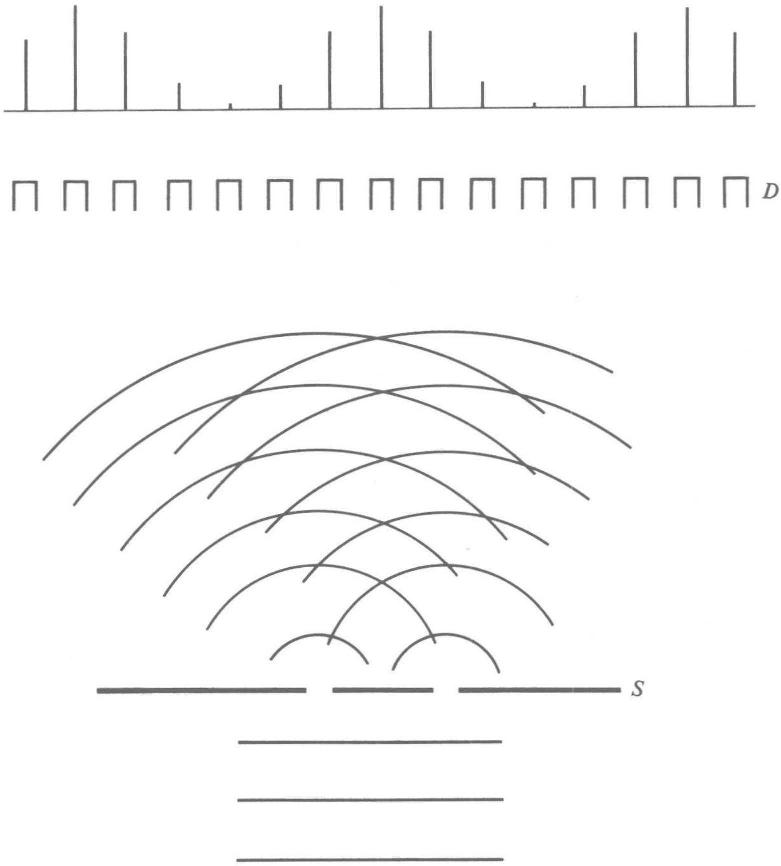

Figure 1.3 A plane electromagnetic wave approaches a screen *S* containing two slits, and the resulting interference pattern is a superposition of two circular waves. The number of photons detected by each of the detectors *D* is proportional to the intensity of the electromagnetic wave at that point, as is shown in the bar graph.

electromagnetic wave at that point (see Fig. 1.3) which is calculated in the usual way by assuming interference between the light waves passing through the separate slits. Moreover, whatever the intensity of the incident light—whether it is so strong that all the photons must have passed through the slits at more or less the same time, or if it is so weak that there could have been only one photon in the apparatus at any one time—the form of the interference pattern after a large number of photons have been detected is the same. Both the wave and particle models of light are necessary to explain these results. Thus the light has been detected as photons each carrying a quantum of energy, but the formation of the interference pattern implies that it had the form of a classical wave while passing through the slits.