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Principles of Quantum Mechanics

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NOTE ON THE AUTHOR

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Principles of Quantum Mechanics, which was first published in 1944, was gradually accepted as one of the most popular graduate textbooks by Russian and other European physicists. A German translation of the second edition was used in this country as well as throughout the Western World. Lasting through a generation of students, its third revised edition was published in the USSR in the summer of 1963. The assistance of several noted pedagogues, chiefly that of Corresponding Academician Markov, served to develop and refine the uniquely readable style of this highly informative text.

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PREFACE

In the last ten years, research in atomic phenomena has created not only one of the most important chapters in modern physics, but has also found wide application for it in engineering.

Even the most cursory glance at the remarkable region (field) of atomic phenomena reveals new features substantially different from those which are characteristic of the macrocosm.

The first aspect encountered in the macrocosm is atomism. The simplest elementary particles are characterized by wholly determined attributes (charge, mass, etc.) which are identical for all particles of a given type.

Such atomicity does not exist in the macrocosm. Microscopic objects are aggregations of a large number of elementary particles. The laws governing macroscopic phenomena are laws which are characteristic of an aggregation of a large number of new particles.

All of this attests that it would be methodologically incorrect to base investigation of microparticles on similarity with macroscopic bodies. Even the material viewpoint of classical mechanics is an abstract idealized form, not of the microparticle at all, but of a macroscopic body whose dimensions are small in comparison with the distance encountered in the problem.

The atomism of the microcosm is not limited by the definiteness(?) of the attributes of the microparticles themselves. It is also expressed in the existence of a certain absolute dimension for mechanical motion. Such a dimension is the Planck constant $h = 1.05 \cdot 10^{-27}$ erg.sec. It is of paramount importance in the mechanics of microparticles. Physics long ignored the law of conversion of quantity to quality and attempted to comprehend atomic phemomena without going beyond the framework of classical, macroscopic theories. The discovery of Planck's constant was the first serious warning of the unsuitability of the mechanical transfer of laws from the macro region to the micro region. During the 1920's, new experimental facts were discovered which finally compelled science to abandon this approach. It was shown that electrons exhibit wave properties: If a stream of electrons is passed through a crystal, the distribution of the particles on a screen is the same as the distribution in intensity of waves of appropriate wavelength. We have a phenomenon of diffraction of microparticles which is foreign to classical mechanics. It was later shown that this phenomenon is characteristic not only of electrons but also of all microparticles in general. Thus a fundamentally new and general law was discovered.

The motion of microparticles, in many respects, proved to be more typical of wave motion than the motion of a particle along a trajectory. The phenomenon of diffraction is incompatible with the hypothesis of a trajectory motion of particles. Hence the principles of classical mechanics, in which the concept of trajectory is fundamental, is not suitable for analysis of the motion of microparticles.

The very term "particle" as applied to the individuals of the microcosm gives us the impression of a vastly greater analogy with the particles of classical mechanics than is actually the case.

This must be kept in mind in all those cases where, for the sake of brevity, we shall employ the term "particle" instead of "microparticle".

Classical mechanics proves to be only a certain approximation which is suitable for the investigation of motion of bodies with large mass moving within fields which vary sufficiently smoothly (macroscopic fields). Under such conditions Planck's constant has no meaning: it may be considered negligibly small. Diffraction phenomena also became very insignificant. In the region of small scales (in the region of the microcosm) quantum mechanics must replace classical mechanics. Thus, the motion of microparticles is the subject of investigation of quantum mechanics.

Quantum mechanics is a statistical theory. Thus, by means of quantum mechanics we may predict the mean distribution on a photographic plate of electrons reflected from a crystal. A similar state of affairs is encountered in statistical mechanics. However, between quantum mechanics and classical statistical mechanics there is a wide difference.

Classical statistical mechanics is based on Newtonian mechanics, permitting a description of the history of each of the particles so that, in principle, it is possible to give a biography for each individual specimen.

Modern quantum mechanics, in contrast to statistical mechanics, is not based on any theory of individual micro-processes. It studies the individual properties of microparticles and individual micro-processes by employing statistical aggregations -- ensembles. These statistical ensembles are determined by attributes borrowed from classical macroscopic physics (e.g., impulse, energy, coordinates, etc.). Hence, in quantum mechanics, when we speak of the reproduction of a microphenomenon (e.g., the repetition of one and the same experiment), we are speaking of the reproduction of macroscopic conditions for a microphysical phenomenon, i.e., the achievement of the same statistical ensemble.

Thus, quantum mechanics studies the statistical ensembles of microparticles in relation to their macroscopic measuring apparatus by means of which we may also determine the so-called "particle state," i.e., obtain the statistical ensemble.

Within the framework of the presented statement of the problem, quantum mechanics is the greatest step in the development of atomic physics in the twentieth century and is now already proceeding beyond the limits of physics into a region of a new engineering art.

Principles of Quantum Mechanics

CONTENTS

CHAPTER I

FOUNDATIONS OF QUANTUM THEORY

1. ENERGY AND MOMENTUM OF LIGHT QUANTA

The development of quantum mechanics began in the first years of this century with the quantum theory of light. Until then it had been believed that the debate over the nature of light had been definitely settled in favor of the wave hypothesis by Maxwell's electromagnetic theory. Hertz's experiments on electromagnetic waves and Lebedev's demonstration of the pressure exerted by light appeared to provide conclusive confirmation of this view. However the triumph of the wave theory was not complete: although problems relating to the propagation of light could be successfully solved, a number of important phenomena connected with emission and absorption could not be dealt with. For example, the spectral distribution of black-body radiation that was predicted on the basis of the wave theory could not be made to agree with experiment, in spite of all the efforts of theoretical physicists. The way out of this impasse was found in 1901 when Planck derived a new spectral distribution based on the assumption that emission and absorption are discrete processes involving finite amounts of energy, known as quanta.

According to Planck's assumption, the energy ε of a quantum is related to the frequency of light ω by the equation

$$\varepsilon = h\omega, \tag{1.1}$$

where $h = 1.05 \cdot 10^{-27}$ erg·sec is the famous Planck's constant.[1] This new hypothesis regarding the nature of light attained its full development when Einstein showed that a momentum $p = \varepsilon/c$ must also be

[1] Planck gave the value of h as $6.61 \cdot 10^{-27}$ erg·sec, a quantity 2π times larger than the one given above. If Planck's value is used, our value is denoted by $\hbar$, and the ordinary frequency $\nu = 1/T$ is used instead of the angular frequency $\omega = 2\pi/T$.

ascribed to a quantum, the direction of this momentum coinciding with the direction of propagation. In terms of the components of the wave vector $\boldsymbol{k}$

$$k_x = \frac{2\pi}{\lambda}\cos\alpha,\ \ k_y = \frac{2\pi}{\lambda}\cos\beta,\ k_z = \frac{2\pi}{\lambda}\cos\gamma,$$

where λ is the wavelength, and $\cos\alpha$, $\cos\beta$, and $\cos\gamma$ are the direction cosines of the normal to the light wave, the equation for the momentum of a light quantum can be written in vector form:

$$\boldsymbol{p} = h\boldsymbol{k}. \tag{1.2}$$

Planck's equation (1.1) and Einstein's equation (1.2) are the fundamental equations of the quantum theory of light. They relate the energy ε and momentum $\boldsymbol{p}$ of a light quantum to the frequency ω and wavelength λ of a plane monochromatic wave whose direction of propagation is determined by the vector $\boldsymbol{k}$.[1]

The significance of the quantum theory of light should not be looked for in a corpuscular picture of light as a gas consisting of particles with energy $h\omega$ and momentum $h\boldsymbol{k}$ (this picture may be useful for visualization, but it has limitations). It lies rather in the conception that the exchange of energy and momentum between a particle (such as an electron, atom, or molecule) and a beam of light involves the creation and annihilation of light quanta. To obtain an exact formulation of this notion, we shall now apply the laws of conservation of energy and of momentum to an arbitrary system interacting with light (or, more precisely, with any type of electromagnetic radiation). We can use the more illustrative term "collision" rather than "interaction" for help in visualizing the problem. Let E and $\boldsymbol{P}$ denote the energy and momentum of the system prior to collision with a light quantum, and E' and $\boldsymbol{P}'$, its energy and momentum after collision. Similarly, let $h\omega$ and $h\boldsymbol{k}$ denote the energy and momentum of the light quantum prior to collision, and $h\omega'$ and $h\boldsymbol{k}'$, these same quantities after collision. Here the precise meaning of the word "collision" is that as a result of an interaction the energy and momentum of an electromagnetic wave of frequency ω and direction $\boldsymbol{k}$ are decreased by $h\omega$ and $h\boldsymbol{k}$ respectively (one light quantum vanishes), and the energy and momentum of another electromagnetic wave of frequency ω' and direction $\boldsymbol{k}'$ are increased by $h\omega'$ and $h\boldsymbol{k}'$ (a second light quantum appears). Expressing ourselves figuratively, as though we were referring to the collision of classical particles, we can say that a light quantum $(h\omega,\ h\boldsymbol{k})$ has "collided" with the system and that

[1] Equations (1.1) and (1.2) are supposed to hold for any frequency ω, and they are just as valid for gamma-rays as for visible light. For this reason, it is generally found more convenient to speak of "photons" rather than light quanta, gamma-ray quanta, or quanta of any other specific kind of electromagnetic radiation.

its energy and momentum have been changed to $(h\omega', hk')$. The laws of conservation of energy and momentum have the following form in our notation:

$$h\omega + E = h\omega' + E', \tag{1.3}$$

$$hk + P = hk' + P'. \tag{1.4}$$

These equations apply to all three fundamental processes: namely, absorption, emission, and scattering. Equations (1.3) and (1.4) describe the absorption of a light quantum $h\omega$ if $\omega' = 0$ $(k' = 0)$. They describe the emission of a quantum $h\omega$ if $\omega = 0$ $(k = 0)$. Finally if both ω and ω' differ from zero, the equations describe the scattering of light, with a quantum characterized by $h\omega$ and hk going over into a quantum characterized by a different energy $h\omega'$ and different momentum hk'.

In the above form the laws of conservation of energy and momentum do not agree with either the wave or the corpuscular hypothesis of light, and they cannot, in general, be interpreted within the conceptual framework of classical physics. According to the wave theory, the energy of a wave field is determined by the amplitudes of the waves and not by their frequency ω. There is no general relationship between the wave amplitude and the frequency which would enable us to relate the energy of an individual quantum to the wave amplitude. To show this, let us imagine that a beam of light impinges on a transparent plate, part of the light being reflected, and part transmitted through the plate. It follows from the wave theory that the amplitudes of the incident, transmitted, and reflected waves are all different. If we relate the energy of the quanta to the wave amplitudes in an arbitrary general manner, we are driven to the conclusion that the energy is different in each of the three beams. According to (1.1), the energy of a quantum cannot be changed without changing the frequency, and consequently, a fraction of a quantum always differs in "color" from the original, undivided quantum. In this way, our assumption that the energy of a quantum is determined by the amplitude must lead us to the conclusion that the incident, reflected, and transmitted beams will differ in color, and this, of course, is simply not the case when light passes through a transparent body.

In similar fashion, inconsistences are obtained if it is assumed that a light quantum is a particle located in space—a sort of "floating object" on a wave. By definition [see (1.1) and (1.2)], a light quantum is associated with a monochromatic plane wave, or in other words a pure periodic disturbance of infinite extent in space and time. The assumption that a quantum has a location cannot be reconciled with the perfect periodicity of the wave, since a sinusoidal wave which is in any way deformed can only be built up from several different pure sinusoidal waves. Thus we see that if we are to adopt the conservation laws (1.3) and (1.4), we must recognize that classical concepts are not adequate. Light has a dual nature, possessing both wave and corpuscular properties. These two aspects of light can be accounted for in modern quantum electrodynamics, but this subject lies outside the scope of this book, which is concerned with nonrelativistic particle mechanics.

2. EXPERIMENTAL VERIFICATION OF THE CONSERVATION LAWS FOR THE ENERGY AND MOMENTUM OF LIGHT QUANTA

With the help of the conservation law (1.3), Einstein was able to explain the photo-electric effect, which had remained a very puzzling phenomenon according to classical views. Essentially, this effect involves the emission of electrons from the surface of a metal under the influence of light.[1] Experiment shows that (for any given metal) the velocity of the photo-electrons depends only on the frequency of the incident light ω and is completely independent of the intensity, which determines only the number of electrons emitted per unit time. However ingenious the classical model devised for this effect, the acceleration of the electron always had to be proportional to the force acting on it, in accordance with Newton's laws of motion. Since this force is equal to the product of the electronic charge e and the electric intensity $\vec{E}$ of the light wave (the effect of the magnetic field of the wave being negligible), all classical models predicted that the velocity acquired by the electron would be proportional to E, and the energy to E^2. This prediction conflicted, however, with what was observed in practice.

It was shown by Ioffe and Dobronravov[2] that the photo-electric effect is observed even at low intensities, the electrons being emitted according to statistical laws, so that only the average number of electrons is proportional to the intensity of the light. Millikan obtained an even more important experimental result, which showed conclusively that the energy of photo-electrons depends only on the frequency of the light, and not on the intensity. This result can be explained only in terms of the law of conservation of energy (1.3). Let us suppose that monochromatic light of frequency ω falls on the metal surface. A certain expenditure of work is required in order to liberate electrons from the metal. If this amount of work is denoted by χ (the electronic work function), the initial energy of an electron in the metal must be taken as $-\chi$. Since a light quantum is completely absorbed in the photo-electric effect, it follows that $h\omega' = 0$. After the absorption of a quantum, the energy of the electron may be taken as $m_0v^2/2$, where m_0 is the mass

[1] The characteristics of the photo-electric effect were first studied by A. G. Stoletov, W. Hallwachs, A. Righi, and others.

[2] See P. S. Tartakovskiy, Kvanty sveta (Light Quanta), Gos. izdatel'stvo, 1928.

of the electron, and v is the velocity with which it escapes from the metal. Accordingly, equation (1.3) reduces to Einstein's well-known equation for the photo-electric effect:[1]

$$\hbar\omega - \chi = \frac{m_0 v^2}{2}. \tag{2.1}$$

It follows from this equation that the energy $m_0v^2/2$ of photo-electrons increases linearly as a function of the light frequency ω. The energy of the electrons is related to the stopping potential V by the equation $eV = m_0v^2/2$, and therefore if V is plotted as a function of ω, the slope of the resulting straight line will be equal to $\hbar/e$. Since the charge e is known and the slope can be found from experiment, it is possible to determine $\hbar$. By conducting the appropriate measurements, Millikan showed that the value obtained for $\hbar$ is the same as in the theory of black-body radiation, thus providing a rigorous corroboration of the applicability of equation (1.3) to the photo-electric effect. It is worth noting that Einstein's equation (2.1) now has important practical applications in photo-electric instruments.[2]

A simultaneous verification of equations (1.3) and (1.4) was provided by Compton's investigations of the dependence of the frequency of scattered x-rays on the scattering angle. The scattering materials used in his experiments were substances in which the electrons are weakly bound to the atom (paraffin and graphite). Because of the high energy of the x-ray quanta, the energy of the electrons in the atoms can be neglected (at least for electrons in the outer shells), and they can be treated as free particles at rest. Accordingly, in our discussion of the experiments, we take the initial energy of the electron E and its momentum P to be equal to zero. Since the energy of an electron may be very high after a collision with an x-ray quantum, it is necessary to use relativistic equations, in order to take into account the dependence of mass on velocity. According to the theory of relativity, the kinetic energy of an electron travelling with a velocity v is

$$E' = \frac{m_0 c^2}{\sqrt{1 - v^2/c^2}} - m_0 c^2, \tag{2.2}$$

where m_0 is the rest mass and c is the velocity of light, whereas the momentum is

$$P' = \frac{m_0 v}{\sqrt{1 - v^2/c^2}}. \tag{2.3}$$

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[1] Equation (1.4) is not important in this case since it simply asserts that the momentum of the light quantum is completely transferred to the piece of metal as a whole.

[2] For an account of Millikan's experiments, see R. A. Millikan, The Electron, The University of Chicago Press, Chicago, 1917; see also P. S. Tartakovskiy, op. cit., and E. Shpol'skiy, Atomnaya Fizika (Atomic Physics), Gos. izdatel'stvo teoret.-tekhn. lit., 1951.

On substituting these expressions into (1.3) and (1.4), and remembering that $E = 0$ and $P = 0$, we obtain

$$h\omega = h\omega' + m_0c^2\left[\frac{1}{\sqrt{1-\beta^2}} - 1\right], \tag{2.4}$$

$$h\boldsymbol{k} = h\boldsymbol{k}' + \frac{m_0\boldsymbol{v}}{\sqrt{1-\beta^2}}, \quad \beta = \frac{v}{c}. \tag{2.4'}$$

where ω and $\boldsymbol{k}$ are, respectively, the frequency and the wave vector of the incident radiation, and ω' and $\boldsymbol{k}'$ are the corresponding quantities for the scattered radiation. It follows directly from equation (2.4) that $\omega > \omega'$ and therefore the scattered radiation should have a greater wavelength than the incident radiation. This particular conclusion was corroborated by Compton's experiments, whereas in the classical theory the frequency of the scattered light would have to be equal to the frequency of the incident light (Rayleigh scattering). It is worth noting here that equations (2.4) and (2.4′) together lead to an important conclusion, namely, a free electron can scatter light, but cannot absorb it. Total absorption would mean that $\omega' = 0$ (and $\boldsymbol{k}' = 0$), and from (2.4′) this would imply that $\boldsymbol{k}$ and $\boldsymbol{v}$ are in the same direction. Consequently, if (2.4′) is written in scalar form

$$hk = \frac{m_0 v}{\sqrt{1-\beta^2}}$$

and combined with (2.4), we find that absorption takes place only if

$$\frac{1}{\sqrt{1-\beta^2}} - 1 = \frac{\beta}{\sqrt{1-\beta^2}}.$$

Hence $\beta = 0$, and therefore it follows that $k = 0$, thus proving the impossibility of absorption. The photo-electric effect, which does involve the complete absorption of a quantum, is possible only because the electron is bound to the metal; this changes the situation in two important respects, in that an energy χ is required to eject the electron and in that the momentum of the quantum can be imparted to the metal.

In order to obtain a method of verifying equations (2.4) and (2.4′) simultaneously, Compton determined the dependence of the frequency of scattered light ω' on the scattering angle θ on the basis of these equations. In deriving Compton's formula, we shall find it convenient to refer to Fig. 1. In this diagram, OA indicates the direction of propagation of the beam of primary x-rays, and OC, the direction of the scattered x-rays. The parallelogram $OCAD$ represents the momentum of the incident quantum $h\boldsymbol{k}$ as the sum of the momentum of the scattered quantum $h\boldsymbol{k}'$ and the momentum of the electron $\boldsymbol{P}$. The angle θ is the scattering angle, and α is the angle