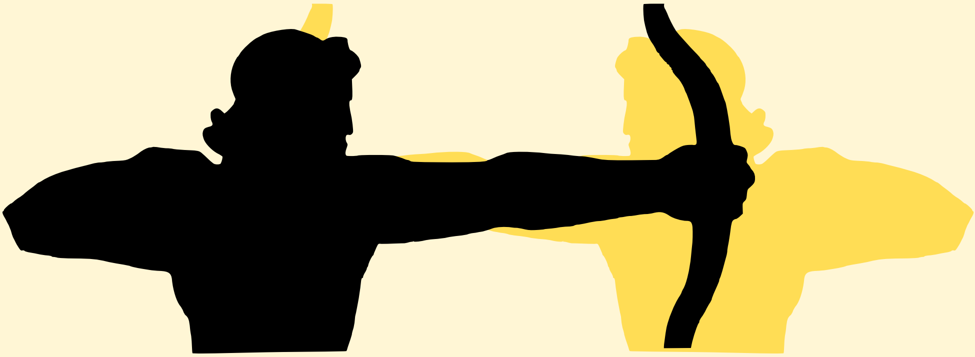
L.V. Tarasov

Basic Concepts of

Although quantum mechanics deals with microparticles, its significance is by no means limited to microphenomena. In our endless quest for understanding and perfecting our knowledge of the laws of nature, quantum mechanics represents an important *qualitative leap*.



Quantum Mechanics

MIR Publishers Moscow

This book gives a detailed and systematic exposition of the fundamentals of non-relativistic quantum mechanics for those who are not acquainted with the subject. The character of the physics of microparticles and the problems of the physics of microphenomena (interference of amplitudes, the principle of superposition, the specific nature of measuring processes, causality in quantum mechanics) are considered on the basis of concepts about probability amplitudes. Besides, the quantum-mechanical systems—microparticles—with two basic states are analyzed in detail. The apparatus of quantum mechanics is considered as a synthesis of concepts about physics and the theory of linear operators. A number of specially worked out problems and examples have been included in order to demonstrate the working of the apparatus.
This book is meant for use by students of engineering and teachers-training institutes. It may also be used by engineers of different profiles.

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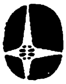

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ОСНОВЫ КВАНТОВОЙ МЕХАНИКИ

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Contents

Preface

Some Preliminary Remarks

Research in physics, conducted at the end of the 19th century and in the first half of the 20th century, revealed exceptionally peculiar nature of the laws governing the behaviour of microparticles—atoms, electrons, and so on. On the basis of this research a new physical theory called *quantum mechanics* was founded.

The growth of quantum mechanics turned out to be quite complicated and prolonged. The mathematical part of the theory, and the rules linking the theory with experiment, were constructed relatively quickly (by the beginning of the thirties). However, the understanding of the physical and philosophical substance of the mathematical symbols used in the theory was unresolved for decades. In Fock's words [1], *The mathematical apparatus of non-relativistic quantum mechanics worked well and was free of contradictions; but in spite of many successful applications to different problems of atomic physics the physical representation of the mathematical scheme still remained a problem to be solved.*

Many difficulties are involved in a mathematical interpretation of the quantum-mechanical apparatus. These are associated with the dialectics of the new laws, the radical revision of the very nature of the questions which a physicist "is entitled to put to nature", the reinterpretation of the role of the observer *vis à vis* his surroundings, the new approach to the question of the relation between chance and necessity in physical phenomena, and the rejection of many accepted notions and concepts. Quantum mechanics was born in an atmosphere of discussions and heated clashes between contradictory arguments. The names of many leading scientists are linked with its development, including N. Bohr, A. Einstein, M. Planck, E. Schrödinger, M. Born, W. Pauli, A. Sommerfeld, L. de Broglie, P. Ehrenfest, E. Fermi, W Heisenberg, P. Dirac, R. Feynman, and others.

It is also not surprising that even today anyone who starts studying quantum mechanics encounters some sort of psychological barrier. This is not because of the mathematical complexity. The difficulty arises from the fact that it is difficult to break away from accepted concepts and to reorganize one's pattern of thinking which are based on everyday experience.

Before starting a study of quantum mechanics, it is worthwhile getting an idea about its place and role in physics. We shall consider (naturally in the most general terms) the following three questions: What is quantum mechanics? What is the relation between classical physics and quantum mechanics? What specialists need quantum mechanics? So, what is quantum mechanics?

The question can be answered in different ways. First and foremost, quantum mechanics is a theory describing the properties of matter at the level of *microphenomena*—it considers the laws of motion of *microparticles*. Microparticles (molecules, atoms, elementary particles) are the main "characters" in the drama of quantum mechanics.

From a broader point of view quantum mechanics should be treated as the theoretical foundation of the modern theory of the structure and properties of matter. In comparison with classical physics, quantum mechanics considers the properties of matter *on a deeper and more fundamental level.* It provides answers to many questions which remained unsolved in classical physics. For example, why is diamond hard? Why does the electrical conductivity of a semiconductor increase with temperature? Why does a magnet lose its properties upon heating? Unable to get answers from classical physics to these questions, we turn to quantum mechanics. Finally, it must be emphasized that quantum mechanics allows one to *calculate* many physical parameters of substances. Answering the question "What is quantum mechanics?", Lamb [2] remarked: *The only easy one* (*answer*) *is that quantum mechanics is a discipline that provides a wonderful set of rules for calculating physical properties of matter.*

What is the relation of quantum mechanics to classical physics? First of all quantum mechanics includes classical mechanics as a limiting (extreme) case. Upon a transition from microparticles to macroscopic bodies, quantum-mechanical laws are converted into the laws of classical mechanics. Because of this it is often stated, though not very accurately, that quantum mechanics "works" in the microworld and the classical mechanics, in the macroworld. This statement assumes the existence of an isolated "microworld" and an isolated "macroworld". In actual practice we can only speak of microparticles (microphenomena) and macroscopic bodies (macrophenomena). It is also significant that microphenomena form the basis of macrophenomena and that macroscopic bodies are made up of microparticles. Consequently, the transition from classical physics to quantum mechanics is a transition not from one "world" to another, but from a shallower to a deeper level of studying matter. This means that in studying the behaviour of microparticles, quantum mechanics considers in fact the same macroparticles, but on a more fundamental level. Besides, it must be remembered that the boundary between micro- and macrophenomena in general is quite conditional and flexible. Classical concepts are frequently found useful when considering microphenomena, while quantum-mechanical ideas help in the understanding of macrophenomena. There is even a special term "quantum macrophysics" which is applied, in particular, to quantum electronics, to the phenomena of superfluidity and superconductivity and to a number of other cases.

In answering the question as to what specialists need quantum mechanics, we mention beforehand that we have in mind specialists training in engineering colleges. There are at least three branches of engineering for which a study of quantum mechanics is absolutely essential. Firstly, there is the field of *nuclear power* and the application of radioactive isotopes to industry. Secondly, the field of *materials sciences* (improvement of properties of materials, preparation of new materials with preassigned properties). Thirdly, the field of *electronics* and first of all the field of *semiconductors* and *laser technology*. If we consider that today almost any branch of industry uses new materials as well as electronics on a large scale, it will become clear that a comprehensive training in engineering is impossible without a serious study of quantum mechanics.

The Structure of the Book

The aim of this book is to acquaint the reader with the concepts and ideas of quantum mechanics and the physical properties of matter; to reveal the logic of its new ideas, to show how these ideas are embodied in the mathematical apparatus of linear operators and to demonstrate the working of this apparatus using a number of examples and problems of interest to engineering students.

The book consists of three chapters. By way of an introduction to quantum mechanics, the *first chapter* includes a study of the physics of microparticles. Special attention has been paid to the fundamental ideas of quantization and duality as well as to the uncertainty relations. The first chapter aims at "introducing" the main "character", i.e. the microparticle, and at showing the necessity of rejecting a number of concepts of classical physics.

The *second chapter* deals with the physical concepts of quantum mechanics. The chapter starts with an analysis of a set of basic experiments which form a foundation for a system of quantum-mechanical ideas. This system is based on the concept of the amplitude of transition probability. The rules for working with amplitudes are demonstrated on the basis of a number of examples, the interference of amplitudes being the most important. The principle of superposition and the measurement process are considered. This concludes the first stage in the discussion of the physical foundation of the theory. In the second stage an analysis is given based on amplitude concepts of the problems of causality in quantum mechanics. The Hamiltonian matrix is introduced while considering causality and its role is illustrated using examples involving microparticles with two basic states, with emphasis on the example of an electron in a magnetic field. The chapter concludes with a section of a general physical and philosophical nature.

The *third chapter* deals with the application of linear operators in the apparatus of quantum mechanics. At the beginning of the chapter the required mathematical concepts from the theory of Hermitian and unitary linear operators are introduced. It is then shown how the physical ideas can be "knitted" to the mathematical symbols, thus changing the apparatus of operator theory into the apparatus of quantum theory. The main features of this apparatus are further considered in a concrete form in the framework of the coordinate representation. The transition from the coordinate to the momentum representation is illustrated. Three ways of describing the evolution of microsystems in time, corresponding to the Schrödinger, Heisenberg and Dirac representation, have been discussed. A number of typical problems are considered to demonstrate the working of the apparatus; particular attention is paid to the problems of the motion of an electron in a periodic field and to the calculation of the probability of a quantum transition.

The book contains a number of *interludes*. These are dialogues in which the author has allowed himself free and easy style of considering certain questions. The author was motivated to include interludes in the book by the view that one need not take too serious an attitude when studying serious subjects. And yet the reader should take the interludes fairly seriously. They are intended not so much for mental relaxation, as for helping the reader with fairly delicate questions, which can be understood best through a flexible dialogue treatment.

Finally, the book contains many quotations. The author is sure that the "original words" of the founders of quantum mechanics will offer the reader useful additional information.

Personal Remarks

The author wishes to express his deep gratitude to Prof. I.I. Gurevich, Corresponding Member of the USSR Academy of Sciences, for the stimulating discussions which formed the basis of this book. Prof. Gurevich discussed the plan of the book and its preliminary drafts, and was kind enough to go through the manuscript. His advice not only helped mould the structure of the book, but also helped in the nature of exposition of the material. The subsection "The Essence of Quantum Mechanics" in Sec. 16 is a direct consequence of Prof. Gurevich's ideas.

The author would like to record the deep impression left on him by the works on quantum mechanics by the leading American physicist R. Feynman [3-5]. While reading the sections in this book dealing with the applications of the idea of probability amplitude, superposition principle, microparticles with two basic states, the reader can easily detect a definite similarity in approach with the corresponding parts in Feynman's "Lectures in Physics" The author was also considerably influenced by N. Bohr (in particular by his wonderful essays *Atomic Physics and Human Knowledge* [6]), V. A. Fock [1, 7], W. Pauli [8], P. Dirac [9], and also by the comprehensive works of L. D. Landau and E. M. Lifshitz [10], D. I. Blokhintsev [11], E. Fermi [12], L. Schiff [13].

The author is especially indebted to Prof. M. I. Podgoretsky, D.Sc., for a thorough and extremely useful analysis of the manuscript. He is also grateful to Prof. Yu. A. Vdovin, Prof. E. E. Lovetsky, Prof. G. F. Drukarev, Prof. V. A. Dyakov, Prof. Yu. N. Pchelnikov, and Dr. A. M. Polyakov, all of whom took the trouble of going through the manuscript and made a number of valuable comments. Lastly, the author is indebted to his wife Aldina Tarasova for her constant interest in the writing of the book and her help in the preparation of the manuscript. But for her efforts, it would have been impossible to bring the book to its present form.

Prelude. Can the System of Classical Physics Concepts Be Considered Logically Perfect?

He who would study organic existence,
First drives out the soul with rigid persistence,
Then the parts in his hands he may hold and class
But the spiritual link is lost, alas!
Goethe (*Faust*)

Participants: the Author and the Classical Physicist (Physicist of the older generation, whose views have been formed on the basis of classical physics alone).

Author: It is well known that the basic contents of a physical theory are formed by a system of concepts which reflect the objective laws of nature within the framework of the given theory. Let us take the system of concepts lying at the root of classical physics. Can this system be considered logically perfect?

Classical Physicist: It is quite perfect. The concepts of classical physics were formed on the basis of prolonged human experience; they have stood the test of time.

Author: What are the main concepts of classical physics?

Classical Physicist: I would indicate three main points: (a) continuous variation of physical quantities; (b) the principle of classical determinism; (c) the analytical method of studying objects and phenomena.

While talking about *continuity*, let us remember that the state of an object at every instant of time is completely determined by describing its coordinates and velocities, which are continuous functions of time. This is what forms the basis of the concept of motion of objects along trajectories. The change in the state of an object may in principle be made as small as possible by reducing the time of observation.

Classical determinism assumes that if the state of an object as well as all the forces applied to it are known at some instant of time, we can precisely predict the state of the object at any subsequent instant. Thus, if we know the position and velocity of a freely falling stone at a certain instant, we can precisely tell its position and velocity at any other instant, for example, at the instant when it hits the ground.

Author: In other words, classical physics assumes an unambiguous and inflexible link between present and future, in the same way as between past and present.

Classical Physicist: The possibility of such a link is in close agreement with the continuous nature of the change of physical quantities: for every instant of time we always have an answer to two questions: "What are the coordinates of an object"? and, "How fast do they change?"

Finally, let us discuss the *analytical method* of studying objects and phenomena. Here we come to a very important point in the system of concepts of classical physics. The latter treats matter as made up of different parts which, although they interact with one another, may be investigated individually. This means that firstly, the object may be *isolated* from its environments and treated as an independent entity, and secondly, the object may be *broken up*, if necessary, into its constituents whose analysis could lead to an understanding of the nature of the object.

Author: It means that classical physics reduces the question "what is an object like?" to "what is it made of?"

Classical Physicist: Yes, indeed. In order to understand any apparatus we must "dismantle" it, at least in one's imagination, into its constituents. By the way, everyone tries to do this in his childhood. The same is applicable to phenomena: in order to understand the idea behind some phenomenon, we have to express it as a function of time, i.e. to find out what follows what.

Author: But surely such a step will destroy the notion of the object or phenomenon as a single unit.

Classical Physicist: To some extent. However, the extent of this "destruction" can be evaluated each time by taking into account the interactions between different parts and relation between the time stages of a phenomenon. It may so happen that the initially isolated object (a part of it) may considerably change with time as a result of its interaction with the surroundings (or interaction between parts of the object). However, since these changes are continuous, the individuality of the isolated object can always be returned over any period of time. It is worthwhile to stress here the internal logical connections among the three fundamental notions of classical physics.

Author: I would like to add that one special consequence of the "principle of analysis" is the notion, characteristic of classical physics, of the mutual independence of the object of observation and the measuring instrument (or observer). We have an instrument and an object of measurement. They can and should be considered separately, independently from one another.

Classical Physicist: Not quite independently. The inclusion of an ammeter in an electric circuit naturally changes the magnitude of the current to be measured. However, this change can always be calculated if we know the resistance of the ammeter.

Author: When speaking of the independence of the instrument and the object of measurement, I just meant that their interaction may be simply "ignored".

Classical Physicist: In that case I fully agree with you.

Author: Born has considered this point in [14]. Characterizing the philosophy of science which influenced "people of older generation", he referred to the tendency to consider that the object of investigation and the investigator are completely isolated from each other, that one can study physical phenomena without interfering with their passage. Born called such style of thinking "Newtonian", since he felt that this was reflected in "Newton's celestial mechanics."

Classical Physicist: Yes, these are the notions of classical physics in general terms. They are based on everyday commonplace experience and it may be confidently stated that they are acceptable to our common sense, i.e. are taken as quite natural. I rather believe that the "principle of analysis" is not only a natural but the only effective method of studying matter. It is incomprehensible how one can gain a deeper insight into any object or phenomenon without studying its components. As regards the principle of classical determinism, it reflects the causality of phenomena in nature and is in full accordance with the idea of physics as an *exact science*.

Author: And yet there are grounds to doubt the "flawlessness" of classical concepts even from very general considerations.

Let us try to extend the principle of classical determinism to the universe as a whole. We must conclude that the positions and velocities of all "atoms" in the universe at any instant are precisely determined by the positions and velocities of these "atoms" at the preceding instant. Thus everything that takes place in the world is *predetermined beforehand*, all the events can be fatalistically predicted. According to Laplace, we could imagine some "superbeing" completely aware of the future and the past. In his *Theorie analytique des probabilités*, published in 1820, Laplace wrote [15]: *An intelligence knowing at a given instant of time all forces acting in nature as well as the momentary positions of all things of which the universe consists, would be able to comprehend the motions of the largest bodies of the world and those of the lightest atoms in one single formula, provided his intellect were sufficiently powerful to subject all data to analysis, to him nothing would be uncertain, both past and future would be present to his eyes.* It can be seen that an imaginary attempt to extend the principle of classical determinism to nature in its entity leads to the emergence of the idea of fatalism, which obviously cannot be accepted by common sense.

Next, let us try to apply the "principle of analysis" to an investigation of the structure of matter. We shall, in an imaginary way, break the object into smaller and smaller fractions, thus arriving finally at the molecules constituting the object. A further "breaking-up" leads us to the conclusion that molecules are made up of atoms. We then find out that atoms are made up of a nucleus and electrons. Accustomed to the tendency of splitting, we would like to know what an electron is made of. Even if we were able to get an answer to this question, we would have obviously asked next: What are the constituents, which form an electron, made of? And so on. We tend to accept the fact that such a "chain" of questions is endless. The same common sense will revolt against such a chain even though it is a direct consequence of classical thinking.

Attempts were made at different times to solve the problem of this chain. We shall give two examples here. The first one is based on Plato's views on the structure of matter. He assumed that matter is made up of four "elements"—earth, water, air and fire.

Each of these elements is in turn made of atoms having definite geometrical forms. The atoms of earth are cubic, those of water are icosahedral, while the atoms of air and fire are octahedral and tetrahedral, respectively. Finally, each atom was reduced to triangles. To Plato, a triangle appeared as the simplest and most perfect mathematical form, hence it cannot be made up of any constituents. In this way, Plato reduced the chain to the purely mathematical concept of a triangle and terminated it at this point.

The other example is characteristic for the beginning of the 20th century. It makes use of the external similarity of form between the planetary model of the atom and the solar system. It is assumed that our solar system is nothing but an isolated atom of some other, gigantic world, and an ordinary atom is a sort of "solar system" for some third dwarfish world for which "our electron" is like a planet. In this case we admit the existence of an infinite row of more and more dwarfish worlds, just like more and more gigantic worlds. In such a system the structure of matter is described in accordance with the primitive "chinese box" principle.

The "chinese box" principle of hollow tubes, according to which nature has a more or less similar structure, was not accepted by all the physicists of older generations. However, this principle is quite characteristic of classical physics, it conforms to classical concepts, and follows directly from the classical principle of analysis. In this connection, criticizing Pascal's views that the smallest and the largest objects have the same structure, Langevin pointed out that this would lead to the same aspects of reality being revealed at all levels. The universe should then be reflected in an absolutely identical fashion in all objects, though on a much smaller scale. Fortunately, reality turns out to be much more diverse and interesting.

Thus, we are convinced that a successive application of the principles of classical physics may, in some cases, lead to results which appear doubtful. This indicates the existence of situations for which classical principles are not applicable. Thus it is to be expected that for a sufficiently strong "breaking-up" of matter, the principle of analysis must become redundant (thus the idea of the independence of the object of measurement from the measuring instrument must also become obsolete). In this context the question "what is an electron made of?" would simply appear to have lost its meaning.

If this is so, we must accept the *relativity* of the classical concepts which are so convenient and dear to us, and replace them with some qualitatively new ideas on the motion of matter. The classical attempts to obtain an endless detailization of objects and phenomena mean that the desire inculcated in us over centuries "to study organic existence" leads at a certain stage to a "driving out of the soul" and a situation arises, where, according to Goethe, "the spiritual link is lost".

Chapter 1

Physics of the Microparticles

Microparticles

Molecules, *atoms*, *atomic nuclei* and *elementary particles* belong to the category of microparticles. The list of elementary particles is at present fairly extensive and includes quanta of electromagnetic field (*photons*) as well as two groups of particles, the *hadrons* and the *leptons*. Hadrons are characterized by a strong (nuclear) interaction, while leptons never take part in strong interactions. The electron, the muon and the two neutrinos (the electronic and muonic) are leptons. The group of hadrons is numerically much larger. It includes nucleons (proton and neutron), mesons (a group of particles lighter than the proton) and hyperons (a group of particles heavier than the neutron). With the exception of photons and some neutral mesons, all elementary particles have corresponding anti-particles.

Among properties of microparticles, let us first mention the *rest mass* and *electric charge*. As an example, we note that the mass m of an electron is equal to 9.1×10^{-28} g; a proton has mass equal to $1836m$, a neutron, $1839m$ and a muon, $207m$. Pions (π-mesons) have a mass of about $270m$ and kaons (K-mesons), about $970m$. The rest mass of a photon and of both neutrinos is assumed to be equal to zero.

The mass of a molecule, atom or atomic nucleus is equal to the sum of the masses of the particles constituting the given microparticle, less a certain amount known as the mass defect. The mass defect is equal to the ratio of the energy that must be expended to break up the microparticle into its constituent particles (this energy is usually called the binding energy) to the square of velocity of light. The stronger the binding between particles, the greater is the mass defect. Nucleons in atomic nuclei have the strongest binding—the mass defect for one nucleon exceeds $10m$.

The magnitude of the electric charge of a microparticle is a multiple of the magnitude of the charge of an electron, which is equal to 1.6×10^{-19} C (4.8×10^{-10} CGSE units). Apart from charged microparticles, there also exist neutral microparticles (for example, photon, neutrino, neutron). The electric charge of a complex microparticle is equal to the algebraic sum of the charges of its constituent particles.

Spin of a Microparticle

Spin is one of the most important specific characteristics of a microparticle. It may be interpreted as the angular momentum of the microparticle not related to its motion as a whole (it is frequently known as the internal angular momentum of the microparticle). The square of this angular momentum is equal to $\hbar^2 s\ (s + 1)$, where s for the given microparticle is a definite integral or semi-integral number (it is this number which is usually referred to as the spin), $\hbar$ is a universal physical constant which plays an exceptionally important role in quantum mechanics. It is called *Planck's constant* and is equal to 1.05×10^{-34} J.s Spin s of a photon is equal to 1, that of an electron (or any other lepton) is equal to $\frac{1}{2}$ while pions and kaons don't have any spin.* Spin is a specific property of a microparticle. It does not have a classical analogue and certainly points to the complex internal structure of the microparticle. True, it is sometimes attempted to explain the concept of spin on the model of an object rotating around its axis (the very word "spin" means "rotate"). Such a mode is descriptive but not true. In any case, it cannot be literally accepted. The term "rotating microparticle" that one comes across in the literature does not by any means indicate the rotation of the microparticle, but merely the existence of a specific internal angular momentum in it. In order that this momentum be transformed into "classical" angular momentum (and the object thereby actually rotate) it is necessary to satisfy the conditions $s \gg 1$. Such a condition, however, is usually not satisfied.

The peculiarity of the angular momentum of a microparticle is manifested, in particular, in the fact that its projection in any fixed direction assumes discrete values $\hbar s,\ \hbar\ (s - 1),\ .\ \ .,\ -\hbar s$, thus in total $2s + 1$ values. It means that the microparticle may exist in $2s + 1$ spin states. Consequently, the existence of spin in a microparticle leads to the appearance of additional (internal) degrees of freedom.

Bosons and Fermions

If we know the spin of a microparticle, we can predict its behaviour in the collective of microparticles similar to it (in other words, to predict the statistical properties of the microparticle). It turns out that all the microparticles in nature can be divided into two groups, according

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* The definition of spin of a microparticle assumes that spin is independent of external conditions. This is true for elementary particles. However, the spin of an atom, for example, may change with a change in the state of the latter. In other words, the spin of an atom may change as a result of influences on the atom which lead to a change in its state.

to their statistical properties: a group with integral values of spin or with zero spin, and another with half-integral spin.

Microparticles of the first group are capable of populating one and the same state in unlimited numbers.* Moreover, the more populated is a given state, the higher is the probability that a microparticle appears in this state. Such microparticles are known to obey the Bose-Einstein statistics, in short they are simply called *bosons.* Microparticles of the second group may inhabit the states only one at a time, if the state under consideration is already occupied, no other microparticle of the given type can be accommodated there. Such microparticles obey Fermi-Dirac statistics and are called *fermions.*

Among elementary particles, photons and mesons are bosons while the leptons (in particular, electrons), nucleons and hyperons are fermions. The fact that electrons are fermions is reflected in the well-known *Pauli exclusion principle.*

Instability of Microparticles

All elementary particles except the photon, the electron, the proton and both neutrinos are *unstable.* This means that they decay spontaneously, without any external influence, and are transformed into other particles. For example, a neutron spontaneously decays into a proton, an electron and an electronic antineutrino ($n \rightarrow p + e^- + \nu_e$). It is impossible to predict precisely at what time a particular neutron will decay since each individual act of disintegration occurs randomly. However, by following a large number of acts, we find a regularity in decay. Suppose there are N_0 neutrons ($N_0 \gg 1$) at time $t = 0$. Then at the moment t we are left with $N(t) = N_0 \exp(-t/\tau)$ neutrons, where τ is a certain constant characteristic of neutrons. It is called the lifetime of a neutron and is equal to 10^3 s. The quantity $\exp(-t/\tau)$ determines the probability that a given neutron will not decay in time t.

Every unstable elementary particle is characterized by its lifetime. The smaller the lifetime of a particle, the greater the probability that it will decay. For example, the lifetime of a muon is 2.2×10^{-6} s, that of a positively charged π-meson is 2.6×10^{-8} s, while for a neutral π-meson the lifetime is 10^{-16} s and for hyperons, 10^{-10} s. In recent years, a large number of particles (about 100) have been observed to have an anomalously small lifetime of about 10^{-22}-10^{-23} s. These are called *resonances.*

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* The concept of the state of a microparticle is discussed in Sec. 3 below.

It is worthnoting that hyperons and mesons may decay in different ways. For example, the positively charged π-meson may decay into a muon and a muonic neutrino ($\pi^+ \to \mu^+ + \nu_\mu$), into a positron (antielectron) and electronic neutrino ($\pi^+ \to e^+ + \nu_e$), into a neutral π-meson, positron and electronic neutrino ($\pi^+ \to \pi^0 + e^+ + \nu_e$). For any particular π-meson, it is impossible to predict not only the time of its decay, but also the mode of decay it might "choose". Instability is inherent not only in elementary particles, but also in other microparticles. The phenomenon of radioactivity (spontaneous conversion of isotopes of one chemical element into isotopes of another, accompanied by emission of particles) shows that the atomic nuclei can also be unstable. Atoms and molecules in excited states are also unstable; they spontaneously return to their ground state or to a less excited state.

Instability determined by the probability laws is, apart from spin, the second special specific property inherent in microparticles. This may also be considered as an indication of a certain "internal complexity" in the microparticles.

In conclusion, we may note that instability is a specific, but by no means essential, property of microparticles. Apart from the unstable ones, there are many stable microparticles: the photon, the electron, the proton, the neutrino, the stable atomic nuclei, as well as atoms and molecules in their ground states.

Interconversion of Microparticles

Looking at the decay scheme of a neutron ($n \to p + e^- + \bar{\nu}_e$), an inexperienced reader might presume that a neutron is made up of mutually bound proton, electron and electronic antineutrino. Such an assumption is wrong. The decay of elementary particles is by no means a disintegration in the literal sense of the word; it is just an act of conversion of the original particle into a certain aggregate of new particles; the original particle is annihilated while new particles are created. The unfoundedness of the literal interpretation of the term "decay of particles" becomes apparent when one considers that many particles can decay in several different ways.

The interconversion of elementary particles turns out to be much more diverse and complicated if we consider particles not only in a free, but also in a bound state. A free proton is stable, and a free neutron decays according to the equation mentioned above. If, however, the neutron and the proton are not free but bound in an atomic nucleus, the situation radically changes. Now the following equations of interconversion are operative: $n \rightarrow p + \pi^-$, $p \rightarrow n + \pi^+$ (here, π^- is a negatively charged π-meson, the antiparticle of the π^+-meson). These equations very well illustrate that an attempt to find out whether the proton is a "constituent" of the neutron, or vice versa is pointless.

Everyday experience teaches us that to break up an object into parts means to reveal its structure. The idea of analysis (or splitting) reflects the characteristic feature of classical methods. When we go over to the microparticles, this idea still holds to a certain extent: the molecules are made up of atoms, the atoms consist of nuclei and electrons, the nuclei are made up of protons and neutrons. However, the idea exhausts itself at this point: for example, "splitting up" of a neutron or a proton does not reveal the structure of these particles. As regards elementary particles, when we say that a particle decays into parts, it does not mean that these particles constitute the given particle. This condition itself might serve as a definition of an elementary particle.

Decay of elementary particles is not the only kind of interconversion of particles. Equally important is the case of interconversion of particles when they collide with one another. As an example, we shall consider some equations of interconversion during collision of photons (γ) with protons and neutrons:

$$\gamma + p \rightarrow n + \pi^+, \qquad \gamma + n \rightarrow p + \pi^-,$$

$$\gamma + p \rightarrow p + \pi^0, \qquad \gamma + n \rightarrow n + \pi^0,$$

$$\gamma + p \rightarrow p + \pi^+ + \pi^-,$$

$$\gamma + n \rightarrow n + \pi^0 + \pi^0,$$

$\gamma + p \rightarrow p + p + \bar{p}$ ($\bar{p}$—denotes an antiproton)

It should be mentioned here that in all the above equations, the sum of the rest masses of the end particles is greater than the rest mass of the initial ones. In other words, the energy of the colliding particles is converted into mass (according to the well-known relation $E = mc^2$). These equations demonstrate, in particular, the fruitlessness of efforts to break up elementary particles (in this case, nucleons) by "bombarding" them with other particles (in this case, photons): in fact, it does not lead to a breaking-up of the particles being bombarded at, but to the creation of new particles, to some extent at the expense of the energy of the colliding particles.

A study of the interconversion of elementary particles permits us to determine certain regularities. These regularities are expressed in the form of laws of conservation of certain quantities which play the role of some definite characteristics of certain particles. As a simple example, we take the electric charge of a particle. For any interconversion of particles, the algebraic sum of electric charges of the initial and end particles remains the same. The law of conservation of the electric charge refers to a definite regularity in the interconversion of particles: it permits one to summarily reject equations where the total electric charge is not conserved.

As a more complicated example, we mention the so-called barionic charge of a particle. It has been observed that the number of nuleons during an interconversion of particles is conserved. With the discovery of antinucleons, it was observed that additional nucleons may be created, but they must be created in pairs with these antinucleons. So a new characteristic of particles, the barionic charge, was introduced. It is equal to zero for photons, leptons and mesons, +1 for nucleons, and —1 for antinucleons. This permits us to consider the above-mentioned regularity as a law of conservation of the total barionic charge of the particles. The law was also confirmed by the discoveries that followed: the hyperons were assigned a barionic charge equal to 1 (as for nucleons) and the antihyperons were given a barionic charge equal to —1 (as for antinucleons).

Universal Dynamic Variables

While going over from macroparticles to microparticles, one would expect qualitatively different answers to questions like: Which dynamic variables should be used to describe the state of the object? How should its motion be depicted? Answers to these questions reveal to a considerable extent the specific nature of microparticles.

In classical physics, we make use of the *laws of conservation of energy, momentum and angular momentum.* It is well known that these laws are consequences of certain properties of the symmetry of space and time. Thus, the law of conservation of energy is a consequence of *homogeneity of time* (independence of the course of a physical process of the moment chosen as the starting point of the process); the law of conservation of momentum is a consequence of the *uniformity of space* (all points in space are physically equivalent); the law of conservation of angular momentum is a consequence of the *isotropy of space* (all directions in space are physically equivalent). To elucidate the properties of symmetry of space and time, we note, for example, that thanks to these properties, Kepler's laws describing the motion of the planets around the sun are independent of the position of the sun in the galaxy, of the orientation in space of the plane of motion of the planets and also of the century in which these laws were discovered. The connection between the properties of symmetry of space and time and the corresponding conservation laws means that the energy, momentum and angular momentum can be considered as *integrals of motion*, whose conservation is a consequence of the corresponding homogeneity of time and the homogeneity and isotropy of space.

The absence of any experimental evidence indicating violation of the above-mentioned properties of symmetry of space and time for microphenomena reveals that such dynamic parameters as energy, momentum and angular momentum should retain their meaning when applied to microparticles. In other words, the connection of these dynamic variables with the fundamental properties of symmetry in space and time makes them universal variables, i.e. variables which are "used" while considering the kind of phenomena occurring in different branches of physics.

When transferring the concepts of energy, momentum and angular momentum from classical physics to quantum mechanics, however, the specific nature of the microparticles must be taken into account. In this connection we recall the well-known expressions for energy (E), momentum ($\vec{p}$) and angular momentum ($\vec{M}$) of a classical object, having mass m, coordinate $\vec{r}$, velocity $\vec{v}$:

$$E=\frac{mv^2}{2}+U(\vec{r}),\ \vec{p}=m\vec{v},\ \vec{M}=m(\vec{r}\times\vec{v}). \tag{1.1}$$

Eliminating the velocity, we get from here the relations connecting energy, momentum and angular momentum of a classical object:

$$E=\frac{p^2}{2m}+U(\vec{r}), \tag{1.2}$$

$$\vec{M}=(\vec{r}\times\vec{p}). \tag{1.3}$$

If we turn to a microparticle, we can go a bit farther, (see Sec. 3) and conclude that relations (1.2) and (1.3) are no longer valid. In other words, the classical connections between the integrals of motion become useless as we go over to microparticles (as regards relations (1.1), they cannot be mentioned at all since the very concept of the velocity of a microparticle, as we shall see below, is meaningless). This is the first qualitatively new circumstance.

In order to consider the other qualitatively new circumstances, we must turn to the fundamental ideas of quantum mechanics, i.e. the idea of *quantization of physical quantities* and the idea of wave-particle duality.

Section 2 Two Fundamental Ideas of Quantum Mechanics

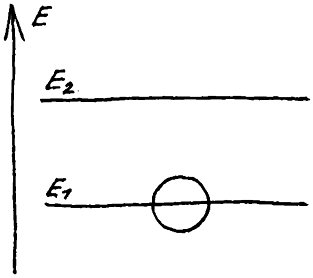
The Idea of Quantization (Discreteness)

The essence of the idea of quantization lies in the fact that certain physical quantities related to the microparticles may assume, under relevant circumstances, only certain *discrete* values. These quantities are said to be *quantized.*

Thus the energy of any microparticle in a bound state, like that of an electron in an atom, is quantized. The energy of a freely moving microparticle, however is not quantized.

Let us consider the energy of an electron in an atom. The system of so-called *energy levels* corresponds to a discrete set of values of electron energy. We consider two energy levels E_1 and E_2 as shown in Fig. 2.1 (the values of electron energy are plotted along the vertical axis). The electron may possess energy E_1 or E_2 and cannot possess any intermediate energy—all values of energy E satisfying the condition $E_1 < E < E_2$ are forbidden for it*. It should be noted that the discreteness of energy does not mean in any case that the electron is "doomed" to remain forever in the initial energy state (for example on level E_1). The electron may go over to another energy state (level E_2 or any other) by acquiring or releasing the corresponding amount of energy. Such a transition is called a *quantum transition.*

Fig. 2.1



The quantum-mechanical idea of discreteness has a fairly long history. By the end of 19th century, it was established that the radiation spectra of free atoms are *line spectra* (i.e. they consist of sets of lines) and contain, for every element, definite lines which form ordered groups (*series*). In 1885, it was discovered that atomic hydrogen emits radiation of frequencies ω_n (henceforth we use the cyclic frequencies ω, related to the normal frequencies ν through the equation $\omega = 2\pi\nu$) which may be described by the formula

$$\omega_n = 2\pi c R \left(\frac{1}{4} - \frac{1}{n^2}\right), \tag{2.1}$$

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* A specific situation in quantum mechanics is possible in which one must assume that an electron occupies level E_1 as well as level E_2 (see Sec. 10).

where n are integral numbers 3, 4, 5, . . ., c is the velocity of light, R is the so-called *Rydberg constant* ($R = 1.097 \times 10^7$ m^{-1}). Formula (2.1) was derived by Balmer, hence the set of frequencies described by this formula is called the *Balmer series*. The frequencies of the Balmer series fall in the visible region of spectrum. Later (in the beginning of 20th century), additional series of radiation from atomic hydrogen falling in the ultraviolet and infrared regions were discovered. The regularities in the structure of these spectra were identical to the regularities in the structure of the Balmer series, which enabled a generalization of formula (2.1) in the following form:

$$\omega_n = 2\pi cR\left(\frac{1}{k^2} - \frac{1}{n^2}\right) \qquad (2.2)$$

The number k fixes the series (in each series $n > k$); $k = 2$ gives the Balmer series, $k = 1$, the *Lyman series* (ultraviolet frequencies), $k = 3$, the *Paschen series* (infrared frequencies), and so on.

Regularity in the structure of series was observed not only in the spectrum of atomic hydrogen, but also in the spectra of other atoms. It definitely indicated the possibility of some generalizations. One such generalization was proposed by Ritz in 1908 in his *combination principle*, which states that if the formulae of series are given and the constants occurring in them are known, any newly discovered line in the spectrum may be obtained from the lines already known by means of combinations in the form of sums and differences. This principle may be applied to hydrogen in the following way: we write the so-called *spectral terms* for different numbers n:

$$T(n) = 2\pi cR/n^2.$$

Then each frequency observed in the hydrogen spectrum may be expressed as a combination of two spectral terms. By combining the spectral terms, it is possible to predict different frequencies.

It is remarkable that at about the same time, the idea of discreteness arose in another direction (not related to atomic spectroscopy). This is the case of radiation within a closed volume or, in other words, *black body radiation*. After analyzing the experimental data, Planck in 1900 proposed his famous hypothesis. He suggested that the energy of electromagnetic radiation is emitted by the walls of a cavity not continuously, but *in portions (quanta)*, the energy of a quantum being equal to

$$E = \hbar\omega \qquad (2.3)$$

where ω is the frequency of radiation and $\hbar$ is a certain universal constant (it later became known as Planck's constant). Planck's hypothesis provided an agreement between the theory and experiment and, in particular, removed the flaws arising in the previous theory when passing to higher frequencies. This had been called the "ultraviolet catastrophe" (see, for example, [17]).

The Idea of Quantization and Bohr's Model of Hydrogen Atom

In 1913, Bohr proposed his theory of the hydrogen atom. This theory was evolved as a "confluence" of the planetary atomic model by Rutherford, the Ritz combination principle, and Plank's ideas of quantization of energy.

According to Bohr's theory, there exist certain states in which the atom does not radiate (*stationary states*). The energy of these states forms a *discrete spectrum*, E_1, E_2, ., E_n, The atom emits (absorbs) during transition from one stationary state to another. The emitted (absorbed) energy is the difference between the energies of the corresponding stationary states. Thus, during a transition from the state with energy E_n to the state with lower energy E_k, a quantum of radiation with energy $(E_n - E_k)$ is emitted. Thus a line with frequency

$$\omega = \frac{E_n - E_k}{\hbar} \tag{2.4}$$

appears in the spectrum. Formula (2.4) expresses the well-known Bohr's *frequency condition*.

In Bohr's theory, the n-th stationary state of hydrogen atom corresponds to a circular orbit of radius r_n along which the electron revolves around the nucleus. In order to compute r_n, Bohr suggested, firstly, using Newton's second law for a charge moving in a circle under the influence of a Coulomb's force:

$$m\frac{v_n^2}{r_n} = \frac{e^2}{r_n^2} \tag{2.5a}$$

(here m and e are the mass and the charge of an electron, v_n is the velocity of the electron in the n-th orbit). Secondly, Bohr suggested the condition of quantization of the angular momentum of the electron:

$$mv_nr_n = n\hbar \tag{2.5b}$$

By using relations (2.5a) and (2.5b), it is easy to find r_n and v_n:

$$r_n = \frac{\hbar^2}{me^2}n^2, \qquad v_n = \frac{e^2}{\hbar n} \tag{2.6}$$

The energy E_n of the stationary state consists of kinetic (T_n) and potential (U_n) terms: $E_n = T_n + U_n$. Assuming that $T_n = mv_n^2/2$, $U_n = -e^2/r_n$ and using (2.6), we find that

$$E_n = -\frac{me^4}{2\hbar^2 n^2} \tag{2.7}$$

The negative sign of the energy means that the electron is in a bound state (energy of a free electron is taken to be equal to zero).

Substituting the result (2.7) into the frequency relation (2.4), and comparing the expression thus obtained with formula (2.2), we may, following Bohr, find an expression for Rydberg's constant:

$$R = \frac{me^4}{4\pi c\hbar^3} \tag{2.8}$$

Bohr's theory (or the old quantum theory, as it is now called) suffered from internal contradictions; in order to determine the radius of the orbit, one had to make use of relations of different kinds—the classical relation (2.5a), and the quantum relation (2.5b). In spite of this, the theory was of great significance as a first step towards the creation of a consistent quantum theory. Moreover, the nature of the spectral terms, and, consequently, the Ritz combination principle, was revealed for the first time and the calculated value of Rydberg's constant was in excellent agreement with its empirical value. The success of the theory proved testimony to the usefulness of the idea of quantization. Having acquainted himself with Bohr's calculations, Sommerfeld wrote Bohr a letter, in which he said:

I thank you very much for sending me your extremely interesting work.... The problem of expressing the Rydberg-Ritz constant by Planck's has been for some time in my thoughts... Although I am for the present still rather sceptical about atom models in general, nevertheless the calculation of the constant is indisputably a great achievement.

On Quantization of Angular Momentum

We must note that in contrast to energy, the angular momentum of a microparticle is always quantized. Thus, the observed values of the square of angular momentum of a microparticle are expressed by the formula

$$M^2 = \hbar^2 l\,(l+1), \tag{2.9a}$$

where l is an integer 0, 1, 2, . If we consider the angular momentum of an electron in the atom in the n-th stationary state, the number l assumes values from 0 to $n-1$.

In the literature, it is customary to refer to the angular momentum as simply *momentum*. Henceforth, we shall follow this practice.

The projection of the momentum of a microparticle in a certain direction (let us denote it as z-direction) assumes the values

$$M_z = \hbar m \tag{2.9b}$$

where $m = -l, -l+1, \ldots, l-1, l$. For a given value of the number l, the number m can assume $2l + 1$ discrete values. We emphasize here that different projections of the momentum of a microparticle in a given direction differ from one another by values which are multiples of Planck's constant.

It was mentioned above that spin is a distinctive "internal" momentum of a microparticle having a definite value for a given microparticle. To distinguish it from the *spin* momentum, ordinary momentum is called *orbital* momentum. Kinematically the spin momentum is analogous to the orbital momentum. Naturally, in order to find the possible projections of the spin momentum we must use a formula of the type (2.9b) (as in the case of orbital momentum, the projections of the spin momentum differ from one another by integral multiples of Planck's constant). If s is the spin of a microparticle (this number was introduced in Sec. 1), then the projection of the spin momentum assumes values $\hbar\sigma$, where $\sigma = -s, -s+1, \ldots, s-1, s$. Thus, the projection of the spin of an electron assumes values $-\frac{\hbar}{2}$ and $+\frac{\hbar}{2}$

The numbers n, l, m, σ considered here determine the different discrete values of the quantized dynamic variables (in this case, energy and momentum), and are called *quantum numbers*; n is called the *principal* quantum number; l, the *orbital* quantum number; m, the *magnetic* quantum number and σ, the *spin* quantum number. There also exist other quantum numbers.

Anomalies of Quantum Transitions

In spite of the resounding success of Bohr's theory, the idea of quantization engendered serious doubts in the beginning. It was noticed that this idea was full of internal contradictions. Thus in his letter to Bohr, Rutherford [19] wrote in 1913:

...Your ideas as to the mode of origin of the spectrum of hydrogen are very ingenious and seem to work out well; but the mixture of Planck's ideas with the old mechanics makes it very difficult to form a physical idea of what is the basis of it. There appears to me one grave difficulty in your hypothesis which I have no doubt you fully realise namely, how does an electron decide what frequency it is going to vibrate at when it passes from one stationary state to the other? It seems to me that you would have to assume

*that the electron knows beforehand where it is going to stop**...

We shall explain the difficulties noticed by Rutherford. Let an electron occupy level E_1 (Fig. 2.1). In order to go over to the level E_2, the electron must absorb a quantum of radiation (i.e. a photon) with a definite energy equal to $(E_2 - E_1)$. Absorption of a photon with any other energy will not result in the indicated transition and is therefore not possible (for simplicity, we shall consider only two levels). The question now arises: In what way does an electron perform a "selection" of the "required" photon out of the photon flux of different energies falling on it? In order to "select" the "required" photon, the electron must be "previously aware" of the second level, i.e. as if it had already visited it. However, in order to visit the second level, the electron must have first absorbed the "required" photon. This gives rise to a vicious circle.

Further contradictions are observed while considering the jump of an electron from one orbit in the atom to another. Whatever the speed at which the transition of the electron from the orbit of one radius to that of another takes place, it has to last for some finite period of time (otherwise it would be a violation of the basic requirements of the theory of relativity). But then it is hard to understand what the energy of the electron should be during this intermediate period—the electron no longer occupies the orbit corresponding to energy E_1 and has not yet arrived at the orbit corresponding to energy E_2.

It is thus not surprising that at one time efforts were made to obain an explanation of experimental results without resorting to the idea of quantization. In this respect, the famous remarks by Schrödinger about "these damned quantum jumps", which, of course, were made in the heat of the moment, are worth noting.

However, experience inevitably pointed to the usefulness of quantization and no place was left for an alternative.

In this case, there is just one way out: new ideas must be introduced, which form a non-contradictory picture of the whole including the ideas of discreteness. The idea of wave-particle duality was just such a new physical concept.

Idea of Wave-Particle Duality

Classical physics acquaints us with two types of motion: *corpuscular* and *wave* motion. The first type is characterized

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* The reader should not be confused by the remarks about the oscillations of electron: uniform motion in a circle is a superposition of two harmonic oscillations in mutually perpendicular directions.

by a localization of the object in space and the existence of a definite trajectory of its motion. The second type, on the contrary, is characterized by delocalization in space. No localized object corresponds to the motion of a wave, it is the motion of a medium. In the world of macrophenomena, the corpuscular and wave motions are clearly distinguished. The motion of a stone thrown upward is something entirely different from the motion of a wave breaking a beach.

These usual concepts, however, cannot be transferred to quantum mechanics. In the world of microparticles, the above-mentioned strict demarcation between the two types of motion is considerably obliterated. The motion of a microparticle is characterized simultaneously by wave and corpuscular properties. If we schematically consider the classical particles and classical waves as two extreme cases of the motion of matter, microparticles must occupy in this scheme a place somewhere in between. They are not "purely" (in the classical sense) corpuscular, and at the same time they are not "purely" wavelike; they are something qualitatively different. It may be said that a microparticle to some extent is akin to a corpuscle, and in some respect it is like a wave. Moreover, the extent depends, in particular, on the conditions under which the microparticle is considered. While in classical physics a corpuscle and a wave are two mutually exclusive extremities (either particle, or wave), these extremities, at the level of microphenomena, combine dialectically within the framework of a single microparticle. This is known as *wave-particle duality.*

The idea of duality was first applied to electromagnetic radiation. As early as 1917, Einstein suggested that quanta of radiation, introduced by Planck, should be considered as *particles* possessing not only a definite energy, but also a definite momentum:

$$E = \hbar\omega, \qquad p = \frac{\hbar\omega}{c}. \tag{2.10}$$

Later (from 1923), these particles became known as *photons.*

The corpuscular properties of radiation were very clearly demonstrated in the *Compton effect* (1923). Suppose a beam of X-rays is scattered by atoms of matter. According to classical concepts, the scattered rays should have the same wavelength as the incident rays. However, experiment shows that the wavelength of scattered waves was greater than the initial wavelength of the rays. Moreover, the difference between the wavelengths depends on the angle of scattering. The Compton effect was explained by assuming that the X-ray beam behaves like a flux of photons which undergo elastic collisions with the electrons of the atoms, in conformity with the laws of conservation of energy and momentum for colliding particles. This led not only to a qualitative but also to a quantitative agreement with experiment (see [17]).

In 1924, de Broglie suggested that the idea of duality should be extended not only to radiation but also to all microparticles. He proposed to associate with every microparticle *corpuscular characteristics* (energy E and momentum p) on the one hand and *wave characteristics* (frequency ω and wavelength λ) on the other hand. The mutual dependence between the characteristics of different kinds was accomplished, according to de Broglie, through the Planck's constant $\hbar$ in the following way:

$$E = \hbar\omega, \qquad p = \frac{2\pi\hbar}{\lambda} \tag{2.11}$$

(the second relation is known as *de Broglie's equation*). For photons, relation (2.11) is automatically satisfied if we substitute $\omega = 2\pi c/\lambda$ in (2.10). The boldness of de Broglie's hypothesis lays in that relation (2.11) was assumed to be satisfied not only for photons, but generally for all microparticles, and in particular, for those which have a rest mass and which were hitherto associated with corpuscles.

De Broglie's ideas received confirmation in 1927, with the discovery of *electron diffraction*. While studying the passage of electrons through thin foils, Davisson and Germer (as well as Tartakovsky) observed characteristic diffraction rings on the detector screen. For "electron waves" the crystal lattice of the target served as a diffraction grating. Measurement of distances between diffraction rings for electrons of a given energy confirmed de Broglie's formula.

In 1949, Fabrikant and coworkers set up an interesting experiment. They passed an extremely weak electron beam through the diffraction apparatus. The interval between successive acts of passage (between two electrons) was more than 10^4 times longer than the time required for the passage of an electron through the apparatus. This ensured that other electrons of the beam do not influence the behaviour of an electron. The experiment showed that for a prolonged exposure, permitting registration of a large number of electrons on the detector screen, the same diffraction pattern was observed as in the case of regular electron beams. It was thus concluded that the wave nature of the electrons cannot be explained as an effect of the electron aggregate; every single electron possesses wave properties.

The Role of Planck's Constant

The idea of quantization introduces discreteness, and discreteness requires a unit of measure. Planck's constant plays the role of such a measure. It may be said that this constant determines the "boundary" between microphenomena and macrophenomena. By using Planck's constant, as well as mass and charge of an electron, we may form the following simple composition having dimensions of length:

$$r_1 = \frac{\hbar^2}{me^2} = 0.53 \times 10^{-8}\,\text{cm} \qquad (2.12)$$

(note that r_1 is the radius of the first Bohr orbit). According to (2.12), a magnitude of about 10^{-8} cm may be considered as the spatial "boundary" of microphenomena. This is just about the linear dimensions of an atom.

If the Planck constant $\hbar$ were, say, 100 times larger, then (other conditions being equal) the "limit" of microphenomena would, according to (2.12), have been of the order of 10^{-4} cm. This would mean that the microphenomena would become much closer to us, to our scale, and the atoms would have been much bigger. In other words, matter in this case would have appeared much "coarser", and classical concepts would have to be revised on a much larger scale.

As was indicated above, the projections of the momentum of a microparticle differ from one another by multiples of $\hbar$ [see (2.9b)]. Consequently, Planck's constant appears here as a *unit of quantization*. If the orbital momentum is much greater than $\hbar$, its quantization may be neglected. We get in this case the classical angular momentum. In contrast to the orbital momentum, spin momentum cannot be very large. It is clear, that it is impossible to neglect its quantization in principle; hence the spin momentum does not have a classical analogue (this circumstance was already indicated in Sec. 1).

Planck's constant is inseparably linked not only with the idea of quantization, but also with the idea of duality. From (2.11) it is evident that this constant plays a fairly important role—it supplies a "link" between the corpuscular and wave properties of a microparticle. This becomes quite clear if we rewrite (2.11) in a form permitting us to take account of the vector nature of momentum:

$$E = \hbar\omega \qquad \vec{p} = \hbar\vec{k}. \qquad (2.13)$$

Here $\vec{k}$ is the wave vector; its direction coincides with the direction of propagation of the wave, and its magnitude is expressed through the wavelength in the following way: $k = 2\pi/\lambda$. The left-hand sides of equations (2.13) describe corpuscular properties of a microparticle, and the right-hand sides wave properties. We note, by the way, that the form of relations (2.13) indicates the relativistic invariance of the idea of duality.

Thus, Planck's constant plays two fundamental roles in quantum mechanics—it serves as a measure of discreteness, and it combines the corpuscular and wave aspects of the motion of matter. The fact that the same constant plays both these roles is an indirect indication of the internal unity of the two fundamental ideas of quantum mechanics.

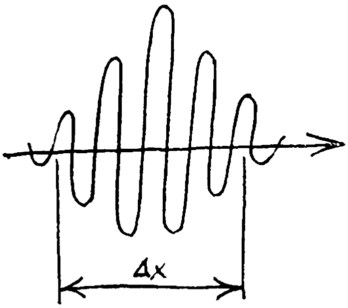
In conclusion, we remark that the presence of Planck's constant in any expression indicates the "quantum-mechanical nature" of this expression.*

Section 3 Uncertainty Relations

Idea of Duality and Uncertainty Relations

Let us consider an aggregate of a large number of plane waves (the nature of waves is not important) propagating, say, along the x-axis. Let the frequencies of the waves be "spread" over a certain interval $\Delta\omega$, and the values of the wave vector, over an interval Δk_x. If all these plane waves are superimposed on one another, we get a wave formation limited in space called a *wave packet* (Fig. 3.1). The spreading of the wave packet in space (Δx) and in time (Δt) is determined by the relations

Fig. 3.1



$$\left.\begin{aligned}\Delta\omega\Delta t &\geqslant 1,\\ \Delta k_x\Delta x &\geqslant 1.\end{aligned}\right\} \qquad (3.1)$$

These relations are well known in classical physics. Those acquainted with radio engineering know that for a more localized signal one must take more plane waves with different frequencies. In other words, to reduce Δx and Δt, one must increase Δk_x and $\Delta\omega$.

Digressing from the wave packet, we shall formally assume that relations (3.1) are valid not only for classical waves, but also for wave characteristics of a microparticle. We stress that this assumption by no means indicates that we shall in fact model a microparticle in the form of

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* The converse statement is not true. It would be incorrect to attempt, as is sometimes done, to reduce the whole "essence" of quantum mechanics to the presence of Planck's constant. This question is considered in [51].

a wave packet. By considering ω and k_x in (3.1) as wave characteristics of a microparticle and making use of relations (2.13), it is easy to go over to an analogous expression for the corpuscular characteristics of a microparticle (for its energy and momentum):

$$\Delta E \Delta t \geqslant \hbar, \tag{3.2}$$

$$\Delta p_x \Delta x \geqslant \hbar. \tag{3.3}$$

These relations were first introduced by Heisenberg in 1927 and are called *uncertainty relations.*

Relations (3.2) and (3.3) should be supplemented by the following uncertainty relation:

$$\Delta M_x \Delta \varphi_x \geqslant \hbar, \tag{3.4}$$

where $\Delta\varphi_x$ is the uncertainty in the angular coordinates of the microparticle (we consider rotation around the x-axis) and ΔM_x is the uncertainty in the projection of the momentum on the x-axis.*

By analogy with (3.3) and (3.4), one may write down relations for other projections of momentum and angular momentum:

$$\Delta p_y \Delta y \geqslant \hbar, \qquad \Delta p_z \Delta z \geqslant \hbar, \tag{3.3a}$$

$$\Delta M_y \Delta \varphi_y \geqslant \hbar, \qquad \Delta M_z \Delta \varphi_z \geqslant \hbar. \tag{3.4a}$$

The Meaning of the Uncertainty Relations

Let us consider relation (3.3). Here Δx is the uncertainty in the x-coordinate of the microparticle and Δp_x, the uncertainty in the x-projection of its momentum. The smaller Δx is, the greater Δp_x is, and vice versa. If the microparticle is localized at a certain definite point x, then the x-projection of its momentum must have arbitrarily large uncertainty. If, on the contrary, the microparticle is in a state with a definite value of p_x, then it cannot be localized exactly on the x-axis.

Sometimes the uncertainty relation (3.3) is interpreted in the following way: it is impossible to measure simultaneously the coordinate and momentum of a microparticle with an arbitrarily high precision; the more accurately we measure the coordinate, the less accurately can the momentum be determined. Such an interpretation is not very good since it might lead to the erroneous conclusion that the essense of the uncertainty relation (3.3) is responsible for limitations associated with the process of measure-

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* Notice that relations (3.4) and (3.4a) are valid only for sm values of the uncertainty in angular coordinate ($\Delta\varphi \ll 2\pi$) or, in other words, for large values of uncertainty in the projection of the momentum.

ment. One might be led to assume that a microparticle itself possesses a definite coordinate as well as a definite momentum, but the uncertainty relation does not permit us to measure them simultaneously.

Actually the situation is quite different. The microparticle itself simply cannot have simultaneously a definite coordinate and a corresponding definite projection of the momentum. If, for example, it is in a state with a more definite value of the coordinate, then in this state the corresponding projection of its momentum is less definite. From this the actual impossibility of simultaneous measurements of coordinates and momenta of a microparticle follows naturally. This is a result of the specific character of the microparticle and is by no means a whim of nature which makes it impossible for us to perceive all that exists. Consequently, the sense of relation (3.3) is not that it creates certain obstacles to the understanding of microphenomena, but that it reflects certain peculiarities of the objective properties of a microparticle. The last remark is, of course, of a general nature: it refers not only to relation (3.3), but also to other uncertainty relations.

Now let us look at relation (3.2). Let us consider two different, though mutually supporting interpretations, of this relation. Suppose that the microparticle is unstable and that Δt is its lifetime in the state under consideration. The energy of the microparticle in this state must have an uncertainty ΔE which is related to the lifetime Δt through inequality (3.2). In particular, if the state is stationary (Δt is arbitrarily large), the energy of the microparticle will be precisely determined ($\Delta E = 0$).

The other interpretation of relation (3.2) is connected with the measurements carried out to ascertain whether the microparticle is located at the level E_1 or E_2. Such a measurement requires a finite time T which depends on the distance between the levels $(E_2 - E_1)$:

$$(E_2 - E_1)\, T \geqslant \hbar. \tag{3.2a}$$

It is not difficult to see the connection between these two interpretations. In order to distinguish the levels E_1 and E_2, it is necessary that the uncertainty ΔE in the energy of the microparticle should not be greater than the distance between the levels: $\Delta E \leqslant (E_2 - E_1)$. At the same time the duration of measurement T should obviously not exceed the lifetime Δt of the microparticle in the given state: $T \leqslant \Delta t$. Consequently, the limiting conditions, under which measurement is still possible, are given by

$$\Delta E \approx E_2 - E_1, \quad T \approx \Delta t.$$

By using (3.2), we can arrive at (3.2a) from these relations.

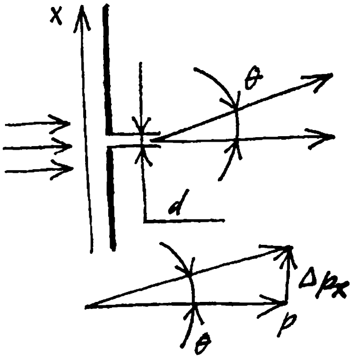
The uncertainty relations (3.2)-(3.4) show how the concepts of energy, momentum and angular momentum should be applied in the case of microparticles. Here, a very important peculiarity of the physics of microparticles is revealed: the energy, momentum and the angular momentum of a microparticle have meaning only within the limitations imposed by the uncertainty relations. Heisenberg [20] writes that we cannot interpret processes on an atomic scale in the same way as processes on a large scale. If we make use of the usual concepts, their applicability is limited by the uncertainty relations.

It should, however, be pointed out that the uncertainty relations do not in any way lead to the above-mentioned restrictions on the applicability of classical concepts of coordinates, momentum, energy, etc. for microparticles. It would be unfair not to mention the considerable "positive aspects" of uncertainty relations after having talked about their "negative aspects" They serve as a working instrument of the quantum theory. By reflecting the specific character of the physics of microparticles, the uncertainty relations allow us to obtain fairly important results through fairly simple means. Some examples are given in Sec. 4 below.

From Diffraction in Microparticles to Uncertainty Relations

The method of deriving the uncertainty relations considered in the beginning of this section might appear too formal and unconvincing to some readers. There are various means of deriving uncertainty relations (see, for example [21]). One such method [which is specifically applied to relations (3.3)] is based on a consideration of the phenomena of diffraction of microparticles.

Fig. 3.2



Suppose (Fig. 3.2) a screen with a narrow slit is placed in the path of a strictly parallel beam of certain microparticles with momentum p. Let d be the width of the slit along the x-axis (the x-axis is perpendicular to the direction of the beam). Diffraction takes place during the passage of microparticles through the slit. Let θ be the angle between the initial direction and the direction of the first (principal) diffraction peak. The classical wave theory gives the following well-known relation for this angle $\sin\theta = \lambda/d$. Assuming angle θ to be sufficiently small, we can rewrite this relation in the following form:

$$\theta \approx \lambda/d \tag{3.5}$$

If by λ we now mean not the classical wavelength, but the length of the de Broglie wave (i.e. the wave characteristic of the microparticle), we may rewrite relation (3.5) in "corpuscular language" by using the expression (2.11):

$$\theta \approx \hbar/pd. \tag{3.5a}$$

But how we are to understand the existence of the angle θ in "corpuscular language"? Obviously, it means that while passing through the slit, the microparticle acquires a certain momentum Δp_x in the direction of the x-axis. It is easy to see that $\Delta p_x \approx p\theta$. Substituting (3.5a) into this, we get $\Delta p_x \approx \hbar/d$. By considering the quantity d as the uncertainty Δx in the x-coordinate of the microparticle passing through the slit, we get $\Delta p_x \Delta x \approx \hbar$, i.e. we arrive at the uncertainty relation (3.3). Thus the attempt to determine in some way the coordinate of a microparticle in a direction perpendicular to the direction of its motion leads to an uncertainty in the momentum of the microparticle in that direction, which also explains the phenomenon of diffraction observed in the experiment.

Uncertainty Relations and the State of Microparticles. The Concept of a Complete Set of Physical Quantities

In order to describe the *state* of a classical object it is necessary to give a definite set of numbers—the coordinates and the velocity components. In doing this other quantities, in particular, energy, momentum and angular momentum of the object will also be determined [see (1.1)]. The uncertainty relations show that this method of defining a state is not applicable to microparticles. Thus, for example, the existence of a definite projection of momentum in a given direction for a microparticle means that the position of the microparticle in this direction cannot be determined unambiguously: according to (3.3), the corresponding spatial coordinate is characterized by an infinitely large uncertainty. The electron in an atom has a definite energy; moreover its coordinates are characterized by an uncertainty of the order of the linear dimensions of the atom. This [according to (3.3)] leads to an uncertainty in the projection of the momentum of the electron equal to the ratio of Planck's constant to the linear dimension of the atom.

We now indicate the following situations, fundamental in quantum mechanics, which arise from the uncertainty relation: (a) various dynamic variables of a microparticle are combined in sets of *simultaneously determined* (simultaneously measurable) quantities, the so-called *complete sets* of quantities; (b) various states of a microparticle are combined in groups of states corresponding to different complete sets of quantities. Each group contains the states of the microparticle in which the values of the corresponding complete sets are known (it is customary to say that every complete set has its own method of defining its states).

We shall give examples of the complete sets employed for determining the states of, say, an electron and a photon. Each of the sets includes four quantities (because of this we say that a microparticle like an electron or a photon has four *degrees of freedom*). To describe the states of an electron, the following sets are employed:

$$x,\ y,\ z,\ \sigma \tag{3.6a}$$

$$p_x,\ p_y,\ p_z,\ \sigma \tag{3.6b}$$

$$E,\ l,\ m,\ \sigma \tag{3.6c}$$

(remember that l, m, and σ are orbital, magnetic and spin quantum numbers, respectively). We emphasize that the coordinates and the momentum components of a microparticle (in this case an electron) fall in different complete sets of quantities; these two physical quantities cannot be measured simultaneously. Hence the classical relations (1.2) and (1.3) are not valid when going over to microparticles, since each of these relations contains the coordinates as well as the momentum.

The set (3.6b) is used, in particular, for a describing the states of a freely moving electron. Moreover, the energy of the electron also turns out to be definable: $E = (p_x^2 + p_y^2 + p_z^2)/2m$*. The set (3.6c) is usually employed for describing the states of an electron in the atom.

To describe the states of a photon, the following sets are most commonly employed:

$$k_x,\ k_y,\ k_z,\ \alpha, \tag{3.7a}$$

$$E,\ M^2,\ M_z,\ P. \tag{3.7b}$$

Here k_x, k_y, k_z are the projections of the wave vector of the radiation; α is the polarization of the photon; M^2 and M_z are the square of the momentum and the projection of the momentum of the photon, respectively; P is a quantum number called the spatial parity. We notice that as soon as the projections of the wave vector of radiation are determined, the projections of the photon momentum are also known (recall that $\vec{p} = \hbar k$). The *polarization* of a photon may take two values corresponding completely to the two independent polarizations of a classical wave (thus, for example, one might talk about a photon having right elliptical polarization).

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* In contrast to relation (1.2), the classical relation $E = p^2/2m$ remains valid for a freely moving particle when going over to microparticles.

The *spatial parity* is a characteristic property of a microparticle; it may be considered as an integral of motion whose conservation is a result of symmetry with respect to the operation of reflection by a mirror. At a later stage (see Sec. 20) we shall discuss it in greater detail. Here, we only mention that parity can assume one of the two values: +1 and —1.

The set (3.7a) is used for describing the states of photons corresponding to plane classical waves, in this case the energy of the photon is also defined (recall that $E = \hbar\omega = \hbar ck$). The states described by the set (3.7a) are called $k\alpha$-states. The set (3.7b) is employed for describing the states of photons belonging to *spherical* classical waves. We note that just as a spherical wave may be represented as a superposition of plane waves, the states of a photon described by the set (3.7b) may be represented as a "superposition" of states described by the set (3.7a). The converse statement regarding the representation of plane waves as a superposition of spherical waves is also true. Here we have touched upon (for the present just touched upon) one of the most important and delicate aspects of the quantum-mechanical description of matter—the specific character of the "interrelations" between states of a microparticle described by different complete sets. This specific character is reflected in the most constructive principle of quantum mechanics—the *principle of superposition of states.* The superposition of states will be considered in detail in the second chapter; here we shall just restrict ourselves to the above-mentioned remarks.

Uncertainty Relations and Quantum Transitions

The main contradiction regarding quantum transitions indicated in Sec. 2 is essentially overcome by making use of the idea of duality or, more precisely, the uncertainty relation (3.2). Let us consider transition of an electron in an atom from level E_1 to level E_2 by absorbing a photon of energy $\hbar\omega = E_2 - E_1$. We recall that the contradiction in transition was connected with the question whether the absorption of the photon precedes the transition of the electron or vice versa. It is easy to see that this question simply loses its meaning now. In fact, if we have a bound electron with energies E_1 and E_2 before and after interaction with radiation, respectively, then during the interaction we have *one quantum-mechanical* system including both the electron and the radiation. This system exists for a definite time (while the interaction with the radiation takes place) and, according to (3.2), cannot have any definite energy. Hence it is meaningless to find out precisely what takes place

in such a system. Strictly speaking, during the interaction of the electron with the photon there is no electron and no photon, but a single entity which must be treated as such, without going into details. This example shows that in quantum mechanics a physical process cannot be infinitely detailed in time. The question "what follows what"? cannot always be posed in the case of microphenomena.*

The uncertainty relation (3.2) allows us to introduce and employ a very important concept in quantum theory, the so-called *virtual transitions*, for explaining quantum transitions. We shall give here a simplified treatment of virtual transitions, but we shall give a detailed explanation later in Sec. 6. According to relation (3.2), an electron may go over from level E_1 to E_2 without getting any energy from outside; what is important is that it should quickly return to its initial level E_1. Such a "journey" ($E_1 \rightarrow E_2 \rightarrow E_1$) is possible if its duration Δt is such that the inequality $\hbar/\Delta t > (E_2 - E_1)$ is satisfied, because in this case the uncertainty in the energy of the electron is greater than the difference in the energies of the levels under consideration. Hence it is clear that the statement "the electron occupies level E_1" may be understood quite specifically—as incessant "transition" of the electron from the given state to others with an inevitable return every time to the starting level E_1. Such transitions cannot be observed experimentally, and are called virtual transitions in contrast to the normal (real) transitions. During interaction of an electron undergoing virtual transitions with radiation, the electron is liable to change its "residence". For example, it might now occupy level E_2 and will in future perform virtual transitions not from level E_1, but from level E_2. If such a thing happens, the electron is said to have absorbed a photon of energy $\hbar\omega = E_2 - E_1$, and undergone a transition from level E_1 to E_2. Virtual transitions don't require any expenditure of energy from outside while a real transition cannot occur without expenditure of energy—the energy of the photons absorbed (or emitted) by electrons during interaction with radiation.

To explain the difference between real and virtual transitions, we note that a real transition from a level E_1 to another level E_2 and back may be broken up into two successive events in time (in between, the electron may be experimentally registered in the intermediate state E_2). However, the virtual transition from level E_1 to E_2 and back cannot be broken up into two events in time—both parts of the transition must be considered as a single, indivisible process in time.

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* The anomaly of quantum transition is completely removed by considering the principle of superposition of states (see Sec. 10).

Uncertainty Relation "Number of Photons-Phase"

The uncertainty relations used in quantum theory are by no means exhausted by relations (3.2)-(3.4). As an example of one more such relation we consider the uncertainty relations for the number of photons and the phase of the wave.

Let there be a monochromatic radiation of frequency ω. On one hand, it may be considered as a collective of photons each having energy $\hbar\omega$; on the other hand, we might treat it as a classical electromagnetic wave. Let N be the number of photons in the volume under consideration and let $\Phi = \omega t$ be the phase of the classical wave. The corpuscular characteristic of the radiation (number of photons N) and its wave characteristic (phase Φ) cannot have definite values simultaneously; there exists the uncertainty relation

$$\Delta N \Delta \Phi \geqslant 1. \tag{3.8}$$

In order to arrive at relation (3.8), we start from the uncertainty relation for energy and time. We recall that for measuring the energy of a quantum object with an accuracy ΔE we must spend time $\Delta t \geqslant \hbar/\Delta E$. If we take the collective of photons as the quantum object, we get

$$\Delta E = \hbar\omega\Delta N,$$

where ΔN is the uncertainty in the number of photons. During the time Δt necessary for measurement of the energy of the object with an accuracy $\hbar\omega\Delta N$, the phase Φ changes by $\Delta\Phi = \omega\Delta t$. Substituting into this the relation $\Delta t \geqslant \hbar/\hbar\omega\Delta N$, we find $\Delta\Phi \geqslant 1/\Delta N$, Q.E.D.

Relation (3.8) reflects the dialectically contradictory unity of corpuscular and wave properties of radiation. The uncertainty $\Delta\Phi$ is small when the wave properties of radiation are clearly exhibited; in this case the density of photons is high (N is large) and so is the uncertainty ΔN. On the other hand, the uncertainty ΔN is small when there are a few photons in the aggregate. In this case the corpuscular properties of radiation are clearly exhibited and therefore the uncertainty $\Delta\Phi$ is large.

Section 4

Some Results Ensuing from the Uncertainty Relations

Evaluation of Energy of Ground State of Hydrogen Atom

The uncertainty relations serve as very useful working tools of quantum theory since they permit one to obtain important results, by fairly simple means.

As an example, we consider the *hydrogen atom in its ground state.* We make use of the well-known classical expression for energy of a charged particle moving in a Coulomb field:

$$E=\frac{p^2}{2m}-\frac{e^2}{r} \tag{4.1}$$

where m and e are the mass and charge of the electron, respectively. In order to use the classical expression (4.1) in the quantum theory, we consider the quantities p and r occurring in it as uncertainties in momentum and coordinates of the electron, respectively. According to relation (3.3), these quantities are connected with each other. We assume $pr \approx \hbar$, or, simply,

$$pr=\hbar. \tag{4.2}$$

Eliminating the quantity r from (4.1) by using (4.2), we get

$$E(p)=\frac{p^2}{2m}-\frac{e^2p}{\hbar}. \tag{4.3}$$

It is easy to see that the function $E(p)$ has a minimum for a certain value $p=p_1$. We denote it as E_1. The quantity E_1 may be considered as the energy of the ground state of the hydrogen atom while the quantity $r_1=\frac{\hbar}{p_1}$ is the estimate of the linear dimensions of the atom (in Bohr's theory this is the radius of the first orbit). By equating the derivative $\frac{d}{dp}E(p)$ to zero, we find $p_1 \quad \frac{me^2}{\hbar}$. This at once gives the required evaluations [cf. (2.6) and (2.7)]:

$$r_1=\frac{\hbar^2}{me^2}, \qquad E_1=-\frac{me^4}{2\hbar^2} \tag{4.4}$$

The values given by (4.4) fully coincide with the results of the rigorous theory*. Of course such a complete coincidence must be considered to some extent as an accidental success. Only the order of the quantities should be taken seriously here. We emphasize that this order can be evaluated quite simply as follows: it is sufficient first to simply replace the precise values of the dynamic variables in expression (4.1) by quantities which characterize the degree of "blurring" of these variables, i.e. by their uncertainties, and then use the quantum-mechanical relations connecting the said uncertainties.

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* In the rigorous theory the quantity r_1 is a characteristic for the ground state of the hydrogen atom and denotes the distance from the nucleus at which an electron is most likely to be observed [see expression (5.4)].

Estimate of the Energy of Zero-Point Oscillations of an Oscillator

We shall proceed exactly in the same way as in the preceding example. The energy of a classical one-dimensional harmonic oscillator is given by the expression

$$E=\frac{p_x^2}{2m}+\frac{m\omega^2x^2}{2} \tag{4.5}$$

Treating p_x and x as uncertainties in the momentum and coordinate of the oscillating microparticle and using the equality $p_x \cdot x = \hbar$ as the uncertainty relation, we get from (4.5)

$$E(p_x)=\frac{p_x^2}{2m}+\frac{m\omega^2\hbar^2}{2p_x^2} \tag{4.6}$$

By equating the derivative $\frac{d}{dp_x}E(p_x)$ to zero we find the value of $p_0 = \pm\sqrt{m\hbar\omega}$ for which the function $E(p_x)$ assumes its minimum value. It is easy to see that this value is

$$E_0 = E(p_0) = \hbar\omega. \tag{4.7}$$

This result is quite interesting. It shows that in quantum mechanics the energy of an oscillator cannot vanish; its minimum value is of the order of $\hbar\omega$. This is the energy of what is called the zero-point oscillation. We note that the estimate (4.7) differs from the exact expression for the energy of the zero-point oscillation just by a factor of 1/2 (exact value $E_0 = \frac{1}{2}\hbar\omega$).

By taking the zero-point oscillations into account, one may arrive at the following interesting conclusion: the energy of the oscillatory motion of atoms in a crystal does not vanish even at absolute zero.

The zero-point oscillations illustrate a basically general circumstance: it is impossible to find a microparticle at the "bottom of the potential well", or, in other words "a microparticle cannot fall to the bottom of the potential well" This conclusion does not depend on the form of the potential well, since it is a direct consequence of the uncertainty relation: "falling to the bottom of the well" is connected with the vanishing of momentum and hence the uncertainty in the momentum of the microparticle. In this case, the uncertainty in the coordinate becomes so large that there is a direct contradiction with the very fact that the microparticle is in a potential well.

Evaluation of the "Blurring" of the Optical Absorption Band Edge in the Franz-Keldysh Effect

The essence of the effect, investigated in 1958 by Keldysh, and independently by Franz, lies in the following: in a uniform external electric field, the minimum of the electron energy in the conduction band of semiconductors shifts downwards on the energy scale, leading to a "blurring" of the edge of the fundamental optical absorption band (as a result the absorption of the photons with energies lower than the forbidden band width becomes possible) [22]. The value of the shift of electronic states characterizing the indicated "blurring" may be obtained in the same way as the preceding evaluations were made. We make use of the classical expression for the energy of a charged particle in the electric field of intensity $\mathscr{E}$:

$$E=\frac{p_x^2}{2m}-\mathscr{E}ex. \tag{4.8}$$

Here m is the effective mass of the electron in the conduction band. Treating p_x and x as uncertainties in the momentum and coordinate of the electron and using the equality $p_x \cdot x = \hbar$ as the uncertainty relation, we get from (4.8)

$$E(p_x)=\frac{p_x^2}{2m}-\frac{\mathscr{E}e\hbar}{p_x}. \tag{4.9}$$

Next, as usual we equate the derivative $\frac{d}{dp_x}E(p_x)$ to zero and obtain the value $p_0 = -\sqrt[3]{\mathscr{E}e\hbar m}$ for which the function $E(p_x)$ assumes its minimum value:

$$E_0=\frac{3}{2}\sqrt[3]{(\mathscr{E}e\hbar)^2/m}\approx\sqrt[3]{(\mathscr{E}e\hbar)^2/m}. \tag{4.10}$$

Expression (4.10) gives an estimate of the extent of the "blurring" of the edge of the fundamental optical absorption band in the Franz-Keldysh effect.

Why does not the Electron Fall into the Nucleus?

While postulating the stationary states, Bohr's theory did not explain why, after all, the electron, moving under acceleration, does not radiate and fall into the nucleus as a result of this. Relation (3.3) explains this fact. The falling of an electron into a nucleus would obviously mean a considerable reduction in the uncertainty of its coordinate. Before the hypothetical falling into the nucleus, the electron is localized within the limits of the atom, i.e. in a region of space with linear dimensions $\hbar^2/me^2 \approx 10^{-8}$ cm [see (4.4)], whereas after falling into the nucleus it would be localized in a region with linear dimensions less than 10^{-12} cm. According to (3.3) a stronger localization of a microparticle in space is linked with a "blurring" of its momentum. Hence upon falling into the nucleus, the mean value of the momentum of the electron must increase, which requires an expenditure of energy. Thus it turns out that effort has to be made not to "hold" the electron from falling into the nucleus, but on the contrary to "force" the electron to be localized within the nucleus.

In the example of the zero-point oscillations it was pointed out that the microparticle in a potential well always possesses a non-zero minimum energy E_0. The magnitude of E_0 depends, in particular, on the spatial dimensions of the well (or on its width a, which determines the extent of localization of the microparticle in space). By taking into account the uncertainty relation, it is easy to see that

$$E_0 \approx \frac{\hbar^2}{ma^2}. \qquad (4.11)$$

If a decreases, E_0 increases. For sufficiently small a, the energy E_0 may become greater than the depth of the potential well. It is obvious that such a well will not hold the microparticle at all.

The falling of an electron into the nucleus corresponds to a decrease in the width of the potential well from 10^{-8} cm to 10^{-12} cm (and even lower). According to (4.11) the minimum energy E_0 should increase in this case from 10 to 10^9 eV (and higher). As a result the minimum energy of the electron turns out to be a few orders higher than the binding energy of a nucleon in the atomic nucleus (the latter being not greater than 10^7 eV). This means that the electron cannot ever be present in the nuclear potential well and hence it can by any means be compelled to be localized within the nucleus, not even by force. This not only eliminates the problem of "an electron falling into the nucleus" but also solves another fundamental question: the *electron is not one of the constituents of the atomic nucleus.*

On the "Trajectory" of Microparticles

In order to draw the trajectory of a particle, it is necessary, strictly speaking, to know the coordinate and momentum of the particle at every moment of time (in fact, in order to depict the dependence $x(t)$, it is necessary to know, for every t, the values x and $\frac{dx}{dt}$). Since, according to the uncertainty relation (3.3), a microparticle cannot simultaneously possess a definite coordinate and a definite projection of the momentum, one can draw the conclusion that the concept of trajectory in case of microparticle, strictly speaking, is not applicable.

The rejection of the trajectory concept is connected with the existence of wave properties in microparticles, which do not permit one to consider microparticles as classical corpuscles. The movement of a microparticle along the x-axis cannot be associated with the differentiable function $x(t)$ which is so widely used when considering the mechanics of classical objects. From a known value of x of the microparticle at a certain time t, it is impossible to predict the value of its coordinate at the time $t + dt$.

As applied to Bohr's theory, this means a rejection of the very concept of "the orbit of an electron in an atom". One may speak about the localization of the electron within the atom as a whole; the orbit requires a much greater spatial localization. Turning to the problem of "the electron falling into the nucleus" discussed above, we can understand the consequence to which such a localization leads. The planetary model of the atom thus turns out to be just an intermediate step in development of our concept of the atom. Much later, in the fifties, Bohr himself amusingly recalled how after one of his lectures a student came up and asked him "Were there really idiots who thought that the electron revolves in an orbit?"

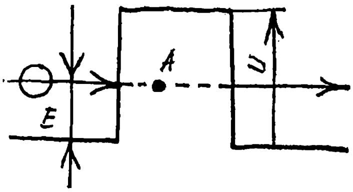
We note that with the rejection of the idea of orbits of the electron in an atom the contradiction regarding the problems of the instantaneous jump of the electron from one orbit into another, discussed in Sec. 2, is automatically eliminated.

There are situations, however, in which one can make use of the idea of "the trajectory of a microparticle" As an example we consider the motion of electrons in the kinescope of a television set. The momentum of the electron along the axis of the tube is $p = \sqrt{2meU}$, where U is the accelerating voltage. The formation of the electron beam means a definite localization of the coordinate in the transverse direction. The degree of this localization is characterized by the diameter d of the beam. According to (3.3), there must be an uncertainty in the electron momentum in a direction perpendicular to the axis of the beam: $\Delta p \approx \hbar/d$. As a result of this uncertainty, the electron may deviate from the axis of the beam within an angle $\Delta\theta \approx \Delta p/p \approx \hbar/pd$. Let L be the path length of the electron in the kinescope. Then the uncertainty in the position of the point of impingement of an electron on the screen will be characterized by the quantity $\Delta x \approx L\Delta\theta \approx L\hbar/pd$. Assuming $U = 20$ kV, $d = 10^{-3}$ cm, $L = 10^{2}$ cm, we get $\Delta x \approx 10^{-5}$ cm. In this way, the blurring of the point of impingement due to the uncertainty relation is considerably less than the diameter of the beam. It is clear that in such cases the motion of the electron may be treated classically.

The Possibility of a Microparticle Sub-Barrier Passage (Tunneling Effect)

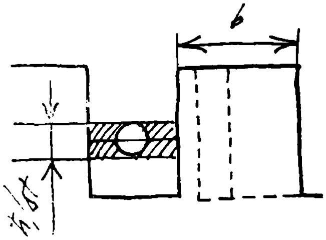
Suppose we have a potential barrier whose height U is greater than the energy of the particle (Fig. 4.1). We ask the question: can a particle, situated somewhere to the left of the barrier, appear after some time to the right of it, without getting any energy from outside? Classical mechanics gives a negative answer—a classical corpuscle cannot pass through the barrier. If this were to happen, then the total energy of the particle, say, at the point A in Fig. 4.1 would be less than its potential energy, which is physically absurd.

Fig. 4.1



Does this ban apply to microparticles as well? It can be shown that it does not—it is removed by relation (3.2). Let the microparticle move from infinity to the right and encounter the potential barrier. Until this encounter it was in a state of free motion for an infinitely long time and hence its energy had a definite value. But now the microparticle interacts with the barrier, or, more precisely, with the objects which caused the appearance of the barrier. Suppose the interaction lasts for a time Δt. According to (3.2), the energy of the microparticle in a state of interaction with the barrier is no longer definite but is characterized by the uncertainty $\Delta E \geqslant \hbar/\Delta t$. If this uncertainty is of the order of the height U of the barrier, the latter stops being an unsurmountable obstacle for the microparticle. Thus the microparticle may pass through the potential barrier. This specific quantum effect is called the *tunneling effect*. It explains, in particular, the α-decay of atomic nuclei. It should be noted that when considering the tunneling effect, the motion of the microparticle cannot be represented by the dotted line in Fig. 4.1. The dotted line corresponds to the classical trajectory, while a microparticle does not have a trajectory. Hence there is no point in trying to "accuse" the microparticle of having been "under the potential barrier" at some moment of time.

Fig. 4.2



It has been noted above that the energy of a freely moving microparticle is not quantized. This may be easily shown by making use of the tunneling effect. Suppose a microparticle is located in a potential well shown in Fig. 4.2. On account of the tunneling effect the microparticle may of its own accord leave the potential well. Consequently, the time for which it stays in the well is not infinite. If we denote this time as Δt, it follows from (3.2) that the energy of the microparticle must have an uncertainty of the order $\hbar/\Delta t$. We reduce the width b of the potential barrier (dotted line in Fig. 4.2). It is clear that as a result the magnitude of Δt will decrease, since the probability of the microparticle leaving the well will increase. With a decrease in Δt, the uncertainty in the energy of the microparticle, $\hbar/\Delta t$, will increase. This may be considered as a larger blurring (further broadening) of the energy levels of the microparticle in the well. In the limiting case of zero thickness of the barrier, the value of Δt vanishes, the microparticle becomes a freely moving particle, and the energy levels broaden up indefinitely, actually transforming into a continuous energy spectrum.

Section 5

Impossibility of Classical Representation of a Microparticle

A Microparticle Is not a Classical Corpuscle

The process of "breaking up" of objects surrounding us into smaller and smaller "fractions" leads to microparticles. Therefore it is but natural to associate microparticles first of all with *corpuscles*. This is also supported by the fact that a microparticle is characterized by a definite rest mass and a definite charge. For instance, it is meaningless to speak of a half-electron having half the mass and half the electric charge of a whole electron. The very terms "microparticle" and "elementary particle" reflect the notion of the microparticle as being some particle (corpuscle).

However, as follows from the preceding discussion, a microparticle is considerably different from a classical corpuscle. Firstly it does not have a trajectory which is an essential attribute of a classical corpuscle. The use of such corpuscular characteristics as coordinate, momentum, angular momentum, energy when considering microparticles is restricted to the framework of the uncertainty relations. Interconversion of microparticles, spontaneous decays, the existence of an indestructible intrinsic moment (spin) and the ability to pass through potential barriers indicate that microparticles are quite dissimilar to classical corpuscles.

Wave concepts are radically different from corpuscular concepts. Hence it is not surprising that the striking contrast between classical corpuscles and microparticle is explained by the existence of wave properties in the latter. Moreover, it is the wave properties which account for the uncertainty relations and all the consequences resulting from them. In this respect, the following remark by de Broglie [23] is worth noting: "for a century, the corpuscular method of analysis in optics was too much neglected in comparison with the wave method. Hasn't the converse been the case in the theory of matter? Haven't we thought too much of the "particle" picture and neglected the wave aspect far too much?" The question raised by de Broglie is fully justified. However, an excessive exaggeration of the wave aspect while considering microparticles should be avoided. We must remember that while on one hand a microparticle is not a classical corpuscle, it is similarly, on the other hand, not a classical wave.

A Microparticle Is not a Classical Wave

The analysis of one mistake which is committed quite often even these days when considering a simplified account of quantum mechanics is quite instructive. We shall demonstrate this mistake through two examples.

Example 1

It is contended that the wave properties of an electron permit one to derive the conditions for the quantization of momentum which are postulated in Bohr's theory. The "derivation" is done in the following way. Let $2\pi r_n$ be the perimeter of the n-th Bohr's orbit. In this orbit, an electron moves with de Broglie's wavelength $\lambda_n = 2\pi\hbar/p_n$. The basic assumption lies in the fact that the perimeter of the orbit should contain n wavelengths λ_n of the electron. Consequently, $2\pi r_n = n\lambda_n$. This at once gives the desired condition for quantization of momentum:

$$p_n r_n = n\hbar. \tag{5.1}$$

Example 2

It is stated that the wave properties of an electron permit a very simple derivation of the formula for the energy levels in a potential well, if we assume that a definite number of de Broglie half-waves are confined in the potential well (in analogy with the number of half-waves contained in the length of a string fixed at both ends) corresponding to different stationary states. Designating the width of the one-dimensional potential well by a, we write $a = n\lambda_n/2$, from which we get the desired result:

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{5.2}$$

Both these final results [(5.1) as well as (5.2)] are correct; they are the same as the result deduced from strict theory. However, the "derivation" of these formulas must be considered to be unsound. In both cases in fact the same fundamental mistake has been committed: they are based on the wrong assumption that the electron in a potential well has a definite de Broglie wavelength, or, in other words, a definite momentum. However, according to (3.3), the momentum of a microparticle in a bound state is characterized by the uncertainty $\Delta p \gtrsim \hbar/a$. Since in the above examples $p \approx \hbar/\lambda \approx \hbar/a$, it follows that the momentum is of the same order of magnitude as the uncertainty in momentum given by relation (3.3). It is clear that in such cases one cannot speak about any value of the electron momentum (and correspondingly of its de Broglie wavelength) even approximately.* These examples demonstrate an obvious exaggeration of the wave aspect. The identification of an electron in a potential well with a classical wave inside a "resonator" is incorrect. The picture of an electron wave in a "resonator" is the same kind of simplification as the picture of an electron-ball moving in a classical orbit. We shall return again to the question of waves in quantum mechanics; however, it is useful to emphasize at this stage that by the term "de Broglie wave" we do not conceal any sort of classical wave. It is just a reflection in our imagination of the fact that microparticles possess wave properties.

Attempts to Represent a Microparticle as a Symbiosis of a Corpuscle and a Wave

If a microparticle is neither a corpuscle nor a wave, then may be it is some kind of a symbiosis of a corpuscle and a wave? Several attempts were made to model such a symbiosis and thus also to visually demonstrate the wave-particle duality. One such attempt represents a microparticle as a formation, limited in space and in time. This may be the wave packet mentioned in Sec 3. This may also be just a "scarp" of a wave, often called a wave train. Another attempt uses a model of a pilot-wave, according to which a microparticle is some sort of a "compound" of a corpuscular "core" with a certain wave which controls the motion of the core.

One of the versions of the pilot wave model is considered by D. Baum in his book [25]: *We first postulate that connected with each of the "fundamental" particles of physics (e.g. an electron) is a body existing in a small region of space.... in most applications at the atomic level the body can be approximated as a mathematical point..*
The next step is to assume that associated with this body there is a wave without which the body is never found. This wave will be assumed to be an oscillation in a new kind of field, which is represented mathematically by the ψ-field of Schrödinger somewhat like the gravitational and the electromagnetic, but having some new characteristics of its own...
We now assume that the ψ-field and the "body" are interconnected in the sense that the ψ-field exerts a new kind of "quantum-mechanical" force on the body, the force is such as to produce a tendency to pull the body into regions where $|\psi|$ is largest.
If the above tendency were all that were present, the body would eventually find itself at the place where the ψ-field had the highest intensity. We now further assume that this tendency is resisted by random motions

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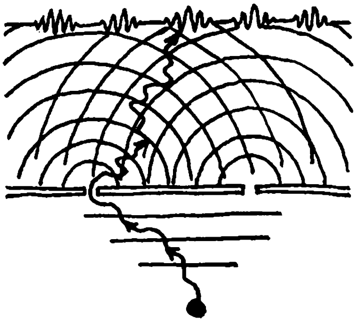
* This question is considered in greater detail in Sec. 23 of this book. See also [24].

undergone by the body, motions which are analogous to the Brownian movement. They could, for example, come from random fluctuations in the ψ-field itself.

Once admitting the existence of these fluctuations, we then see that they will produce a tendency for the body to wander in a more or less random way over the whole space accessible to it. But this tendency is opposed by the "quantum force" which pulls the body into the places where the ψ-field is most intense. The net result will be to produce a mean distribution in a statistical ensemble of bodies, which favours the regions, where the ψ-field is most intense. ....

Figure 5.1 illustrates the given model as applied to the passage of a microparticle through the screen with slits: the ψ-wave is diffracted on both the slits, while the "body" passes through one slit and is registered on the screen in accordance with the result of the interference of ψ-waves.

Fig. 5.1



It is not denied that such models could appear attractive at first glance if only because of their intuitive appeal. It must be emphasized at once, however, that all these models are baseless. We shall not explain at this stage the reasons for worthlessness of the pilot-wave model considered above, but shall just mention that it is cumbersome since it uses artificial notions such as the ψ-field which is "to some extent similar to gravitational end electromagnetic fields", or the "quantum force" which reflects the interaction of certain "object" with the ψ-field. The reader will later realize that the worthlessness of such models is not because of some specific feature, but because of deep fundamental reasons. He will understand that any attempt at a literal interpretation of the wave-particle duality, any attempt to model a symbiosis of corpuscle and a wave, should be considered fruitless from the very start. A microparticle is not a symbiosis of a corpuscle and a wave.

How to Understand the Wave-Particle Duality?

At present the wave-particle duality is considered as the potential ability of a microparticle to exhibit its different properties depending on external conditions, in particular, on the conditions of observation. As Fock [1] wrote, *Thus under certain conditions an atomic object may exhibit wave properties and under other conditions corpuscular properties; conditions are also possible when both kinds of properties appear simultaneously but not sharply. We can state that it is potentially possible for an atomic object to manifest itself either as a wave or as a particle or in an intermediate fashion, according to the external condition prevailing. It is just this potential possibility of exhibiting various properties inherent in an atomic object that constitutes the wave-corpuscular duality. Any other, more literal meaning attached to this duality,* *such as a wave-particle model of any kind, is incorrect.* Let us consider a simple example. Let a beam of electrons pass through a screen with slits and then hit a detector screen. While passing through the slits, the electrons realize their wave properties which leads to a distribution for electrons beyond the slit characteristic of interference. When impinging on the detector screen, the electrons exhibit their corpuscular properties—each of them is registered at a certain point on the screen. It may be said that the electron passes through the slit as a "wave", and is registered on the detector screen as a "particle" In this connection, it is sometimes said that a microparticle is a wave under some circumstances, and a microparticle is a particle under other circumstances. Such a treatment of wave-particle duality is incorrect. Whatever the conditions, a microparticle is neither a wave, nor a particle, not even a symbiosis of a wave and a particle. It is a quite specific object, capable of exhibiting corpuscular or wave properties to some extent or other depending on the circumstances. The understanding of wave-particle duality as the potential capability of the microparticle to exhibit different properties in different external conditions is the only correct one. Hence, in particular, follows an important conclusion: *it is impossible to give a definite visual model of a microparticle.*

Electron in an Atom

The absence of a visual model of a microparticle does not in any way prevent us from using tentative models quite suitable for representing a microparticle under different conditions. As an example, let us consider an electron in an atom.

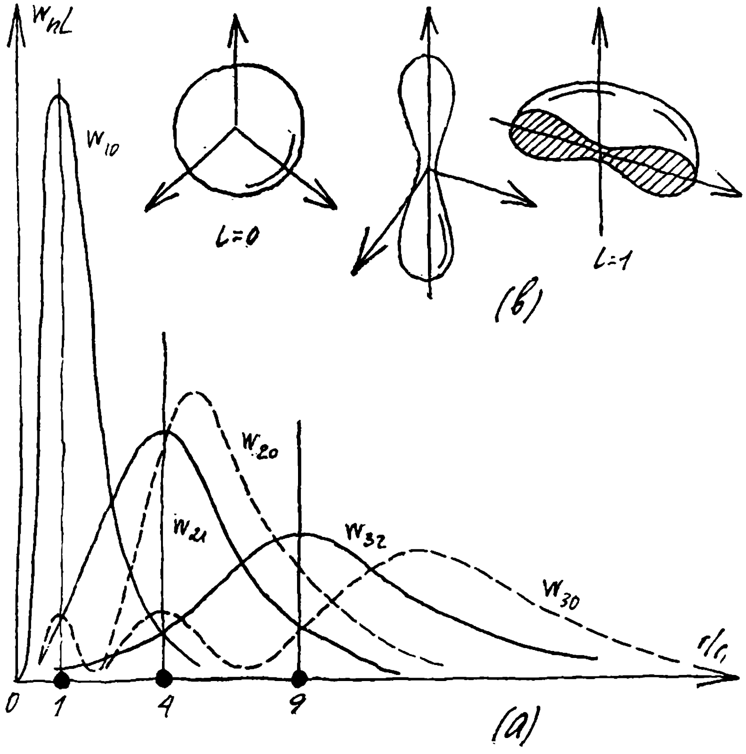
We recall that the state of an electron in an atom is described by a set of quantum numbers n, l, m, σ. A given state is characterized by a definite energy, while in the particular case of the hydrogen atom, it depends only on the number n [see (2.7)], and in a more general case on the numbers n and l. An electron in an atom is delocalized in space—its coordinates have an uncertainty of the order of the size of the atom. Usually, when considering an electron in an atom, it is customary to introduce the concept of an *electron cloud* which may be interpreted in this case as a tentative image of the electron. The form and the effective size of an electron cloud depend on the quantum numbers n, l, m and, consequently, vary from one state of the electron in the atom to another.

In order to describe the dimensions and the form of the electron cloud, we introduce a certain function

$$u_{nlm}(r, \theta, \varphi) = v_{nl}(r)\, Z_{lm}(\theta, \varphi), \qquad (5.3)$$

where r, θ, φ are the spherical coordinates of the electron. The function u_{nlm} is interpreted in the following way: $u_{nlm}(r, \theta, \varphi)\, dV$ is the *probability* of finding an electron in a state with quantum numbers n, l, m in an element of volume dV in the vicinity of point (r, θ, φ). In other

Fig. 5.2



words, $u_{nlm}(r, \theta, \varphi)$ is the corresponding *probability density* of finding the electron. Remember that $dV = r^2 dr d\Omega$, where $d\Omega = \sin\theta d\theta d\varphi$ is the element of solid ngle. The function

$$w_{nl}(r)\, dr = v_{nl}(r)\, r^2 dr \tag{5.3a}$$

is thus the probability of finding the electron with quantum numbers n, l at a distance between r and $r + dr$ from the nucleus.

In Fig. 5.2*a* are shown forms of functions $w_{nl}(r)$ for different states of the electron in a hydrogen atom. Notice that the functions w_{10}, w_{21}, w_{32} have maxima corresponding to the radii of first, second and third orbits in Bohr's theory. Figure 5.2*b* shows forms of function Z_{lm} for some states of the electron. For $l = 0$ (for the so-called s-electron) we have a spherical electron cloud. For $l = 1$ (for p-electron) the electron cloud has a form of either a spindle or a toroid depending on the quantum number m. Thus in order to imagine an electron in atom, one may use conventional forms like the models of a sphere, spindle, toroid, etc.

The ground state of the hydrogen atom is characterized by a spherical electron cloud. Theory shows (see, for example, [11]) that in this case

$$w_{nl}(r) = 4\frac{r^2}{r_1^3}\exp\left(-\frac{2r}{r_1}\right). \tag{5.4}$$

The parameter r_1 characterizing the effective radius of the cloud is determined by relation (4.4); in Bohr's theory it occurs as the radius of the first orbit.

In conclusion we note that during quantum transitions in an atom, there occurs not only a change in energy, but also a "redistribution" of electron clouds—a change of their shape and size.

Section 6 Rejection of Ideas of Classical Physics

General Remarks

As has been asserted, a transition from macrophenomena to microphenomena presupposes a rejection of the basic ideas of classical physics. The notion of a strict continuity in the spectrum of values of physical quantities is no longer valid, the classical concept of a trajectory is rejected, the principle of classical determinism is in question. At the root of this viewpoint lie ideas of quantization (discreteness) and wave-particle duality which are alien to classical physics.

On the basis of a number of examples that we have considered, we could see the need to reject the classical principle of unlimited detailing of objects in space, and of phenomena in time. Thus the question of the internal structure of elementary particles turns out to be groundless. Likewise the efforts towards a detailed development in time of the process of the quantum jump (quantum transition) have no meaning.

The concepts of energy momentum, angular momentum which are widely used in classical physics are carried over to quantum mechanics as well. However, these concepts are now seen differently with a reconsideration of the previous interconnections, taking into account the possibility of quantization, and the limitations imposed by the uncertainty relations. In particular, there arises the question, unknown to classical physics, of the simultaneous measurement of physical quantities, and questions about the state and the methods of describing a state are put in a new light. In conclusion we stress the impossibility of the classical interpretation of a microparticle, and the loss of the clarity of classical physics.

Identity of Microparticles

The rejection of the classical individualization of an object is quite fundamental. In classical mechanics objects are known to have individuality since it is always possible in principle to enumerate them and observe the behaviour of any one of them. In this case, however alike two classical objects may be, they are never identical and can always be distinguished. But in quantum mechanics two microparticles of the same type should be treated as absolutely identical. Thus, all electrons are identical and so are all unexcited hydrogen atoms, helium nuclei, etc.

Suppose we have several electrons, one of which is "assigned" the number 1 at the moment of time $t = 0$. Can this electron be identified after a certain time t? Such an identification could have been easily done if we could put some "label" on this isolated object. We could get by without "labelling" this electron if we could simply keep a watch over the isolated object, i.e. if we could "mentally" follow it (in our imagination) along its trajectory. This is precisely what we would have done in the case of isolated classical objects. However, none of this holds in the case of an electron; it is in principle impossible to "label" it. Strictly speaking, it has no trajectory. The electron "isolated" by us at the instant $t = 0$, cannot be isolated in actual practice: it does not have the individuality which would allow it to be identified in the assembly of electrons after a certain time t. Two electrons are much more "like each other" than the proverbial "two peas in a poll"; since the latter are classical objects, they could differ in size or in chemical composition in some way.

It is understood that the identity of microparticles does not exclude the possibility of their differentiation on the basis of different states in which these particles may be found. Two electrons belonging to two different atoms are, of course, identical but at the same time distinguishable. The affiliation of an electron to one atom or another permits its "isolation". However, nothing changes physically if the electrons interchange places. It is clear that if such an exchange is possible, for example, by combining the atoms under consideration into a molecule, the distinguishability of the electrons vanishes.

Chance and Necessity in the Behaviour of a Microparticle

Laplacian determinism excludes the element of chance from the behaviour of an isolated object; in classical mechanics, *necessity* completely dominates. Because of this, the laws of classical mechanics are *dynamic* and *not statistical*. The element of *chance* (and, consequently, *statistical laws* also) appear in classical physics only when considering aggregates of objects or assemblies of particles.

From this point of view, it is important to stress that in quantum mechanics we are dealing with a qualitatively different situation concerning the behaviour of individual microparticles: here, elements of necessity, as well as chance, are present. An excited atom *spontaneously* returns to the ground state without any external influence. This is associated with the spontaneous transitions of electrons in the atom from one set of energy levels to another. It is impossible in principle to indicate precisely when a particular excited atom will return to its ground state; such a return is a random act. Precisely in the same way, it is impossible to predict exactly when a given elementary particle, for example, a neutron, will decay spontaneously. In this case also an element of chance is present.

In addition to elements of chance, there are also present the elements of necessity in the behaviour of a microparticle. As has already been indicated in Sec. 1, if we have N_0 neutrons at the instant $t = 0$, $N_0 \gg 1$, we can confidently state that at the time t we will be left with only $N_0 \exp(-t/\tau)$ neutrons, τ being a constant called the lifetime of the neutron. Here, the necessity is obvious. In the case of an individual neutron this necessity is replaced by a definite probability of keeping the neutron intact until time t, once it has managed to survive to time $t = 0$. This probability is equal to $\exp(-t/\tau)$. It should be noted that this probability is independent of the time for which the given neutron has survived up to the time $t = 0$. Necessity is also manifested in the conservation laws which govern decay processes as well as the processes of interconversion of microparticles in general. We may also mention the fact that there are definite modes of decay; for example, a free neutron may decay into a proton, an electron and an electronic neutrino.

The existence of chance as well as necessity in the behaviour of an individual microparticle has very important consequences. It leads to the fact that quantum mechanics turns out to be in principle a *statistical theory* with probability as one of its basic attributes. As Fock [1] has remarked, *in quantum physics the concept of probability is a primary concept and plays a fundamental* *role.* It could be said that the behaviour of an individual microparticle is random, but the probability of this behaviour is necessary*. The electronic cloud considered in Sec. 5 may serve as a good example of this. The occurrence of an electron at some point near the nucleus is a random event, but the probability of its being found at a given point (r, θ, φ) is definite—it is described by a function of the type (5.3) or, in other words, is determined by the shape and size of the corresponding electron cloud.

In the end, we note that the element of chance in the behaviour of an individual microparticle is due to the uncertainty relations. In Sec. 4, we concluded on the basis of relation (3.3) that it is impossible to "aim a microparticle to hit a given point" In other words, the registration of a particular electron at some point of a detector screen is random; we can only speak of the probability of such a fact. In Sec. 3, we introduced on the basis of relation (3.2) the concept of the virtual transitions of a microparticle. It is easy to see that such transitions also point, towards the existence of randomness in the behaviour of a microparticle. When discussing the specific nature of the physics of microparticles, it is necessary to discuss in greater detail the idea of virtual transitions and of virtual microparticles associated with them.

Virtual Transitions and Virtual Microparticles

Perhaps there is nothing more alien to classical physics than the idea of *virtual transitions and virtual microparticles*. The virtual transition of an electron from level E_2 to level E_1 and back (the transition $E_2 \to E_1 \to E_2$) may be considered as a process in which the electron emits and absorbs a photon of energy ($E_2 - E_1$). Such a photon is called virtual. In contrast to the photons participating in real transitions, virtual photons cannot be observed experimentally. The creation of a virtual photon is not connected with an absorption of energy from outside, and its annihilation is not connected with a release of energy. The law of conservation of energy is not violated since a virtual photon exists for a very short time Δt and, according to uncertainty relation (3.2), the energy of an electron emitting the virtual photon is characterized by the uncertainty $\Delta E \geqslant \hbar/\Delta t$, which may be of the order of, or greater than, the energy of the photon ($E_2 - E_1$). The emission or absorption by an electron of virtual photons corresponds, from a

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* Here, it is quite appropriate to recall the words of F. Engels: *Necessity emerges from within the framework of randomness.*

physical point of view, to the process in which an electron undergoes virtual transitions.

Taking into consideration the emission and absorption of virtual photons by an electron, one may imagine that each electron is surrounded by a photon cloud. This "cloud" should be compared with the electron's own electromagnetic field. Two electrons may exchange virtual photons. In quantum field theory, the interaction of electrons is seen as a result of the exchange of virtual photons between electrons. For this we frequently make use of Feynman's diagrams, which enable us to consider the various processes of photon exchange.

Fig. 6.1

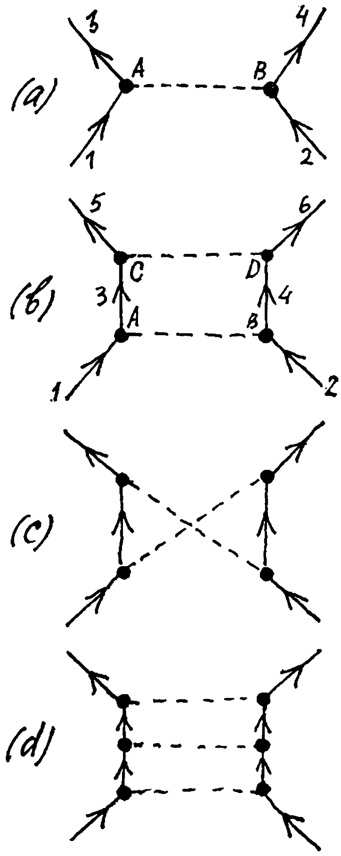

Figure 6.1 shows four Feynman's diagrams demonstrating the scattering of one electron by another. The solid lines "show" electrons and the dotted one—photons. The intersections of solid and dotted lines are called the *vertices* of the diagram. Let us consider the diagram (*a*). Here *1* and *2* are the electrons before interaction with each other (before scattering), *AB* is a virtual photon which is exchanged by the electrons during the process of interaction (note that all the particles indicated in the diagram by lines connecting two vertices are virtual); *3* and *4* are the electrons after scattering. Let us turn to the diagram (*b*). Here *1* and *2* are electrons before scattering, *AB* and *CD* are virtual photons exchanged by the electrons, *3* and *4* are virtual electrons, *5* and *6* are electrons after scattering. The diagram (*c*) is of the same type as diagram (*b*); here the electrons exchange two photons. The diagram (*d*) shows one of the processes in which the electrons exchange three photons. It is obvious that there is an infinite number of such diagrams which become more and more complicated (with the participation of more and more photons).

In order to calculate the probability of scattering of an electron by an electron, one must consider in principle the contribution of the various processes indicated by the various diagrams. Fortunately, the contribution of different processes is different: it is less if the number of vertices is greater (i.e. if more virtual photons take part in a process). Theory shows that this contribution is quantitatively determined by the dimensionless quantity $(e^2/\hbar c)^{n/2}$, where e is the charge of the electron, c is the velocity of light, $\hbar$ is Planck's constant and n is the number of vertices in the diagram. Since $e^2/\hbar c = 1/137$, it follows that the main contribution to the scattering of one electron by another must come from the diagram (*a*) with two vertices (exchange of one photon). The four vertices diagrams (*b*) and (*c*) (exchange of two photons) should provide the next approximation; their contribution will be two orders of magnitude lower. Thus, in actual practice there is no need to consider a very large number of diagrams, it is sufficient to limit ourselves to diagrams with a relatively small number of vertices.

Fig. 6.

Of course, a systematic study of Feynman's diagrams and calculations based on them is beyond the scope of this book. These questions are related not to quantum mechanics, but to *quantum field theory* (quantum electrodynamics)*. However, a general introduction to the ideas forming the bases of Feynman's diagrams is quite appropriate at this point, since they permit us to emphasize the specific nature of the physics of microparticles and also demonstrate some fundamental quantum-mechanical principles (the latter will be considered below, in particular, in Sec. 25).

Before ending this discussion on Feynman's diagrams, we consider the so-called effect of *polarization of a vacuum*. Figure 6.2 shows a diagram describing one of the processes responsible for this effect. A photon is transformed into a virtual electron-positron pair, which is annihilated and transformed again into a photon (one of the solid lines between the vertices of the diagram "shows" a virtual electron, and the other, a virtual positron). The members of this pair during their lifetime may obviously generate virtual photons and, consequently, new virtual electron-positron pairs, and so on. As a result of this, the vacuum turns out to be not "empty" but "filled" with virtual electric charges which must exercise a screening effect on external (real) charges. Experimental confirmation of this effect is the best evidence of the usefulness of our concept of virtual particles.

The Microparticle and Its Surroundings

As we have already mentioned, the existence of the element of chance in the behaviour of a microparticle is one of its most specific properties. As a result of this, quantum mechanics turns out in principle to be a statistical theory operating with probabilities. But what is the *reason* for the existence of an element of chance in the behaviour of a microparticle?

This question can be answered as follows: The existence of chance in microphenomena is explained by the fact that a microparticle, figuratively speaking, interacts with all its surroundings. The specific nature of quantum

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* A simple and detailed account of Feynman's diagrams is given, for example, in [26].

mechanics is such that, strictly speaking, not a single object in it can be considered to be fully isolated, completely independent of its surroundings. It has been remarked [27] that the cause of the statistical nature of quantum mechanics is the same as in classical statistical mechanics, i.e. the existence of a large number of bonds affecting the motion of the object. A particle treated as free in quantum mechanics is in fact free only from influences of a dynamic nature. But it remains under the influence of random forces which cause quantum fluctuations in its behaviour, as reflected by the uncertainty relation.

What is the *nature* of the random influences on a microparticle? In quantum field theory, it manifests itself in an explicit form as the interaction of a microparticle with a vacuum (recall that a vacuum is not "empty"; it is "filled" with virtual charges). It may be said that a microparticle interacts with its surroundings through virtual microparticles.

The reader should now find it quite natural to interpret wave-particle duality as the potential ability of a microparticle to exhibit one kind of property or another, depending on the external conditions, i.e. on the microparticle's surroundings. This envisages a close connection between the microparticle and its surroundings—in fact, the very nature of a microparticle is displayed in one form or another depending on specific conditions and circumstances.

The impossibility of an unlimited detailization of objects and phenomena being displayed in quantum mechanics should also be explained by the interaction of a microparticle with its surroundings. This means that after a certain stage of investigation, physical objects cannot be considered as being isolated. Here it is appropriate to recall the statement given in Sec. 3 regarding the discussion on quantum transition: "During the interaction of an electron with photons there is, strictly speaking, no electron and no photon but a single entity which must be considered as such without going into details."

Quantum mechanics re-establishes the idea acquired through everyday experience regarding the unity of the universe and general connections among phenomena. This idea received a setback in the classical theory. The sharp boundaries that existed between waves and particles, particles and fields, object under investigation and the medium are all obliterated and the concept of the interconversion of matter is introduced. We find ourselves in full agreement with the following appropriate remark made by Bohm [28]: *It seems necessary to give up the idea that the world can correctly be analysed into distinct parts, and to replace it with the assumption that the entire universe is basically a single, indivisible unit. Only in the classical limit can the description in terms of component parts be correctly applied without reservations. Wherever quantum phenomena play a significant role, we shall find that the apparent parts can change in a fundamental way with the passage of time, because of the underlying indivisible connections between them. Thus, we are led to picture the world as an indivisible, but flexible and everchanging, unit.*

Interlude. Is a "Physically Intuitive" Model of a Microparticle Possible?

Participants: (same as in Prelude).

It may well be that these electrons
Are worlds just like our very own,
With kings and scholars, arts and armies,
And memories of ages flown.
And atoms—cosmic systems, spinning
Around a central spinning sphere.
Where things are just like ours, but smaller,
Or nothing like what we have here.

Bryusov (*The World of the Electron*)

Author: The impossibility of the classical interpretation of a microparticle predetermines a negative answer to the question "Is it possible to have a "physically intuitive" model for a microparticle?"

Classical Physicist: It is still not clear why a "physically intuitive" model of a particle explaining its various properties including spin, instability, wave properties, etc. cannot be created. Such a model may turn out to be complicated. Or, it may be possible that we still do not know enough about a microparticle to create such a model. But why can't we believe in the very possibility of this model?

Author: There are very sound reasons for this. I shall indicate just two of them. Firstly, any modelling envisages in the long run a detailization irrespective of whether it is a model of an object or a process. However, the impossibility of an unlimited detailization is characteristic of microparticles and microphenomena, as we have already mentioned. This important situation was persistently stressed by Bohr. He wrote, in particular (see his article *Quantum Physics and Philosophy*—[6]): *A new epoch in physical science was inaugurated, however, by Planck's discovery of the elementary quantum of action, which revealed a feature of wholeness inherent in atomic divisibility of matter. Indeed, it became clear that the pictorial description of classical physical theories represents an idealization valid only for phenomena in the analysis of which all actions involved are sufficiently large to permit the neglect of the quantum....* It is appropriate to mention here that this feature of wholeness indicated by Bohr is closely linked with the identity of a microparticle. Secondly, as we have already indicated, a characteristic property of microparticles is their inavoidable interaction with surroundings leading, in particular, to a dependence of some of the properties of microparticle on definite external circumstances. These properties should be treated as certain possibilities which can be realized depending on the external circumstances. One may ask, in what way can these possibilities be reflected in the framework of a definite "physically intuitive" model?

Classical Physicist: It must be admitted that these ideas serve as strong arguments against a "physically intuitive" model of a microparticle. However, I don't like the very spirit of quantum mechanics which rejects graphic representations. In my view it introduces subjectiveness in describing real world. Take, for example, the statement: "The electron may present itself as a wave or as a particle, depending on circumstances". Now, everything depends on circumstances, especially on the circumstances of observation. Involuntarily, one gets the idea that the electron is not something objective, but rather something subjective depending on how we "look" at it.

Author: Of course, this is not true. First of all, you overlook the fact that the electron has quite definite characteristics like rest mass, electric charge, spin, etc. It is stable and is a fermion. As regards a "physically intuitive" model of an electron, well, it simply does not exist. However, in rejecting a "physically intuitive" model of a microparticle, quantum mechanics in no way sacrifices objectivity in favour of subjectivity. It is just that the electron is a very complicated physical object, and depending on the external circumstances, including circumstances of observation, it exhibits its different aspects, which objectively existed in potential form (I stress this) even before the observer was born. A sober assessment of this complex situation is that a "physically intuitive" model of the electron is not possible.

Classical Physicist: Can one seriously speak about an object without having an idea of what it looks like? Isn't it strange that we study, for example, the behaviour of an electron in a crystal while we don't even know what an electron actually is?

Author: I don't agree that we don't even know what an electron is. I have just indicated a number of precisely determined characteristics and properties of an electron. More detailed properties of microparticles in general and electrons in particular were considered in the preceding sections of the book (and will be considered in the following sections). In fact, we know quite a lot about the electron and know, in particular, about its behaviour in a crystal. This is evidenced by the large number of semiconducting devices fabricated and used by us in practice. As you will see, the absence of a "physically intuitive" model of the electron has in no way turned out to be a serious obstacle. We may even go a step further and state that an understanding of natural phenomena in which Planck's constant plays an important role is possible only through a significant rejection of a graphic description. By the way, this idea was given by Heisenberg, in whose works much attention was given to questions of the use of physically intuitive methods.

Classical Physicist: But by rejecting models, isn't quantum mechanics running the risk of losing its material basis? Won't we be finally left with only equations and abstract mathematical symbols?

Author: I can understand your doubts. For you, apparently, only the *extremes* matter: either graphic models, or mathematical abstraction. To you, either a model should reflect everything or almost everything, otherwise it is quite useless. The doubts arising in your mind are a consequence of precisely this type of viewpoint. However, the quantum-mechanical approach to such questions is more flexible, or rather, *dialectical*.

Classical Physicist: I don't understand what exactly you mean by that.

Author: I want to stress two points. Firstly, although there is no "physically intuitive" model for a microparticle, this does not stand in the way of the "model representations" in quantum mechanics.

Classical Physicist: That means I was right after all?

Author: This is something different. Quantum mechanics believes that even the most refined model cannot reflect the specific characteristics of a microparticle. Hence quantum mechanics makes use of *tentative* models (tentative images)—sometimes one, sometimes another, admitting the *relativity* of every model. The only thing that is important is that each of the models employed should reflect some side of the nature of the object or phenomenon. Thus, when considering electronic transitions through the forbidden band in a semiconductor, we unhesitatingly imagine electrons as some kind of corpuscles, which "jump" on the energy scale. When considering the propagation of electrons through an ideal crystal lattice we use wave concepts. It is convenient to study the scattering of electron waves by the elastic waves of a crystal in a "corpuscular language", using the picture of collisions of corpuscles of two types—electrons and phonons. Similarly, the image of the electron cloud used for describing electrons in an atom also serves as a good example of tentative modelling. As you see, modelling in quantum mechanics is used quite extensively and flexibly. Moreover, all models are not interpreted literally but tentatively.

Classical Physicist: All right. And what is your second point?

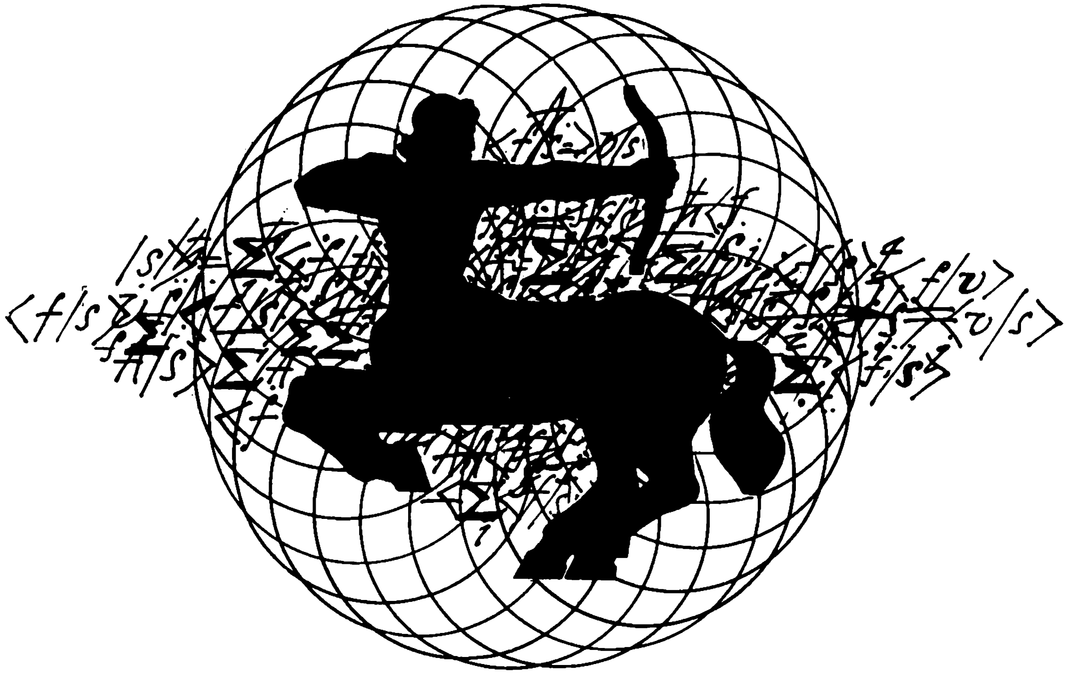
Author: The second point is as follows: Quantum mechanics makes use of both tentative models and mathematical abstractions on an equal footing. Just on equal footing! At this point modern physics breaks off quite radically from classical concepts. Stressing the great heuristic (and leading) significance acquired by mathematics in the new physics, which was not the case earlier in the epoch of the domination of "physically intuitive" concepts, Vavilov [29] writes: *we don't have enough accepted ideas and concepts for a physically intuitive model interpretation, but logic with its immense perspectives represented in mathematical form continues to be valid, thereby creating order in the new, unexplored world and opening possibilities for physical predictions.*

Classical Physicist: As a matter of fact, there is nothing definite in all this.

Author: To be more precise, there is nothing predetermined beforehand. The new physics turns to a study of the objective world, if one may say so, "without classical prejudices". It flexibly makes use of different media: models and mathematical abstractions. Figuratively speaking, it is not "alien to anything that is human". Summing up, we may say that firstly, when studying microphenomena, we do make use of visual models quite extensively. Secondly, models are by no means taken literally in quantum mechanics; their relativeness and arbitrariness are considered. Thirdly, getting acquainted with microphenomena is based on the *dialectic unity of model concepts and mathematical abstractions.*

Chapter 2

Physical Foundations of Quantum Mechanics



Section 7 Some Basic Experiments

Actual Experiments and the System of Basic Experiments

The concepts of quantum mechanics are based on a vast collection of experimental data gathered over a period of more than fifty years at the end of the 19th century and in the first half of the 20th century. Among the large number of experiments, a few stand out as being definite "milestones" and can hence be called decisive. They include the experiments of Lummer and Pringsheim on black body radiation coupled with Planck's theoretical works (1900), the experiments of Frank and Hertz (1914) on inelastic collision of electrons with atoms, Millikan's experiments (1914) on the photoelectric effect, confirming the laws predicted ealier by Einstein, the experiments conducted by Stern and Gerlach (1921) on the splitting of atomic beams in non-uniform magnetic fields, the measurements of wavelengths of X-rays scattered by matter carried out by Compton (1923), and the experiments of Davisson and Germer, and Tartakovsky (1927) on electron diffraction*. These experiments (and many others which did not become so famous) constitute the foundation on which, over a number of decades, quantum theory was built, perfected, freed from various paradoxes, and finally brought to its present harmonious structure.

Looking now from the position of the existing quantum theory at the experimental quest which led to it, it is worth generalizing the actual experimental picture by omitting the details that do not play a significant role and trying to conceive the simplest system of basic experiments which describe the fundamental aspects of the quantum-mechanical viewpoint. In this section an attempt has been made to consider such a system of experiments. This system is built on the basis of actual experiments but one should not look for a one-to-one correspondence between the basic experiments and actual experiments conducted at a certain time in a certain laboratory. Basic experiments must be seen as a sort of generalization of several actual experiments. Hence, the experimental details concerning a certain apparatus or various details of a historical nature do not play a significant role here.

In our view, resorting to the system of basic experiments is motivated by two circumstances. Firstly, being free

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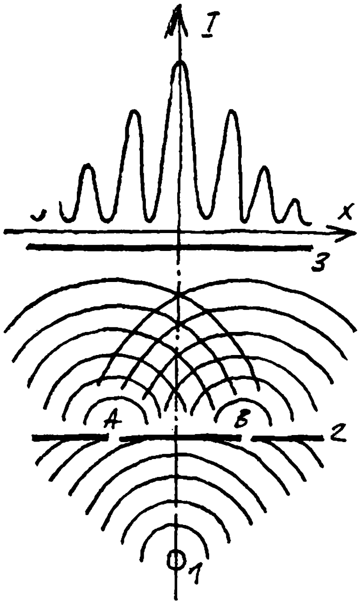
* A description of these experiments may be found, for example, in [30].

from the details of actual experimental researches and their unavoidable "zigzags" and "deadends", such a system of experiments permits one to isolate the main events prominently, and clearly show the experimental foundations of the theory. Secondly, quantum-mechanical ideas have so radically changed our views on the structure and properties of matter that it would not be proper to draw final conclusions on the basis of particular individual experiments (even on "decisive" experiments) but only on their totality. It is essential to consider the totality of experiments as a whole, and for this purpose it is useful to conceive a system of basic experiments.

Experiment 1 (Microparticles in an Interferometer)

Let us begin by considering the well-known experiment on the interference of light waves. Figure 7.1 schematically shows the simplest *interferometer*. Here, *1* is a point source of monochromatic light, *2* is a screen with two small slits A and B, and *3* is a detector screen registering the intensity of light impinging it. This intensity is indicated on the diagram by the curve $I(x)$. The interference character of the curve $I(x)$ is fairly simply explained within the framework of classical wave theory of light: the light wave from source *1* upon reaching the screen *2* converts the slits A and B into sources of new light waves, which add up to give on screen *3* the characteristic *interference pattern* of intensity distribution.

Fig. 7.1



We recall that the interference of light was observed in the middle of the 17th century by Grimaldi, and its explanation on the basis of wave concepts was given in the beginning of the 19th century by Young. Since then, the experiment shown in Fig. 7.1 is called Young's experiment.

One might ask what relation can the phenomenon of the interference of light, discovered and explained long ago, have with quantum mechanics? It turns out that the two are directly related.

Let us gradually reduce the intensity of light from source *1*. The illumination of screen *3* as a result will naturally decrease. However, the interference character of the curve $I(x)$ will be retained. By increasing the time of exposure, it is possible in principle to obtain the interference curve $I(x)$ for even the smallest light intensities. This is not trivial since with decreasing intensity of the light beam the number of photons in it will decrease and so, obviously, a situation should arise when individual photons will have to be considered in place of light waves. However, as has been shown experimentally, the nature of the interference curve $I(x)$ obviously remains unchanged no matter how much the light intensity is decreased. The distribution of the individual photons falling on the detector screen gives the same interference pattern on the screen as is produced by light waves.

Moreover, the interference is observed even if at point *1* (Fig. 7.1) we place a source of monochromatic electrons (all having the same energy). In this case also the intensity of the electron beam may be reduced indefinitely. We can even perform an experiment in which the electrons pass through the interferometer one by one. By studying the distribution of the electrons falling on the detector screen over a sufficiently long exposure time we get in this case also the characteristic interference pattern [curve $I(x)$]. Experiments repeated with other microparticles (protons, neutrons, etc.) lead to similar results.

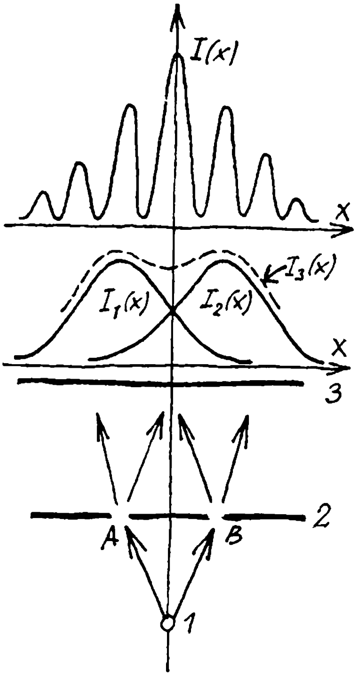
From an observation of the behaviour of microparticles in the interferometer it should be concluded that, firstly, the phenomenon of interference is inherent in *all* microparticles and, secondly, it should be explained by the properties not of *ensembles* of microparticles but of *individual* microparticles.

We shall try to "follow" the motion of an individual microparticle (say, electron) in the interferometer shown in Fig. 7.1. The electron emerges from point *1*, passes through the slits in screen *2* and is finally registered at a certain point x on screen *3*. By repeating the experiment for a large number of single electrons we notice two fairly interesting facts.

The first fact is the impossibility of predicting precisely at what point x a particular electron will be registered. The experimental conditions are the same for each electron (remember that the electrons pass through the interferometer one by one) and yet each electron "behaves in its own way"; moreover, one cannot predict the way in which it will behave. This remark applies to every single electron. However, by following a large number of electrons, we observe a pattern in the distribution of their incidence on the screen *3*, shown by a kind of the interference curve $I(x)$. Moreover it is immaterial whether we observe the distribution of the incidences of a large number of single electrons or the distribution of the incidences of electrons from a beam. Thus, the unpredictability concerning the behaviour of an individual microparticle is associated with the predictability concerning the behaviour of a large number of microobjects.

The second fact is connected with the specific nature of the passage of an electron through the slits in the screen. Let us close slit B; in this case we observe the distribution of incidences on the screen, as described by curve $I_1(x)$ (Fig. 7.2). Let us open slit B but close slit A; in this case the distribution $I_2(x)$ is observed. By opening both slits, we do not get the additive distribution $I_1(x) + I_2(x)$ described by the curve $I_3(x)$ in the diagram but the *interference* distribution $I(x)$ which was noted earlier. It is this fact that is especially remarkable. If we suppose that each electron passes through any one of the slits, the appearance of the interference distribution $I(x)$ forces us to admit that the electron in some way "perceives" the other slit, otherwise, it does not matter for an electron passing through one slit whether the neighbouring slit is open or closed and thus the distribution of incidences with both slits open must be described not by the interference curve but by the additive curve $I_3(x) = I_1(x) + I_2(x)$. The electrons passing through slit A should give the distribution $I_1(x)$, while those passing through slit B should give the distribution $I_2(x)$. The detector screen should then register the sum of these distributions. Since it is meaningless to talk about the electron "perceiving" we have to admit that the interference distribution $I(x)$ observed with both the slits open is associated with the passage of the electron somehow simultaneously through the two slits.

Fig. 7.2



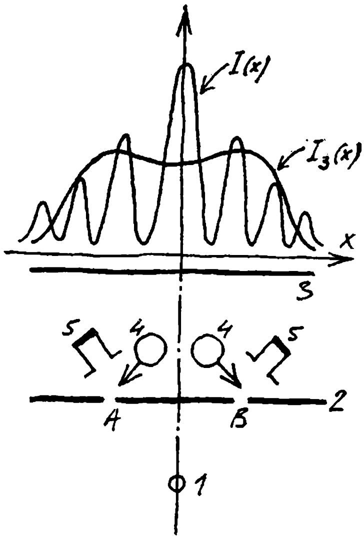
However, this admission does not simplify matters since it is not clear exactly in what way a single electron can pass simultaneously through two slits. Of course, we may assume that the electron at first passes through one slit, then it somehow returns through the other slit and again passes through the first slit (we get a sort of loop encompassing both the slits). Finally, we may assume that near the slits the electron is "spread out" (delocalized) in space, partially passing through one slit and partially through the other, and while impinging on the detector screen, it is again localized in space (we get a temporary splitting of the electron into two "halves"). There is no special need to prove that both the attempts made above to model the passage of electron through two holes are artificial. This becomes quite obvious if we turn to more complicated interferometers. Thus, in Michelson's interferometer, for example, one "half" of the microparticle will have to move towards one reflecting mirror and the other "half", towards the other (in completely the opposite direction).

Thus, the interference curve $I(x)$ greatly complicates the problem about the nature of the passage of a microparticle through a screen with two slits. If the microparticle passes through one slit, then either there should be no interference, or we must admit that the microparticle has a hidden ability to "perceive" the neighbouring slit. The only logical conclusion arising from the existence of interference is that the microparticle passes simultaneously through two slits, though the mechanism of such an unusual passage is not clear. In such a situation, obviously, a direct experiment could be helpful. Why shouldn't we try to "spy" on the electron to see exactly in what way an electron passes through the slits in the screen? Such experiments were actually conducted. Let us see what they led to.

Experiment 2 ("Observing" a Microparticle in the Interferometer)

Let us imagine that near the slits A and B of screen *2* we have light sources *4* and photodetectors *5* (Fig. 7.3), designed for "observing" the passage of electron through the screen with slits (the photodetectors register light scattered by the electron). If the electron simultaneously passes through both the slits both the photodetectors are activated simultaneously. But if the electron passes through either one of the slits, only one detector is activated; in this case we shall also know through which slit the given electron passes.

Fig. 7.3



So, we place an electron source at point *1*, switch on the light sources *4* and watch the photodetectors *5*. We shall assume that the electrons pass through the apparatus one by one: the source emits an electron only after the preceding one has reached the detector screen. What does the experiment show? It always turns out that *only one* photodetector (either left or right) is activated and both photodetectors are never activated simultaneously. It means that the electron passes not through two slits but only through one. Moreover, we can always indicate the slit through which any electron passes.

The reader may surmise that to explain interference we again have to start talking about an electron "perceiving" the neighbouring slit by some secret means, while passing through a slit. We shall not jump to conclusions but shall first carry out the experiment to the end; we obtain a sufficiently large number of events of electron incidence on the detector screen *3* and see how they are distributed. Here, we get a surprise. On screen *3* we get not the interference curve $I(x)$ but the additive curve $I_3(x)$.

We repeat the experiment after switching off the light sources (thus depriving ourselves of the possibility of "observing" the passage of the electrons through the slits). In this case we again observe the interference curve $I(x)$.

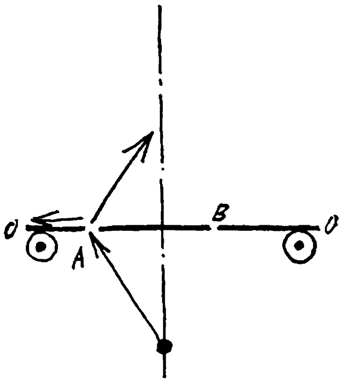
The situation is such that interference occurs when light sources are switched off and is absent when they are switched on. As soon as we try to control the process of passage of electrons through two open slits, the interference disappears. In other words, our observation of the behaviour of electrons near the slits destroys the interference!

A change in the nature of the motion of electrons upon the switching on of the light sources has a simple physical explanation: this change is the result of collision of photons with the electrons "being controlled" In the process of measurement some influence on the object under investigation is inevitable. Here only one thing is important—can this influence be made sufficiently small? Maybe the experiment considered above was too crude? Maybe we should somehow try to observe the electrons more delicately, so that the interference picture is not destroyed by this.

But how to reduce the influence of a photon on an electron? It is obvious that a reduction in the light intensity of the sources would not yield anything—light intensity is associated with the number of photons in a beam, thus a reduction in the intensity will simply result in an increase in the number of "unregistered" electrons. We must reduce the energy of a single photon. But for this we shall have to increase the wavelength of the radiation and this will lead to an increase in the spatial delocalization of the photon (a photon is localized in space with an accuracy not exceeding its wavelength) and thus for a wavelength exceeding the distance between the slits the photon will no longer be in a position to register a particular slit.

But, may be, we could think of some other experiment—without resorting to the scattering of photons by electrons? For example, isn't it possible to try to construct an extremely light screen with slits in such a way, that it could move to the left or right upon being struck by individual electrons? The screen deflects to the left if an electron passes through the left slit and to the right if it passes through the right slit (Fig. 7.4). But if the electron passes through two slits simultaneously, the screen will not move at all. Thus, we just have to follow the movement of the screen. It would appear that at least in principle the aim has been achieved—the required

Fig. 7.4



delicate experiment has been conceived. But it is meaningless to set up such an experiment. To make sure that this is so, we recall the uncertainty relation for momentum and coordinate. It follows from this relation that if the experimental conditions really permit us to register the momentum of the screen due to a recoil from the electron impingement, the same condition must lead to an uncertainty in the position of the screen on the line *OO* (Fig. 7.4). Consequently, the shift in such a screen does not permit one to draw any conclusion on the nature of passage of an electron through the slits. If, on the other hand, we fix the position of the screen on the line *OO*, then it is easy to see that a measurement of the momentum of its recoil will become impossible.

Several attempts were made to devise such an experiment in which the passage of electrons through a screen with slits could be "controlled" without seriously influencing the electrons themselves (so that the interference is not destroyed). But all these attempts proved futile. As a result, we must admit that the above conclusion regarding the destruction of interference caused by observing the behaviour of electrons near the slit, is of a fundamental nature. In other words, the effect of observation (measurement) destroying interference cannot be eliminated in principle.

A Brief Interlude

He was going into one room
And by mistake entered another...
Griboiedoff (*Gore ot Ouma*)

Reader: This means we were not able to determine exactly how an electron passes through a screen with slits—through one slit or simultaneously through both the slits?

Author: Indeed, we couldn't.

Reader: But then experiment 2 did not attain its goal. Was it necessary to consider it?

Author: Yes, it was. The experiment did not answer the question posed by us. So what? It just means that the question was not formulated properly. We see that we cannot question all the phenomena of nature.

Reader: Does the whole idea of the experiment lie in its negative result?

Author: This is not to be ignored. However, as we shall see later, it also contains a positive result of utmost importance. In fact, we were looking for one thing, but we found another.

Reader: And what is that?

Author: Let us not make haste. We shall first consider our system o fundamental experiments to the end.

Experiment 3 (Passage of Photons Through Polarizers)

Let us pass a beam of light through a polarizer, say, a tourmaline crystal. A *linearly polarized* light beam emerges from the crystal. The direction of polarization of the beam is determined by the orientation of the polarizer with respect to the beam (the direction of polarization coincides with the direction of the axis of the polarizer). Let us denote the intensity of the linearly polarized light beam through I.

Further, we place a second polarizer in the path of the linearly polarized light beam and consider the following three cases: (a) the axis of the second polarizer is parallel to the axis of the first; (b) the axis of the second polarizer is perpendicular to the axis of the first; (c) the axis of the second polarizer makes an angle α with the axis of the first. We shall measure the intensity of light emerging from the second polarizer. In case (a) we get intensity I, in case (b) we do not get anything, while in case (c) we get a light beam of intensity $I \cos^2 \alpha$, polarized along the axis of the second polarizer. These cases are shown in Fig. 7.5, where AA and BB are the directions of the axis of the first and the second polarizers, respectively.

The above experiment is well known in classical optics. However, like the Young experiment on interference, it has a direct relation to quantum mechanics. As in the case of interference we shall reduce the intensity of the light beam till the photons pass one by one through our

Fig. 7.5

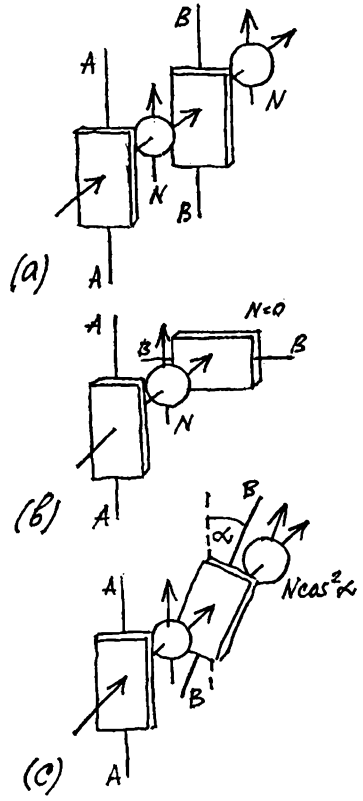
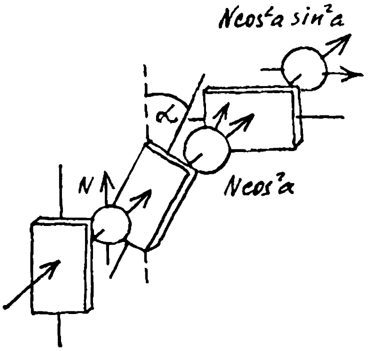


Fig. 7.6



set-up. We shall consider the cases illustrated in Fig. 7.5 as applied to single photons.

First of all, we recall that a photon is characterized by a definite *polarization*. Moreover, this polarization corresponds to the polarization of the classical light wave from which the photon under consideration has been "taken" In particular, this means that after the first polarizer we shall have linearly polarized (polarized in the direction of the axis of the polarizer) photons. In the following we shall "deal" only with these photons and shall call them "initial photons"

In case (a) the initial photon always passes through the second polarizer; in case (b), on the contrary, it never passes the second polarizer. These results are not unexpected. But what happens in case (c)? It turns out that in this case the photon may pass through the second polarizer or it may not. Moreover, it is absolutely impossible to predict which of the two alternatives (passing or not passing) will be realized for a given initial photon. If it so happens that the photon passes through the second polarizer, its polarization will change—it will be polarized in the direction of the axis of the second polarizer. Thus, the fate of any particular individual photon is, in principle, unpredictable!

Let us assume further that there are N initial photons. We observe their passage through the second polarizer in the case (c) and see what happens. We find that if N is sufficiently large, the number of photons passed can be predicted fairly accurately; it will be about $N \cos^2 \alpha$. In this connection, we recall our earlier remark that the unpredictability in the behaviour of an individual microparticle is related to the predictability in the behaviour of a large number of microparticles (see Experiment 1). We can say that there is a definite probability of the initial photon passing through the second polarizer. This probability is equal to $\cos^2 \alpha$.

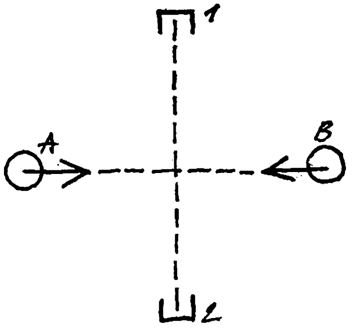
Let us now complicate the experiment. We use the situation shown in Fig. 7.5 (*c*) and add yet another (i.e. a third) polarizer, whose axis is perpendicular to the axis of the first polarizer. The three-polarizer system under consideration is shown in Fig. 7.6. Let N be the number of initial photons (i.e. photons passing through the first polarizer). After the second polarizer, as we already know, we shall have $N \cos^2 \alpha$ photons, the polarization of these photons coinciding with the axis of the second polarizer. Analysing further in the same way, we conclude that after the third polarizer, we must have $N \cos^2 \alpha \sin^2 \alpha$ photons; moreover, the polarization of these photons must coincide with the axis of the third polarizer. The experiment certainly confirms this conclusion.

There is nothing that appears astonishing in this (that is, of course, if we assume that our astonishment over the existence of two unpredictable possible behaviours of an individual photon has somewhat diminished). And yet there is something here which contradicts our usual concepts. Let us remove the second polarizer. Then no photons will be observed after the third polarizer. This creates a fairly interesting situation. Photons pass through this apparatus, as if they are "filtered" first through the second polarizer and then through the third. As a result, we at first have N photons, then $N \cos^2 \alpha$, and we are finally left with $N \cos^2 \alpha \sin^2 \alpha$ photons. We remove one of the "filters" and thus, it would appear, improve the conditions for passage of photons through the given apparatus. However, in actual practice it turns out quite differently—now the photons do not pass through the apparatus at all!

Experiment 4 (Scattering of Microparticles by Microparticles)

We shall consider *elastic collisions* of microparticles and use for convenience the centre of mass system for the colliding particles. Figure 7.7 shows experimental diagram related to the system of the centre of mass of the particles. Here, A and B are particle beams, *1* and *2* are the counters for scattered particles, deployed on the line perpendicular to the direction of motion of the particles before collision. Thus, we consider here the scattering of particles through an angle of 90° in the centre of mass system.

Fig. 7.7



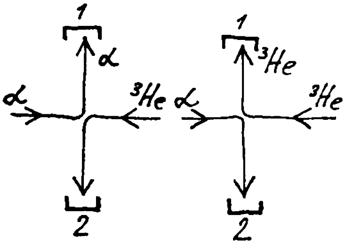
We note that the picture of the process in the centre of mass system may considerably differ from the analogous picture in the laboratory system. Thus, for example, in the laboratory system the counters *1* and *2* may not be on the same line. Besides, in actual practice only one beam of particles (for example, particles of type A) may be used while the particles of the other type (type B) constitute the stationary target. It is assumed that every time the experiment in the laboratory system is conducted in such a way that the diagram shown in Fig. 7.7 is applicable for the centre of mass system of the particles.

We shall consider different examples as applied to the above diagram, measuring each time the probability of scattering of particles by the number of simultaneous activations of counters *1* and *2*.

First example. Particles of type A are α-particles (^{4}He nuclei), particles of type B are ^{3}He nuclei; counter *1* registers only α-particles, counter *2*, only ^{3}He nuclei. Let w be the probability of scattering measured in this case.

Second example. The particles are the same, but now each counter can register both α-particles and ^{3}He nuclei. In this case the measured probability of scattering turns out to be $2w$. This result appears quite natural—the doubling of the probability w is associated with the realization of the two alternatives shown in Fig. 7.8.

Fig. 7.8



Third example. We replace ^{3}He nuclei by α-particles. Let the α-particles be scattered now by α-particles. It would appear that in this case the scattering probability must be the same (or nearly the same) as in the previous case, i.e. $2w$. The experiment, however, yields quite a different result, $4w$. A "mere" replacement of ^{3}He nuclei by ^{4}He nuclei has doubled the scattering probability! Still more unexpected results are observed by taking into account the spin states of the colliding particles (in the case of α-particles the question of taking spin into account did not arise since α-particles do not have spin). In this connection let us consider scattering of electrons by electrons. We recall that an electron may exist in two spin states ($\sigma = 1/2, -1/2$). Electrons created as a result of photoelectric emission, for example, appear in one spin state or the other with same probability. Such electron beams are termed nonpolarized; half the electrons in them have $\sigma = 1/2$ and the other half, $\sigma = -1/2$. If we take special measures, we may obtain a polarized electron beam in which all electrons are in the same spin state. Having made these remarks, let us now return to the diagram in Fig. 7.7 and continue the list of examples under consideration. Moreover, we shall assume that the energies of the colliding particles are considerably small, hence, the possibility of an electron changing its spin state upon collision need not be taken into consideration.

Fourth example. The two electron beams are nonpolarized. Let the scattering probability measured in this case be w_e.

Fifth example. The electron beams are polarized but in both directions. For example, *A*-electrons have spin $\sigma = 1/2$ and *B*-electrons, $\sigma = -1/2$. In this case the scattering probability turns out to be $2w_e$.

Sixth example. The electron beams are polarized in the same direction. In this case the counters *1* and *2* are "silent" —the scattering probability is zero!

As will be seen later, the results of experiments on the scattering of microparticles reveal fundamental quantum-mechanical laws.

Conclusion

We have thus considered a system of four fairly simple experiments. While considering them we emphasized the unexpectedness of the results, which indicates the impossibility of their classical explanation. The system of basic experiments could have been enlarged and supplemented by more complex experiments. However, we shall not do this. We content ourselves with considering the four experiments, as we think that all the basic principles of quantum mechanics are fairly clearly revealed in them. On the basis of the experiments considered, we move on to build up in the following sections a system of quantum-mechanical concepts which essentially expresses the physical foundations of quantum mechanics.

Section 8 Amplitudes of Transition Probabilities (Formulation of Basic Principles)

Introduction to the Concept of Amplitude of Transition Probability

We suppose that for a certain microparticle definite *initial* and *final* states (s-state and f-state, respectively) are considered. The specific characteristics of these states as well as the nature of the microparticle are immaterial for the present. As has been pointed out earlier, the transition of the microparticle between the two given states has, as a rule, a *probabilistic* character. We therefore introduce into the picture the *transition probability* $w_{s\to f}$. In quantum mechanics, apart from transition probability, the concept of the *amplitude of the transition probability* $\langle f \mid s\rangle$* is also introduced. Generally speaking, it is a complex number, the square of whose modulus is equal to the transition probability:

$$w_{s\to f} = |\langle f \mid s\rangle|^2. \tag{8.1}$$

Note that the amplitude of the transition probability is written so that the initial state is on the right and the final one on the left (as if it were read from right to left). Henceforth for brevity we shall call the amplitude of the transition probability the transition amplitude (and sometimes even more briefly simply the amplitude).

Besides introducing the concept of the transition amplitude, which is of utmost importance to quantum mechanics, we shall devote this section to a formulation of a number of basic principles in their most general form. The reader should not be perplexed over the formality of the exposition in this section. It will be compensated for in the next section where we shall demonstrate the principles indicated in this section using specific examples. Moreover, among other things, we shall consider the con-

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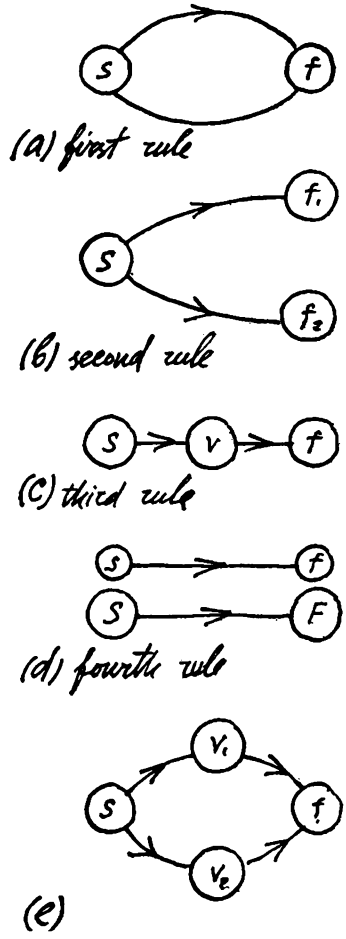
* The treatment of quantum mechanics on the basis of probability amplitudes is given in books by Feynman [3-5] and Dirac [9].

nection between these principles and the experiments discussed in Sec. 7. This will provide, on one hand, grounds for the formal description of the principles and, on the other hand, an explanation of the astonishing experimental results.

Basic Rules of Working with Amplitudes

We shall indicate four basic rules of working with transition amplitudes. These rules should be considered as postulates forming the basis of a system of quantum-mechanical concept which are in conformity with experiment.

Fig. 8.1



First Rule. We assume (Fig. 8.1(a)) that there are several *physically indistinguishable* ways (paths) in which a microparticle can move from s-state to f-state. In this case, the resulting transition amplitude is the sum of the amplitudes corresponding to the different modes of transition:

$$\langle f \mid s\rangle = \sum_i \langle f \mid s\rangle_i \qquad (8.2)$$

(the index i denotes the i-th mode of transition).

Second Rule. We assume (Fig. 8.1(b)) that there are several *final* states (f_1, f_2, ., f_i, . .) and that we are considering the probability of transition to *any* of these states, no matter which state it is. In this case, the resulting transition probability $|\langle f \mid s\rangle|^2$ is the *sum of the transition probabilities* to the various final states:

$$|\langle f \mid s\rangle|^2 = \sum |\langle f \mid s\rangle_i|^2. \qquad (8.3)$$

Third Rule. Let us assume (Fig. 8.1(c)) that the transition $s \rightarrow f$ takes place through some intermediate state (v-state). In this case we introduce the idea of the amplitude of the successive transitions $s \rightarrow v$ and $v \rightarrow f$ (corresponding to the amplitudes $\langle v \mid s\rangle$ and $\langle f \mid v\rangle$); the resulting amplitude is the product of these amplitudes:

$$\langle f \mid s\rangle = \langle f \mid v\rangle\langle v \mid s\rangle. \qquad (8.4)$$

In other words, if the transition is broken up into successive steps, the transition amplitude is expressed by the product of the amplitudes of the separate steps. It should be noted that if the notation in (8.4) is read from right to left, then the states will be designated in proper sequence: first the initial state, followed by the intermediate state and then the final state.

Fourth Rule. Suppose (Fig. 8.1(d)) we have two independent microparticles. Suppose one microparticle undergoes a transition $s \rightarrow f$ and the other simultaneously undergoes a transition $S \rightarrow F$. In this case the resulting transition amplitude for the system of microparticles is given by the *product* of the transition amplitudes for the individual microparticles:

$$\langle fF \mid sS\rangle = \langle f \mid s\rangle\langle F \mid S\rangle \qquad (8.5)$$

We can see that the second, third and fourth rules appear quite natural since, together with (8.1), they represent well-known theorems, i.e. the theorem of addition of probabilities (second rule) and the theorem of multiplication of probabilities of independent events (third and fourth rules). Only the first rule, which may be called the *rule of addition of amplitudes*, appears unusual. In a certain sense, the entire system of quantum-mechanical concepts is based on the rule of the addition of amplitudes.

Distinguishable and Indistinguishable Alternatives. Interference of Amplitudes

Suppose that the transition of a microparticle from the initial to the final state ($s \to f$ transition) always takes place through one of the intermediate states (v_1, v_2, . . ., v_i, . . .) (Fig. 8.1(*e*)). In this case, one or the other mode of transition $s \to f$ (one alternative or the other) is determined by the "participation" of the corresponding intermediate state in the transition.

We take two different cases. Suppose in the first case the intermediate state through which a given transition takes place is known. This is the case of *physically distinguishable alternatives.* To describe this we must combine the second and the third rules. The transition probability that we obtain as a result will be of the form

$$|\langle f \mid s\rangle|^2 = \sum_i |\langle f \mid v_i\rangle \langle v_i \mid s\rangle|^2. \qquad (8.6)$$

One might ask: where does the second rule come in if it only involves the various final states? As a matter of fact, if we know the intermediate state at which the microparticle arrives, it may be treated as the final state of the first step of the transition. We fix the microparticle in this state and temporarily stop the experiment here. One microparticle will be fixed in one state, the others in various other states, so, a situation with different final states actually arises. We stress here that distinguishability of alternatives is connected with the actual existence of different final states (even if in the given experiment they play the role of intermediate states).

In the second case, we don't know the intermediate state through which a particular transition takes place. This is the case of physically indistinguishable alternatives. To describe this case we should combine the first and the third rules. The resulting transition probability will be of the form

$$\langle f \mid s\rangle = \sum_i \langle f \mid v_i\rangle \langle v_i \mid s\rangle. \qquad (8.7)$$

The result (8.7) is a specifically quantum-mechanical one. When it holds, we speak of the *interference of amplitudes of transitions* through different intermediate states. We emphasize that the interference of amplitudes is possible only under conditions of the physical indistinguishability of the alternatives corresponding to the given experiment (the microparticle is not fixed in the intermediate state, hence we are actually dealing only with one final state). Changing over from amplitude in (8.7) to the probability of transition, we get

$$|\langle f \mid s\rangle|^2 = \sum_i |\langle f \mid v_i\rangle \langle v_i \mid s\rangle|^2. \tag{8.8}$$

The difference between the cases of physically distinguishable and indistinguishable alternatives becomes clear from a comparison of probabilities (8.6) and (8.8). While in the first case the probabilities of the alternatives are added, in the second case it is the amplitudes of the probabilities of alternatives which are added.

Transition Involving Two Microparticles

It is interesting to expand somewhat the fourth rule regarding the simultaneous transition of two microparticles. Let us suppose (Fig. 8.2(*a*)) that one microparticle undergoes a transition $s \rightarrow f$ through the intermediate v-state and that another microparticle simultaneously undergoes the transition $S \rightarrow F$ through the intermediate V-state. By combining the third and fourth rules we represent the transition amplitude for the system of microparticles in the following form:

$$\langle fF \mid sS\rangle = \langle f \mid v\rangle \langle v \mid s\rangle \langle F \mid V\rangle \langle V \mid S\rangle. \tag{8.9}$$

Let us assume further (Fig. 8.2(*b*)) that both the microparticles in the process of their transitions pass through one and the same intermediate v_1-state. Then (8.9) must take the form

$$\langle fF \mid sS\rangle = \langle f \mid v_1\rangle \langle v_1 \mid s\rangle \langle F \mid v_1\rangle \langle v_1 \mid S\rangle. \tag{8.10}$$

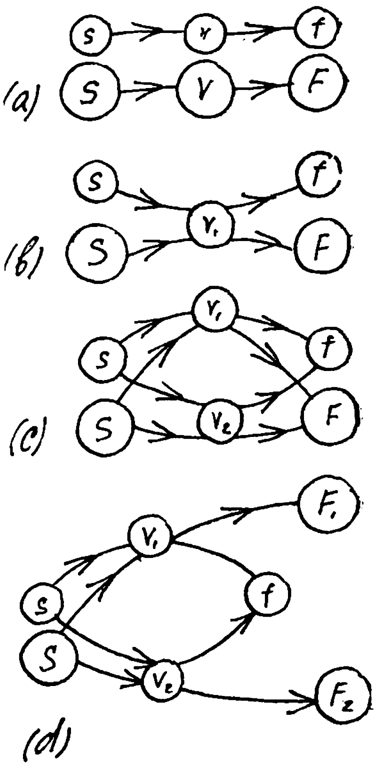
Finally, we assume (Fig. 8.2(*c*)) that each microparticle realizes a number of physically indistinguishable alternatives through different intermediate states (v_1, v_2, . . ., v_i). Moreover, every intermediate state is common to both the microparticles. In this case generalizing result (8.10) by combining it with the first rule, we get

$$\langle fF \mid sS\rangle = \sum_i \langle f \mid v_i\rangle \langle v_i \mid s\rangle \langle F \mid v_i\rangle \langle v_i \mid S\rangle. \tag{8.11}$$

Destruction of the Amplitude Interference

The interference of amplitudes is destroyed when the alternatives become distinguishable. We shall show how this happens by using transitions involving two microparticles [by using the result (8.11)].

Fig. 8.2



For brevity, we shall call the microparticle undergoing the $s \to f$ transition the s-particle and the one performing $S \to F$ transition as the S-particle. We assume that S-particles are used to "control" (observe) through which intermediate state the transition of the s-particle takes place in each specific case. To exercise this control, we must have as many final F-states (denoted by F_1, F_2, . . ., F_i) as there are intermediate v-states to be "controlled" and arrange it so that an S-particle passing, for example, through the v_i-state, goes just to the F_i-state. This is schematically shown in Fig. 8.2 (*d*). Here each intermediate state appears to be "bound" to a definite final F-state. We simply have to watch the final state in which a "controlled" S-particle appears in each case. Whereas earlier (in the absence of S-particles) the alternatives were indistinguishable, so that it was not known in each case through which intermediate state the transition of the s-particle took place, the different alternatives now become physically distinguishable. An S-particle observed in any F-state unambiguously indicates the intermediate state through which a given transition took place. According to the remarks made above, the use of S-particles for distinguishing intermediate states must lead to a destruction of the interference of amplitudes. Let us verify this now.

If only the S-particle which has passed through the intermediate v_i-state comes to the F_i-state, then we have as a result $\langle F_i \mid v_k \rangle = 0$ for $k \neq i$. Using (8.11) we get from this

$$\langle fF_i \mid sS \rangle = \langle f \mid v_i \rangle \langle v_i \mid s \rangle \langle F_i \mid v_i \rangle \langle v_i \mid S \rangle. \qquad (8.12)$$

Since the F_i-states are the various final states, we get, according to second rule, the following expression for the resulting transition probability of the "controlled" s-particle:

$$|\langle f \mid s \rangle|^2 = \sum_i |\langle fF_i \mid sS \rangle|^2$$

$$= \sum_i |\langle f \mid v_i \rangle \langle v_i \mid s \rangle \langle F_i \mid v_i \rangle \langle v_i \mid S \rangle|^2. \qquad (8.13)$$

If we further assume that the amplitude $\langle F_i \mid S \rangle$ is the same for all i (which is often the case in practice), then, denoting this amplitude by a for brevity, we rewrite (8.13) in the form

$$|\langle f \mid s \rangle|^2 = |a|^2 \sum_i |\langle f \mid v_i \rangle \langle v_i \mid s \rangle|^2. \qquad (8.14)$$

Thus while result (8.8) is obtained in the absence of S-particles (in the absence of "control"), we now have the result (8.14). It is easy to see that it corresponds to (8.6)—

we destroy the interference of amplitudes by establishing a "control" over the intermediate states, i.e. by turning the physically indistinguishable alternatives into distinguishable ones.

Section 9

Amplitudes of Transition Probabilities (Demonstration of Basic Principles)

Behaviour of a Microparticle in the Interferometer and Interference of Amplitudes

Using the concept of the transition amplitude and the rules relating to the amplitudes, let us turn to experiment 1 discussed in Sec. 7. An electron emerges from the initial s-state, passes through a screen with slits A and B, each of which corresponds to its intermediate state (A-state and B-state, respectively) and is finally registered in its final x-state, i.e. at the point with coordinate x on the detector screen.

Suppose that slit A is open and slit B is closed. In this case $\langle x \mid s\rangle_A = \langle x \mid A\rangle\langle A \mid s\rangle$. The probability of transition $s \rightarrow x$, i.e. the probability of the electron being registered at point x of the detector screen, is of the form

$$|\langle x \mid s\rangle_A|^2 = |\langle x \mid A\rangle \langle A \mid s\rangle|^2. \qquad (9.1)$$

We denote this probability by $I_1(x)$, and recall that this is how we denoted the distribution of electron incidences on the detector screen in experiment 1 (Sec. 7) under the conditions that slit A is open and slit B is closed. For the probability of an electron being registered at point x in the case when slit B is open and slit A is closed, we may write the analogous expression

$$|\langle x \mid s\rangle_B|^2 = |\langle x \mid B\rangle \langle B \mid s\rangle|^2 = I_2(x). \qquad (9.2)$$

Now let us open both the slits. Since it is impossible to indicate through which slit any electron passes (the alternatives are indistinguishable), we have, consequently,

$$\langle x \mid s\rangle = \langle x \mid A\rangle\langle A \mid s\rangle + \langle x \mid B\rangle\langle B \mid s\rangle. \qquad (9.3)$$

Denoting the transition probability $|\langle x \mid s\rangle|^2$ by $I(x)$ (we denoted the interference curve observed on the detector screen with both slits open in the same way in Sec. 7), and taking into account (9.1) and (9.2) we get from this

$$I(x) = |\langle x \mid A\rangle \langle A \mid s\rangle + \langle x \mid B\rangle \langle B \mid s\rangle|^2$$
$$= I_1(x) + I_2(x) + \langle x \mid s\rangle_A \langle x \mid s\rangle_B^* + \langle x \mid s\rangle_A^* \langle x \mid s\rangle_B. \qquad (9.4)$$

It is easy to see that the resulting probability of transition is not equal to the sum of probabilities of the transitions through slits A and B $[I(x) \neq I_1(x) + I_2(x)]$.

In addition to the components $I_1(x)$ and $I_2(x)$, the right-hand side of expression (9.4) contains two additional terms caused by the interference of amplitudes. It is these terms that account for the difference of the interference curve $I(x)$ from the additive curve $I_3(x) = I_1(x) + I_2(x)$.

Thus, the interference distribution of the electron incidences on the detector screen observed with both the slits open in experiment 1 in Sec. 7 is a consequence of the result (9.4), i.e. a consequence of the interference of the amplitudes of two possible transitions of the electron from the given initial state to the given final state.

Destruction of Interference of Amplitudes upon "Controlling" the Behaviour of a Microparticle in the Interferometer

Fig. 9.1

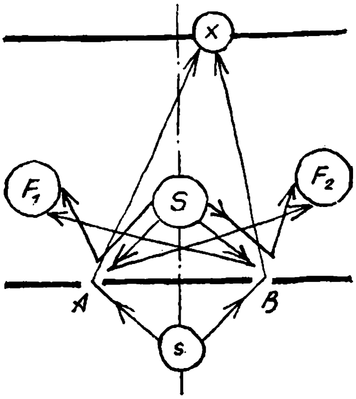


Figure 9.1 depicts schematically the fundamental experiment 2 considered in Sec. 7. Here s is the electron source, S is the photon source, F_1 and F_2 are photoelectric counters which fix the two final states of photons scattered by electrons in the vicinity of slits A and B. To begin with, we shall assume that the photons scattered in the vicinity of either of the slits may be registered in the F_1-state as well as the F_2-state (which corresponds to the use of radiation with a sufficiently large wavelength). In this case, obviously, the photons don't "control" the passage of electrons through the screen with slits. We denote the transition amplitudes thus:

for electrons

$$\langle x \mid A\rangle\langle A \mid s\rangle = \varphi_1, \quad \langle x \mid B\rangle\langle B \mid s\rangle = \varphi_2, \tag{9.5}$$

for photons (taking into account the symmetry of the photon transition which can be clearly seen from Fig. 9.1)

$$\begin{aligned}\langle F_1 \mid A\rangle\langle A \mid S\rangle &= \langle F_2 \mid B\rangle\langle B \mid S\rangle = \psi_1,\\ \langle F_2 \mid A\rangle\langle A \mid S\rangle &= \langle F_1 \mid B\rangle\langle B \mid S\rangle = \psi_2.\end{aligned} \tag{9.6}$$

Using these notations and result (8.11), we write the following expression for the probability amplitude of simultaneously registering an electron at point x and a photon in the F_1-state

$$\langle xF_1 \mid sS\rangle = \varphi_1\psi_1 + \varphi_2\psi_2. \tag{9.7}$$

Correspondingly, for the probability amplitude of simultaneously registering the electron at point x and the photon in the F_2-state, we write

$$\langle xF_2 \mid sS\rangle = \varphi_1\psi_2 + \varphi_2\psi_1. \tag{9.8}$$

The probability of an electron being registered at point x, independent of where the photon is registered, is of the form (according to second rule from Sec. 8)

$$|\langle x \mid s\rangle|^2 = |\langle xF_1 \mid sS\rangle|^2 + |\langle xF_2 / sS\rangle|^2. \tag{9.9}$$

Substituting (9.7) and (9.8) into this, we find

$$|\langle x \mid s\rangle|^2 = (|\varphi_1|^2 + |\varphi_2|^2)(|\psi_1|^2 + |\psi_2|^2) + (\varphi_1\varphi_2^* + \varphi_1^*\varphi_2)(\psi_1\psi_2^* + \psi_1^*\psi_2). \tag{9.10}$$

Thus the resulting probability of the electronic transition $s \to x$ is made up of two components. The first is the sum of the probabilities of transitions through slits A and B (considered separately) multiplied by $(|\psi_1|^2 + |\psi_2|^2)$. The second component has an interference character; it is due to the interference of amplitudes. Because of the existence of this component, we observe the interference distribution of the impingements of electrons on the detector screen.

Thus, when the photons don't "control" the passage of electrons through a screen with slits, we observe the interference effect described by the expression (9.10).

Remember that in the example considered here we assumed a sufficiently long wavelength for the radiation. Let us now reduce the wavelength. This will lead to a reduction in the probability of a photon scattered by an electron falling in the "alien" counter (for example, the probability of a photon scattered near slit A being detected by counter F_2). This means that with a decrease in the radiation wavelength, the amplitude ψ_2 must decrease. A decrease in the amplitude ψ_2 will also decrease the relative contribution of the interference component as is seen clearly from (9.10). As a result, the interference pattern observed on the detector screen gets blurred.

For a sufficiently small radiation wavelength, it is possible to accurately "control" the passage of electrons through a screen with slits. In this extreme case a photon scattered near either of the slits arrives only at its "own" detector. This means that $\psi_2 = 0$. Substituting this result in (9.10) we get

$$|\langle x \mid s\rangle|^2 = |\psi_1|^2 (|\varphi_1|^2 + |\varphi_2|^2). \tag{9.11}$$

Thus, "control" of the passage of electrons through a screen with slits leads to a destruction of the interference amplitudes, and consequently to a disappearance of the interference distribution of the electrons impingements on the detector screen. The result (9.11) is in complete accord with (8.14). "Control" makes the alternatives corresponding to the passage of an electron through different slits distinguishable.

From this example we see that there is a subtle point involved in the question of the distinguishability of alternatives: in addition to the complete indistinguishability and complete distinguishability, there is a continuous spectrum of intermediate situations which should be identified with partial distinguishability. The result (9.11) describes the limiting case of complete indistinguishability of the alternatives under consideration ($\psi_2 = 0$). The opposite extreme case of the complete indistinguishability of alternatives envisages equal probabilities for a photon falling on its "own" or the "other" detector: $\psi_1 = \psi_2$. In this case it is easy to see that expression (9.10) assumes the form

$$|\langle x \mid s\rangle|^2 = 2 \mid \psi_1 \mid^2 \mid \varphi_1 + \varphi_2 \mid^2. \tag{9.12}$$

Results (9.11) (the squares of the moduli of electron amplitudes are added) and (9.12) (the electron amplitudes themselves are added up) are obtained from (9.10) as particular (limiting) cases. The general expression (9.10) describes the intermediate situation corresponding to partial distinguishability of the alternatives under consideration, differing from one another by the magnitude of the interference component. The less the interference component is the greater is the degree of distinguishability of alternatives.

Thus, distinguishability and indistinguishability are by no means discrete. Complete indistinguishability is continuously transformed into complete distinguishability through *intermediate* situations corresponding to *partial distinguishability*. In Sec. 10 we shall return to the question of partial distinguishability from the point of view of the principle of superposition.*

Scattering of Microparticles and Interference of Amplitudes

We turn to experiment 4 of Sec. 7. Let s_1 and s_2 be the initial states of the colliding microparticles and f_1 and f_2 be the final states registered by the corresponding counters. In Sec. 7 we considered the scattering through an angle of 90° in the centre of mass system of the colliding particles. For a more general approach, we shall consider scattering through an angle θ. In this case the counters are arranged along a straight line at an angle θ with the initial direction of the colliding particles—see Fig. 9.2(*a*) (the analysis is carried out, as before, in the centre of mass system of particles).

If upon scattering one microparticle undergoes a transition $s_1 \rightarrow f_1$, and the other a transition $s_2 \rightarrow f_2$ (Fig. 9.2(*b*)), the scattering amplitude has the form

$$\varphi(\theta) = \langle f_1 \mid s_1\rangle\langle f_2 \mid s_2\rangle. \tag{9.13}$$

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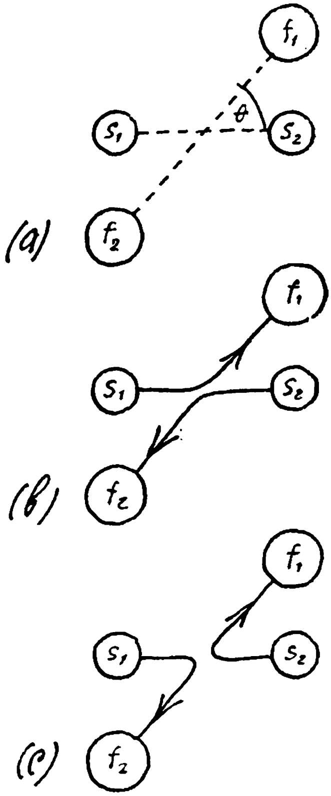
* Partial distinguishability of alternatives is described in detail in [31].

Another alternative is also possible: one microparticle undergoes a transition $s_1 \to f_2$ and the other, $s_2 \to f_1$ (Fig. 9.2(c)). In this case the scattering amplitude has the form

$$\varphi(\pi-\theta)=\langle f_2 \mid s_1\rangle\langle f_1 \mid s_2\rangle. \tag{9.14}$$

Fig. 9.2



Suppose that the microparticles are *completely distinguishable*. This may mean, for example, that different kinds of microparticles, or the same kind of microparticles with different spin states are colliding. We first consider a situation when counter f_1 registers microparticles from s_1 only and counter f_2 from s_2 only. In this case the probability of a simultaneous activation of both counters is

$$|\varphi(\theta)|^2=|\langle f_1 \mid s_1\rangle\langle f_2 \mid s_2\rangle|^2. \tag{9.15}$$

Second situation: each counter registers any of the microparticles participating in the collision (the situation corresponds to the second example in experiment 4 of Sec. 7). We should now consider two possible alternatives. Since these alternatives are also completely distinguishable for completely distinguishable microparticles, the probability of simultaneous activation of both counters will be given in this case by the expression

$$|\varphi(\theta)|^2+|\varphi(\pi-\theta)|^2=|\langle f_1 \mid s_1\rangle\langle f_2 \mid s_2\rangle|^2 + |\langle f_2 \mid s_1\rangle\langle f_1 \mid s_2\rangle|^2. \tag{9.16}$$

For $\theta=\pi/2$, we get the probability $2|\varphi(\pi/2)|^2$—it is this doubling of probability which we mentioned in the second example in experiment 4 of Sec. 7.

Further, we assume that the microparticles are *completely indistinguishable*. This means that microparticles of the same type and in the same identical state are considered. Note that the identity of microparticles mentioned in Sec. 6 is a *necessary* condition for complete indistinguishability.

If the microparticles are completely indistinguishable, so are the alternatives shown in Fig. 9.2(b), (c). In this case we should sum not the probabilities of the alternatives, but their amplitudes. The probability of simultaneous activation of the counters should be determined by the expression

$$w=|\varphi(\theta)+\varphi(\pi-\theta)|^2. \tag{9.17}$$

When applied to the third example in experiment 4 of Sec. 7 (when we considered the scattering of α-particles by α-particles), the result assumes the form

$$w=|\varphi(\pi/2)+\varphi(\pi/2)|^2=4|\varphi(\pi/2)|^2. \tag{9.18}$$

It is this four-fold increase in the probability $|\varphi(\pi/2)|^2$ which was observed in the experiment.

Interference of scattering amplitudes is just one of the consequences of the complete indistinguishability of microparticles. Another consequence is that the probability of the simultaneous activation of counters should not change if we interchange s_1 and s_2, or, in other words, if we interchange the scattering amplitudes $\varphi(\theta)$ and $\varphi(\pi-\theta)$. If we proceed from these consequences, the probability may be formally written in the form

$$w = |\varphi(\theta) \pm \varphi(\pi-\theta)|^2. \tag{9.19}$$

The alternative with the "+" sign (interfering amplitudes have the same sign) is already familiar to us—it is the expression (9.17). The other alternative, when the amplitude with opposite signs interfere, is also formally possible. It is remarkable that nature "employs" this alternative as well; this can be verified by studying the results of experiments on scattering of electrons by electrons.

Thus, we assume that amplitudes with opposite signs interfere:

$$w_e = |\varphi(\theta) - \varphi(\pi-\theta)|^2 \tag{9.20}$$

and turn to the results of the indicated experiments. For $\theta = \pi/2$, the probability (9.20) vanishes. This corresponds to the sixth example in experiment 4 of Sec. 7. We recall that this example concerned the collision of electrons in the same spin state. It is in this case that we have two completely indistinguishable alternatives for the electrons*

If the colliding electrons are in different spin states (the fifth example in experiment 4), the alternatives are distinguishable. In this case the probability of the activation of the counters is given (as for distinguishable particles) by expression (9.17), which for $\theta = \pi/2$ leads to the familiar result $2|\varphi(\pi/2)|^2$. In the case of non-polarized electron beams (the fourth example in experiment 4), it should be remembered that the probability of collision between two electrons in similar spin states is 1/2. From this, taking (9.20) and (9.16) into account, we get the following expression for the probability of activation of

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* We shall henceforth omit the word "completely", but shall always mean it while speaking of distinguishable and indistinguishable alternatives. Partial distinguishability will be specially mentioned.

the counters

$$w_e = \frac{1}{2} \,|\, \varphi(\theta) - \varphi(\pi - \theta) |^2$$

$$+ \frac{1}{2} [\,| \varphi(\theta) |^2 + | \varphi(\pi - \theta) |^2]. \qquad (9.21)$$

Result (9.21) includes the summing of amplitudes (for cases characterized by indistinguishable alternatives) as well as the summing of probabilities (for cases characterized by distinguishable alternatives). For $\theta = \pi/2$, (9.21) gives the probability $w_e = |\varphi(\pi/2)|^2$. This is half the “classical probability” (i.e. the probability taking place in the case of indistinguishable alternatives) in complete agreement with the results of the experiments considered in Sec. 7.

Interference of Amplitudes and Division of Microparticles into Bosons and Fermions

Thus, we have found that the experiments on the scattering of microparticles described in Sec. 7 provide a good experimental background for the concept of the interference of amplitudes. Moreover, these experiments indicate the necessity for using not one but two different laws of interference, (9.17) and (9.20). We shall discuss the meaning of these two laws, assuming that $\theta = \pi/2$. According to (9.17), we have for α-particles

$$w = 4 \,|\, \varphi(\pi/2) |^2, \qquad (9.22)$$

and from (9.20) we have for the electrons in the same spin state

$$w_e = 0. \qquad (9.23)$$

The use of angle $\theta = \pi/2$ makes the scattering diagram symmetrical. If in addition we also take into account that the electrons are in similar spin states (α-particles do not have spin), we may conclude that expressions (9.22) and (9.23) describe the probabilities of α-particle pairs and electron pairs, respectively, appearing in the same state. Comparing this expression with the “classical probability” $2\,|\varphi(\pi/2)|^2$, we can come to the conclusion that one kind of microparticles (α-particles in this case) exhibits a tendency to “populate” a given state densely, while other microparticles (electrons in this case), on the contrary, may “populate” states only one at a time.

The fact that all microparticles in nature are divided, according to their behaviour in assemblies of similar particles, into two groups—*bosons* (with a tendency to densely “populate” the same state) and *fermions* (“populating” the states only one at a time) has already been mentioned in Sec. 1. Now we see that this fundamental fact is associated with the existence of two different laws for the interference of amplitudes. In the case of bosons, the amplitudes with like signs interfere; in the case of fermions, it is the amplitudes with opposite signs that interfere.

Bosonic Nature of Photons and Processes of Spontaneous and Induced Emission of Light

Let us consider an example: there are three atoms emitting photons (s_1, s_2, s_3) and three photon counters (f_1, f_2, f_3). The amplitude of probability that three transitions $s_1 \rightarrow f_1$, $s_2 \rightarrow f_2$, $s_3 \rightarrow f_3$ take place simultaneously is $\langle f_1 \mid s_1\rangle \langle f_2 \mid s_2\rangle \langle f_3 \mid s_3\rangle$. We assume that the photons are registered in the same state. We then have $3! = 6$ indistinguishable alternatives. Besides the one indicated above, the remaining five amplitudes are given by

$$
\begin{aligned}
&\langle f_1 \mid s_2\rangle \langle f_2 \mid s_1\rangle \langle f_3 \mid s_3\rangle, \\
&\langle f_1 \mid s_1\rangle \langle f_3 \mid s_2\rangle \langle f_2 \mid s_3\rangle, \\
&\langle f_3 \mid s_1\rangle \langle f_2 \mid s_2\rangle \langle f_1 \mid s_3\rangle, \\
&\langle f_1 \mid s_2\rangle \langle f_2 \mid s_3\rangle \langle f_3 \mid s_1\rangle, \\
&\langle f_1 \mid s_3\rangle \langle f_2 \mid s_1\rangle \langle f_3 \mid s_2\rangle.
\end{aligned}
$$

Assuming that the amplitude of each transition $s_i \rightarrow f_k$ is the same (we denote it by a), and taking into account the indistinguishability of alternatives, we get, for the amplitude of a transition with the emission of three photons, the expression $3!a^3$, and for the probability of the transition $(3!)^2 | a^3 |^2$. If the alternatives were distinguishable (if distinguishable microparticles were emitted), the probability would be expressed by $3! | a^3 |^2$. Generalizing these results for the case of n microparticles, we get for emission probabilities the expressions $(n!)^2 | a^n |^2$ and $n! | a^n |^2$, respectively.

Let w_n be the probability of the emission of n bosons (photons in this case) in the same state, and W_n the probability of the emission of n distinguishable microparticles in the same state. It is easy to see that

$$w_n = n! W_n. \tag{9.24}$$

Consequently, the probability of the combined detection of n bosons is $n!$ times greater than the probability of the combined detection of n distinguishable microparticles. We rewrite the result (9.24), replacing n by $n + 1$:

$$w_{n+1} = (n+1)!\, W_{n+1}. \tag{9.25}$$

Dividing (9.25) by (9.24) we get

$$w_{n+1}/w_n = (n+1)\, W_{n+1}/W_n. \tag{9.26}$$

This means that the probability of getting one more boson in a state where there are already n bosons is $(n + 1)$ times greater than the probability of getting one more distinguishable microparticle in a state where there are already *n* such microparticles. We note further that for distinguishable microparticles the degree of prior "population" of the state is not important. When applied to bosons, it is analogous to the situation when a boson appears in a state which was not occupied earlier. Hence result (9.26) may also be interpreted in a different way. The probability of getting another boson in a state having *n* bosons is $n+1$ times greater than the probability of a boson appearing in a state which was hitherto unoccupied. In accordance with this interpretation we can rewrite result (9.26) in the form

$$|\langle n+1 \mid n\rangle|^2 = (n+1)\,|\langle 1 \mid 0\rangle|^2. \tag{9.27}$$

Here we consider a particular state, and $\langle 1 \mid 0\rangle$ is the amplitude of the transition:
(unoccupied state) → (state with one boson), $\langle n+1 \mid n\rangle$ is the amplitude of the transition:
(state with *n* bosons) → (state with $n+1$ bosons). When applied to amplitudes and not probabilities, result (9.27) means

$$\langle n+1 \mid n\rangle = \sqrt{n+1}\,\langle 1 \mid 0\rangle. \tag{9.28}$$

Let us analyse the result (9.27) by considering photon emission (emission of light). It is easy to see that the probability of emission is split into two components:

$$|\langle n+1 \mid s\rangle|_s^2 = |\langle 1 \mid 0\rangle|^2, \tag{9.29}$$

$$|\langle n+1 \mid n\rangle|_i^2 = n|\langle 1 \mid 0\rangle|^2. \tag{9.30}$$

The component (9.29) describes the probability of *spontaneous* emission of light and the component (9.30) that of *induced emission of light.* In the case of spontaneous emission, the transitions in a substance (to be more precise, in the radiating atoms) are spontaneous. They are mutually unrelated and are independent of external radiation. In contrast to spontaneous emission, induced emission depends on the existence of photons near the radiating atom—the more photons there are, the greater is the probability of induced emission. It turns out that on account of their bosonic nature, the photons "extract" as it were, new photons from the substance. To be more precise, they stimulate transitions in a substance which lead to the emission of new photons. We stress that a "stimulated" photon is created in the same state in which the "stimulating" photon was.

Absorption of Light and Connection Between the Amplitudes of Direct and Reverse Transitions

Experiment shows that the probability of the absorption of light by a substance depends upon the number of photons in the radiation. In this respect the process of absorption of light is an induced process. By using the analogy with (9.30) we can write the following expression for the probability of the annihilation of a photon in a state having n photons: $|\langle n-1 \mid n\rangle|^2 = n\,|\langle 0 \mid 1\rangle|^2$. We rewrite this result, replacing n by $(n+1)$:

$$|\langle n \mid n+1\rangle|^2 = (n+1)\,|\langle 0 \mid 1\rangle|^2. \tag{9.31}$$

Comparing (9.31) with (9.27), we conclude that the probabilities of direct and reverse transitions are equal to each other: $|\langle n+1 \mid n\rangle|^2 = |\langle n \mid n+1\rangle|^2$.
Thus, using a specific example, we have demonstrated the so-called *principle of microscopic reversibility*:

$$|\langle f \mid s\rangle|^2 = |\langle s \mid f\rangle|^2. \tag{9.32}$$

When applied to transition amplitudes, this principle means

$$\langle f \mid s\rangle = \langle s \mid f\rangle^*. \tag{9.33}$$

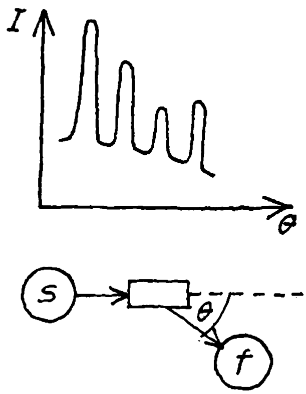
Result (9.33) supplements the set of four rules applicable to transition amplitudes, which we have considered in Sec. 8. It may be treated as an additional, fifth rule.

Supplementary Examples

We shall consider two useful examples which demonstrate the amplitude concepts very clearly.

Scattering of neutrons by a crystal. We shall consider the scattering of very slow neutrons (with energies of the order of 0.1 eV and lower) by atomic nuclei. It is well known that for such low energies, the scattering amplitude φ, considered in the centre of mass system for a neutron and a nucleus, is independent of the scattering angle. So, it would appear, the scattering probability should also be isotropic. However, experiments on the scattering of very slow neutrons by crystals reveal a strong angular dependence of the scattering probability. A typical curve is shown in Fig. 9.3: sharp peaks are observed against a smooth background. These peaks are a visual demonstration of the effect of the interference of amplitudes. We shall see how this is so.

Fig. 9.3



Suppose a neutron emerges from its initial s-state and is registered in its final f-state. The intermediate i-state corresponds to the i-th nucleus in the scattering crystal lattice. According to the third rule of Sec. 8,

$$\langle f \mid s\rangle_i = \langle f \mid i\rangle\,\varphi\,\langle i \mid s\rangle. \tag{9.34}$$

We assume that all the N nuclei of the crystal are alike, have zero spin, and are located strictly at the lattice points.

In this case it is impossible in principle to indicate precisely which nucleus causes the scattering of the neutron—the alternatives corresponding to the scattering by differently "numbered" nuclei are indistinguishable. Hence, we must take into account the interference of the amplitudes:

$$\langle f \mid s\rangle=\sum_{i}^{N}\langle f \mid s\rangle_i=\sum_{i}^{N}\langle f \mid i\rangle\, \varphi\, \langle i \mid s\rangle. \tag{9.35}$$

Taking (9.35) into account, the probability of scattering of the neutron has the form

$$|\langle f \mid s\rangle|^2=|\varphi|^2\left|\sum_{i}^{N}\langle f \mid i\rangle\langle i \mid s\rangle\right|^2. \tag{9.36}$$

On account of the addition of the amplitudes of the scattering at the nuclei, which are distributed in space in a definite order, a mutual "cancelling" of amplitudes is possible in some directions and a mutual "enhancement" in some others; this interference effect is manifested in the form of sharp peaks for definite scattering angles.

We further assume that nuclei in the crystal have a spin (let it be equal to 1/2, as for neutrons). In this case we should distinguish between the amplitude of scattering by the nucleus *with spin inversion* (in accordance with the law of conservation of momentum, the neutron spin must also be inverted in this case), and *without spin inversion* of the nucleus (and the neutron), i.e. between χ and φ, respectively. If the scattering of the colliding microparticles is accompanied by spin inversion, the corresponding alternative is distinguishable—it is clear that in such an act of scattering only that nucleus participates whose spin has been inverted. Now the probabilities and not the amplitudes should be summed.

Taking account of the amplitudes φ and χ we can represent the scattering probability of neutrons from s-state to f-state in the following form:

$$|\langle f \mid s\rangle^2=|\varphi|^2\left|\sum_{i}^{N}\langle f \mid i\rangle\langle i \mid s\rangle\right|^2$$

$$+|\chi|^2\sum_{i}^{N}|\langle f \mid i\rangle\langle i \mid s\rangle|^2. \tag{9.37}$$

The first term on the right-hand side of (9.37) accounts for the characteristic interference peaks in Fig. 9.3, while the second term is responsible for the smooth background. It is customary to say that the first term describes the probability of the *coherent* scattering, and the second that of the *incoherent* scattering of neutrons.

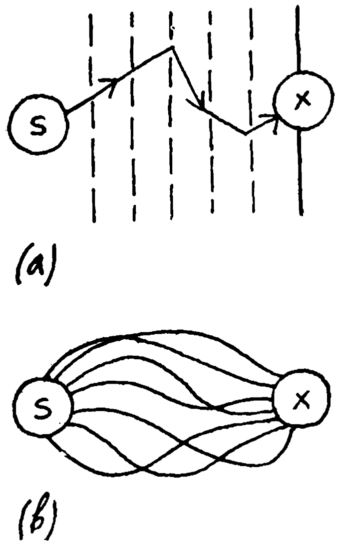
Atomic beam in inhomogeneous fields. Let us assume that a beam of atoms occupying a certain initial s-state (this is a definite spin state) passes first through one region of non-uniform magnetic field (B_1), then through another (B_2) and is finally registered in its final spin state f. Non-uniform magnetic fields are used here as factors capable of changing the spin state of the atoms in the beam. Experiment shows that the probability of the $s \to f$ transition is different in the cases when (a) observations are carried out to find the state of the atoms in the beam between fields B_1 and B_2, and when (b) such observations are not carried out. The difference in probabilities $|\langle f \mid s\rangle|^2$ in these two cases is easily explained if we take into account that in case (a) the intermediate i-spin states are fixed each time and, consequently, the alternatives corresponding to them are distinguishable; hence:

$$|\langle f \mid s\rangle|^2 = \sum_i |\langle f \mid i\rangle\langle i \mid s\rangle|^2. \qquad (9.38)$$

In case (b) the intermediate i-states are not fixed and, consequently, the alternatives corresponding to them are indistinguishable. Hence

$$|\langle f \mid s\rangle|^2 = \left|\sum_i \langle f \mid i\rangle\langle i \mid s\rangle\right|^2 \qquad (9.39)$$

Fig. 9.4



FEYNMAN'S PATH INTEGRALS. In conclusion we shall indicate the possibility of a somewhat unusual formulation of quantum mechanics, based on amplitude concepts. In the beginning of this section, we considered an interferometer in the form of a screen with two slits. There were two indistinguishable alternatives corresponding to the two interference amplitudes. Let us now assume that instead of a screen with two slits, we have a screen with n slits. The number of alternatives (and, correspondingly, amplitudes) will be equal to n. Further, we place another screen with n slits parallel to the first screen; the number of alternatives (amplitudes) will rise to n^2. We shall continue this process by placing more and more screens in the space between the source of microparticles and the detector screen; moreover, we shall simultaneously keep on increasing the number of slits in each screen. In the limiting case of an infinitely large number of screens and an infinitely large number of slits, we arrive at a situation when the entire space between the source and detector screen will turn out to be "filled" by different 'paths' of the microparticle, each corresponding to a definite alternative and a corresponding definite amplitude (one such path is indicated in Fig. 9.4(a)). The total amplitude of $s \to x$ transition is the sum (more exactly, the integral) over all the possible amplitudes. Finally, we assume that the system of screens with slits was introduced only fictitiously; in fact there are no screens and the entire space between points s and x is "filled" by all the possible paths. If we can write the transition amplitude for each such trajectory, then the probability of the $s \rightarrow x$ transition may be found as the square of the modulus of the integral summing up all the given amplitudes (called the path integrals). In this sense, the quantum-mechanical motion from s to x is nothing but the superposition of a set of classical motions (classical trajectories) almost in the same way as indicated in Fig. 9.4(*b*). The transition from quantum to classical mechanics corresponds to the reduction of the given superposition of paths to a certain individual trajectory.

The concept of the motion of a microparticle along classical path integrals (in other words, through interference of amplitudes corresponding to the classical trajectories) is discussed in detail in Sec. 5.

Section 10 Superposition of States

In the previous section, while studying the problem of the probability of the transition of a microparticle from one state to another, we introduced and discussed the concepts of the transition probability amplitude, distinguishable and indistinguishable alternatives of transition, the interference of amplitudes corresponding to indistinguishable alternatives, all of which are specifically quantum-mechanical concepts. On the basis of a number of examples the reader should convince himself of the importance of the concept of interfering amplitudes, which gives an explanation of the results of various experiments with microparticles.

The interference of transition amplitudes is inseparably linked with one of the most fundamental principles of quantum mechanics—the *principle of superposition of states*, which reflects the specific nature of the "interrelations" among the states of a microparticle. We shall now consider this principle.

Principle of Superposition of States

Earlier, in Sec. 3, we studied the uncertainty relations. In this connection it was remarked, in particular, that the states of a microparticle were combined in groups each of which contained the definite values of any one complete set of physical quantities. We also gave examples of complete sets of values for an electron and a photon.

Continuing the discussion commenced in Sec. 3, we shall introduce notations for the various complete sets: the α-set, the β-set, the γ-set, etc. In this context we shall speak of the group of α-states, the group of β-states, etc.

We suppose that the microparticle is in one of the α-states. It means that the quantities in the α-set have definite values. But what can we say about the values of the quantities in any other complete set, for example, the β-set? According to the uncertainty relations, the quantities in the β-set do not have definite values in the state under consideration. The reader is justified in taking this as a negative fact. But, fortunately, this is fully "compensated" by a positive circumstance—the principle of the superposition of states.

According to the principle of superposition, there exists a link between the states of the microparticle, corresponding to different complete sets: any state from one set may be represented in the form of a *superposition of states* from another set. Thus, for example, a given α-state may be represented in the form of a superposition of β-states. If we arbitrarily adopt the symbol $\langle \mid$ to indicate the state of a microparticle, the principle of superposition may be written in the form

$$\langle \alpha \mid = \sum_{\beta} \Phi_{\alpha\beta} \langle \beta \mid . \qquad (10.1)$$

The expression (10.1) appears as an "expansion" of the given state $\langle \alpha \mid$ into the sum of β-states, the numbers $\Phi_{\alpha\beta}$ playing the role of coefficients in the expansion. More concretely, the number $\Phi_{\alpha\beta}$ is the amplitude of the probability that we shall obtain values corresponding to the state $\langle \beta \mid$ while measuring the quantities from the β-set in the state $\langle \alpha \mid$. In other words, it is the amplitude of the probability that a microparticle in state $\langle \alpha \mid$ may also be found in the state $\langle \beta \mid$. If we denote this amplitude by the usual symbol $\langle \alpha \mid \beta \rangle$, expression (10.1) assumes the following form:

$$\langle \alpha \mid = \sum_{\beta} \langle \alpha \mid \beta \rangle \langle \beta \mid . \qquad (10.2)$$

In the preceding sections we considered the amplitudes of the transition probability (in short, transition amplitudes). At first glance, the principle of superposition "brings into play" a new type of amplitudes of probability. Actually, the above-mentioned expression "$\langle \alpha \mid \beta \rangle$ is the amplitude of the probability that a microparticle in state $\langle \alpha \mid$ may also be found in state $\langle \beta \mid$" allows another obvious interpretation: "$\langle \alpha \mid \beta \rangle$ is the amplitude of the probability of a microparticle arriving in state $\langle \beta \mid$, if it is known that the given particle actually exists in state $\langle \alpha \mid$" In short, the latter statement means that $\langle \alpha \mid \beta \rangle$ is the amplitude of the probability with which any β-state is "represented" in a given α-state. This produces the impression that the amplitudes $\langle\alpha\mid\beta\rangle$ don't have anything to do with any transitions or processes. Considering this impression, we introduce a new term for $\langle\alpha\mid\beta\rangle$—the *amplitude of probability of state* (in brief, the *amplitude of state*).

The reader must be warned at once that the above impression is erroneous. However, in order to be convinced of this, we must analyse the process of measurement. Measurement in quantum mechanics will be discussed in Sec. 11. This discussion will necessitate some correction in the above definition of the amplitudes $\langle\alpha\mid\beta\rangle$ and will enable us to actually reduce the amplitudes of states to the already familiar amplitudes of transitions.

But everything has its own time, and so, for the time being, we shall operate with the concept of "amplitude of state" as an independent concept, without ascertaining the practical meaning of, say, the phrase "a particle in state $\langle\alpha\mid$ can also be found in state $\langle\beta\mid$".

As has been noted earlier, the principle of superposition "supplements", as it were, the uncertainty relations; its positive content "compensates" the well-known negative aspect of these relations. Figuratively speaking, the uncertainty relations indicate the "old" concept which must be rejected while we go over from macrophenomena to microphenomena. In particular, they require a rejection of the simultaneous measurability of all physical quantities characterizing a given object. At the same time, the principle of superposition indicates the "new" concept which is applicable when considering microparticles; superposition (10.2) means that if a microparticle is in a state in which the quantities of the α-set are measurable, then the value of the quantities in the β-set may be predicted with a *probability* equal to $|\langle\alpha\mid\beta\rangle|^2$.

Superposition in Classical Physics and Quantum Mechanics

In classical physics one comes across superposition quite frequently, the foremost example being the well-known superposition of classical waves. From a mathematical point of view, the classical superposition and superposition in quantum mechanics are analogous. This circumstance greatly stimulated the development of quantum theory. At the same time, it certainly complicated the interpretation of the physical content of theoretically obtained results since it tempted one to draw erroneous analogies with classical waves. In the words of Dirac [9] *the assumption of superposition relationships between the states leads to a mathematical theory in which the equations that define a state are linear in the unknowns. In consequence of this, people have tried to establish analogies with systems in classical mechanics, such as vibrating strings* *or membranes, which are governed by linear equations and for which, therefore, a superposition principle holds....* (remember the criticism in Sec. 5 of the attempts to represent the motion of a bound microparticle with the help of classical waves in a resonator—*author's remarks*). *It is important to remember, however, that the superposition that occurs in quantum mechanics is of an essentially different nature from any occurring in the classical theory, as is shown by the fact that the quantum superposition principle demands indeterminacy in the results of observations.*

Speaking of the difference between quantum and classical superpositions, remember that a superposition of two classical waves leads to the generation of a new wave having, of course, new characteristics. However, a superposition of two states $\langle\beta_1 |$ and $\langle\beta_2 |$, characterized by the values β_1 and β_2, respectively, of quantities in the β-set, by no means leads to a state having any new value of β. As an example, let us consider a certain superposition of states

$$\langle\alpha | \beta_1\rangle\langle\beta_1 | + \langle\alpha | \beta_2\rangle\langle\beta_2 |.$$

We shall measure the β-quantity in this state. As a result, we get every time one of the earlier values, β_1 or β_2. Moreover, it is impossible to accurately predict which of the two states will be obtained in any particular measurement. We can only indicate the probability of getting β_1 or β_2. These probabilities are equal to $|\langle\alpha | \beta_1\rangle|^2$ and $|\langle\alpha | \beta_2\rangle|^2$, respectively. It is this specific *uncertainty in the results of measurements* that determines the fundamental difference between quantum and classical superpositions.

Taking into consideration the quantum-mechanical principle of superposition, let us return to the question of quantum transitions discussed in Sec. 2. Suppose we consider, as before, two energy levels E_1 and E_2 of the microparticle. We denote the corresponding states of the particle in which it has energy E_1 or E_2 (i.e. is on the first or second level) through $\langle 1 |$ and $\langle 2 |$ respectively. According to the principle of superposition, in addition to states $\langle 1 |$ and $\langle 2 |$ we can also get the state

$$\langle f | = \langle f | 1\rangle\langle 1 | + \langle f | 2\rangle\langle 2 |. \tag{10.3}$$

Measurement of energy of the microparticle in this state leads either to the result E_1 or to the result E_2 (as if the microparticle were on the level E_1 and simultaneously on the level E_2). The first result is obtained with the probability $|\langle f | 1\rangle|^2$, and the second, with the probability $|\langle f | 2\rangle|^2$. The possibility of the existence of such a specific quantum-mechanical situation immediately removes the basic contradiction of the quantum transition, mentioned in Section 2. It is sufficient to assume that an interaction of a microparticle with radiation leads to a superposition state of the type (10.3). Then the probability of finding a particle on one energy level or another (on its earlier level or on a new one) will be described simply by the square of the modulus of the corresponding amplitude of state.

Mutually Orthogonal States; Total and Partial Distinguishability of States

In order to finally convince ourselves that the quantum-mechanical principle of superposition has in fact nothing in common with the classical superposition we turn to expression (10.2) and see how it changes upon the transition to classical physics. Since in classical physics all the quantities can be simultaneously measured, they form together one "complete set". Considering that the superposition bonds described by relation (10.2) operate between different complete sets, we arrive at the conclusion that in the classical case such bonds simply do not exist and, consequently, all formally composed amplitudes of states must be taken as being equal to zero:

$$\langle \alpha \mid \beta \rangle = 0. \tag{10.4}$$

In quantum mechanics condition (10.4) also exists, but only "within the limits" of the given complete set (for states belonging to the same set). Thus, for example,

$$\langle \alpha_i \mid \alpha_j \rangle = 0, \text{ if } i \neq j. \tag{10.5}$$

The amplitude of a state is equal to zero if and only if the two corresponding states are *mutually independent* (if an object is in one of these states, it cannot be found in the other). Such states are called *mutually orthogonal.* In this respect all the states of a classical particle are mutually orthogonal, while in quantum mechanics only the states belonging to the same complete set are orthogonal and the states belonging to different sets are non-orthogonal. This last fact is reflected in the principle of superposition of states.

The idea of mutually orthogonal states permits us to define more precisely the concept of complete and partial distinguishability. For this purpose it is convenient to make use of the above-mentioned example of the scattering of microparticles of one type by one another. Since such particles are identical, their distinguishability is determined by the distinguishability of states (states $\langle s_1 \mid$ and $\langle s_2 \mid$; see Sec. 9). We recall that in Sec. 9 we discussed, in particular, microparticles of the same kind but in different spin states, as examples of completely distinguishable microparticles. We thus tacitly assumed that different spin states are completely distinguishable. We can now clearly indicate the criterion of complete and partial distinguishability of states: if $\langle s_1 | s_2 \rangle = 0$, the states $\langle s_1 |$ and $\langle s_2 |$ are completely distinguishable; there are no superposition bonds between them. But if $\langle s_1 | s_2 \rangle \neq 0$, the states under consideration are partially distinguishable. In other words, orthogonality of states is the criterion of their complete distinguishability.

Suppose we are considering scattering of two bosons of the same type. The result (9.16) will hold good if the initial states are mutually orthogonal (let these states be $\langle \alpha_1 |$ and $\langle \alpha_2 |$). The result (9.17) will be valid if the initial states are similar (say, $\langle \alpha_1 |$ and $\langle \alpha_1 |$). Both these results are just two extreme cases corresponding to complete distinguishability and complete indistinguishability of microparticles, respectively. However, different intermediate situations corresponding to partial distinguishability are possible, when the initial states of microparticles are a superposition of several mutually orthogonal states:

$$\langle s_1 | = \langle s_1 | \alpha_1 \rangle \langle \alpha_1 | + \langle s_1 | \alpha_2 \rangle \langle \alpha_2 |,$$
$$\langle s_2 | = \langle s_2 | \alpha_1 \rangle \langle \alpha_1 | + \langle s_2 | \alpha_2 \rangle \langle \alpha_2 |. \tag{10.6}$$

It can be shown (see [31]) that in this case the probability of simultaneous activation of detectors is determined by the expression

$$w = | \varphi(\theta) |^2 + | \varphi(\pi - \theta) |^2$$
$$+ | \langle s_1 | s_2 \rangle |^2 [\varphi(\theta) \varphi^*(\pi - \theta) + \varphi^*(\theta) \varphi(\pi - \theta)]. \tag{10.7}$$

For $| \langle s_1 | s_2 \rangle |^2 \to 0$, the result (10.7) turns into (9.16) (we come to the limiting case of complete distinguishability). For $| \langle s_1 | s_2 \rangle |^2 \to 1$, the result (10.7) turns into (9.17) (we come to the limiting case of complete indistinguishability).

Thus, we find that the question of the complete and partial distinguishability of alternatives in quantum mechanics is closely linked with the quantum-mechanical principle of superposition, more precisely, with the mutual orthogonality or non-orthogonality of states.

Basic States

The different states corresponding to the same complete set of quantities are called *basic* states (eigenstates). The amplitudes of elementary states satisfy the condition

$$\langle \alpha_i | \alpha_j \rangle = \delta_{ij}, \tag{10.8}$$

where δ_{ij} is the so-called Kronecker delta symbol; it is equal to zero for $i \neq j$ and unity for $i = j$. The expression (10.8) is called the *condition of orthonormalization of basic states*. It is obtained by taking into consideration (10.5) and the fact that the probability of getting the value α_i in the state $\langle \alpha_i \mid$ is obviously equal to unity. The important property of the system of basic states is its *completeness*: any state may be expanded in a system of elementary states.

Basic states may be selected in different ways depending on the complete set under consideration. Thus, different systems of basic states may be used: $\{\langle \alpha_i \mid\}$, $\{\langle \beta_i \mid\}$, etc. It is said that *different representations* are possible. For a more general approach, the principle of superposition of states signifies the fact that any state $\langle f \mid$ of a microparticle may be expanded in any system of basic states:

$$\begin{gathered} \langle f \mid = \sum_i \langle f \mid \alpha_i \rangle \langle \alpha_i \mid, \\ \langle f \mid = \sum_i \langle f \mid \beta_i \rangle \langle \beta_i \mid, \end{gathered} \tag{10.9}$$

Superposition of States and Passage of Photons Through Polarizers

The principle of superposition permits an explanation of the results of experiment 3 in Sec. 7. Using this principle, we shall consider the passage of individual photons through the system of three polarizers shown in Fig. 7.6. We denote the state of polarization of a photon after the first polarization by $\langle s \mid$. According to the principle of superposition, the state $\langle s \mid$ may be considered as a superposition of the basic states $\langle 1 \mid$ and $\langle 2 \mid$, corresponding to two independent polarizations of the photon—along and perpendicular to the axis of the second polarizer, respectively:

$$\langle s \mid = \langle s \mid 1 \rangle \langle 1 \mid + \langle s \mid 2 \rangle \langle 2 \mid \tag{10.10}$$

(note that in this example, the system of basic states contains only two states). The amplitudes of the states may be written in this case in the form $\langle s \mid 1 \rangle = \cos \alpha$ and $\langle s \mid 2 \rangle = \sin \alpha$. Thus,

$$\langle s \mid = \cos \alpha \ \langle 1 \mid + \sin \alpha \ \langle 2 \mid. \tag{10.11}$$

The second polarizer lets through photons from the state $\langle 1 \mid$ only. Since according to (10.11) the state $\langle 1 \mid$ is "represented" in state $\langle s \mid$ with a probability $\cos^2 \alpha$, out of N photons only $N \cos^2 \alpha$ photons will pass through the second polarizer. Moreover, all the photons that pass will appear in the state $\langle 1 \mid$ (i.e. they will be polarized along the axis of the second polarizer). Thus, in front of the second polarizer, the photon exists as if partially in the state $\langle 1 |$ and partially in the state $\langle 2 |$. At the instant when the photon passes through the polarizer, this "duality" vanishes. In some cases a photon exists in the state $\langle 2 |$ and so cannot pass through the polarizer, while in some other cases it is in the state $\langle 1 |$ and can thus pass through the polarizer. Further, for any individual photon it is impossible to predict in which state it will appear (hence it is impossible to predict whether a given photon will pass through the polarizer or not).

While studying the passage of photons through the third polarizer, we proceed in a similar way. The state $\langle 1 |$ is expanded into a system of basic states $\langle 1' |$ and $\langle 2' |$ corresponding to a polarization of photon along or perpendicular to the axis of the third polarizer:

$$\langle 1 | = \sin\alpha \, \langle 1' | + \cos\alpha \, \langle 2' | . \tag{10.12}$$

The third polarizer lets through photons in the state $\langle 1' |$ only. This state is "represented" in the state $\langle 1 |$ with a probability $\sin^2\alpha$. Hence out of $N\cos^2\alpha$ photons only $N\cos^2\alpha\sin^2\alpha$ photons will pass through the third polarizer, all these photons being in the state $\langle 1' |$.

If we now remove the second polarizer, then in place of (10.11) and (10.12) we get

$$\langle s | = \langle s | 1' \rangle \langle 1' | + \langle s | 2' \rangle \langle 2' | , \tag{10.13}$$

where, as can be easily seen, $\langle s | 1' \rangle = 0$ and $\langle s | 2' \rangle = 1$, so that $\langle s | = \langle 2' |$. Naturally, in this case, at the outlet of the system of polarizers no photons are observed at all.

Principle of Superposition of States and Interference of Transition Amplitudes

Let the transition from state $\langle s |$ to state $\langle f |$ take place through certain intermediate v-states. We suppose that the microparticle is not fixed in the intermediate state so that a case of physically indistinguishable alternative takes place. In this case, as we know, the transition amplitude $\langle f | s \rangle$ is given by the expression

$$\langle f | s \rangle = \sum_i \langle f | v_i \rangle \langle v_i | s \rangle , \tag{10.14}$$

where $\langle f | v_i \rangle$ and $\langle v_i | s \rangle$ are the amplitudes of the respective transitions. The intermediate v-states must be completely distinguishable, since otherwise there is no point in introducing the concept of distinguishable or indistinguishable alternatives, since the very concept of alternatives loses its meaning. Consequently, the v-states must form a system of mutually orthogonal basic states. Taking this into consideration, we make use of the principle of superposition and express the state $\langle f |$ in the form

$$\langle f | = \sum_i \overline{\langle f | v_i \rangle} \langle v_i | , \tag{10.15}$$

where the amplitudes $\overline{\langle f \mid v_i \rangle}$ are essentially the amplitudes of the states (the bar is used to distinguish the amplitude of the state from the transition amplitude $\langle f \mid v_i \rangle$). If superposition (10.15) exists, there is actually no need to perform a transition from $\langle s \mid$ to $\langle f \mid$. Since the state $\langle f \mid$ is a superposition of states $\langle v_i \mid$, it is sufficient to simply accomplish transitions from the state $\langle s \mid$ to each of the states $\langle v_i \mid$. This means that the transition amplitude $\langle f \mid s \rangle$ is a superposition of the transition amplitudes $\langle v_i \mid s \rangle$:

$$\langle f \mid s \rangle = \sum_i \overline{\langle f \mid v_i \rangle} \langle v_i \mid s \rangle. \tag{10.16}$$

Comparing (10.16) and (10.14) we conclude that

$$\overline{\langle f \mid v_i \rangle} = \langle f \mid v_i \rangle. \tag{10.17}$$

This means that at the level of mathematical apparatus, we have accomplished a reduction of the amplitudes of the states to transition of amplitudes. In other words, the amplitudes of the states in fact play the same role in the apparatus of quantum mechanics as the transition amplitudes. Incidentally, we have also established that relations (10.14) and (10.15) are closely related to each other and hence the effect of the interference of transition amplitudes and the principle of the superposition of states are directly interrelated.

In conclusion, we mention an important method which is widely applied in quantum mechanics. It is easy to see that if we delete the sign of the initial and final states in the expression for the interference of amplitudes, we automatically obtain the superposition expression for the undeleted state. Thus, if in (10.14) we delete $\mid s \rangle$ on the left- and right-hand sides of the equation, we obtain the superposition expression (10.11) for the state $\langle f \mid$ (note that in addition to the symbol $\langle \ \mid$, the symbol $\mid \ \rangle$ is used for denoting a state).

"Mechanics of Quantum Mechanics"

We shall demonstrate the basic methods reflecting, in Feynman's words, the "mechanics of quantum mechanics". Let us delete the state $\langle f \mid$ from the left- and right-hand sides of equation (10.14). This gives

$$\mid s \rangle = \sum_i \mid v_i \rangle \langle v_i \mid s \rangle. \tag{10.18}$$

Let us further assume that some apparatus converts state $\mid s \rangle$ into some other state $\mid s' \rangle$. We express this in the general form as

$$A \mid s \rangle = \mid s' \rangle. \tag{10.19}$$

We shall say that the *operator* A has acted on the state $|s\rangle$ giving rise to state $|s'\rangle$. We shall apply the operator A to both sides of equation (10.18). Using (10.19), we get

$$|s'\rangle = \sum_i A\,|v_i\rangle\langle v_i|s\rangle \tag{10.20}$$

Further, in place of the state $\langle f|$ deleted earlier, we restore the state $\langle v_j|$ belonging to the system of basic states:

$$\langle v_j|s'\rangle = \sum_i \langle v_j|A|v_i\rangle\langle v_i|s\rangle \tag{10.21}$$

(the notation $\langle v_j|A|v_i\rangle$ should be taken as $\langle v_j|v_i'\rangle$, where $|v_i'\rangle = A\,|v_i\rangle$). Finally, we rewrite (10.14), replacing $|s\rangle$ by $|s'\rangle$:

$$\langle f|s'\rangle = \sum_i \langle f|v_j\rangle\langle v_j|s'\rangle \tag{10.22}$$

Substituting (10.21) into (10.22) we get

$$\langle f|A|s\rangle = \sum_j\sum_i \langle f|v_j\rangle\langle v_j|A|v_i\rangle\langle v_i|s\rangle. \tag{10.23}$$

Summarizing the methods demonstrated above, we write the equations obtained so far and leave it to the reader to follow the logic and appreciate the beauty of the transformations:

$$\boxed{\begin{aligned}
\langle f|s\rangle &= \langle f|s\rangle,\\
\langle f|s\rangle &= \sum_i \langle f|v_i\rangle\langle v_i|s\rangle,\\
|s\rangle &= \sum_i |v_i\rangle\langle v_i|s\rangle,\\
A\,|s\rangle &= \sum_i A\,|v_i\rangle\langle v_i|s\rangle,\\
\langle v_j|A|s\rangle &= \sum_i \langle v_j|A|v_i\rangle\langle v_i|s\rangle,\\
\sum_j \langle f|v_j\rangle\langle v_j|A|s\rangle &\\
&= \sum_j\sum_i \langle f|v_j\rangle\langle v_j|A|v_i\rangle\langle v_i|s\rangle,\\
\langle f|A|s\rangle &= \sum_j\sum_i \langle f|v_j\rangle\langle v_j|A|v_i\rangle\langle v_i|s\rangle.
\end{aligned}}$$

Finally, we assume that operator A acts on the state $|s\rangle$, and is followed by operator B. If the reader has mastered the logic of the "mechanics of quantum mechanics" (it would have been more accurate to call it the "algebra of quantum mechanics"), he will at once surmise that

$$\langle f \mid BA \mid s\rangle = \sum_k \sum_j \sum_i \langle f \mid v_k\rangle \langle v_k \mid B \mid v_j\rangle \langle v_j \mid A \mid v_i\rangle \langle v_i \mid s\rangle \qquad (10.24)$$

(the notation $\langle f \mid BA \mid s\rangle$ should be taken as $\langle f \mid s''\rangle$, where $\mid s''\rangle = B \mid s'\rangle$ and $\mid s'\rangle = A \mid s\rangle$).

This formal structure of the mathematical "manipulations" is characteristic for quantum mechanics. In what follows, this structure will assume a definite meaning on the basis of definite examples. Here it has been given in its most general form, which also allows us to follow its internal logic. We emphasize that the basis of this structure is the idea of quantum-mechanical interference (superposition) and the use of a certain system of basic states in terms of which the expansions are carried out.

Section 11 Measurement in Quantum Mechanics

The question of carrying out measurements in quantum-mechanical systems and an interpretation of the results so obtained is rightly considered to be very complicated, requiring even today further research. We shall not give a detailed analysis of the problem of quantum-mechanical measurements, but shall try to describe a number of fundamental statements which have been explained clearly, and demonstrate them using some examples*.

The Origin of the Superposition of States and the Meaning of the Amplitudes of States

Suppose that a microparticle is in a certain state $\langle\alpha\mid$. According to the principle of superposition, the state $\langle\alpha\mid$ may be expanded in terms of any system of basic states, for example, in the $\{\langle\beta_i\mid\}$ system:

$$\langle\alpha\mid = \sum_i \langle\alpha\mid\beta_i\rangle\langle\beta_i\mid. \qquad (11.1)$$

The numbers $\langle\alpha\mid\beta_i\rangle$ in the superposition (11.1) are essentially the amplitudes of the states $\langle\beta_i\mid$ or, more accurately, the amplitudes of the probabilities with which the various basic states $\langle\beta_i\mid$ are "represented" in the state $\langle\alpha\mid$.

The reader who has read the previous section is already familiar with all this. It is appropriate now to make things more precise.

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* The problem of measurement in quantum mechanics has been dealt with, in particular, in [2, 28, 32].

Firstly, we shall note that any definite superposition of states in a microparticle arises as a result of its interaction with the surroundings. The latter may be some macroscopic body (which is either produced artificially or is a part of the natural external conditions). This macroscopic body is referred to as the *analyzer*. The expression (11.1) should be interpreted in the following way: as a result of the interaction with a particular analyzer (in this case, we may speak of a β-analyzer), a microparticle lying in state $\langle\alpha\mid$ is transformed into the superposition state $\sum_i\langle\alpha\mid\beta_i\rangle\langle\beta_i\mid$. Taking into account the quantum-mechanical nature of the superposition state, it may be said that by interacting with the β-analyzer, the microparticle in some sense is "transformed" at once into all the states $\langle\beta_i\mid$. Here, the amplitude $\langle\alpha\mid\beta_i\rangle$ should be treated as the amplitude caused by the indicated interaction of the transition $\langle\alpha\mid\to\langle\beta_i\mid$. The quantity $\mid\langle\alpha\mid\beta_i\rangle\mid^2$ is the probability of finding the microparticle finally in just the $\langle\beta_i\mid$ state.

One can anticipate at least three questions from the reader. *First question*: What do we really mean by the expression "the microparticle is at once transformed into all the $\langle\beta_i\mid$ states"? The answer to this question will be given below in the subsection "Potentialities and their realization in the measuring process". Here, we just remark that although the microparticle is "simultaneously transformed into all the $\langle\beta_i\mid$ states" as a result of its interaction with the β-analyzer, it can be found in principle each time in only one β-state. Hence it may be said that no confusion arises. By the way, the reader has already come across a similar situation when considering experiments 1 and 2 in Sec. 7. Here we once again remind the reader that quantum-mechanical logic does not always have a corresponding graphic model.

Second question: If the amplitude of state is really the transition amplitude, what about the definitions of amplitudes of states given in Sec. 10? Answering this question we recall the following definition given in Sec. 10: "$\langle\alpha\mid\beta\rangle$ is the probability amplitude of a microparticle existing in state $\langle\alpha\mid$ being also registered in state $\langle\beta\mid$". In this definition the word "existing" should be replaced by a more accurate word "existed", since after interaction with the analyzer the microparticle no longer exists in the state $\langle\alpha\mid$. Now the word "also" becomes redundant. The definition then assumes the following form: "$\langle\alpha\mid\beta\rangle$ is the amplitude of probability of a microparticle that existed in state $\langle\alpha\mid$ being registered in state $\langle\beta\mid$" Registering is a kind of measuring process and $\langle\alpha \mid \beta\rangle$ plays the role of the amplitude of the transition $\langle\alpha \mid \to \langle\beta \mid$ which takes place in this process. Here we remark that in the above-mentioned interaction of the microparticle with the analyzer is just one part of the measuring process. A more detailed treatment of the measuring process will be given at a later stage.

Third question: It was agreed earlier (see Sec. 8) to read the transition amplitudes from right to left. If $\langle\alpha \mid \beta_i\rangle$ is also transition amplitude, it should also be read in the reverse direction (from left to right). Isn't it confusing? Actually, if we strictly follow the condition of writing the preceding states to the right of the ones that follow, then (11.1) should be written as

$$\sum_i \mid \beta_i\rangle\langle\beta_i \mid \alpha\rangle = \mid \alpha\rangle. \tag{11.1a}$$

However, such a notation, as a rule, is not used. Hence we decided to allow some inconsistency, and in order to avoid possible confusion in this connection we shall in future retain the term amplitude of state along with the term transition amplitude. When using both these terms the reader must remember that from the point of view of physical meaning, the amplitude of state is nothing but the transition amplitude (this has already been shown from a mathematical point of view in the previous section).

Examples of Analyzers

The reader has in fact already come across analyzers each time the interference of transition amplitudes was considered. We shall give a few examples.

First example: [see (9.3)]—the analyzer is a screen with two slits. It gives rise to the superposition

$$\langle s \mid = \langle s \mid A\rangle\langle A \mid + \langle s \mid B\rangle\langle B \mid. \tag{11.2}$$

Second example: [see (9.35)]—the analyzer is a crystal lattice consisting of nuclei of the same type with zero spin. It generates the superposition

$$\langle s \mid = \sum_i^N \langle s \mid i\rangle \varphi \langle i \mid. \tag{11.3}$$

Third example: [see (9.39)]—the analyzer is a nonuniform magnetic field B_1. It gives rise to the superposition

$$\langle s \mid = \sum_i \langle s \mid i\rangle\langle i \mid. \tag{11.4}$$

It may be said that an analyzer, generating a certain superposition of states, in fact ensures the emergence of indistinguishable alternatives. Moreover, the number of alternatives is equal to the number of basic states in the given superposition. In the first example this number is just equal to two (i.e. to the number of slits in the screen); in the second example, it is equal to the number of nuclei in the crystal, while in the third example it is equal to the number of spin states (i.e. to $2s + 1$, if s is the spin of the atom).

The Essence of Measuring Process

The process of measurement in quantum mechanics consists of three successive stages: (1) a *preparatory stage* when the microparticle is "prepared" in a certain state $\langle \alpha |$, considered below as the *initial state*; (2) a *working stage* in which the "prepared" microparticle interacts with a certain analyzer and goes over to the *superposition state*, and (3) a *registering stage* in which the microparticle is registered in one of the basic states forming the superposition. In this stage the microparticle interacts with some macroscopic body, capable of changing its state under the influence of the microparticle. This macroscopic body is called the detector.

If for the sake of simplicity we do not consider the preparatory stage, the abstract "scheme" of the measurement process may be written in the following way:

$$\langle s | \xrightarrow{1} \sum_i \langle s | \beta_i \rangle \langle \beta_i | \xrightarrow{2} \langle \beta_i | . \qquad (11.5)$$

Here the arrow 1 corresponds to the working stage, and the arrow 2 to the registering stage.

The basic elements of the measuring instrument (measuring apparatus) are thus the analyzer and the detector. The role of the analyzer has already been explained. We shall now consider the role of the detector. Figuratively speaking, its role boils down to "spying" on how the microparticle "behaves itself" in the superposition state which was created by the analyzer. If we make use of the above examples of analyzers, this "spying" could provide an answer to the question: Which slit did a particular electron pass through? Which nucleus of the crystal lattice scattered a particular neutron? What is the spin state of a particular atom? The reader who is familiar with the results of similar "spying" (in particular, with the results of the experiment 2 in Sec. 7) may foresee that an "intervention" by the detector leads to the destruction of the superposition of states. The detector registers the microparticle each time in one of the states which constitute the superposition. This is done at the expense of the *destruction of superposition*. From the point of view of the ideas considered in Secs. 8 and 9, this means that the detector converts indistinguishable alternatives into distinguishable ones and thus destroys the interference of the transition amplitudes.

We separate from the "scheme" (11.5) the registering stage corresponding to the interaction of the microparticle with the detector:

$$\sum_i \langle s \mid \beta_i\rangle\langle\beta_i \mid \to \langle\beta_i \mid . \tag{11.6}$$

It is often said that a "scheme" of the type (11.6) describes a "construction" of the superposition $\sum_i \langle s \mid \beta_i\rangle\langle\beta_i \mid$ to the state $\langle\beta_i \mid$. This process is also known as "reduction of the wave packet"

Thus, while the analyzer creates a definite superposition of states, the detector destroys it by confining this superposition of states to one of the states constituting it. It is obvious that if the "scheme" (11.5) is tried on a single microparticle, it is difficult to say anything about getting any useful information. It is necessary to repeat the measuring process for a sufficiently large number of microparticles. In this case the observer may find out, firstly, the values of the quantities of the β-set encountered in practice, and, secondly, the frequency with which the microparticle is found in one β-state or another. This allows us to experimentally determine, firstly, the spectrum of the values of the quantities in a β-set and, secondly, the probabilities $|\langle s \mid \beta_i\rangle|^2$.

Some Peculiarities of the Quantum-Mechanical Measuring Process

In the first place we note that the process of measurement has a radical influence on a microparticle. It is enough to point out that a change in the initial state of the microparticle in the measuring process is a circumstance of fundamental importance. It is well known that while carrying out measurements with macroscopic bodies it is possible to isolate the object to a certain extent from the means of measurement. In quantum mechanics this is in principle impossible to do so. In other words, it is impossible to neglect the interaction of the microparticle with its surroundings.

The "scheme" of the measuring process, and more concretely that part which is described by expression (11.6), is a demonstration of the existence of the element of chance in the behaviour of a microparticle. Indeed, it is impossible to predict unambiguously in which β-state a certain microparticle will be finally found.

The impossibility of a graphic representation of the first stage of the process (when the analyzer creates a superposition of states) or the final stage (when the detector "confines" this superposition to a single state) is also a specific feature of the quantum-mechanical measuring process. Thus, obviously, in the first stage of the process of measurement it must not be assumed that a microparticle is literally "spread" over various states of superposition (for example, that it passes partially through one slit and partially through the other in the well-known two-slit experiment). Similarly, it is impossible to assume that as soon as a detector is activated (as soon as the act of registering occurs) the microparticle which is spread over various states suddenly assembles itself in one of these states. It should be noted that the treatment of final stage of the measuring process gave rise to many arguments. Supporters of a model (classical) interpretation of microparticles and microphenomena naturally were at a loss when they tried to visualize a "reduction of wave packets". Inasmuch as the states making up a superposition may be spread in space, in this case the "reduction of a wave packet" should actually indicate a momentary spatial localization of the microparticle. In particular, the following example was extensively used. A wave packet interacts with a semitransparent mirror (the mirror plays the role of analyzer), is partially reflected and partially transmitted (which corresponds to a spreading of the microparticle into the two states comprising the superposition). Detectors are placed in the path of each of the wave packets. It is known that each time only one detector is activated. Suppose that at a certain instant the detector placed in the path of the reflected part of the wave packet is activated. This means that the other part of the wave packet momentarily disappears from that part of the space where the unactivated detector is placed, and reappears in front of the second detector the moment before the act of registration. The absurdity of such "behaviour" of the microparticle, which, by the way, "cannot know" which detector is activated in a given case, is quite obvious.

Persisting in the efforts to retain the classical interpretation, attempts are sometimes made to turn to the classical interpretation of superposition. Such an interpretation assumes that the microparticle after interaction with the analyzer, will actually appear in one of the basic states. The role of the detector is simply reduced to revealing the accomplished fact, i.e. in which basic state the microparticle appears upon interaction with the analyzer. Now everything appears very easy: activation of the detector in the example cited above reveals the fact that the given wave packet upon interaction with the mirror was reflected and not transmitted.

However, such a course has already been precluded. It is enough to remind the reader of the argument put forward in the discussion of experiment 1 in Sec. 7. If it were possible to assume that a microparticle passes through one slit in the screen in some cases and through the other in some other cases, then, as has been remarked earlier, we would not have observed the interference pattern on the detector screen. In other words, the classical concept of superposition of states is equivalent to a destruction of superposition. It must be admitted that until the detector registers the microparticle, the latter exists in the supposition state $\sum \langle s \mid \beta_i \rangle \langle \beta_i \mid$ and not in any of the states $\langle \beta_i \mid$. As to the question of how this can be visually represented, we simply have to give up looking for an answer. It may be said that a discussion of quantum-mechanical measuring process (especially the problem of "reduction of a wave packet") gives a specially convincing proof of fundamental impossibility of a classical interpretation of the microparticle.

Comments on Detectors

A detector in a quantum-mechanical measuring instrument is, as a rule, a macroscopic system in a state which is so unstable that a microscopic influence, or the influence of the microparticle, is enough to change it. In order to be "seen" by an observer, the microparticle causes a complete "catastrophe", an "explosion" on the scale of microphenomena.

Examples of such "catastrophes" include events like the formation of a droplet in Wilson's cloud chamber, or a bubble in a bubble chamber, chemical processes involving photoemulsion grains, avalanche processes of generation of secondary electrons in a photomultiplier, etc. The "observable" microparticle might perish in the "catastrophe" caused by it (as, for example, in the case of the registration of a photon in a photomultiplier or of an electron on a detector screen). However, an even more interesting situation is possible when a microparticle "entrusts" the task of causing the catastrophe to other microparticles. Thus, for example, in Wilson's chamber, the electron "under observation" creates various ions in its wake each of which in turn serves as a centre for the condensation of the supersaturated vapour filling the chamber. It is these ions that cause the "catastrophes" which the observer sees as mist droplets. A multitude of such droplets forms the track which is left by the electron "under observation" We emphasize that an electron track is nothing but a multitude of successively occurring microscopic events, a totality of "catastrophes" on the level of microphenomena.

Potentialities and Their Realization in the Measuring Process

When discussing the idea of quantum-mechanical principle of superposition we come to a situation which is analogous to the one encountered when discussing the idea of wave-particle duality (see Sec. 5). In both cases, a visual (classical) interpretation is not possible. In both cases we come to a problem connected with potentialities and with their realization.

The *possibility* and the *actuality* are the well-known categories of materialistic dialectics. The contradiction that exists between them disappears every time a possibility is realized in one way or the other. Every particular situation is characterized by a set of possibilities out of which only one is realized. The realization process is *irreversible*; as soon as it is accomplished, the initial situation qualitatively changes (one of the possibilities is realized at the expense of all the other possibilities). The possibility that has been realized corresponds to a new situation with new possibilities. The process of resolving the contradictions between the possible and the actual thus turns out to be endless.

In classical mechanics (as also in all theories of dynamic type) the problem of distinguishing between the possible and the actual does not arise because of the absence of the elements of chance in such theories. This problem arises in theories of statistical type. The basically statistical nature of quantum mechanics (where, as has been mentioned earlier, an element of chance is present in the behaviour of an individual object) indicates the importance of the problem of the possible and the actual when considering microparticles and microphenomena.

It is from this point of view of resolution of contradiction between the possible and the actual that the measuring process in quantum mechanics should be considered. The presence of a microparticle in the superposition state corresponds to a situation where the microparticle is characterized by a definite set of possibilities. The quantum-mechanical principle of superposition of states should be interpreted in this way only. In the interaction process of a microparticle with the detector [in the process (11.6)], the above-mentioned resolution of distinction between the possible and the actual takes place, the superposition of probabilities is destroyed and is replaced by one of the alternatives realized. It may be said that the "formula" of measuring process [formula (11.6)] is the mathematical expression for the process in which the dialectical contradiction between the possible and the actual is resolved. The nature of this resolution is that of an *irreversible* and *uncontrollable jump*.

Before concluding this section, it should be stressed that the problems of the interference of amplitudes, the superposition of states and of measurement are not isolated from one another, but form a single entity. Taking this into consideration, we recommend that the reader should pause a little, go back and read through Secs. 7-11 once again, in order to get a general idea about the physical foundations of quantum mechanics.

Interlude. Are These the Same Waves?, Or, Again on Waves in Quantum Mechanics

Participants: the Author and the Reader.

Call it then, what thou wilt—
Call it bliss! Heart! Love! God!
I have no name to give it!
Feeling is all in all:
The Name is sound and smoke,
Obscuring Heaven's clear glow.

Goethe (*Faust*)

Reader: I would like to return to the question of classical superposition. Sometimes I get a seditious idea: what is wrong with such a superposition? In any case it explains the interference effect more clearly than the superposition of amplitudes. I have due regard for the structure of quantum-mechanical concepts based on working with probability amplitudes, but still this idea keeps on haunting me from time to time.

Author: Classical superposition certainly does explain interference. But what about the result of the experiment involving "spying" on the behaviour of a microparticle in the interferometer (for example, in the case of a screen with slits)? The experiment indicates a destruction of interference. Classical interference does not explain this destruction.

Reader: But suppose it were possible to give a classical interpretation of the destruction of the interference pattern?

Author: No, such an interpretation is impossible in principle. This inference can be drawn from a consideration of the problem of the "reduction of a wave packet". A classical interpretation of the microparticle is impossible, and hence a classical interpretation of the interference observed in experiments with microparticles is also excluded.

Reader: This means that the de Broglie waves have nothing in common with classical waves?

Author: At least they are not classical waves.

Reader: Consequently, the diffraction of electrons is also not associated with classical wave processes?

Author: Of course, it is not.

Reader: In that case it is quite surprising that one so often comes across the term "wave" in quantum mechanics: "wave-particle duality", "de Broglie waves", "wave function", "wave equation", etc. Even quantum mechanics itself is sometimes called wave mechanics.

Author: Terminology is created under definite historical circumstances; it is not always quite correct. It is possible that the term "wave" is used too often and even without justification when considering microphenomena. We have become accustomed to treating interference as a specific wave phenomenon. Hence it is not surprising that when in 1927 experimenters observed interference patterns in experiments involving electrons, they immediately started using the term "electron waves". Actually electron interference has a more "subtle" origin; it arises because, generally speaking, the probability laws of nature don't follow the law of addition of probabilities, but require the summing of probability amplitudes. At first, of course, this was not known. And meanwhile the rather erroneous terminology took root in the literature.

Reader: And what about wave quantities such as the electron wave vector or its wavelength? They also appear in mathematical expressions.

Author: They are wave characteristics of a microparticle, but are by no means parameters of any classical wave.

Reader: But we also have the classical light waves, or, in other words, photon waves. Aren't the wave vector and the wavelength the parameters of a wave in this case also?

Author: Here we have a qualitatively different situation. You have raised quite an important question. We recall that photons are bosons and hence have a tendency to densely "populate" states. Suppose we are considering a photon state characterized by the quantities $\vec{k}$, ω, α (α is the photon polarization). This state is called the $k\alpha$-state. Suppose there is only one photon in this state. We don't have any classical wave yet. But suppose this state is "populated" by more and more photons. In the limiting case of a sufficiently large number of photons, we shall get a classical light wave whose parameters coincide with the characteristics of the photon state. We can now speak of the parameters of the classical wave, i.e. of the wave vector $\vec{k}$, frequency ω, polarization α. A peculiar "transformation" of the wave characteristics of a photon into the parameters of a wave has taken place. It must be emphasized that this is the result of an accumulation of photons in one state. The classical wave has been generated as a collective effect.

In the case of electrons, however, such a collective effect is in principle impossible. Electrons are fermions and hence can only "populate" states one at a time. Consequently, classical electronic (and in general fermionic) waves simply can not exist.

Reader: I think now I understand the position of waves in quantum mechanics. But if I am not mistaken, classical interference (classical superposition) may take place in boson ensembles.

Author: You are right. By the way, that is the reason why the interference of light was discovered long before the interference of electrons.

Reader: It turns out that there are two kinds of interference phenomena in nature: classical interference resulting from a summation of waves, and quantum-mechanical interference where the probability amplitudes are summed.

Author: In normal conditions, the classical interference (if we are talking of an ensemble of bosons) "masks" the quantum-mechanical interference. But in the case of electrons, for example, this "masking" does not take place. In this respect we have a "pure" situation.

Reader: Since any mention of waves in quantum mechanics is valid only for bosons and that too only when they "populate" the states fairly densely, don't you think it would be worthwhile to water down the "wave terminology" a bit?

Author: I would prefer not to uproot the established terminology. First of all, it is not the terminology itself that is important but rather the meaning concealed behind it. However, if there is a choice, then one must certainly choose the most appropriate term. That is why we are using here the term "probability amplitude" instead of "wave function". The former is more appropriate, though the latter is used more frequently.

Reader: I have already pointed out that so far, you have said nothing about the wave function, although it is widely used in all books on quantum mechanics.

Author: For the same reason we shall also introduce the wave function at a later stage. In fact we have already introduced it since the "wave function" and "probability amplitude" are terms describing the same thing. However, when speaking of the physical foundations of quantum mechanics, it is better to use the term "probability amplitude" We can go over to the wave function when we consider the mathematical apparatus of the theory.

In conclusion I would like to stress that it is not the terms that are important, but the way they are used. We can use the term "wave" for a microparticle, but we must not forget its specific nature. Here it is worthwhile recalling the remark made in Sec. 5 about the impropriety of using the model of a classical wave in a resonator for a bound electron.

Section 12

Causality in Quantum Mechanics

The impossibility of predicting exactly how a certain microparticle will behave in the measuring process at one time gave rise to talk of "indeterminacy" in quantum mechanics. In particular, it was suggested that causality is absent in microphenomena and in its place the uncontrollable event reigns. In time these ideas were replaced by a deeper understanding of the specific nature of time development of processes involving microparticles. The complaints about the indeterminacy of quantum mechanics proved groundless. It was realized that causality in microphenomena certainly is present although it is considerably different from the classical determinism which is characteristic for "old physics"

The Specific Nature of the Quantum-Mechanical Concept of Causality

In quantum mechanics the principle of causality refers to the possibilities of the realization of events (properties). In other words, in quantum mechanics it is not individually realized events that are causally related, but only the possibilities of the realization of these events. This is the essence of the quantum-mechanical meaning of causality. As Pauli stated in his Nobel lecture, ...*the statements of quantum mechanics are dealing only with possibilities, not with actualities. They have the form, 'This is not possible', or 'Either this or that is possible', but they can never say, 'that will actually happen then and there.*

Considering the specific nature of the quantum-mechanical meaning of causality, we stress the difference between *possible* and *realized* events in quantum mechanics. We also emphasize the objective nature of possibilities determined by the properties of the microparticles and the external conditions.

Since possible and actually realized events are identical in classical mechanics, it is clear that upon a transition from the quantum to the classical description of the world, the causal relation between the possible events must be converted into causal relation between realized events. In this sense the quantum-mechanical principle of causality is a generalization of the principle of classical determinism—it turns into the latter when going over from microphenomena to macrophenomena.

The Manifestation of Causality in Microphenomena

One may ask: If in quantum mechanics it is not the realized events but rather the possibilities of their realization that are causally related, then how can the observer make use of such a causality? In an experiment one always has to deal with events that have been realized.

The answer to this question is as follows: the observer must repeat a set of similar acts of measurements (for this he must have a sufficiently large number of similar microparticles, ensuring each time the same external conditions for each of them). In each act of measurement a random value of the quantity being measured will be realized. However, a set of these random values will allow us to find the *law of distribution* and the *mean value* of the quantity, which can be predicted *a priori*. The existence of a causal relationship between possible events is expressed through the possibility of such predictions.

We shall consider an example. Let the quantities of the β-set be measured in the $\langle\alpha|$ state. By carrying out a large number of identical measurements, the observer gets a whole set of values $\beta_1, \beta_2, \beta_3, \ldots$ Having got N values, the mean value may be determined:

$$\langle\beta\rangle = \frac{1}{N}\sum_{i}^{N} \beta_i. \tag{12.1}$$

Suppose that the observer decides to repeat his observations the next day (or the next year). He will get a certain set of values β'_1, β'_2, β'_3, . . The new set of values will be different from the old set, yet the new mean value determined by a formula of the type (12.1) will be close to the mean value $\langle\beta\rangle$ obtained earlier (provided, of course, that N is sufficiently large). This means that there was no need for the observer to toil on the second day. The mean value could be predicted on the basis of the previous day's measurements.

Moreover, the value $\langle\beta\rangle$ could have been computed beforehand without carrying out any measurement. True, for this the observer would have to have known the amplitudes $\langle\alpha \mid \beta_i\rangle$ in the superposition

$$\langle\alpha \mid = \sum_i \langle\alpha \mid \beta_i\rangle \langle\beta_i \mid . \qquad (12.2)$$

For computing $\langle\beta\rangle$ we must use the relation

$$\langle\beta\rangle = \sum_i \beta_i \mid \langle\alpha \mid \beta_i\rangle \mid^2. \qquad (12.3)$$

We assume that the reader has already understood the crux of the problem. This lies in the fact that the causal relationship among possible events signifies a causal relationship among the probabilities of the realization of these events. In short, prediction in quantum mechanics has a *probability character*! In order to predict the quantity $\langle\beta\rangle$ in the state $\langle\alpha\mid$, we must know the probability $\mid\langle\alpha \mid \beta_i\rangle\mid^2$ of the realization of values β_i in the given state. But if these probabilities are not known beforehand one must collect the corresponding *statistics* of the measurements of β-quantities which allow us to find the required probability.

Summing up the remarks made above, we quote Fock's words: *The probability of a given behaviour of an object in given external conditions is determined by the internal properties of the individual object and by the nature of these external conditions. It is a number characterizing the potential possibilities of this or that behaviour of the object. This possibility manifests itself in the frequency of occurrence of the given behaviour of the object; the relative frequency is its numerical measure. The probability thus belongs to the individual object and characterizes its potential possibilities; at the same time, to determine its numerical value from experiment one must have the statistics of realization of these possibilities, so that many repetitions of the experiment are necessary.*

Causality in Statistical Theories

It has already been remarked in Sec. 6 when discussing the problem of necessity and chance in microphenomena that quantum mechanics is a *statistical theory*. Hence, the question of causality in quantum mechanics may be seen first of all from the point of view of the manifestation of causality in general in statistical theories (as statistical mechanics, physical kinetics, microscopic electrodynamics).

In any statistical theory necessity and chance appear as *dialectical categories*. The relationship between them is that of unity and conflict of opposites. The velocities of molecules in a gas are random (any instantaneous velocity distribution of molecules is random) but the average velocity of a molecule can always be determined. The incidence of any electron passing through a screen with slits at any particular point of the detector screen is random, but the resulting interference pattern can always be determined. Necessity, like chance, is present in every statistical theory. It expresses causal relationships. Consequently, *causality* in statistical theories leads to *necessity* in these theories.

While in dynamic theories necessity dominates, thus making *exact* predictions of the values of physical quantities possible, it appears in statistical theories through *distribution laws* which give only the *probabilities* of various values of physical quantities.

As an additional (quite important) manifestation of necessity in statistical theories, we mention the *conservation laws*. It is well known that conservation laws may be seen as *exclusion principles*. From this point of view, the role of conservation laws in statistical theories is fairly obvious: they serve as conditions which reduce the probability of definite processes to zero.

Statistical Nature of Quantum Mechanics

When treating quantum mechanics as a statistical theory, one must remember that it occupies a special place among these theories. Within the framework of classical physics the laws describing the behaviour of large number of objects are of statistical nature, while the laws relating to the behaviour of an individual object are dynamic. By considering the element of chance in the behaviour of a single object, quantum mechanics places itself in a special position—that of a *statistical theory of an individual object*. That is why we earlier called quantum mechanics a statistical theory in principle.

This circumstance predetermines the specific nature of *statistical ensembles* in quantum mechanics.

According to Fock [1], *the elements of statistical collectives considered in quantum mechanics, are not the microobjects* *themselves, but the results of experiments with them, a definite experimental arrangement corresponding to a definite collective.*

Previously we considered an example in which measurements of quantities in the β-set were carried out on a microparticle in the state $\langle \alpha \mid$. A large number of repeated measurements gives a certain set of numbers β_1, β_2, β_3, This set of numbers is an example of statistical ensemble in quantum mechanics. Looking at the expression (12.3) we may conclude that $|\langle \alpha \mid \beta_i \rangle|^2$ plays the role of a *distribution function* for the given statistical ensemble. By changing the experiment (for example, by going over to the measurement of quantities in the γ-set) the observer will be dealing with another statistical ensemble γ_1, γ_2, γ_3, . It follows from this that it is in fact possible to have several statistical ensembles corresponding to a single microparticle.

Classical and quantum-mechanical ensembles, as can be easily seen, are different in nature. In classical physics a statistical ensemble is made up of a set of many objects, while in quantum mechanics, it is the set of the many possible ways of realizing properties of a microparticle, that forms an ensemble. Any change in the conditions will lead to a new ensemble. In particular, this difference manifests itself in that in classical physics averaging is performed over *different* states of the system, whereas in quantum mechanics we speak of mean values in a *given* state in the system (thus, in the example cited above, we spoke about the mean value $\langle \beta \rangle$ in the $\langle \alpha \mid$-state).

Naturally, in quantum theory we also have to carry out averaging over different states and consider statistical ensembles formed by a set of microparticles. Such problems, however, are beyond the scope of quantum mechanics itself and form a separate discipline called *quantum statistics*. Quantum statistics deals with two types of statistical ensembles and in this sense it is a doubly statistical theory.

Quantum-Mechanical Equation Expressing the Principle of Causality

Consider the following amplitude of state:

$$C_j(t) = \langle s(t) \mid j \rangle. \tag{12.4}$$

This is the probability amplitude of finding a microparticle in its basic j-state while it is located in the s-state at time t (at time t the detector is activated and thus the microparticle is observed in some particular state). The causal relationship among the probabilities of realizing events, which is a characteristic property of quantum mechanics, must be manifested in the existence of a mutual relationship between amplitudes considered at the moments of time t and $t + \Delta t$. Taking into account the principle of superposition we express the relationship between amplitudes as a linear equation

$$C_i(t+\Delta t)=\sum_i U_{ij}(t, \Delta t)\, C_j(t) \qquad (12.5)$$

(On the right-hand side the sum is taken over all the basic states.) The expansion coefficients $U_{ij}(t, \Delta t)$ for small values of Δt will be represented in the form

$$U_{ij}(t, \Delta t)=\delta_{ij}+\frac{i}{\hbar} H_{ij}(t)\, \Delta t. \qquad (12.6)$$

This representation is justified by the fact that for $\Delta t \to 0$ the coefficient U_{ij} will obviously be transformed into δ_{ij} (δ_{ij} is the Kronecker delta symbol).
Substituting (12.6) into (12.5), we get

$$-i\hbar \frac{C_i(t+\Delta t)-C_i(t)}{\Delta t}=\sum H_{ij}(t)\, C_j(t). \qquad (12.7)$$

In the limit as $\Delta t \to 0$ we find the equation

$$-i\hbar \frac{d}{dt} C_i(t)=\sum_j H_{ij}(t)\, C_j(t). \qquad (12.8)$$

This is the fundamental quantum-mechanical equation representing the principle of causality. Here H_{ij} are certain matrix elements describing the physics of the problem under consideration.

Hamiltonian Matrix

The matrix H_{ij} is called the *Hamiltonian matrix.* We make the following remarks concerning the Hamiltonian matrix:

1. The time dependence of the Hamiltonian matrix reflects the dependence of physical conditions on time (for example, a microparticle situated in a magnetic field which varies with time). If the conditions do not change, the matrix does not depend on time.
2. If the Hamiltonian matrix is *diagonalized* (only its diagonal elements are non-zero) then in this case the elements of the matrix have a simple physical meaning: they are the possible values of the energy of the microparticle* Because of this the Hamiltonian matrix may also be called the *energy matrix.*
3. The elements of the Hamiltonian matrix satisfy the relation

$$H_{ij}=H^*_{ji}. \qquad (12.9)$$

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* This remark will be explained later (see Sec. 13).

This relation is associated with the fact that the probability of the presence of a microparticle in at least one of the basic states obviously cannot change with time (the probabilities $\sum C_i C_i^*$). In order to prove this relation, we shall proceed from the equation

$$\frac{d}{dt}\sum C_i C_i^* = 0. \qquad (12.10)$$

Taking into account that

$$\frac{d}{dt}\sum C_i C_i^* = \sum \frac{dC_i}{dt} C_i^* + \sum_i C_i \frac{dC_i^*}{dt},$$

and using expression (12.8), we find that equation (12.10) assumes the form

$$\sum_i \sum_j (H_{ij} - H_{ji}^*) C_j C_i^* = 0, \qquad (12.11)$$

from which the result (12.9) follows directly.

Finally, we note that from (12.9) one can deduce that the diagonal elements of the Hamiltonian matrix are real numbers. This circumstance is in conformity with the above-mentioned role of the diagonal elements as values of the energy of a microparticle.

What Are the Requirements for a Causal Description of Phenomena in Quantum Theory?

The answer to this question may be given by considering expression (12.8) for the basic quantum-mechanical equation. The gist of the answer is as follows. Firstly, we must choose a set of basic states $\{\langle i\,|\}$; secondly, we must find the form of the Hamiltonian matrix considered in the system of chosen basic states. After this we can make definite predictions by using equation (12.8).

It is especially simple to consider cases when the number of basic states is equal to *two*. We can further simplify these by assuming that the Hamiltonian matrix is invariant with time. In Secs. 13 and 14 we shall consider such cases. The use of equation (12.8) which forms the basis of a causal description of microphenomena will be demonstrated by particular examples.

Section 13

Microparticles with Two Basic States

Examples of Microparticles with Two Basic States

The number of basic states of a microparticle is usually greater than two. However, there are situations when it is possible to consider only two basic states. Taking an example already familiar to the reader we shall consider the passage of a photon through a polarizer. The photon is in a state with definite momentum $\hbar\vec{k}$ (and definite energy $\hbar\vec{k}c$). In this case we shall only consider the possible changes in the polarization of the photon. Hence, one may speak of just two basic states of the photon, having in mind its polarization states.

So, every time when we talk about a microparticle with two basic states, it is assumed that we only consider the possible changes in some particular "parameter" of the microparticle (for example, its polarization). All the other "parameters" are assumed to be known. We shall now cite some examples where one can speak of a microparticle with two basic states. These states are denoted by $\langle 1 \,|$ and $\langle 2 \,|$, respectively.

The *ammonia molecule* consists of one nitrogen atom and three hydrogen atoms. The nitrogen atom does not lie in the plane passing through the hydrogen atoms (for brevity, we shall call this plane the H-plane). The state $\langle 1 \,|$ corresponds to the nitrogen atom being on one side of the H-plane, and the state $\langle 2 \,|$ corresponds to this atom being on the other side of the H-plane.

The *hydrogen molecule* is made up of two protons and two electrons, the spin states of the latter being different. Suppose we single out one of these spin states. Then the basic state $\langle 1 \,|$ may be defined as the state of the molecule in which the electron with the singled out spin is localized near one proton, and the state $\langle 2 \,|$ as the state with the localization of this electron near the other proton. Moreover, the second electron is localized each time near the corresponding "vacant" proton (the possibility of the localization of both electrons near one proton need not be considered in view of the strong Coulomb repulsion between electrons).

The Role of Non-Diagonal Elements in the Hamiltonian Matrix

We represent an arbitrary state $\langle s \,|$ of a microparticle in the form of a superposition of basic states $\langle 1 \,|$ and $\langle 2 \,|$:

$$\langle s \,| = \langle s \,|\, 1 \rangle \langle 1 \,| + \langle s \,|\, 2 \rangle \langle 2 \,|,$$

or, taking into account relation (12.4),

$$\langle s \,| = C_1 \langle 1 \,| + C_2 \langle 2 \,|. \tag{13.1}$$

According to (12.8), the amplitudes C_1 and C_2 satisfy the system of equations

$$\left.\begin{aligned} -i\hbar \frac{d}{dt} C_1 &= H_{11} C_1 + H_{12} C_2, \\ -i\hbar \frac{d}{dt} C_2 &= H_{21} C_1 + H_{22} C_2. \end{aligned}\right\} \tag{13.2}$$

We shall consider two cases:

First case. The non-diagonal elements H_{12} and H_{21} are equal to zero (the Hamiltonian matrix is diagonalized). In this case the system of equations (13.2) splits into two independent equations

$$-i\hbar \frac{d}{dt} C_1 = H_{11}C_1, \qquad -i\hbar \frac{d}{dt} C_2 = H_{22}C_2. \tag{13.3}$$

It follows from (13.3) that if at a certain time the microparticle is, for example, in the state $\langle 1 \mid$, it will never appear in the state $\langle 2 \mid$. Here, the basic states $\langle 1 \mid$ and $\langle 2 \mid$ are in fact the *stationary states* of the microparticle characterized by the energy values H_{11} and H_{22} respectively.

Second case. The non-diagonal elements H_{12} and H_{21} are non-zero. In this case, we have a system of two mutually related equations [system (13.2)]. Hence if at a given moment the microparticle is, for example, in the state $\langle 1 \mid$, it may appear in the state $\langle 2 \mid$ at another instant of time. The presence of non-diagonal elements in the Hamiltonian matrix means the existence of *transitions* of the microparticle within various basic states.

While considering examples of microparticles with two basic states, we note that in the ammonia molecule, the nitrogen atom undergoes transitions changing its position with respect to the H-plane. The protons in the hydrogen molecule "exchange" electrons. Note that this very "exchange" of the electron pair forms the basis of a *chemical bond.* It may be said that a valency bond between two atoms arises as a result of each of these atoms "contributing for common use" one electron. It is these "shared" electrons that are responsible for the appearance of a bond between the atoms.

A Brief Interlude

> *—You understand, and are acquainted with Latin, without doubt?*
>
> *—Yes; but act as if I were not acquainted with it.*
>
> Molièr (*The Cit Turned Gentleman*)

Reader: Earlier, in Sec. 10, it was stated that "if an object is in one basic state, it cannot be found in another basic state". Isn't this in contradiction with the possibility just mentioned of transitions between basic states?

Author: In Sec. 10, we were talking about the principle of superposition of states. During the course of the discussion we did not take into account the possibility of the development in time of transition between the states giving rise to the superposition.

Reader: Please clarify this.

Author: First of all, let us expand (13.1) in the following form:

$$\langle s(t)| = C_1(t)\langle 1| + C_2(t)\langle 2|. \tag{13.1a}$$

We have the microparticle in the superposition state $\langle s(t)|$. If the detector is activated at time t, the microparticle will be found in the state $\langle 1|$ or $\langle 2|$, the probability of these events being $|C_1(t)|^2$ and $|C_2(t)|^2$, respectively. It is significant that one event excludes the other—this is what we mean by the statement you quoted.

Reader: I understand the crux of the matter. If the microparticle is found, for example, in the state $\langle 1|$ at time t, this excludes the possibility of its being found in the state $\langle 2|$ at the same time. However, the microparticle may be found in the state $\langle 2|$ at another instant of time.

Author: It is important that the non-diagonal elements of the Hamiltonian matrix should be non-zero in this case. Otherwise, if you find the microparticle in the state $\langle 1|$, you will never find it in the state $\langle 2|$.

Reader: I understand that the superposition states and transitions between basic states are different "subjects".

Author: That is true but don't forget that when considering transitions we should take into acount not only the nondiagonality of the Hamiltonian matrix, but also the superposition relation (13.1a). In this case, everything depends on the nature of the time dependence of the amplitudes C_1 and C_2. In one case it so happens that $|C_1|^2$ and $|C_2|^2$ do not vary with time; in this case there are no transitions between the basic states. In the other case $|C_1|^2$ and $|C_2|^2$ vary with time and then we do have transitions. In short, the question of the nature of the time dependence of the amplitudes C_1 and C_2 requires a more detailed consideration.

We shall consider two cases exhibiting the time dependence of the amplitudes C_1 and C_2.

First case. The non-diagonal elements of the Hamiltonian matrix are equal to zero. By solving equation (13.3), we find

$$C_1(t) = C_1(0)\exp(iH_{11}t/\hbar),$$
$$C_2(t) = C_2(0)\exp(iH_{22}t/\hbar). \quad (13.4)$$

This is the nature of the dependence on time of the amplitudes describing stationary states.

From (13.4) it can be seen that the probability of finding the microparticle in any basic state is invariant in time:

$$|C_1(t)|^2 = |C_1(0)|^2, \quad |C_2(t)|^2 = |C_2(0)|^2. \quad (13.5)$$

If at time $t = 0$ the microparticle is in the state $\langle 1|$, then $|C_1(t)|^2 = 1$ and $|C_2(t)|^2 = 0$. As expected, the lifetime of a microparticle in a stationary state turns out to be indefinitely long.

Second case: The non-diagonal elements of the Hamiltonian matrix are different from zero. We assume that we can put*

$$H_{11} = H_{22} \equiv E_0. \quad (13.6)$$

Besides, if we assume that non-diagonal elements of the Hamiltonian matrix are real and take (12.9) into account, we can denote

$$H_{12} = H_{21} \equiv -A. \quad (13.7)$$

By using (13.6) and (13.7) we rewrite (13.2) in the form

$$\left.\begin{aligned} -i\hbar\frac{d}{dt}C_1 &= E_0C_1 - AC_2, \\ -i\hbar\frac{d}{dt}C_2 &= E_0C_2 - AC_1, \end{aligned}\right\} \quad (13.8)$$

This system of equations is equivalent to the following system:

$$\left.\begin{aligned} -i\hbar\frac{d}{dt}(C_1+C_2) &= (E_0-A)(C_1+C_2), \\ -i\hbar\frac{d}{dt}(C_1-C_2) &= (E_0+A)(C_1-C_2). \end{aligned}\right\}$$

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* This can be done if the problem under consideration is characterized by a certain symmetry; thus in the example with the ammonia molecule, the states $\langle 1|$ and $\langle 2|$ correspond to positions of the nitrogen atom which are symmetrical with respect to the H-plane.

The solutions of the latter system are of the form

$$C_1+C_2=a\exp[i(E_0-A)t/\hbar]$$

$$C_1-C_2=b\exp[i(E_0+A)t/\hbar]$$

from which we obtain

$$C_1(t)=\frac{a}{2}\exp[i(E_0-A)t/\hbar]+\frac{b}{2}\exp[i(E_0+A)t/\hbar], \qquad (13.9a)$$

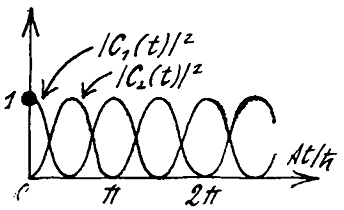
$$C_2(t)=\frac{a}{2}\exp[i(E_0-A)t/\hbar]-\frac{b}{2}\exp[i(E_0+A)t/\hbar]. \qquad (13.9b)$$

Suppose that at $t = 0$ the microparticle is in the state $\langle 1\,|$. Then $C_1(0) = 1$ and $C_2(0) = 0$, from which $a = b = 1$. In this case expressions (13.9) assume the form

$$C_1(t)=\exp(iE_0t/\hbar)\cos(At/\hbar), \qquad (13.10a)$$

$$C_2(t)=-i\exp(iE_0t/\hbar)\sin(At/\hbar). \qquad (13.10b)$$

Fig. 13.1



From these expressions it is obvious that the probability of the microparticle remaining in the state $\langle 1\,|$ at time t is equal to

$$|C_1(t)|^2=\cos^2(At/\hbar), \qquad (13.11a)$$

and the probability of its appearing at time t in the state $\langle 2\,|$ is equal to

$$|C_2(t)|^2=\sin^2(At/\hbar). \qquad (13.11b)$$

It is useful to compare (13.5) and (13.11). While in the first case the probabilities $|C_1|^2$ and $|C_2|^2$ are invariant in time, their dependence on time in the second case is quite obvious. The time dependence of the probabilities $|C_1(t)|^2$ and $|C_2(t)|^2$ determined by relations (13.11) is shown in Fig. 13.1.

Diagonalization of the Hamiltonian Matrix

Let us compare the expressions for $C_1 + C_2$ and $C_1 - C_2$, obtained in the previous section, with (13.4). This comparison allows us to conclude that the amplitudes $C_1 + C_2$ and $C_1 - C_2$ describe the stationary states of the microparticle with energies equal to $E_0 - A$ and $E_0 + A$, respectively. Further, we introduce a new pair of basic states

$$\begin{aligned}\langle \mathrm{I}\,| &= \frac{1}{\sqrt{2}}(\langle 1\,|-\langle 2\,|),\\ \langle \mathrm{II}\,| &= \frac{1}{\sqrt{2}}(\langle 1\,|+\langle 2\,|)\end{aligned} \qquad (13.12)$$

[it is easy to see that if the states ⟨1 | and ⟨2 | satisfy the orthonormalization condition (10.8), the states ⟨I | and ⟨II | also satisfy this condition]. By using (13.12), we rewrite (13.1) in the form

$$\langle s \| = \frac{C_1 - C_2}{\sqrt{2}} \langle \mathrm{I} | + \frac{C_1 + C_2}{\sqrt{2}} \langle \mathrm{II} |. \qquad (13.13)$$

It can be seen from here that a transition from the basic states ⟨1 | and ⟨2 | to the basic states ⟨I | and ⟨ II | corresponds to a transition from amplitudes C_1 and C_2 to amplitudes $(C_1 - C_2)/\sqrt{2}$ and $(C_1 + C_2)/\sqrt{2}$. Since the latter describe the stationary states of the microparticle, it follows that the transition under consideration is associated with a diagonalization of the Hamiltonian matrix.

$$\begin{bmatrix} E_0 & -A \\ -A & E_0 \end{bmatrix} \to \begin{bmatrix} E_0 + A & 0 \\ 0 & E_0 - A \end{bmatrix}.$$

Thus, suppose we have a certain microparticle under certain external conditions. Let us choose a certain system of basic states. The attempt is usually made to choose basic states which have a clear physical meaning (as we did, for example, in the case of the ammonia molecule or the hydrogen molecule). The basic states chosen on the basis of such considerations lead, in the general case, to a Hamiltonian matrix whose non-diagonal elements are different from zero (the microparticle undergoes transitions between the basic states). Further, it is possible to go over to a new system of basic states for which the Hamiltonian matrix is diagonal. The new basic states describe the stationary states of the microparticle; the elements of the diagonalized Hamiltonian matrix are essentially the values of the energy in these states.

General Case

In the general case the non-diagonal elements of the Hamiltonian matrix are different from zero and so the simplifying conditions (13.6) and (13.7) are not applicable. In this case one must solve not the simplified system of equations (13.8), but the more general system of equations (13.2) for a microparticle with two basic states. We suggest that the reader, if he so desires, solves the system (13.2) himself, assuming for the sake of simplicity that the Hamiltonian matrix is invariant in time*. We shall limit ourselves here giving some results.

The energy of the stationary states of a microparticle is

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* Such a solution is given, for example, in [3].

determined by the expression

$$E_{\mathrm{I,\,II}}=\frac{H_{11}+H_{22}}{2}\pm\sqrt{\left(\frac{H_{11}-H_{22}}{2}\right)^2+H_{12}H_{21}}. \qquad (13.14)$$

The basic states $\langle \mathrm{I}\mid$ and $\langle \mathrm{II}\mid$ corresponding to these energy values are expressed in terms of the elementary states $\langle 1\mid$ and $\langle 2\mid$ describing the equation system (13.2) in the following manner:

$$\left.\begin{aligned}\langle \mathrm{I}\mid &= a_1\langle 1\mid+b_1\langle 2\mid,\\ \langle \mathrm{II}\mid &= a_2\langle 1\mid+b_2\langle 2\mid,\end{aligned}\right\} \qquad (13.15)$$

where

$$\left.\begin{aligned}\mid a_1\mid^2+\mid b_1\mid^2=\mid a_2\mid^2+\mid b_2\mid^2=1,\\ a_1/b_1=H_{12}/(E_{\mathrm{I}}-H_{11}),\\ a_2/b_2=H_{21}/(E_{\mathrm{II}}-H_{22}).\end{aligned}\right\} \qquad (13.16)$$

It can be easily seen that if $H_{11}=H_{22}=E_0$ and $H_{12}=H_{21}=-A$, the result (13.14) gives $E_{\mathrm{I,II}}=E_0\pm A$, the superpositions (13.15) turn into (13.12). In other words, we arrive at the simplified case of the non-diagonal Hamiltonian matrix discussed above in detail. But if $H_{12}=H_{21}=0$, the result (13.14) gives $E_{\mathrm{I}}=H_{11}$, $E_{\mathrm{II}}=H_{22}$—we arrive at the case of the diagonal Hamiltonian matrix ($\langle \mathrm{I}\mid=\langle 1\mid$, $\langle \mathrm{II}\mid=\langle 2\mid$).

Example of the Ammonia Molecule

We recall that the basic states $\langle 1\mid$ and $\langle 2\mid$ of the ammonia molecule were chosen using graphic physical considerations: they correspond respectively to the position of the nitrogen atom on one side of the H-plane and on the other. Since these positions are symmetrical, we may take $H_{11}=H_{22}\equiv E_0$. Assuming further that the elements H_{12} and H_{21} are real ($H_{12}=H_{21}\equiv -A$), which, as it turns out, does not involve the loss of generality in this case, we arrive at the situation to which the simplified system of equation (13.8) corresponds. It follows from this that the energy levels of a molecule are essentially E_0+A and E_0-A. We emphasize that if no transitions took place between the states $\langle 1\mid$ and $\langle 2\mid$, there would have been only one level E_0 in place of the levels E_0+A and E_0-A. It would have been doubly degenerate since there would be two states corresponding to it. It may be said that transitions between the states $\langle 1\mid$ and $\langle 2\mid$ (associated with "pushing" of the nitrogen atom through the H-plane) correspond to a removal of degeneracy, i.e. to a splitting of the level E_0 into two levels E_0+A and E_0-A.

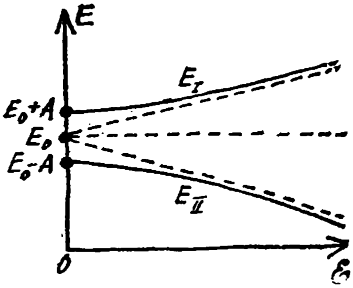
Further, let us assume that the ammonia molecule is placed in a static electric field with intensity $\mathcal{E}$ which is perpendicular to the H-plane. Denoting the electric dipole moment of the molecule by d, we write

$$H_{11}=E_0+\mathscr{E}d, \quad H_{22}=E_0-\mathscr{E}d. \tag{13.17}$$

Now the positions of the nitrogen atom on either side of the H-plane are no longer physically symmetrical ($H_{11} \neq H_{22}$). Assuming that $H_{12}=H_{21}=-A$ as before, we write the system of equations (13.2) for the case under consideration:

$$\left.\begin{aligned} -i\hbar\frac{d}{dt}C_1&=(E_0+\mathscr{E}d)C_1-AC_2,\\ -i\hbar\frac{d}{dt}C_2&=-AC_1+(E_0-\mathscr{E}d)C_2. \end{aligned}\right\} \tag{13.18}$$

Fig. 13.2



By using (13.14), we obtain the following expressions for the energy levels of the molecule in a static electric field:

$$E_{\mathrm{I}}=E_0+\sqrt{A^2+\mathscr{E}^2d^2}, \quad E_{\mathrm{II}}=E_0-\sqrt{A^2+\mathscr{E}^2d^2}. \tag{13.19}$$

Figure 13.2 shows the qualitative dependence of the energy levels of ammonia molecule on the field intensity. It can be easily seen that the effect of "throwing" the nitrogen atom through the H-plane is important for relatively small field intensities. In strong fields, when the levels diverge considerably, this effect becomes insignificant.

Section 14 The Electron in a Magnetic Field

It is well known that the projection of the electron spin momentum in any direction may assume only two values ($-\hbar/2$ and $+\hbar/2$). This allows us to treat the electron as a microparticle with two basic states. The problem of an electron in a magnetic field is of great practical interest. Besides, this problem is also quite interesting from a methodical point of view: its analysis enables one to get acquainted with not only the general nature of a system with two basic states, or, in other words, the two-level system, through a physically suggestive example, but also with the general approach to the analysis of such systems.

The Hamiltonian Matrix for an Electron in a Magnetic Field

Let us first fix the direction of the coordinate axes (including the direction of the z-axis). For the basic states $\langle 1 \mid$ and $\langle 2 \mid$ we choose states for which the projections of the electron spin on the z-axis are equal to $\hbar/2$

and $-\hbar/2$, respectively. We switch on a static magnetic field (we denote the value of the magnetic induction by B) and consider the following two cases.

First case: the magnetic field is directed along the z-axis ($B_x = B_y = 0$). In this case the basic states $\langle 1 \mid$ and $\langle 2 \mid$ are stationary; the state $\langle 1 \mid$ has energy $-\mu B_z$ and the state $\langle 2 \mid$ has energy μB_z (μ denotes the magnetic moment of the electron). The amplitudes C_1 and C_2 satisfy two independent equations of the type (13.3):

$$-i\hbar \frac{dC_1}{dt} = -\mu B_z C_1, \quad -i\hbar \frac{dC_2}{dt} = \mu B_z C_2. \tag{14.1}$$

The Hamiltonian matrix of the electron is of the form

$$[H] = \begin{bmatrix} -\mu B_z & 0 \\ 0 & \mu B_z \end{bmatrix}. \tag{14.2}$$

Second case: the magnetic field is in an arbitrary direction. In the first place, we note that irrespective of the direction of the field (in other words, irrespective of the choice of the direction of the coordinate axes) the energy levels of the electron are determined by the expressions $-\mu B$ and μB; while in the previous case we had to take $B = B_z$, in this case we must have $B = (B_x^2 + B_y^2 + B_z^2)^{1/2}$. Thus

$$E_{\mathrm{I}} = -\mu \sqrt{B_x^2 + B_y^2 + B_z^2}, \quad E_{\mathrm{II}} = \mu \sqrt{B_x^2 + B_y^2 + B_z^2}. \tag{14.3}$$

Note that

$$E_{\mathrm{I}} = -E_{\mathrm{II}}. \tag{14.4}$$

Further we make use of relation (13.14). By taking (14.4) into account, we may assume that $H_{11} + H_{22} = 0$. As a result, by combining (14.3) and (12.9), we get

$$\left(\frac{H_{11} - H_{22}}{2}\right)^2 + |H_{12}|^2 = \mu^2 (B_x^2 + B_y^2 + B_z^2). \tag{14.5}$$

We shall assume a linear relationship between the elements of the Hamiltonian matrix and the field. It turns out that this fairly natural assumption allows us to derive the following relations from (14.5): $H_{11} = -\mu B_z$, $H_{22} = \mu B_z$, $H_{21} = H_{12}^* = -\mu (B_x + iB_y)$. Thus, the Hamiltonian matrix of an electron in a magnetic field has the following general form:

$$[H] = \begin{bmatrix} -\mu B_z & -\mu (B_x - iB_y) \\ -\mu (B_x + iB_y) & \mu B_z \end{bmatrix} \tag{14.6}$$

It can be easily seen that when $B_x = B_y = 0$, the matrix (14.6), as expected, coincides with the matrix (14.2).

By using (14.6) we write the system of equation (13.2) for the case under consideration:

$$\left.\begin{aligned} -i\hbar\frac{d}{dt}C_1 &= -\mu\,[B_zC_1+(B_x-iB_y)\,C_2],\\ -i\hbar\frac{d}{dt}C_2 &= -\mu\,[(B_x+iB_y)\,C_1-B_zC_2]. \end{aligned}\right\} \qquad (14.7)$$

In conclusion, we note that although the above argument was conducted for the case when the Hamiltonian matrix is invariant in time, the results (14.6) and (14.7) are valid even when the magnetic field varies with time.

Projection Amplitudes

Let the direction of the magnetic field be determined by the polar angle θ and azimuth φ (Fig. 14.1). We shall assume that the electron spin is directed along the field; consequently, the electron is in the stationary state $\langle \mathrm{I}\,|$ with energy $E_{\mathrm{I}} = -\mu B$. According to (13.15), the state $\langle \mathrm{I}\,|$ can be represented as a superposition:

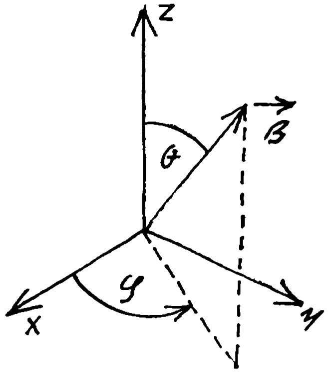


Fig. 14.1

$$\langle \mathrm{I}\,| = a_1\langle 1\,| + b_1\langle 2\,|, \qquad (14.8)$$

where, as we recall, $\langle 1\,|$ and $\langle 2\,|$ are the states in which the projections of the electron spin on the z-axis are equal to $\hbar/2$ and $-\hbar/2$, respectively, and the coefficients a_1 and b_1 are determined by the relations (13.16):

$$a_1/b_1 = H_{12}/(E_{\mathrm{I}}-H_{11}), \quad |a_1|^2+|b_1|^2=1. \qquad (14.9)$$

By using (14.6) we write

$$\left.\begin{aligned} H_{11} &= -\mu B_z = -\mu B\cos\theta,\\ H_{12} &= -\mu\,(B_x-iB_y) = -\mu B\sin\theta\exp(-i\varphi). \end{aligned}\right\} \qquad (14.10)$$

Substituting (14.10) into (14.9), we find that

$$a_1/b_1 = \sin\theta\exp(-i\varphi)/(1-\cos\theta).$$

Taking into account that $|\,a_1\,|^2 + |\,b_2\,|^2 = 1$, we arrive at the following final result:

$$\begin{aligned} a_1 &= \cos(\theta/2)\exp(-i\varphi/2);\\ b_1 &= \sin(\theta/2)\exp(i\varphi/2). \end{aligned} \qquad (14.11)$$

Thus, we have determined the amplitudes of the probabilities that the electron has its spin directed along the z-axis (amplitude a_1) or in the opposite direction (amplitude b_1) by assuming that the electron spin is directed along the field (i.e. in the direction determined by the angles θ and φ).

Note that (14.11) does not contain the magnetic induction B. It is obvious that the result (14.11) must be valid in the limiting case $B \to 0$. In other words, we may exclude the field from consideration and interpret (14.11) in the following way. It is clear that the direction of the electron spin is determined by the angles θ and φ. In this case the amplitude of the probability that the electron spin is along the z-axis is a_1 and the amplitude of the probability that the electron spin is in the opposite direction is b_1. Expression (14.8) should be treated in this case as an expansion of the spin state $\langle\theta, \varphi\,|$ in terms of the spin states $\langle z\,|$ and $\langle -z\,|$:

$$\langle\theta, \varphi| = \cos(\theta/2)\exp(-i\varphi/2)\langle z| + \sin(\theta/2)\exp(i\varphi/2)\langle -z|. \qquad (14.12)$$

The amplitudes of the states occurring in (14.12)

$$\begin{aligned}\langle\theta, \varphi|z\rangle &= \cos(\theta/2)\exp(-i\varphi/2);\\ \langle\theta, \varphi|-z\rangle &= \sin(\theta/2)\exp(i\varphi/2)\end{aligned} \qquad (14.13)$$

are called *projection amplitudes.*

By using projection amplitudes, we may predict the result of the following experiment. Let an electron beam, polarized in a direction given by the angles θ and φ, pass through some "filter" which only allows through electrons whose spin is along the z-axis. In this case the amplitude of probability of an electron passing through the apparatus (through the "filter") is $\langle\theta, \varphi\,|\,z\rangle$. The projection amplitude here plays the role of the amplitude of the electron transition from the state $\langle\theta, \varphi\,|$ to the state $\langle z\,|$.

Precession of the Electron Spin

Let the direction of the electron spin be given by the angles θ and φ (the electron is in the state $\langle\theta, \varphi\,|$). This state can be represented in the form of superposition (14.12) of the states $\langle z\,|$ and $\langle -z\,|$. Suppose that at time $t = 0$ we switch on a magnetic field B which is directed along the z-axis. Now the states $\langle z\,|$ and $\langle -z\,|$ become stationary states. Using this, we write [see (13.4)]

$$\left.\begin{aligned}\langle\theta, \varphi|z\rangle &= C_1(0)\exp(-i\mu B_z t/\hbar),\\ \langle\theta, \varphi|-z\rangle &= C_2(0)\exp(i\mu B_z t/\hbar).\end{aligned}\right\} \qquad (14.14)$$

Comparing (14.14) with (14.13), we conclude that

$$\begin{aligned}C_1(0) &= \cos(\theta/2)\exp(-i\varphi/2);\\ C_2(0) &= \sin(\theta/2)\exp(i\varphi/2).\end{aligned} \qquad (14.15)$$

It follows from this that in time t after the magnetic field has been switched on the projection amplitudes assume the form

$$\langle\theta,\ \varphi(t)\,|\,z\rangle=\cos(\theta/2)\exp\left[-\frac{i}{2}(\varphi+2\mu B_z t/\hbar)\right],$$
$$\langle\theta,\ \varphi(t)\,|-z\rangle=\sin(\theta/2)\exp\left[\frac{i}{2}(\varphi+2\mu B_z t/\hbar)\right] \tag{14.16}$$

Thus, the switching on of a magnetic field along the z-axis does not change the polar angle θ but changes the azimuth φ, the change in φ being proportional to the time interval t which elapses after switching on the field. This means that the spin of an electron *precesses* around the z-axis (around the direction of magnetic field) with a constant angular velocity. It can be easily seen that the angular velocity of the spin precession is given by the relation

$$\omega = 2\mu B_z/\hbar. \tag{14.17}$$

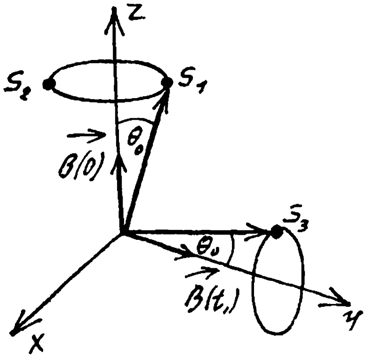
We move one step further by ignoring coordinate axes. Suppose that at time $t = 0$ the direction of electron spin forms an angle θ with the direction of the magnetic field. This angle will remain constant with time, but the electron spin will precess around the field direction with an angular velocity

$$\omega = 2\mu B/\hbar. \tag{14.17a}$$

We further suppose that the magnetic field is varying with time (in the general case, both the direction and the magnitude of the vector $\vec{B}$ are varying). A change in the field leads to a corresponding change in the electron spin precession: a change in the magnitude of the magnetic field results in a change in the angular velocity of precession, while a change in the direction of the field causes a change in the direction around which the precession takes place.

A knowledge of the precession enables one to predict changes in the electronic state over a given period of time. We shall consider a simple example (Fig. 14.2). Suppose that at the instant $t = 0$ the field is directed along the z-axis [vector $\vec{B}$ (0)], and the electron spin is in the zy-plane and forms an angle θ_0 with the direction of the field. Thus the initial state of the electron $\langle\theta(0), \varphi(0)\,|$ is determined by the angles $\theta(0) = \theta_0$ and $\varphi(0) = \pi/2$. We shall assume that the magnitude of the field does not change with time, but that the direction of the field changes. Suppose after time $t_1 = \pi\hbar/2\mu B$ the field becomes directed along the y-axis [vector $\vec{B}$ (t_1) in Fig. 14.2]. What will be the state of the electron at the

Fig. 14.2



time t_1? It is clear that if the field direction had remained unchanged, the end point of the electron spin vector, while precessing around the z-axis, would have described a semicircle during the time $\pi\hbar/2\mu B$, thus shifting from point s_1 to point s_2. If we take into account the variation in field direction, we shall find that it has shifted not to the point s_2 but to the point s_3. Consequently, the required state of the electron $\langle\theta(t_1), \varphi(t_1) \mid$ would be determined by the angles $\theta(t_1) = \pi/2 - \theta_0$ and $\varphi(t_1) = \pi/2$.

Generalization of the Problem of an Electron in a Magnetic Field to an Arbitrary Two-Level System

According to Feynman [3], *it is interesting that the mathematical ideas we have just gone over for the spinning electron in a magnetic field can be applied to any two-state system. That means that by making a mathematical analogy to the spinning electron, any problem about two-state systems can be solved by pure geometry.... If we can solve the electron problem in general, we have solved all two-state problems.* Let us clarify these remarks.

We shall consider some two-level system with the basic states $\langle 1 \mid$ and $\langle 2 \mid$. We assign some vector to each state of the microparticle. A choice of the basic states $\langle 1 \mid$ and $\langle 2 \mid$ in this case is equivalent to a choice of the z-axis (as if these two states correspond to the two z-projections of the electron spin). Suppose that the microparticle is in the state $\langle s(0) \mid$ at the initial moment of time. We assign to this state a vector whose direction is determined by the angles $\theta(0)$ and $\varphi(0)$:

$$\langle s(0) \mid \longleftrightarrow \langle \theta(0), \varphi(0) \mid. \qquad (14.18)$$

In order to find the angles $\theta(0)$ and $\varphi(0)$, we must expand the state $\langle s(0) \mid$ in terms of the basic states $\langle 1 \mid$ and $\langle 2 \mid$ and use for the coefficients of expansion expression (14.13) for the projection amplitudes. This expansion is of the form

$$\langle s(0)| = \cos[\theta(0)/2]\exp[-i\varphi(0)/2]\langle 1| + \sin[\theta(0)/2]\exp[i\varphi(0)/2]\langle 2|. \qquad (14.19)$$

Further, let us turn to the Hamiltonian matrix of the microparticle. First of all we shift the zero point of the energy in such a way that it is located precisely half-way between the two energy levels or, in other words, so that the condition (14.4) is satisfied. In this case

$$H_{11} + H_{22} = 0. \qquad (14.20)$$

We now formally introduce a vector $\mu\vec{B}$ (it is in no way associated with any magnetic field!) such that its projections on the coordinate axes (remember that the axes are determined by the choice of the basic states) satisfy the conditions

$$H_{11} = -\mu B_z, \quad H_{12} = -\mu (B_x - iB_y). \tag{14.21}$$

By using (14.21) we determine

$$\omega = 2\mu (B_x^2 + B_y^2 + B_z^2)^{1/2}/\hbar. \tag{14.22}$$

In order to solve this two-level problem, i.e. in order to determine the change in the $\langle s\,|$-state during certain time t, we must consider the precession of the vector $\langle \theta, \varphi\,|$ around the direction $\vec{B}$ with an angular velocity ω. If the Hamiltonian matrix is time dependent, both the direction of $\vec{B}$ and the magnitude of the angular velocity of precession will change accordingly. After a time t, the microparticle will be in the state $\langle s\,(t)\,|$, defined by the angles $\theta\,(t)$ and $\varphi\,(t)$, which may be determined if we know the initial values $\theta\,(0)$ and $\varphi\,(0)$ and the precession (in exactly the same way as was done in the example given at the end of the preceding subsection). The transition from the angles $\theta\,(t)$ and $\varphi\,(t)$ to the required final state $\langle s\,(t)\,|$ is accomplished by using the familiar superposition:

$$\begin{aligned}\langle s\,(t)\,| = {} & \cos[\theta\,(t)/2] \exp[-i\varphi\,(t)/2] \langle 1\,| \\ & + \sin[\theta\,(t)/2] \exp[i\varphi\,(t)/2] \langle 2\,|.\end{aligned} \tag{14.23}$$

Applying these remarks to the example of the ammonia molecule considered in Sec. 13, we must shift the zero point of the energy by an amount E_0, and go over (for the sake of convenience) from the basic states $\langle 1\,|$ and $\langle 2\,|$ to the basic states $\langle \mathrm{I}\,|$ and $\langle \mathrm{II}\,|$. As a result, we get in place of (13.18) the following system of equations:

$$\left.\begin{aligned} -i\hbar \frac{d}{dt} C_{\mathrm{I}} &= AC_{\mathrm{I}} + \mathscr{E} dC_{\mathrm{II}}, \\ -i\hbar \frac{d}{dt} C_{\mathrm{II}} &= \mathscr{E} dC_{\mathrm{I}} - AC_{\mathrm{II}}. \end{aligned}\right\} \tag{14.24}$$

This system is convenient for drawing the analogy with the electron in a magnetic field. Comparing (14.24) and (14.7), we find that the quantity A corresponds to $-\mu B_z$ and the quantity $\mathscr{E}d$ to $-\mu B_x$. Consequently, we have to consider the precession of the vector describing the state $\langle s\,|$ of the molecule in the "magnetic field" which is made up of two components: a constant component along the z-axis, associated with the effect of the "throwing" of a nitrogen atom through the H-plane, and a component along the x-axis, associated with the electric field. The latter component may, obviously, vary with time.

PAULI SPIN MATRICES. In conclusion, we shall mention the ***Pauli spin matrices*** which are widely used in the quantum mechanics of two-level systems. These matrices are of the form

$$\sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \quad \sigma^y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}; \quad \sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{14.25}$$

By using these matrices, we can rewrite the expression for the elements of Hamiltonian matrix of an electron in a magnetic field (14.6) in the following form:

$$H_{ij} = -\mu\, (\sigma^x_{ij} B_x + \sigma^y_{ij} B_y + \sigma^z_{ij} B_z). \tag{14.26}$$

By considering σ^x, σ^y, σ^z as components of some matrix vector $\vec{\sigma}$, we can rewrite (14.26) in a form which is independent of the choice of the coordinate axes:

$$H_{ij} = -\mu \vec{\sigma}_{ij} \vec{B}. \tag{14.27}$$

Pauli spin matrices are useful because any second-order matrix (in particular, the Hamiltonian matrix of any microparticle with two basic states) may be represented as a superposition of these matrices. The Pauli spin matrices introduced for an electron in a magnetic field have proved to be convenient for considering a wide range of two-level problems. This is not surprising when we consider the possibility, discussed above, of generalizing the problem of an electron in a magnetic field to arbitrary two-level systems.

Section 15 The Wave Function

At the very outset, let us make it clear that this section hardly adds anything new to the physical foundations of quantum mechanics considered in this chapter. In fact, we are already able to summarize the physical aspects of the theory and go over to its mathematical side, based on the use of linear operators. However, before doing so, it is worthwhile to introduce the concept of the *wave function*. Wave functions are widely used in the existing literature on quantum mechanics; hence it is important that the reader should be aware of the "position" of the wave function in the above description of amplitude concepts. Until now, the wave function, being essentially the amplitude of state, existed in this picture in an implicit form; we shall now make it explicit. Besides, one must remember that while changing over to the mathematical apparatus of quantum mechanics, it is more convenient to use the wave function rather than the amplitude of state.

The Wave Function as the Amplitude of State

Let $\langle x|$ be the state of a microparticle corresponding to its localization at a point in space with the coordinate x (for simplicity we consider the *one-dimensional* case). Then $\langle s \mid x\rangle$ may be considered as the probability amplitude that a microparticle in the state $\langle s \mid$ has the coordinate x.

However, we must make this a little more precise. When considering the probability of any spatial localization of a microparticle, we must take into account the *continuity* in the variation of a spatial coordinate. Hence, instead of the probability of finding a microparticle precisely at the point x, we must consider the probability of finding it on the interval from x to $x + dx$. Denoting this probability by $dw_s(x)$, we have

$$dw_s(x) = |\langle s | x\rangle|^2 \, dx. \tag{15.1}$$

Consequently, the quantity $\langle s \mid x\rangle$ is, strictly speaking, not the amplitude of probability, but the *amplitude of probability density.*

In literature, the quantity $\langle s \mid x\rangle$ is referred to as the *wave function* and is expressed, for example, by $\psi_s(x)$. Thus,

$$\psi_s(x) = \langle s \mid x\rangle. \tag{15.2}$$

Using (15.2) we can rewrite (15.1) as

$$dw_s(x) = |\psi_s(x)|^2 \, dx. \tag{15.3}$$

It follows from (15.3) that $|\psi_s(x)|^2$ is the probability density of finding a microparticle with the state $\langle s|$ at the point x.

From a mathematical point of view, the wave function in $\psi_s(x)$ is a *parametric function*, the parameters being the quantities which are precisely defined in the state $\langle s \mid$. Taking into account the earlier remarks on the structure of amplitudes of states, we may state that the quantities of one complete set serve as the *argument* for the wave function, its *parameter* being the quantities of another set. It is often said that the wave function $\psi_s(x)$ is an *eigenfunction* of the quantities of the s-set, given in the representation determined by the quantities of the x-set (or simply, in the x-representation).

Generalization of the Concept of the Wave Function

Wave functions are frequently used in practice in the x-representation (*coordinate representation*). However, apart from the x-representation, other representations are obviously also possible. In this connection, the concept of the wave function must be generalized:

$$\psi_\alpha(\beta) = \langle \alpha | \beta\rangle. \tag{15.4}$$

The function $\psi_\alpha(\beta)$ is the eigenfunction of the quantities of the α-set, given in the β-representation. If the values of the β-set change discretely, $\psi_\alpha(\beta)$ is the amplitude of the probability that the state $\langle\beta\mid$ is represented in the state $\langle\alpha\mid$. In the case of continuously changing values of the β-set, $\psi_\alpha(\beta)$ is the amplitude of the given probability density.

By giving the wave function $\psi_\alpha(\beta)$ we give the exact values of the quantities in the α-set and *probable* values of the quantities in the β-set. Correspondingly, by giving the function $\varphi_\alpha(\gamma)$ we give the exact values of the α-set and probable for the values of the γ-set. It could be said that the function $\psi_\alpha(\beta)$ describes the state $\langle\alpha\mid$ in the β-representation, while the function $\varphi_\alpha(\gamma)$ describes the same state, but in the γ-representation. The fact that different functions $\psi_\alpha(\beta)$ and $\varphi_\alpha(\gamma)$ are used for describing the same state $\langle\alpha\mid$ indicates that there must be some connection between them. This connection is expressed through the *principle of superposition of states*. Assuming that γ-values change discretely, we can write

$$\psi_\alpha(\beta)=\sum_i \varphi_\alpha(\gamma_i)\,\chi_{\gamma i}(\beta) \tag{15.5}$$

It can be easily seen that (15.5) is the expression for the superposition of amplitudes of states:

$$\langle\alpha\mid\beta\rangle=\sum_i \langle\alpha\mid\gamma_i\rangle\,\langle\gamma_i\mid\beta\rangle. \tag{15.5a}$$

If the γ-values vary continuously, we get in place of (15.5)

$$\psi_\alpha(\beta)=\int \varphi_\alpha(\gamma)\,\chi_\gamma(\beta)\,d\gamma. \tag{15.6}$$

Let us consider the eigenfunction of the quantities of a certain set given in the representation of the quantities of the same set. If these quantities change discretely, we have, according to (10.8),

$$\Psi_{\alpha_i}(\alpha_j)=\delta_{ij}. \tag{15.7}$$

If, however, the quantities vary continuously, we get in place of (15.7)

$$\Psi_{\alpha'}(\alpha)=\delta(\alpha-\alpha'). \tag{15.8}$$

where $\delta(\alpha-\alpha')$ is the so-called *Dirac delta function*, which is a generalization of the Kronecker's symbol for the case of continuously varying quantities.*

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* The delta function is discussed in detail, for example, in [13].

The delta function is determined in the following way:

$$\delta(\alpha-\alpha')=0 \quad \text{at} \quad \alpha\neq\alpha'; \qquad \int_{-\infty}^{\infty}\delta(\alpha-\alpha')\,d\alpha'=1. \quad (15.9)$$

Strictly speaking, it is impossible to plot the function $\delta(\alpha-\alpha')$ because it would involve drawing an infinitely narrow and infinitely high peak at the point $\alpha=\alpha'$ with a finite "area" under it equal to unity. One of the most important properties of the delta function, which can be easily derived from its definition (15.9), can be written as follows:

$$\int_{-\infty}^{\infty} f(\alpha)\,\delta(\alpha-\alpha')\,d\alpha=f(\alpha'), \quad (15.10)$$

where $f(\alpha)$ is a bounded function, continuous at the point $\alpha=\alpha'$.

Condition of Orthonormalization of Eigenfunctions

Assuming that the α-values are discrete and the β-values vary continuously we rewrite (15.6) in the form

$$\Psi_{\alpha_i}(\alpha_j)=\int\psi_{\alpha_i}(\beta)\,\Phi_\beta(\alpha_j)\,d\beta. \quad (15.11)$$

By using (9.33), we can write

$$\Phi_\beta(\alpha_j)=\psi^*_{\alpha_j}(\beta). \quad (15.12)$$

From (15.12) and (15.7), we obtain from (15.11) the condition for the orthonormalization of the eigenfunctions $\psi_{\alpha_i}(\beta)$:

$$\int\psi_{\alpha_i}(\beta)\,\psi^*_{\alpha_j}(\beta)\,d\beta=\delta_{ij}. \quad (15.13)$$

If the α-quantities vary continuously, we must use (15.8) instead of (15.7). In this case the condition of orthonormalization of the eigenfunctions assumes the form

$$\int\psi_\alpha(\beta)\,\psi^*_{\alpha'}(\beta)\,d\beta=\delta(\alpha-\alpha'). \quad (15.14)$$

The Wave Function of a Freely Moving Microparticle

As an example, we consider the case of a freely moving microparticle. For simplicity, we assume that it has zero spin. The wave function in coordinate (three-dimensional) representation has the form*

$$\psi_{\vec{p}_0}(\vec{r})=\langle\vec{p}_0\,|\,\vec{r}\rangle=(2\pi\hbar)^{-3/2}\exp\left(i\vec{p}_0\vec{r}/\hbar\right), \quad (15.15)$$

where $\vec{p}_0$ is the momentum of the microparticle and $\vec{r}$ is its spatial coordinate. The function $\psi_{\vec{p}_0}(\vec{r})$ is an eigen-

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* We shall derive this result later (see Sec. 20).

function of the momentum, given in the coordinate representation. It describes the state in which the momentum components of a microparticle have definite values, while the spatial coordinates may be assigned only probable values.

Switching over from the *coordinate* to the *momentum* representation and making use of (9.33) we get

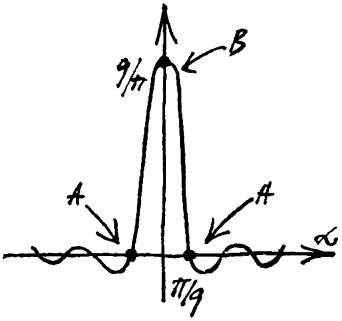
$$\varphi_{\vec{r}_0}(\vec{p}) = \langle \vec{r}_0 \mid \vec{p} \rangle = \langle \vec{p} \mid \vec{r}_0 \rangle^* = (2\pi\hbar)^{-3/2} \exp(-i\vec{p}\vec{r}_0/\hbar). \tag{15.16}$$

The function $\varphi_{\vec{r}_0}(\vec{p})$ is an eigenfunction of the coordinate of the microparticle given in the momentum representation.

It can be seen from (15.15) and (15.16) that the states of a freely moving microparticle are described by wave functions in the form of *plane waves* (in coordinate or momentum space).

The functions $\psi_{\vec{p}_0}(\vec{r})$ and $\varphi_{\vec{r}_0}(\vec{p})$ satisfy the condition (15.14) of orthonormalization. This can be verified by using the integral representation of the delta function*

Fig. 15.1



$$\delta(\alpha) = \frac{1}{2\pi} \int_{+\infty}^{\infty} \exp(i\alpha\beta)\, d\beta \tag{15.17}$$

(the quantities α and β represent the components of the spatial coordinate and the momentum of the microparticle).

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* Let us consider the function $\sin(g\alpha)/\pi\alpha$ (Fig. 15.1). Irrespective of the value of parameter g, $\int_{-\infty}^{\infty} d\alpha \sin(g\alpha)/\pi\alpha = 1$. Let us increase g. This will bring the points A in the figure closer to $\alpha = 0$, and raise the point B on the ordinate axis. In the limit as $g \to \infty$ we get an infinitely narrow and high peak whose integral is equal to unity. This is just the delta function. Thus, $\delta(\alpha) = \lim_{(g\to\infty)} \sin(g\alpha)/\pi\alpha$. We can easily get (15.17) from this since

$$\sin(g\alpha)/\pi\alpha = \frac{1}{2\pi} \int_{-g}^{g} \exp(i\alpha\beta)\, d\beta.$$

Section 16

Quantum Mechanics as a Qualitative Leap in Man's Knowledge of the Laws of Nature

> *Of course it is impossible to distinguish sharply between natural philosophy and human culture. The physical sciences are, in fact, an integral part of our civilization, not only because our ever-increasing mastery of the forces of nature has so completely changed the material conditions of life, but also because the study of these sciences has contributed so much to clarify the background of our own existence.*
>
> N. Bohr

Although quantum mechanics deals with microparticles, its significance is by no means limited to microphenomena. In our endless quest for understanding and perfecting our knowledge of the laws of nature, quantum mechanics represents an important *qualitative leap*. Without a comprehension of the importance, and radical (we could even say revolutionary) nature of this leap, it is impossible to understand the *modern physical picture of the world.* In this section, an attempt has been made to look at quantum mechanics from this point of view. This may serve as a logical conclusion to the chapter, which has been devoted to the physical foundations of this astonishing theory.

"Crazy Ideas"

The expression "crazy theory" as one which is "crazy enough to be true" was once coined by Bohr. This expression reflects the stunning impression produced on Bohr's contemporaries by the astonishing physical discoveries made at the beginning of the 20th century, discoveries which could not be confined within the framework of classical concepts. It became obvious that an explanation of these discoveries required radically new ideas and a new approach.

In Sec. 2 we considered two fundamental ideas of quantum mechanics—the *idea of discreteness* and the *idea of duality.* Returning, in our imagination, to the beginning of the century, we could call the first idea "incomprehensible" and the second, "not properly understood" The introduction of discreteness to the physical picture of the world led to incomprehensible and, apparently, logically controversial quantum "jumps" The idea of duality, which asserts the specific nature of microparticles, eliminated the contradiction of quantum "jumps" by suggesting a "manoeuvring" between the "particle" and the "wave" concepts. But the meaning of the wave concept introduced here remained in fact unclear for a very long time. These two "absurd" ideas led to the emergence of the extravagant "uncertainty relations" which resulted in a different outlook on even such fundamental concepts as "energy", "momentum" and "angular momentum"

Quantum mechanics was born under circumstances of a significant breaking up of physical traditions. It called for a rejection of many usual and accepted notions such as the strict continuity of the spectra of values of physical quantities, the trajectory as an essential attribute of the motion of an object, Laplace determinism as the basic form of expression of the principle of causality, the possibility of an infinite detailization of the structure of an object or of a phenomenon with respect to time, the possibility of distinguishing between two objects, however similar to each other, under any circumstances, the belief that it is always possible, at least in principle, to disregard the measuring instrument when conducting any measurements, etc. (all these questions have been analysed in detail in the preceding sections).

It is difficult to recall any other period in the history of physics when such a serious and large-scale revision of physical concepts was carried out. According to Bohr, *...the new lesson which has been impressed upon physicists stresses the caution with which all usual conventions must be applied as soon as we are not concerned with everyday experience... In the study of atomic phenomena we have repeatedly been taught that questions which were believed to have received long ago their final answers had most unexpected surprises in store for us.*

The Essence of Quantum Mechanics

The revision of the concepts and the rejection of many accepted notions could well be considered as a "negative aspect" of quantum mechanics. Let us now consider its "positive aspect".

If we try to summarize the main positive knowledge imparted by quantum mechanics to man in his search for learning about his surroundings, the following two important points stand out:

First: quantum mechanics showed that the *basic laws of nature are not dynamic but are statistical*, and that the *probabilistic form of causality is the fundamental form while the classical* determinism is just its limiting (degenerate) case.

Second: quantum mechanics revealed that *probability in nature should not be dealt with as in classical statistical theories*. It was found that in certain cases it is not the probabilities of events that should be summed, but rather the amplitudes of these probabilities. This leads to the *interference of probability amplitudes.*

Thus we emphasize firstly the *probabilistic character of the laws of nature* (the pre-eminence of statistical laws) and, secondly, the *special relations among the probabilities*, which assume not only the summation of the latter, but also the specific interference effects. In our view, it is in this that the main importance of the information one gets from quantum mechanics is to be found.

As Born pointed out in [14], the statistical methods found wider applicability with the development of physics. As regards modern physics, it is completely based on statistical foundations. In Born's view, it is the quantum theory that established the closest links between statistics and the basic aspects of physics. This should be considered as an important event in the history of human knowledge, with consequences reaching far beyond the limits of science.

It is sometimes said that the fundamental difference between quantum mechanics and classical mechanics is determined by the statistical nature of the former and dynamic nature of the latter. Upon careful consideration, this apparently bland and irrefutable statement turns out to be incorrect. While revealing the pre-eminence of statistical laws in physics, quantum mechanics shows at the same time that dynamic laws with their unique predictions are, as a matter of fact, a special (degenerate) case of probability laws. In this respect not only quantum mechanics, but classical mechanics as well, must be, strictly speaking, formulated in the language of probabilities* The qualitative difference between quantum mechanics and classical mechanics (or classical physics in general) depends on how the relations among probabilities are considered. It has been mentioned in [27] that the main difference between quantum mechanics and classical mechanics does not lie in the statistical nature of the former. It lies in the fact that it is not the probability but its amplitude, the wave function, that is of primary importance in quantum mechanics. This leads to the interference of probabilities, an effect which does not have an analogy in classical mechanics.

Developing the above ideas, let us single out the following points: (a) the special interrelations among quantum-mechanical states and the resulting specific nature of quantum-mechanical description of phenomena; (b) the

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* This point of view is systematically analysed in [27], where it is stated, in particular, that Feynman's concepts of path integrals in fact converts the principle of least action into the principle of maximum probability, i.e. it proves that the fundamental dynamic principle is essentially statistical in nature.

specific nature of the application of probabilities in quantum mechanics; (c) the special role of interference in quantum mechanics; (d) the complementarity principle as a logical foundation of quantum mechanics, and (e) the dialectical nature of quantum mechanics. We shall consider these questions one by one.

The Specific Nature of Quantum-Mechanical Description of Phenomena

According to Feynman, one of the most outstanding achievements of quantum mechanics lies in the fact that it allows so much to be extracted from so little.

The reader has already found out how much can be achieved from the phenomenon of interference of amplitudes (see Sec. 9), on the basis of the principle of superposition of states (see Sec. 10), and from a consideration of the simplest quantum-mechanical systems, i.e. microparticles with two basic states (see Secs. 13, 14). The relative formal simplicity of the description of microphenomena is connected with the specific nature of this description. Remember that for a quantum-mechanical description we must know firstly the *basic states* and, secondly, the *Hamiltonian matrix*, which reflects the physics of the phenomena under consideration. A simplification in the description can be achieved because of the following two circumstances.

Firstly, it is important that the number of basic states, and consequently the number of elements of the Hamiltonian matrix required for describing a definite phenomenon, should not be large. Thus, in the examples given in Secs. 13 and 14, this number was equal to two. Here the contradiction regarding the diversity in the possible states of the microparticle does not arise, since according to the principle of superposition either of them may be represented in the form of some superposition of basic states. The principle of superposition itself is the deciding factor, which permits us to manage usually with a small number of states selected as the basic states. As Dirac wrote [9], *...in departing from the determinacy of the classical theory a great complication is introduced into the description of Nature, which is a highly undesirable feature. This complication is undeniable, but it is offset by a great simplification provided by the general principle of superposition of states...* .

It has been noted earlier (see Sec. 10) that in classical physics all states of a particle should be considered as mutually orthogonal, or, in other words, as basic states. Because of this, the above-mentioned simplifying situation is impossible here in principle.

Secondly, the relative simplicity of superposition relations allows us to draw analogies among microparticles having the same number of basic states and reduce all the real problems in practice to a consideration of the two-level problem, three-level problem, etc. It has been shown in Sec. 14 how an arbitrary problem with two basic states can be reduced formally to the problem of an electron in a magnetic field.

Of course, it cannot be deduced from all this that in general "quantum mechanics is simpler than classical mechanics". Certainly it is simpler in the above-mentioned sense. However, it has sufficient problems of its own, especially problems connected with a rational choice of the system of basic states and with finding the form of the Hamiltonian matrix. It is hardly necessary to recount all the difficulties which invariably result from the necessity of departing from graphic representations of accustomed concepts. That is the way things are. Hence it wouldn't be wise to say that "quantum mechanics is simple!" And yet one must remember that the peculiar relations that exist among different states of a microparticle and appear in the specific principle of superposition of states considerably simplify the quantum-mechanical description of phenomena.

Probability in Quantum Mechanics

Quantum mechanics forces us to take a fresh look at the well-known theorem of addition of probabilities for incompatible events. We have to consider not only the incompatibility but also the distinguishability of the events. This is where the novelty of the approach lies. It is well known that in the probability theory used in classical physics, as well as in engineering, it is always implied that events are distinguishable.

In order to demonstrate the specific nature of the application of probability in quantum mechanics, we make use of the example considered in Secs. 9 and 10 of the scattering of bosons of the same type by each other. We recall the notations introduced in these sections: $\varphi(\theta) = \langle f_1 \mid s_1 \rangle \langle f_2 \mid s_2 \rangle$—the probability amplitude of one event (one transition), $\varphi(\pi - \theta) = \langle f_2 \mid s_1 \rangle \langle f_1 \mid s_2 \rangle$—the probability amplitude of the other event, w — the probability of simultaneous activation of both detectors. Since microparticles of the same type are scattered by each other, the question of their distinguishability leads to the distinguishability of the initial states $\langle s_1 \mid$ and $\langle s_2 \mid$. In this connection three cases may be isolated:

First case. The events are completely indistinguishable. This means that the initial states are the same, and

$$| \langle s_1 \mid s_2 \rangle | = 1. \tag{16.1}$$

In this case, we get [see (9.17)]

$$w = |\varphi(\theta) + \varphi(\pi - \theta)|^2. \tag{16.2}$$

Second case. The events are partially distinguishable. This means that the amplitude $\langle s_1 \mid s_2 \rangle$ satisfies the condition

$$0 < |\langle s_1 \mid s_2 \rangle| < 1. \tag{16.3}$$

In this case, we get [see (10.7)]

$$w = |\varphi(\theta)|^2 + |\varphi(\pi - \theta)|^2 + |\langle s_1 | s_2 \rangle|^2 [\varphi(\theta)\varphi^*(\pi - \theta) + \varphi^*(\theta)\varphi(\pi - \theta)]. \tag{16.4}$$

Third case. The events are completely distinguishable. This means that the amplitude $\langle s_1 \mid s_2 \rangle$ satisfies the condition

$$\langle s_1 \mid s_2 \rangle = 0. \tag{16.5}$$

This gives us [see (9.16)]

$$w = |\varphi(\theta)|^2 + |\varphi(\pi - \theta)|^2. \tag{16.6}$$

Thus we find that the theorem of the addition of probabilities "holds" only in the third of the above-mentioned cases, i.e. in the case of completely distinguishable events. From (16.5) it follows that the states $\langle s_1 |$ and $\langle s_2 |$ must be *mutually orthogonal** in this case. In the remaining cases the theorem of the addition of probabilities does not hold. If the events are completely indistinguishable, the amplitudes of the probabilities should be summed. But if the events are partially distinguishable, we must use the more complicated relation (16.4). When deriving this relation, both the law of the addition of amplitudes and the theorem of the addition of probabilities have been used in the same way as in Sec. 9 when deriving (9.10).

It can be easily seen that the result (16.4) based on the addition of probabilities as well as the addition of amplitudes is the most general one. When the condition (16.5) is satisfied, it at once leads to the "purely" classical case of addition of probabilities while condition (16.1) is fulfilled "purely" in the case of addition of amplitudes of probabilities.

It should be emphasized that the very possibility of the existence of the general result (16.4) is caused by the presence of superposition bonds between the states $\langle s_1 |$

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* It is worthwhile mentioning here that the mutual orthogonality of all states of a classical object stipulates a complete distinguishability of events and, as a result, leads to the theorem of addition of probabilities.

and $\langle s_2 \mid$ [see (10.6) in this connection]. Thus we track the active connection between the quantum-mechanical principle of superposition of states and the specific nature of the application of probability in quantum mechanics. The superposition relations among states and the interference of probability amplitudes have the same physical nature.

Quantum Mechanics and Interference

We draw the reader's attention to the following fact. In order to explain the interference results in experiments with microparticles (for example, the interference pattern on the detector-screen in Experiment 1 of Sec. 7), we can formally proceed in two different ways. One way corresponds to the "conservation" in quantum mechanics of the theorem of the addition of probabilities for any incompatible events. This way, however, requires a comparison of the microparticle with some classical wave. The other way corresponds to the addition of probability amplitudes. In this case an explanation of interference results no longer requires the introduction of any visual wave model.

The specific nature of microparticles, which has been discussed in detail in the preceding sections, precludes the first way and so puts the question of interference and wave processes in a new light. Before the appearance of quantum mechanics, interference was always considered as an example of a typical wave effect. If a characteristic interference pattern was observed in any experiment, it was considered sufficient evidence to draw conclusions on the presence of waves. In this sense, *waves* were considered as being "*primary*", and *interference* as being *secondary*. Quantum mechanics shows that the reverse order of emphasis is more correct.

In revealing that the probability laws of nature involve the addition of probability amplitudes and not of the probabilities themselves, quantum mechanics revealed the fundamental role of interference in physical phenomena. Simultaneously, it showed that classical wave processes need not essentially be at the root of an interference pattern. *In the general case, interference is a specifically quantum-mechanical effect associated with the addition of probability amplitudes.*

Traditions, however, die hard. This explains attempts to "translate" the interference of probability amplitudes into the graphic language of classical waves, which inevitably leads to a definite misuse of wave terminology (see the above interlude "Are these the same waves?"). In a number of cases the "translation" into wave language is not justified even from a formal point of view. For example, the division of microparticles into fermions and bosons, which is such an important consequence of the interference of amplitudes, is fairly difficult to explain on the basis of wave processes. The analysis of the process of the destruction of interference of amplitudes in the measuring process ("the reduction of the wave packet") directly indicates the impropriety of using classical wave concepts when considering microphenomena. All this indicates that an explanation of interference obviously does not come within the framework of the traditional wave model.

By the way, the last fact may be taken as the starting point for a generalization of the very concept of "wave process". Such a generalization assumes a transition from visual classical waves with real amplitudes to some sort of generalized waves with *complex amplitudes*. The classical waves must appear as an extreme (degenerate) case of such generalized waves. In other words, quantum-mechanical interference may be used for an extension of the framework of the accepted wave picture (which, incidentally, is invariably accompanied by rejection of a graphic representation) and for creating a theory for the generalized wave processes which would reflect not only the probability nature of physical laws but also the special relations among probabilities in nature.

By demonstrating the fundamental nature of the phenomenon of interference, quantum mechanics naturally arises an interest in the study of this phenomenon in different branches of physics. In our view, it raises definite hopes that modern physics, stimulated by the *effect of interference*, will develop in future into a study of the *interference of effects* in the fields of both microphenomena and macrophenomena.

The idea of "addition" (summation, accumulation) of different phenomena is familiar to us. In a way, this can be compared with the "addition of probabilities" It is likely that quantum mechanics tells us (indicates in its own way) that such a picture is the result of a certain "averaging", approximation or simplification of a finer and better picture in which we "add up" not the effects themselves, but something different (corresponding to probability amplitudes in the language of quantum mechanics), thereby arriving at the phenomenon of interference of effects.

A Brief Interlude

Fairy tales, though oft untrue,
Teach good lads a thing or two.

Pushkin

Reader: It is not clear what you wanted to say in the last sentences which, though quite eloquent, are tentative. Please explain them, if possible.

Author: Gladly. Let us take a definite example. It is well known that if a substance is placed in a condenser, its optical properties will change under the influence of the external electric field. Such effects are called *electro-optical effects.* If the substance is subjected to a light field of sufficient intensity (generated, say, by a high-power laser), the optical properties change in this case also. These effects are called *nonlinear optical effects.* It so happens that if a condenser field and an intense light field are *simultaneously* switched on, then in addition to the familiar electro-optical and nonlinear optical effects we observe qualitatively different effects which may be explained only as a *unique interference* of electro-optics and nonlinear optics. This is an example of the interference of effects.

Reader: But can one perceive in this example any tendency towards the development of modern physics?

Author: Let us take another example, that of a *laser.* We shall not discuss the principle of its working here; it is just sufficient to mention that it is based on some nonlinear effect, called the *saturation effect.* Let us take another instrument, the *second-harmonic generator* (that is what a transformer of coherent light which doubles the frequency is called in quantum mechanics). We shall simply state that this instrument also is based on the principle of nonlinear optical effect called the *generation of second harmonics.* Thus, the laser produces coherent light of a definite frequency, while the second-harmonic generator partially transforms the frequency of this light. We can say that we first use the saturation effect and then the effect of second-harmonic generation. Such is a general situation corresponding to a simple "summing" of these effects. Now, suppose that both these effects are used *simultaneously.* In order to do so, we must place a special crystal, which causes a trans formation of the frequency of light passing through it, inside the laser (or, more precisely, inside the resonator of the laser). Here, we are speaking of a qualitatively different situation corresponding to the *interference of two nonlinear optical effects.* It is quite significant that this and other similar situations have been increasingly drawing the attention of specialists engaged in the field of quantum electronics. Intraresonator generation of second harmonic is already being put into practice; it has been proved that it can ensure a more effective transformation of optical frequency.

Reader: This really sounds interesting. It is possible that some tendency is indicated here. But what has this got to do with quantum mechanics?

Author: When studying reality on a fundamental level, quantum mechanics highlighted some important points. It showed that the question of interference is *deeper* than it was considered, and that this question can be posed independently of wave questions; and finally, that interference is an example of *qualitatively new interrelations*, i.e. relations which obviously have more prospects than the traditional interrelations corresponding to a simple summing, adding, or accumulation.

Complementary Principle

The *dialectical nature* of quantum mechanics is reflected in its very initial principles. In this connection the *principle of complementarity*, put forth by Bohr, is of special interest. This principle forms in fact the logical foundation of the entire system of quantum-mechanical ideas.

The essence of the principle of complementarity lies in the following: it is stated that in any experiment with microparticles, the observer gets information not about the "properties of the particles themselves" but about the properties of the particles associated with some particular situation including, among other things, the measuring instruments. The information about the object obtained under *some definite* conditions should be considered as *complementary* to the information obtained under *different* conditions. Essentially, the information obtained under different circumstances cannot be added, accumulated or combined into a single picture; it reflects various sides (complementing one another) of a single reality, to wit the object under investigation. The principle of complementarity finds a direct expression, in particular, in the idea of wave-particle duality and in the uncertainty relations.

According to Bohr, the term 'complementarity' is used *in order to stress that in the contrasting phenomena we have to do with equally essential aspects of all well-defined knowledge about the object* (N. Bohr, "On the Notions of Causality and Complementarity").

...In atomic physics the word 'complementarity' is used to characterize the relationship between experiences obtained by different experimental arrangements and visualizable only by mutually exclusive ideas... (N. Bohr, "Natural Philosophy and Human Cultures").

...Evidence obtained under different experimental conditions cannot be comprehended within a single picture, but must be regarded as complementary... (N. Bohr, "Discussion with Einstein on Epistemological Problems in Atomic Physics").

In quantum physics, however, evidence about atomic objects obtained by different experimental arrangements exhibits a novel kind of complementary relationship. Indeed, it must be recognized that such evidence which appears contradictory when combination into a single picture is attempted, exhausts all conceivable knowledge about the object (N. Bohr, "Quantum Physics and Philosophy").

We advise the reader to carefully read the words of Bohr once again. Thus, data about a microparticle may be "*graphically interpreted*" only on the basis of "ideas mutually excluding one another" In this sense they cannot be added in a simple way, and "*cannot be contained in a single picture*". Various data have "peculiar" (the reader must not let this epithet go unnoticed) relations with one another, hence the term "complementarity". The peculiarity of the "complementarity" relations lies in the fact that data "complementary" to one another may be obtained only "under different experimental conditions"

The specific nature of quantum-mechanical ideas, emphasized frequently in the foregoing, and their somewhat unusual logic rests to a considerable extent on the principle of complementarity. A microparticle is neither a corpuscle, nor a wave, but still we employ both these images, which mutually exclude each other, for describing a microparticle. Just imagine the situation: the corpuscle and wave pictures are used for describing an object which is neither a corpuscle, nor a wave, nor even a symbiosis of them! Naturally, this could give rise to a ticklish question: Doesn't this mean an alienation of the image from the object, which is fraught with a transition to the position of subjectivism? A negative answer to this question is given by the principle of complementarity itself. From the position of this principle, pictures mutually excluding one another are used as *mutually complementary pictures*, adequately representing various sides of the objective reality called the microparticle. According to Bohr, *this point is of great logical consequence, since it is only the circumstance that we are presented with a choice of either tracing the path of a particle or observing interference effects, which allows us to escape from the paradoxical necessity of concluding that the behaviour of an electron or a proton should depend on the presence of a slit in the diaphragm through which it could be proved not to pass.*

The Dialectical Nature of Quantum Mechanics

It is true that dialectical nature is inherent in every physical science to some extent. Still it may be stated that classical physics, because of the very style of its philosophy (unambiguous predictions in theories of dynamic type, the approach to any object as a "combination" of certain "details", and to any phenomenon as a succession of certain elementary events, etc.) is drawn towards *metaphysics*. In this sense the significance of quantum mechanics cannot be overestimated. It has convincingly shown that a higher level of knowledge of the laws of nature is inevitably linked with a deeper and more serious knowledge and application of the methods of *materialistic dialectics*.

In considering the cases in which the dialectical character of quantum mechanics is especially manifested, we single out two points which appear most important to us. These are the statement of relations of dialectical type and the application of the categories of dialectics.

Statement of Relations of Dialectical Type. Simple *accumulation*, or *summation* of data, properties and concepts are characteristic (we shall say that *summation relations* are characteristic) of a metaphysical method. These relations to a considerable extent form the logical foundations of classical physics. Quantum mechanics lays emphasis on relations of a qualitatively different, dialectical type, like the *relations of complementarity* and *relations of interference*. Thus, it shows that data about an object, strictly speaking, do not simply add up but *complement* one another, that the probabilities of different events, strictly speaking, are not summed, but *interfere* with one another. We have discussed these specific relations above when considering the principle of complementarity and the specific nature of the application of probability in quantum mechanics. When evaluating complementarity and interference as new relations, or new interrelations corresponding to a higher level of knowledge of the laws of nature, it can't be denied that quantum mechanics really determines the direction for the development of modern physics.

Application of the Categories of Materialistic Dialectics. In classical theories of dynamic type the concepts of necessity and chance, possibility and actuality do not appear as dialectical categories. Necessity here is absolutely (metaphysically) the opposite of chance. The latter is simply banished from the theory, which immediately leads to an *identification* of the concepts of the possibility and actuality. As *dialectical categories*, relations among which is unity and struggle of opposites, these concepts appear in statistical theories, primarily in quantum mechanics. It is essential that in quantum mechanics the dialectical categories of necessity and chance, possibility and actuality are applied not only to the ensembles of objects but also to an *individual microparticle*. The application of dialectical categories in quantum mechanics has been considered throughout this book when discussing certain questions. We remind the reader that an analysis of the problem of causality in quantum mechanics could be accomplished only on the basis of the dialectical categories of necessity and chance. An explanation of the quantum-mechanical superposition of states and its destruction in the process of measurement was made possible only by using the dialectical categories of possibility and actuality.

In conclusion, we note that quantum mechanics has clearly demonstrated the dialectical struggle between form and content. In Bohr's words, *the lesson we have hereby received would seem to have brought us a decisive step further in the neverending struggle for harmony between content and form, and taught us once again that no content can be grasped without a formal frame and that any form, however useful it has hitherto proved, may be found to be too narrow to comprehend new experience.*

Interlude. Do Quantum-Mechanical Concepts Contradict Our Common Sense?

In this unusual discussion the author is joined by two physicists (Bohr and Cooper) and two literateurs (Dobrolyubov and Perrault).
Excerpts from the following works have been used in the discussion: N. Bohr, "Natural philosophy and human cultures" in "Atomic Physics and Human Knowledge", 1958; N. Bohr, "The Unity of Knowledge", 1955; N. A. Dobrolyubov, "What Is Oblomovshchina?" 1948; L. N. Cooper, "An Introduction in the Meaning and Structure of Physics", 1968; C. Perrault, "The Sunshine Book" 1946.

Common sense is that layer of prejudice we acquire before we are 16.
A. Einstein

In the balance between seriousness and humour, characteristic of all truly artistic achievements, we are reminded of complementary aspects conspicuous in children's play and no less appreciated in mature life.
N. Bohr

Cooper: There have been bitter complaints from some of our contemporaries, that physics in the twentieth century has become too abstract, has lost touch with those things ordinary people can understand, has lost contact with common sense and substituted instead constructs so abstract that the ordinary mind can never attain them.

Author: That is why I want to talk about quantum mechanics and "common sense". I have many times heard the complaint that quantum mechanics is hard to follow because its concepts are in "contradiction to common sense". Unfortunately nobody knows precisely the meaning of "common sense". If I am not mistaken, you are of the view that "common sense" is a relative concept, and that its meaning changes significantly with the development in science.

Cooper: Yes, it is a cliché that the commonsense of the new generation is formed from concepts laboriously constructed by their elders, that what is avant-garde for one generation is common sense and prosaic for the next. It seems dubious that the Newtonian conception of the world would have been common sense to the Greeks in the time of Aristotle, for that matter to the scholastic scholars. It was not even so for many of his contemporaries. And those so enamored of common sense (at present Newton's world) are often just those who complain that the mechanical Newtonian view destroyed the magical medieval world.

Author: It is difficult to counter such a point of view. By the way, it immediately solves the question posed by us at the very beginning. Isn't it?

Cooper: I think so, for the present generation of physicists it is quantum physics that is common sense. It is the structure of the quantum theory that is closest to them, relations of the quantum theory that have an immediacy and an intuitive correctness....

Author: However, without denying the justification of the point of view mentioned above, let us try to solve the question of common sense and look at this question from a more open position. Moreover, we would like to speak of the commonsense not of physicists, but of "ordinary people", those who "bitterly complain" that the "ordinary mind can never attain" the ideas of modern physics.

An approach from a more open position to the "common sense" in quantum mechanics was strongly advocated by one of our honoured participants. It would be nice to hear in this connection his remarks on the complementarity principle, for example.

Bohr: Using the word "complementarity" much as it is used in atomic physics, to characterise the relationship between experiences obtained by different experimental arrangements, and visualizable only by mutually exclusive ideas, we may truly say that different human cultures are complementary to each other. Indeed, each such culture represents a harmonious balance of traditional conventions by means of which latent potentialities of human life can unfold themselves in a way which reveals to us new aspects of its unlimited richness and variety.

Author: What is there that an ordinary person cannot comprehend? And yet the complementarity principle finally boils down to uncertainty relations as well as wave-particle duality of microparticles. Meanwhile, all these incomprehensible ideas find their due place not only in questions linked with human cultures but even in quite common questions, for example questions linked with psychology.

Bohr: We all know the old saying that, if we try to analyse our own emotions, we hardly possess them any longer, and in that sense we recognise between physical experiences, for the descriptions of which words such as "thoughts" and "feelings" are adequately used, a complementary relationship similar to that between the experiences regarding the behaviour of atoms obtained under different experimental arrangements.

Author: But can't we go one step further, and try to draw some analogies between modern ideas in physics and ideas contained in famous literary works? It would be quite interesting to compare poetical truth and scientific truth.

Bohr: In other words, is there a poetical or spiritual or cultural truth distinct from scientific truth?

Author: Precisely.

Bohr: We are indeed directly confronted with the relationship of science and art. The enrichment which art can give us originates in its power to remind us of harmonies beyond the grasp of systematic analysis.

Author: I am extremely grateful to you. You have helped dispel some of my doubts. I would now turn to particular examples, the first example being Oblomov, a novel by I. A. Goncharov. Let us recall what one of our distinguished participants has written about the image of Oblomov.

Dobrolyubov: Well, take for example this: Oblomov's wishes always assume the form "how good it would be if this were done", but how this can be done he does not know. That is why he is so fond of dreaming and dreads the moment when his dreams may come in contact with reality.

Author: I remember that you drew analogy between Oblomov and such literary heroes as Onegin, Pechorin, Rudin.

Dobroluybov: Yes, indeed. But the point is that they all have one common feature—a fruitless striving for activity, the consciousness that they could do a great deal but will do nothing.

Author: (to Bohr): And what would you say to this?

Bohr: I would say that the relation between the experience of a feeling of volition and conscious pondering on motives for action is especially instructive.

Author: I should state that the ideas expressed by my learned friends pertain to different situations and were profounded at different times. And yet they do have something in common. To a certain extent the personal tragedy of Oblomov lies in his inability to overcome the dialectical contradiction between the possible and the actual. Potentially, much is vested in Oblomov; this is an evidence of the considerable superposition of possibilities. But the "act of measurement", which would allow Oblomov to realize some aspect of his nature at the cost of this superposition is missing. This act does not occur, the superposition is not destroyed and everything remains as it was.

Let us now consider the second literary example, the famous fairy-tale "Cinderella" by Charles Perrault. Will you please narrate the scene in which the fairy godmother sees Cinderella off to the ball at King's palace.

Perrault: Here you are: The fairy godmother then said to Cinderella, "Here is a coach fit for the ball, and coachman and footmen" As Cinderella stepped into the carriage, her fairy godmother said, "Remember, you must not stay a minute after twelve, for if you do, your coach will become a pumpkin again, the horses will turn back into mice; the footmen will become lizards, and the coachman will become a rat; and your dress will turn to rags."

Author: Thank you. I wanted to draw your attention to the fact that the omnipotent fairy godmother gave the coach and the dress to Cinderella only for a while, until midnight. And why not for good? It is clear that she could have done that but it would be against the inherent logic and the central idea of the tale. It would, so to say, take away the "charm". If it is for a while, well and good; but if it is for ever, there is no charm. Doesn't it remind us of a model of virtual transitions? The conservation laws are violated, treasures are created out of "nothing" with the help of a magic wand, but all this is allowed only for a finite interval of time—"until midnight" After this, Cinderella must return to her previous state, and without the beautiful dress. Just compare: a quantum system visits a new level without any expenditure of energy from outside, only for a limited interval of time after which the system must return to its previous level. In the same way, Cinderella performs "virtual transitions" between her house and the royal palace, enjoys and dances but is careful not to overstep the agreed time limit.

Then a messenger with the crystal slipper appears on the scene. Please narrate what happened after this.

Perrault: The messenger, who had been sent with the slipper, said that everyone was to try it. He looked at Cinderella and saw that she was beautiful. He ordered her to sit down and put the slipper on It fitted her perfectly... Just then the fairy godmother appeared and touched Cinderella with her wand and her rags became a dress more beautiful than any she had yet worn.

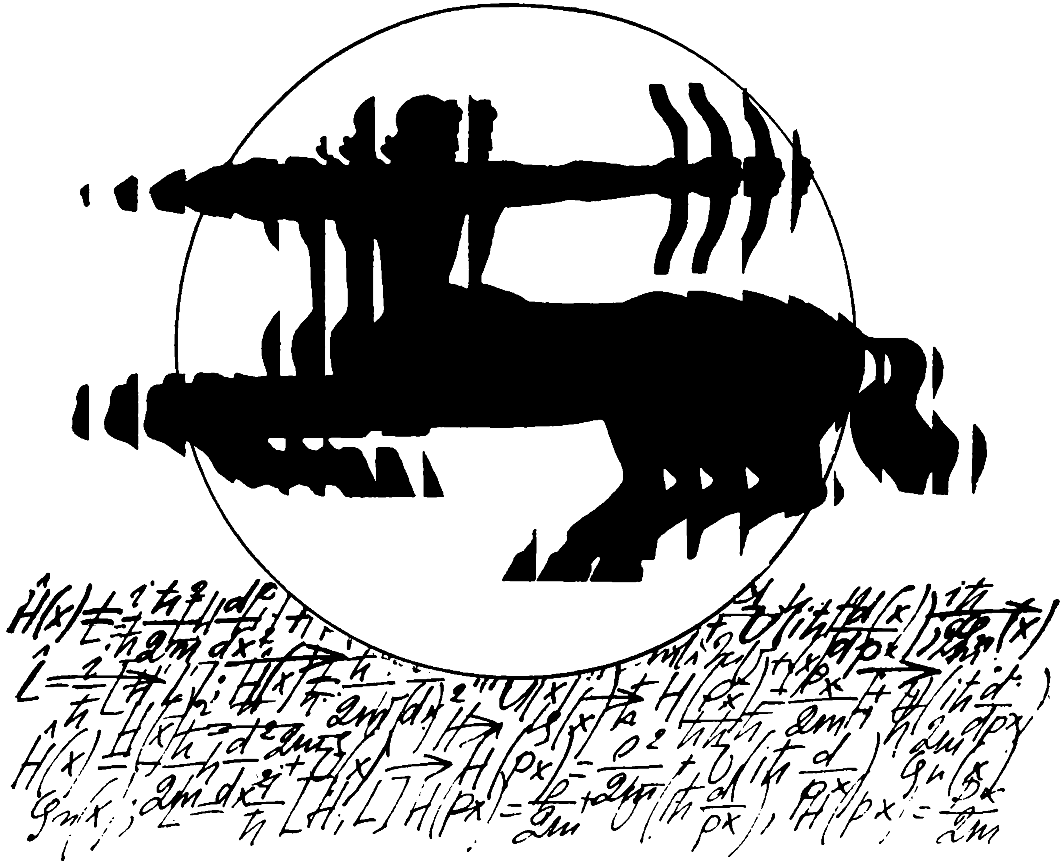
Author: And so, it came true. The fairy godmother gave Cinderella the dress to keep for ever. The virtual transition led to a real transition by Cinderella to "a new level". The prince, the slipper, the messenger—all played the role of the photon which, by interacting with the system undergoing virtual transitions, has led to a real transition. Of course, the Cinderella story should not be seriously taken as an illustration of the idea of virtual transitions, as an explanation of quantum jumps. In the same way the novel *Oblomov* should not be seriously taken as an illustration of the principle of superposition of states or as an explanation of the problem of destruction of superposition in the act of measurement. However, it is easy to see the general internal logic in the comparison drawn above.

Bohr: It may not be irreverent to remark that even at the climax of his work the artist relies on this common human foundation on which we stand.

Author: With this interesting discussion we come to the end of our consideration of the basic concepts of quantum mechanics. Of course, quantum-mechanical ideas are quite unusual and peculiar. And yet they did not appear from nothing but rather arose on the basis of a solid foundation of concepts and ideas which are a result of the entire human experience. Hence the analogies between physical models and literary images are not incidental, but rather inevitable.

Chapter 3

Linear Operators in Quantum Mechanics



Some General Remarks

Every physical theory is a synthesis of certain physical ideas (advanced on the basis of experiment) and a certain mathematical apparatus. The building-up of a theory is a complicated and controversial process developing according to successive approximations. However, in this controversial process, at least in its initial stage, a completely definite logical structure is envisaged, including three logically successive stages: (1) a stage in which the basic ideas are formulated and interpreted, and the physical foundation of the theory is built; (2) a stage in which an adequate mathematical aparatus for the physical ideas is found and the physical ideas and the mathematical apparatus are linked together, i.e. it is postulated exactly what physical meaning corresponds to the various mathematical symbols (as a result, the mathematical relations acquire the meaning of physical laws), and (3) a stage in which the "physicized" mathematical apparatus is "set to work" The new results thus obtained are checked experimentally where this is possible. This leads to a further understanding of the physical content of theory and to a further development of its apparatus.

At the time of creation of a theory the mathematical apparatus adequate for the description of physical ideas may or may not be available. When Newton created his mechanics, he also had to work out the corresponding mathematical apparatus—the method of fluxions which later developed into differential and integral calculus. But when quantum mechanics was created, the appropriate mathematical apparatus was already available in the form of *theory of linear operators.*

In *Quantum Physics and Philosophy* [6], Bohr writes ... *in quantal formalism, the quantities by which the state of a physical system is ordinarily defined are replaced by symbolic operators subjected to a non-commutative algorism involving Planck's constant. This procedure prevents a fixation of such quantities to the extent which would be required for the deterministic description of classical physics, but allows us to determine their spectral distribution as revealed by evidence about atomic processes. In conformity with the non-pictorial character of the formalism, its physical interpretation finds expression in laws, of an essentially statistical type...*

Turning to the mathematical aspect of quantum theory, we shall consider below how quantum-mechanical ideas "are introduced into" the apparatus of linear operators. We shall demonstrate the working of this apparatus by a number of specially selected examples and problems.

Section 17. A Brief Look at the Theory of Linear Operators

This section is essentially mathematical in nature. It includes different questions on the theory of linear operators. In other words, it describes the fundamentals of the mathematical apparatus which proved to be suitable for the creation of quantum theory. We emphasize that in this section none of the mathematical symbols is "loaded" with any physical meaning.

Linear Operators (Basic Definitions)

An *operator*, when applied to some function, transforms it into a new function. The notation

$$L\psi(x) = \varphi(x) \tag{17.1}$$

means that the operator denoted by the symbol $\hat{L}$ acts on the function $\psi(x)$, as a result of which we get function $\varphi(x)$.

The operator $\hat{L}$ is called *linear* if it satisfies the conditions

$$\hat{L}(\psi_1+\psi_2)=\hat{L}\psi_1+\hat{L}\psi_2; \qquad \hat{L}(a\psi)=a\hat{L}\psi, \tag{17.2}$$

where a is some number. We shall be using only linear operators below.

The effect of an operator acting on a function may be represented as a definite or an improper integral:

$$\hat{L}\psi(x) = \int L(x, y)\psi(y)\,dy. \tag{17.3}$$

The quantity $L(x, y)$ is called the *kernel of the operator*. If the variable is discrete, we will have instead of (17.3)

$$\hat{L}\psi_n = \sum_m L_{nm}\psi_m. \tag{17.4}$$

The totality of coefficients L_{nm} forms the *matrix of the operator* $\hat{L}$, and we speak of the matrix representation of the operator. A matrix representation is always possible because the kernel $L(x, y)$ in (17.3) may obviously be treated as a continuous matrix.

Suppose $\hat{L}\psi = \varphi$; the operator $\hat{L}^*$ is called the *complex conjugate* of the operator L, if by the action of this operator on the function ψ^* we get the function φ^*:

$$\hat{L}^*\psi^*(x)=\varphi^*(x). \tag{17.5}$$

The operator $\tilde{\hat{L}}$ is said to be the *transpose* of the operator $\hat{L}$ if the following condition is satisfied:

$$\int \Psi(x)\hat{L}\psi(x)\,dx=\int \psi(x)\tilde{\hat{L}}\Psi(x)\,dx. \tag{17.6}$$

The kernel of the transposed operator satisfies the condition

$$\tilde{L}(x, y) = L(y, x). \tag{17.7}$$

while the matrix satisfies the condition

$$\tilde{L}_{nm} = L_{mn}. \tag{17.8}$$

Let us consider some linear operator $\hat{L}$. Let us find its complex conjugate operator $\hat{L}^*$. We then find the transposed operator $\tilde{\hat{L}}^*$ for the operator $\hat{L}^*$. This operator is denoted by $\hat{L}^+$ and is said to be *conjugate* to the operator $\hat{L}$. By using the concept of the conjugate operator, two important types of linear operators are defined: Hermitian operators and unitary operators. If

$$\hat{L} = \hat{L}^+, \tag{17.9}$$

the operator $\hat{L}$ is called *Hermitian* (*self-adjoint*). If

$$\hat{L}\hat{L}^+ = \hat{L}^+\hat{L} = 1, \tag{17.10}$$

the operator $\hat{L}$ is said to be a *unitary* operator. Note that unitary operators are usually denoted by the symbol $\hat{U}$. The matrix of a unitary operator satisfies the condition

$$\sum_m U_{nm}U^+_{mk} = \delta_{nk}. \tag{17.11}$$

Note an important property of unitary operators. Suppose $\sum\limits_m U_{nm}\psi_m = \varphi_n$. It can be easily seen that

$$\sum_n \varphi^*_n\varphi_n = \sum_m \psi^*_m\psi_m. \tag{17.12}$$

The basic equation of the theory of linear operators has the form

$$\hat{L}\psi = \lambda\psi. \tag{17.13}$$

The numbers λ for which the equation (17.13) has finite solutions, form the *spectrum of eigenvalues* of the operator $\hat{L}$. The spectrum of eigenvalues of an operator may be continuous, discrete or mixed. The solutions $\psi(x)$ of equation (17.13) are called the *eigenfunctions* of the operator $\hat{L}$. One or more *eigenfunctions* may correspond to a given eigenvalue. If s linearly independent eigenfunctions correspond to a certain value λ_1, it is said that the eigenvalue λ_1 is s-fold *degenerate*.

We shall state three theorems concerning the basic properties of Hermitian operators. (The proofs of the first two theorems are given in Appendix A.)

First Theorem

An operator has real eigenvalues if and only if it is Hermitian.

Second Theorem

The eigenfunctions of a Hermitian operator, corresponding to different eigenvalues, are mutually orthogonal.

Let $\hat{L}\psi_n = \lambda_n\psi_n$. The theorem states that for $\lambda_n \neq \lambda_m$,

$$\int \psi_m^*(x)\,\psi_n(x)\,dx = 0. \tag{17.14}$$

Since (17.13) is homogeneous, the eigenfunctions are determined upto an arbitrary constant multiplier. We choose this multiplier so that the normalization condition is satisfied:

$$\int \psi_n^*(x)\,\psi_n(x)\,dx = 1. \tag{17.15}$$

By combining (17.14) and (17.15), we get the condition of orthonormalization of the eigenfunctions of a Hermitian operator:

$$\int \psi_m^*(x)\,\psi_n(x)\,dx = \delta_{mn}. \tag{17.16}$$

If the spectrum of the operator is continuous, we get instead of (17.16)

$$\int \psi_{\lambda'}^*(x)\,\psi_\lambda(x)\,dx = \delta(\lambda - \lambda'). \tag{17.17}$$

Let us consider the case of the s-fold degeneracy of an eigenvalue. The eigenfunctions corresponding to this eigenvalue are, generally speaking, not orthonormalized. However, we can form s linear combinations of the given functions which satisfy the condition of orthonor, malization.

Third Theorem

Any bounded function may be expanded in a series (integral) of eigenfunctions of a Hermitian operator. In other words, the system of eigenfunctions of a Hermitian operator is a closed (complete) one.

Using the last theorem, we represent any particular function $\Phi(x)$ in the form of a series of eigenfunctions $\psi_n(x)$: $\Phi = \sum\limits_n c_n\psi_n$. In order to find c_n, we multiply this equation by $\psi_m^*(x)$ and integrate with respect to x:

$$\int \psi_m^*(x)\,\Phi(x)\,dx = \sum_n c_n \int \psi_m^*(x)\,\psi_n(x)\,dx.$$

Using (17.16), we get from this

$$\int \psi_m^*(x)\,\Phi(x)\,dx = \sum_n c_n \delta_{mn} = c_m.$$

Thus,

$$\left.\begin{aligned} &\Phi(x) = \sum_n c_n \psi_n(x),\\ &\text{where}\\ &\quad c_n = \int \psi_n^*(x)\,\Phi(x)\,dx. \end{aligned}\right\} \qquad (17.18)$$

In the case of a continuous spectrum, we must use the condition (17.17). As a result, we get instead of (17.18)

$$\left.\begin{aligned} &\Phi(x) = \int c(\lambda)\,\psi_\lambda(x)\,d\lambda,\\ &\text{where}\\ &c(\lambda) = \int \psi_\lambda^*(x)\,\Phi(x)\,dx. \end{aligned}\right\} \qquad (17.19)$$

We shall mention one of the results which is a direct consequence of the completeness of the system of eigenfunctions of a Hermitian operator. Suppose $\Phi(x) = \int c(\lambda)\,\psi_\lambda(x)\,d\lambda$ and $\Psi(x) = \int b(\lambda')\,\psi_{\lambda'}(x)\,d\lambda'$ By using (17.17), it can be easily seen that

$$\int \Psi^*(x)\,\Phi(x)\,dx = \int b^*(\lambda)\,c(\lambda)\,d\lambda. \qquad (17.20)$$

Representations

Suppose that the Hermitian operator M transforms the function $\Phi(x)$ into the function $\Psi(x)$:

$$\Psi(x) = \hat{M}\Phi(x). \qquad (17.21)$$

Let us expand the functions Φ and Ψ in terms of eigenfunctions $\psi_\lambda(x)$ of another Hermitian operator (the operator $\hat{L}$). Assuming that the spectrum of the operator $\hat{L}$ is continuous, we have

$$\Phi(x) = \int c(\lambda)\,\psi_\lambda(x)\,d\lambda; \qquad \Psi(x) = \int b(\lambda)\,\psi_\lambda(x)\,d\lambda \qquad (17.22)$$

The transformation (17.21) will then have some corresponding transformation of the function $c(\lambda)$ to the function $b(\lambda)$. We write this transformation in the form

$$b(\lambda) = \hat{M}(\lambda)\,c(\lambda). \qquad (17.23)$$

It is said that (17.21) and (17.23) are two different representations of the same transformation. The nature of the representation is determined by the variables on which the initial and final functions depend. Hence we speak of x-representation in the case of (17.21) and of λ-representation (representation of the operator $\hat{L}$) in the case of (17.23). Correspondingly, the operator $\hat{M}$ in (17.21) is the operator of the given transformation, defined in the x-representation [for convenience, we shall henceforth write it as $\hat{M}(x)$], while the operator $\hat{M}(\lambda)$ occurring in (17.23) is the operator of the given transformation, defined in λ-representation.

Let us see what the Hermitian operator looks like in eigen representation. Let $\varphi_\mu(x)$ be the eigenfunctions of the operator $\hat{M}$. In this case, we can write (17.22) in the following form:

$$\Phi(x) = \int c(\mu)\,\varphi_\mu(x)\,d\mu; \qquad \Psi(x) = \int b(\mu)\,\varphi_\mu(x)\,d\mu. \tag{17.24}$$

Applying the operator $\hat{M}(x)$ to the function $\Phi(x)$, we get

$$\hat{M}(x)\,\Phi(x) = \int c(\mu)\,\hat{M}(x)\,\varphi_\mu(x)\,d\mu = \int \mu c(\mu)\,\varphi_\mu(x)\,d\mu.$$

Comparing this result with the second equality in (17.24), we have

$$b(\mu) = \mu c(\mu), \tag{17.25}$$

whence we get

$$\hat{M}(\mu) = \mu. \tag{17.26}$$

Thus in its eigen representation, the Hermitian operator coincides with its eigenvalues.

We shall now consider a more general situation: the operator $\hat{M}(x)$ is known; it is required to find out the form of this operator in the λ-representation. Using (17.21) and (17.22) we write

$$\Psi(x) = \hat{M}(x)\,\Phi(x) = \int c(\lambda')\,\hat{M}(x)\,\psi_{\lambda'}(x)\,d\lambda'$$
$$= \int b(\lambda')\,\psi_{\lambda'}(x)\,d\lambda'.$$

Multiplying both sides of the last of these equalities by $\psi_\lambda^*(x)$ and integrating with respect to x, we get

$$\int c(\lambda')\left[\int \psi_\lambda^*(x)\,\hat{M}(x)\,\psi_{\lambda'}(x)\,dx\right]d\lambda'$$
$$= \int b(\lambda')\left[\int \psi_\lambda^*(x)\,\psi_{\lambda'}(x)\,dx\right]d\lambda'.$$

By using (17.17), we find that

$$b(\lambda)=\int\left[\int \psi_{\lambda}^{*}(x)\,\hat{M}(x)\,\psi_{\lambda'}(x)\,dx\right]c(\lambda')\,d\lambda'$$

Lastly, by taking (17.23) into account, we finally get the result [compare with (17.3)]:

$$\hat{M}(\lambda)\,c(\lambda)=\int M(\lambda,\ \lambda')\,c(\lambda')\,d\lambda',$$

where

$$M(\lambda,\ \lambda')=\int \psi_{\lambda}^{*}(x)\,\hat{M}(x)\,\psi_{\lambda'}(x)\,dx. \qquad (17.27)$$

Thus, if the form of the operator is known, say, in the x-representation, we can find the matrix of this operator in the λ-representation by using the eigenfunctions of the operator $\hat{L}$, given in the x-representation, by (17.27).

In conclusion, we mention a situation where the eigenfunctions of one Hermitian operator are given in the representation of another operator. In this case, the following relation is valid:

$$\psi_{\lambda}(\mu)=\varphi_{\mu}^{*}(\lambda). \qquad (17.28)$$

Transition from One Representation to Another as Unitary Transformation

A transition from the λ-representation to the x-representation is determined with the help of (17.22). In operator form, these relations can be written as

$$\Phi(x)=U(x,\ \lambda)\,c(\lambda);\qquad \Psi(x)=U(x,\ \lambda)\,b(\lambda). \qquad (17.29)$$

Next, we put

$$\int \Psi^{*}(x)\,\Phi(x)\,dx=\int \Psi^{*}(x)\,\hat{U}(x,\ \lambda)\,c(\lambda)\,dx$$
$$=\int c(\lambda)\,[\hat{U}^{+}(\lambda,\ x)\,\Psi(x)]^{*}\,d\lambda.$$

Using (17.20), we get

$$b(\lambda)=\hat{U}^{+}(\lambda,\ x)\,\Psi(x).$$

Two important results follow from the last formula. Firstly,

$$\Psi(x)=\hat{U}(x,\ \lambda)\,b(\lambda)=\hat{U}(x,\ \lambda)\,\hat{U}^{+}(\lambda,\ x)\,\Psi(x)$$

and, consequently,

$$\hat{U}(x,\ \lambda)\,\hat{U}^{+}(\lambda,\ x)=1. \qquad (17.30)$$

This means that the transition from one representation to another is accomplished with the help of a unitary transformation. Secondly, if

$\Psi(x)=\hat{M}(x)\Phi(x)$, then $\hat{U}(x, \lambda)b(\lambda)=\hat{M}(x)\hat{U}(x, \lambda)c(\lambda)$ and, according to (17.30),

$$b(\lambda)=\hat{U}^{+}(\lambda, x)\hat{M}(x)\hat{U}(x, \lambda)c(\lambda). \qquad (17.31)$$

Comparing (17.31) and (17.23), we get

$$\hat{M}(\lambda)=\hat{U}^{+}(\lambda, x)\hat{M}(x)\hat{U}(x, \lambda). \qquad (17.32)$$

It should be explained here that a product of operators means the successive action of the operators on the functions to their right. In the present case we should first apply the operator $U(x, \lambda)$ to the function $c(\lambda)$, thus getting the function $\Phi(x)$. Operator $M(x)$ then acts on the function $\Phi(x)$, resulting in the function $\Psi(x)$. Finally, the function $\Psi(x)$ is acted on by the operator $\hat{U}^{+}(\lambda, x)$.

Thus, the relations (17.29) describe the transition from one representation of functions to another carried out with the help of a unitary operator. Relation (17.32) describes the same transition for operators.

Unitary Invariants

Quantities and properties which do not change with unitary transformations and are, consequently, independent of the choice of representation are called *unitary invariants*. Unitary invariants include: (a) the Hermitian property of an operator (if an operator is Hermitian in one representation, it will be Hermitian in any other representation); (b) the spectrum of eigenvalues of a Hermitian operator; (c) the condition of orthonormalization of eigenfunctions [this is immediately seen from (17.12)]; (d) integrals of the type $\int \Psi^{*}(x)\Phi(x)\,dx$ [this directly follows from (17.20)]; (e) integrals of the type $\int \Psi^{*}(x) \times \hat{M}(x)\Phi(x)\,dx$ and of the more general type $\int \Psi^{*}(x)\hat{M}^{n}(x)\Phi(x)\,dx$, where n is a positive integer. Note that unitary invariance of these integrals means that the following relations hold:

$$\int \Psi^{*}(x)M(x)\Phi(x)\,dx=\int b^{*}(\lambda)\hat{M}(\lambda)c(\lambda)\,d\lambda, \qquad (17.33)$$

$$\int \Psi^{*}(x)\hat{M}^{n}(x)\Phi(x)\,dx=\int b^{*}(\lambda)\hat{M}^{n}(\lambda)c(\lambda)\,d\lambda. \qquad (17.34)$$

As an example we shall prove (17.33). Using (17.29) and (17.32), we successively transform the left-hand side of (17.33):

$$\int [\hat{U}^* b^* (\lambda)] \hat{U} \hat{M} (\lambda) \hat{U}^+ \hat{U} c (\lambda)\, dx$$

$$= \int [\hat{U}^* b^* (\lambda)] \hat{U} M (\lambda) c (\lambda)\, dx$$

$$= \int b^* (\lambda) \hat{U}^+ \hat{U} \hat{M} (\lambda) c (\lambda)\, d\lambda = \int b^* (\lambda) \hat{M} (\lambda) c (\lambda)\, d\lambda.$$

Thus, as a result, we get the right-hand side of (17.33), Q.E.D.

Commutation of Operators and the System of Common Eigenfunctions

Two operators $\hat{L}$ and $\hat{M}$ are called *commutative* if for any bounded function $\Phi (x)$ they satisfy the following condition:

$$\hat{M} \hat{L} \Phi (x) = \hat{L} \hat{M} \Phi (x). \qquad (17.35)$$

If there is even one function for which (17.35) does not hold, the operators $\hat{L}$ and $\hat{M}$ are called non-commutative. The notation $[\hat{M}, \hat{L}] = \hat{M}\hat{L} - \hat{L}\hat{M}$ is called the *commutator operator* of $\hat{L}$ and $\hat{M}$. If the operators commute, this fact is often expressed thus: $[\hat{M}, \hat{L}] = 0$.

The following *theorem* holds: If the operators $\hat{L}$ and $\hat{M}$ have common eigenfunctions forming a closed system, the operators commute. We shall prove this theorem.

We denote the eigenfunctions of the operators $\hat{L}$ and $\hat{M}$ by $\psi_{\lambda\mu} (x)$. (The double subscript $\lambda\mu$ indicates the fact that these functions are common). Obviously,

$$\hat{M} \hat{L} \psi_{\lambda\mu} = \lambda \hat{M} \psi_{\lambda\mu} = \lambda\mu\psi_{\lambda\mu},$$

$$\hat{L} \hat{M} \psi_{\lambda\mu} = \mu \hat{L} \psi_{\lambda\mu} = \mu\lambda\psi_{\lambda\mu}.$$

It follows from this that

$$(\hat{M}\hat{L} - \hat{L}\hat{M}) \psi_{\lambda\mu} = 0,$$

and since the functions $\psi_{\lambda\mu} (x)$ are known to form a closed system, for any function $\Phi (x)$ we can write

$$(\hat{M}\hat{L} - \hat{L}\hat{M}) \Phi (x) = \sum c_{\lambda\mu} (\hat{M}\hat{L} - \hat{L}\hat{M}) \psi_{\lambda\mu} (x) = 0,$$

Q.E.D.

We stress the importance of the fact that common eigenfunctions must form a closed system. It may so happen that two operators have only one common eigenfunction. In this case it is impossible to draw any conclusion about the commutativity of the operators.

The above theorem means that commutativity of operators is a necessary property of the commonness of the system of eigenfunctions of these operators. But is this property a sufficient condition also? The answer to this question is in the affirmative in the case when there is no degeneracy in the eigenvalues of the operators. In the more general case, taking into account the possibility of degeneracy, the following *theorem* is valid. If the operators $\hat{L}$ and $\hat{M}$ commute, we can find their common eigenfunctions. For example, suppose the eigenvalue λ_1 is s-fold degenerate. From the s solutions of the equation $\hat{L}\psi = \lambda_1\psi$, we can choose s linear combinations which are also the eigenfunctions of the operator $\hat{M}$. In this case, λ_1 will in general correspond to s different eigenvalues of the operator $\hat{M}$.

With this we conclude our degression in the field of "pure" mathematics. The information contained here is sufficient for further use of the apparatus of linear operators without referring to special literature.

Section 18 From Hamiltonian Matrix to Energy Operator

The Influence of the Choice of Basic States

We turn to equation (12.8) discussed in Sec. 12. There we chose a certain system of basic states of microparticle $\{\langle i \mid\}$. An arbitrary state $\langle s(t) \mid$ of this microparticle at time t was represented as a superposition of these basic states:

$$\langle s(t) \mid = \sum_i \langle s(t) \mid i \rangle \langle i \mid. \tag{18.1}$$

The notation $C_i(t)$ was employed for the amplitudes $\langle s(t) \mid i \rangle$ It was shown that the amplitudes $C_i(t)$ satisfy the equation

$$-i\hbar \frac{d}{dt} C_i(t) = \sum H_{ij}(t) C_j(t), \tag{18.2}$$

which permits one to find, from a knowledge of the amplitudes $C_i(t)$ and the Hamiltonian matrix $H_{ij}(t)$ at time t, the amplitudes C_i at any subsequent moments of time.

The expression (18.1) clearly shows that the set of amplitudes $\{C_i(t)\}$ depends on the choice of the system of basic states $\{\langle i \mid\}$. Suppose we have to go over to a new system of basic states $\{\langle m \mid\}$. In order to accomplish this transition, we represent the earlier basic states in the form of superposition of new basic states:

$$\langle i \mid = \sum_m \langle i \mid m \rangle \langle m \mid \tag{18.3}$$

Substituting this superposition in (18.1), we get

$$\langle s(t)| = \sum_i \sum_m C_i(t) \langle i|m\rangle \langle m|,$$

or

$$\langle s(t)| = c_m(t) \langle m|, \tag{18.4}$$

where

$$c_m(t) = \sum_i C_i(t) \langle i|m\rangle. \tag{18.5}$$

The new amplitudes $c_m(t)$, corresponding to the system of basic states $\{\langle m|\}$, satisfy an equation of the type (18.2) but obviously with a new Hamiltonian matrix $H_{mn}(t)$:

$$-i\hbar \frac{d}{dt} c_m(t) = \sum_n H_{mn}(t) c_n(t). \tag{18.6}$$

We shall show how the old Hamiltonian matrix can be expressed in terms of the new one. Substituting (18.5) in (18.6), we find

$$-i\hbar \frac{d}{dt} \sum_{j'} C_{j'}(t) \langle j'|m\rangle = \sum_n \sum_j H_{mn}(t) C_j(t) \langle j|n\rangle.$$

Multiplying both sides of the last equation by $\langle m|i\rangle$ and summing with respect to m, we get

$$-i\hbar \frac{d}{dt} \sum_{j'} C_{j'}(t) \Big[\sum_m \langle j'|m\rangle \langle m|i\rangle\Big] = \sum_j \Big[\sum_n \sum_m H_{mn}(t) \langle j|n\rangle \langle m|i\rangle\Big] C_j(t).$$

Taking into account that $\sum_m \langle j'|m\rangle \langle m|i\rangle = \langle j'|i\rangle = \delta_{j'i}$, we can simplify the left-hand side of the last equation. As a result, we get

$$-i\hbar \frac{d}{dt} C_i(t) = \sum_j H_{ij}(t) C_j(t),$$

where

$$H_{ij}(t) = \sum_n \sum_m H_{mn}(t) \langle j|n\rangle \langle m|i\rangle. \tag{18.7}$$

Thus the choice of any system of basic states of a microparticle influences both the form of the amplitudes of states satisfying (12.8) as well as the form of the Hamiltonian matrix.

It was mentioned in Sec. 13 that the system of basic states is usually chosen in such a way that these states could have a direct physical meaning. However, for the sake of greater convenience when considering equation (12.8), we go over to new, specially selected basic states in a number of cases. Thus, in Sec. 13, the transition from the basic states $\langle 1 |$ and $\langle 2 |$ to the basic states $\langle \mathrm{I} |$ and $\langle \mathrm{II} |$ was motivated by a desire to diagonalize the Hamiltonian matrix, while in Sec. 14 it was done in order to express the Hamiltonian matrix in a form convenient for drawing an analogy with an electron in magnetic field.

Transformation of an Equation Expressing Causality Into a Form Independent of the Choice of Basic States

Let us consider operator $\hat{H}(t)$ satisfying the following relation:

$$H_{ij}(t)=\langle j|\hat{H}(t)|i\rangle. \tag{18.8}$$

The operator $\hat{H}(t)$, acting on the basic state $\langle i |$, gives rise to a new state $\langle \psi(t) | = \hat{H}(t) | i\rangle$, which is not basic. The element of the Hamiltonian matrix $H_{ij}(t)$ here plays the role of the amplitude $\langle j | \psi(t)\rangle$, i.e. of the amplitude probability that a microparticle in the basic state $\langle j |$ may be found in the state $\langle \psi(t) |$. Substituting (18.8) in (18.2), we get

$$-i\hbar \frac{d}{dt}\langle s(t)|i\rangle=\sum_{j}\langle s(t)|j\rangle\langle j|H(t)|i\rangle \tag{18.9}$$

or

$$-i\hbar \frac{d}{dt}\langle s(t)|i\rangle=\langle s(t)|\hat{H}(t)|i\rangle. \tag{18.10}$$

Taking the complex-conjugate of the equation and considering (9.33) and (12.9), we get

$$i\hbar \frac{d}{dt}\langle i|s(t)\rangle=\langle i|\hat{H}(t)|s(t)\rangle \tag{18.11}$$

or

$$i\hbar \frac{d}{dt}|s(t)\rangle=\hat{H}(t)\,|s(t)\rangle. \tag{18.12}$$

Note that while going over from (18.9) to (18.10) or from (18.11) to (18.12), we have made use of the rules given in Sec. 10 under the heading "The Mechanics of Quantum Mechanics". The final equation (18.12) is analogous to equation (18.2), but unlike the latter, it is independent of the choice of basic states.

Vector Analogy

In order to express the causal relationship mathematically [(18.2)] in the above discussion, we had to use information about the state under consideration, the physical meaning of the problem and the system of basic states. But now [Eq. (18.12)] it is sufficient to have information about the state under consideration and the physical meaning of the problem. This means that a transition from (18.2) to (18.12) leads to a more abstract level of analysis.

We emphasize that such an abstraction is made possible by the use of operators. Operators help us to get quantum-mechanical relations that are more abstract and are *independent* of the choice of the system of basic states.

The more abstract analysis, enabled by the introduction of operators is, to a certain extent, analogous to the more abstract analysis connected with the introduction of vectors. We shall consider this analogy in detail.

This analogy is not unexpected. Remember that in Sec. 14 it was suggested that a state should be treated as a vector in some arbitrary space. The concept of projection amplitudes was also introduced there.

The essence of the *vector analogy* is as follows. In order to perform operations with components of vectorial quantities one always has to choose a definite system of coordinate axes. In quantum mechanics we make a corresponding choice of a definite system of basic states. By using vectors, one can perform operations with vector

Quantum-mechanical expression	Vector analogy
$\sum_i \langle f \mid i\rangle \langle i \mid s\rangle = 0$ $\langle f \mid s\rangle = 0$ (mutually orthogonal states)	$\sum_i a_i b_i = 0$ $(\vec{a}\vec{b}) = 0$ (mutually orthogonal vectors)
$i\hbar \frac{d}{dt} \langle i \mid s(t)\rangle =$ $= \sum_j H_{ji} \langle j \mid s(t)\rangle$ $i\hbar \frac{d}{dt} \mid s(t)\rangle = \hat{H} \mid s(t)\rangle$ (operation on a state)	$c_i = \sum_j H_{ij} a_j$ $\vec{c} = \hat{H}\vec{a}$ (operation on a vector)

quantities without resorting to a choice of any particular system of axes. Similarly, by using vectors of states and their operators in quantum mechanics, one can avoid having to choose a system of basic states. Let us illustrate the vector analogy with the help of the table (p. 174).

Each cell of the table contains two expressions having the same meaning (indicated in brackets). However, the upper expression depends on the choice of the system of basic states or coordinate axes, while the lower one is independent of any such choice.

It is worthwhile giving an example for the lower right cell of the above table, which shows how one can imagine an operator acting on a vector. As an example of this (to which, of course, no "quantum-mechanical meaning" should be assigned) let us consider the case when the matrix H_{ij} is of the form

$$(H)=\begin{pmatrix} 0 & -\frac{\partial}{\partial r_3} & \frac{\partial}{\partial r_2} \\ \frac{\partial}{\partial r_3} & 0 & -\frac{\partial}{\partial r_1} \\ -\frac{\partial}{\partial r_2} & \frac{\partial}{\partial r_1} & 0 \end{pmatrix}$$

where r_1, r_2, r_3 are three Cartesian coordinates in space. In this case the relation $\vec{c} = \hat{H}\vec{a}$ acquires the form which is familiar to those who have studied vector analysis: $\vec{c} = \text{curl}\ \vec{a}$.

In conclusion let us reiterate the various aspects of the vector analogy: (a) corresponding to the choice of basic states, we have a choice of the system of coordinate axes; (b) a transition from one set of basic states to another corresponds to a transition from one system of axes to another (note that such a transition does not involve the physics of the problem being considered); (c) the expansion into basic states corresponds to a representation of the vector in terms of its projections on the coordinate axes. The analogy with vectors is a good example of abstraction and of the representation of relations in a form taking into account only strictly physical information.

Average Energy

Let us demonstrate some of the advantages of the operator approach. We shall show how the mean value $\langle E \rangle$ of the energy of a microparticle in some state $\langle s \mid$ is determined. Let $\{\langle i \mid\}$ be the basic states with energies E_i. This means (see Sec. 13) that the Hamiltonian matrix is diagonal. Hence,

$$\langle j|\hat{H}|i\rangle = \delta_{ij}E_i,$$

or

$$\langle j|\hat{H}|i\rangle = \langle j|i\rangle E_i. \qquad (18.13)$$

We expand the state $\langle s|$ in terms of the system of basic states $\{\langle i|\}$ $\langle s| = \sum_i \langle s|i\rangle\langle i|$, and try to find the mean value of the energy $\langle E\rangle$ with the help of a formula of the type (12.3):

$$\langle E\rangle = \sum_i |\langle s|i\rangle|^2 E_i. \qquad (18.14)$$

By taking (9.33) into account, we rewrite (18.14) in the form

$$\langle E\rangle = \sum_i \langle s|i\rangle E_i \langle i|s\rangle \equiv \langle s|\varphi\rangle, \qquad (18.15)$$

where

$$|\varphi\rangle = \sum_i |i\rangle E_i \langle i|s\rangle. \qquad (18.16)$$

From (18.13) it follows that

$$\hat{H}|i\rangle = |i\rangle E_i. \qquad (18.17)$$

Substituting (18.17) in (18.16), we get

$$|\varphi\rangle = \sum_i \hat{H}|i\rangle\langle i|s\rangle = \hat{H}|s\rangle,$$

after which we get the required result from (18.15):

$$\langle E\rangle = \langle s|\hat{H}|s\rangle. \qquad (18.18)$$

It can be seen from (18.18) that mean value of the energy of a microparticle in the state $\langle s|$ is expressed only through the operator $\hat{H}$. Basic states do not enter this relation. The convenience of the relation (18.18) is due to its independence from the choice of basic states, which allows one to use freely any system of basic states when carrying out calculations. For example, suppose it is convenient to use the basic states $\{\langle m|\}$. In this case the operator relation (18.18) immediately acquire the corresponding form

$$\langle E\rangle = \sum_m \sum_n \langle s|m\rangle\langle m|\hat{H}|n\rangle\langle n|s\rangle. \qquad (18.19)$$

Energy Operator (Hamiltonian)

It has been mentioned above that the Hamiltonian matrix could be called the energy matrix (remember that the elements of the diagonalized Hamiltonian matrix are essentially the possible values of the energy of the microparticle). The connection between the operator $\hat{H}$ and the Hamiltonian matrix as well as relation (18.18), expressing the average energy of a microparticle in terms of the operator $\hat{H}$, justify the name *energy operator* given to it. In the literature the operator $\hat{H}$ is also called the *Hamiltonian.*

We write expressions derived above in which the Hamiltonian of a microparticle is present (we emphasize the exceptional importance of these expressions):

$$i\hbar \frac{d}{dt} |s(t)\rangle = \hat{H} |s(t)\rangle, \tag{18.12}$$

$$\langle E\rangle = \langle s|\hat{H}|s\rangle, \tag{18.18}$$

$$\hat{H}|f\rangle = |f\rangle E. \tag{18.20}$$

In expression (18.20), $\langle f|$ denotes some stationary state and E is the energy in this state.

Finally, we note that the Hamiltonian (as well as any other operator) may act not only on the state $|s\rangle$, but also on its amplitude $\langle i|s\rangle$, since we always have the representation [see (17.4)]

$$\hat{H}C_i(t) = \sum_j H_{ij}C_j(t). \tag{18.21}$$

Using (18.21) and taking into account that $\langle i|s\rangle = C_i^*$, we can rewrite (18.2) in a form which, as can be easily seen, is completely analogous in form to (18.12):

$$i\hbar \frac{d}{dt} \langle i|s(t)\rangle = \hat{H} \langle i|s(t)\rangle. \tag{18.22}$$

Correspondingly, (18.20) may be written in the form

$$\hat{H}\langle i|f\rangle = E\langle i|f\rangle. \tag{18.23}$$

Section 19 Linear Operators in Quantum Mechanics

We now come to the main problem of this chapter, i.e. that of imparting physical meaning to the mathematical apparatus of linear operators in order to convert it into the apparatus of quantum mechanics. In this sense the previous section should be considered as a preliminary step towards solving this problem.

Role of Operators in Quantum Mechanics

The following two points must be noted when considering the role of linear operators in quantum mechanics. *Firstly*, in quantum mechanics to every dynamic variable (spatial coordinate, energy, momentum, angular momentum, etc.), there is assigned a definite Hermitian operator.

Secondly, the transition from one representation to another without changing the physical meaning of the problem is achieved with the help of unitary operators.

Let us consider the first point in detail. It means that besides the energy operator $\hat{H}$, other "physical operators" like the coordinate operator $\hat{\vec{r}}$, the momentum operator $\hat{\vec{p}}$, the angular momentum operator $\hat{\vec{M}}$, etc. must be introduced. In this respect, it is significant that the well-known dynamic relations of classical mechanics may be transferred to quantum mechanics in the same form, if *we replace the physical quantities in these relations by the corresponding Hermitian operators.* In other words, the apparatus of quantum mechanics may be built up in analogy with the apparatus of classical mechanics, if we replace the dynamic variables with their corresponding Hermitian operators. As an example, let us compare the following expressions:

In classical mechanics	In quantum mechanics	
$E=\frac{p^2}{2m}+U$	$\hat{H}=\frac{\hat{p}^2}{2m}+\hat{U}$	(19.1)
$\vec{M}=(\vec{r}\times\vec{p})$	$\hat{\vec{M}}=(\hat{\vec{r}}\times\hat{\vec{p}})$	(19.2)

It should be remembered, however, that a complete formal analogy between the apparatus of classical and quantum mechanics does not exist. We point out (for details see Sec. 20) that in the algebraic manipulation of operator relations we must remember that operators may not commute. Thus if $\hat{A}$ and $\hat{B}$ do not commute, then $(\hat{A}+\hat{B})^2 \neq \hat{A}^2+2\hat{A}\hat{B}+\hat{B}^2$. In this case $(\hat{A}+\hat{B})^2=\hat{A}^2+\hat{A}\hat{B}+\hat{B}\hat{A}+\hat{B}^2$. Besides, there are operators in quantum mechanics which do not have classical analogies (for example, the spin operator).

Note that we may formally assign corresponding operators to all classical dynamical variables including those which do not have any meaning in the microworld. Thus, we may introduce the operators of velocity $\hat{\vec{v}}$, of potential energy $\hat{U}$, kinetic energy $\hat{T}$, etc., though neither velocity nor the breaking-up of total energy into kinetic and potential components which is characteristic for classical mechanics, have any meaning for microparticles.

Basic Postulates

Let us consider the question: In exactly what way can we compare a physical quantity with a Hermitian operator? In other words, what is the meaning of the word "compare" here? The following two basic postulates provide an answer to this question.

Postulate 1. If the operator $\hat{L}$ is compared with a physical quantity l, it means that the eigenvalues λ of the operator are identified with the values of the physical quantity under consideration obtained by measurement.

Postulate 2. If operator $\hat{L}$ is compared with a physical quantity l, it means that the eigenfunctions $\psi_\lambda(\alpha)$ of the operator are identified with the eigenfunctions of the quantities from the λ-set, expressed in α-representation. By the remarks made in Sec. 15, this means that the eigenfunctions $\psi_\lambda(\alpha)$ of the operator are identified with the amplitudes of states $\langle\lambda|\alpha\rangle$, often called the wave functions.

Thus a study of the fundamental equation of the theory of linear operators [see (17.13)]

$$\hat{L}(\alpha)\langle\lambda|\alpha\rangle=\lambda\langle\lambda|\alpha\rangle \tag{19.3}$$

includes physical problems such as finding the spectrum of possible values λ of a physical quantity l, and finding the amplitudes of states $\langle\lambda|\alpha\rangle$ in which the corresponding values of λ occur.

When applied to the energy operator, (19.3) takes the form of (18.23). A study of equation (18.23) permits us to find the possible values of the energy of a microparticle and the corresponding amplitude values of the stationary states.

Mathematical Results and Their Physical Meaning

The postulates formulated above "knit together" the physical and mathematical aspects; they "load" the mathematical symbols and inferences with a definite physical meaning. We shall demonstrate this with a number of observations.

1. The eigenvalues of a Hermitian operator are real. From a physical point of view this means that the values of quantities obtained during measurements are real.
2. The spectrum of the eigenvalues of a Hermitian operator may be discrete or continuous. This corresponds to *quantization* or a *continuous variation* of the physical quantities characterizing a microparticle.
3. The eigenfunctions of a Hermitian operator satisfy the condition of orthonormalization. This mathematical fact becomes the condition of orthonormalization of eigenfunctions of physical quantities and, in particular, the

condition of orthogonality of basic states of a microparticle. In other words, the mathematical result (17.16) is converted into physical relations (15.13) and (10.8), while the mathematical result (17.17) is converted into the physical relation (15.14).

4. The system of eigenfunctions of a Hermitian operator is a closed (complete) one. From a physical point of view, this means that it is possible to expand any amplitude in terms of amplitudes which are eigenfunctions of a physical quantity, i.e. in terms of basic amplitudes. In other words, the completeness of a system of eigenfunctions of a Hermitian operator is converted into the physical *principle of superposition of states.*

5. The eigenvalues of a Hermitian operator may be degenerate. Physically this means that one value of a quantity may correspond to several different states.

6. The mathematical result (17.28) for the eigenfunctions of operators corresponds to the physical result (9.33) for amplitudes of states.

7. Unitary transformations corresponding to the transition from one representation to another, physically correspond to a transition from one complete set of quantities to another and, in particular, from one system of basic states of a microparticle to another.

8. The existence of a common complete system of eigenfunctions means that the operators commute. This mathematical fact corresponds to the possibility of *simultaneous measurement* of the corresponding physical values. Note that the impossibility of the simultaneous measurement of such physical quantities as the coordinate and momentum of a microparticle means that the operators of coordinate and momentum do not commute.

9. The mathematical fact of commutativity of the Hamiltonian $\hat{H}$ and the operator $\hat{L}$ means that physically the quantity l corresponding to the operator $\hat{L}$ is an integral of motion. In other words, the condition

$$[\hat{H}, \hat{L}] = 0$$

from the physical point of view is the *law of conservation* of the quantity l.

The last remark will be rigorously proved below. Here, we shall just mention some ideas of a qualitative nature for this purpose. If operators $\hat{H}$ and $\hat{L}$ commute, the quantities E and l can be simultaneously measured since there are states in which both these quantities have definite values. A state in which energy has a definite value is stationary, i.e. has an infinitely long "life" time. But this means that the quantity l must also be conserved for an infinitely long time, just like any other physical quantity for which the given state is an eigenfunction.

Mean Value of a Quantity

If the quantity l is measured in a state described by the amplitude $\langle\lambda|\alpha\rangle$, then, according to basic postulates, the measured value will be λ. We assume now that the quantity l is measured not in its eigenstate, but in some "other" state, for example, in the state described by the amplitude $\Phi_s(\alpha) = \langle s|\alpha\rangle$. In this case the result of a single measurement cannot be predicted unambiguously; probabilistic predictions enter into the picture now, thus permitting an estimation of the *mean value* $\langle\lambda\rangle$ from a relatively large number of measurements (in this connection see Sec. 12). We shall show how to compute the mean value $\langle\lambda\rangle$ in the state $\langle s|$, if we know the Hermitian operator $\hat{L}$ corresponding to the quantity l. Note that in the particular case when energy is used in place of the quantity l, this problem was considered in Sec. 18, where the following result was obtained:

$$\langle E\rangle = \langle s|\hat{H}|s\rangle. \qquad (18.18)$$

In the general case, (18.18) takes the form

$$\langle\lambda\rangle = \int \Phi_s^*(\alpha)\,\hat{L}(\alpha)\,\Phi_s(\alpha)\,d\alpha \qquad (19.4)$$

(we assume for definiteness in this case that the variable α which characterizes the representation varies continuously). Let us prove this.

We expand the amplitudes $\Phi_s(\alpha)$ and $\Phi_s^*(\alpha)$ in terms of eigenfunctions $\psi_n(\alpha) = \langle\lambda_n|\alpha\rangle$ of the operator $\hat{L}$ (we assume that the spectrum of the operator $\hat{L}$ is discrete):

$$\Phi_s(\alpha) = \sum_n \langle s|\lambda_n\rangle\,\psi_n(\alpha),$$

$$\Phi_s^*(\alpha) = \sum_m \langle s|\lambda_m\rangle^*\,\psi_m^*(\alpha).$$

Substituting these superpositions in (19.4) and using (19.3) and (17.16), we get

$$\int \Phi_s^*(\alpha)\,\hat{L}(\alpha)\,\Phi_s(\alpha)\,d\alpha$$

$$= \sum_n \sum_m \langle s|\lambda_n\rangle\langle s|\lambda_m\rangle^* \int \psi_m^*(\alpha)\,\hat{L}(\alpha)\,\psi_n(\alpha)\,d\alpha$$

$$= \sum_n \sum_m \langle s|\lambda_n\rangle\langle s|\lambda_m\rangle^*\,\lambda_n \int \psi_m^*(\alpha)\,\psi_n(\alpha)\,d\alpha$$

$$= \sum_n \sum_m \langle s|\lambda_n\rangle \langle s|\lambda_m\rangle^* \lambda_n \delta_{mn} = \sum_n |\langle s|\lambda_n\rangle|^2 \lambda_n.$$

By (12.3), the last sum is equal to $\langle\lambda\rangle$, Q.E.D.
The result (19.4) is very important. In fact this one result is sufficient to demonstrate the usefulness of the application of operators in quantum mechanics.
In analogy with (18.18), the result (19.4) can be written in a more abstract form which avoids a choice of representation:

$$\langle\lambda\rangle = \langle s \mid \hat{L} \mid s\rangle. \tag{19.5}$$

The Variation of the Mean Value of a Quantity with Time

Using (19.5) and assuming at the outset that the operator $\hat{L}$ is independent of time, let us write

$$\frac{d}{dt}\langle\lambda\rangle = \frac{d}{dt}\langle s(t)\,|\hat{L}|\,s(t)\rangle$$

$$= \left(\frac{d}{dt}\langle s(t)|\right)|\hat{L}|\,s(t)\rangle + \langle s(t)\,|\hat{L}|\left(\frac{d}{dt}|s(t)\rangle\right). \tag{19.6}$$

Further, we turn to (18.12) and transform it into the form

$$-i\hbar\frac{d}{dt}\langle s(t)| = \langle s(t)|\hat{H}^+,$$

or, taking into account the hermiticity of the Hamiltonian,

$$-i\hbar\frac{d}{dt}\langle s(t)| = \langle s(t)|\hat{H}. \tag{19.7}$$

Substituting (18.12) and (19.7) into (19.6), we get

$$\frac{d}{dt}\langle\lambda\rangle = \frac{i}{\hbar}\langle s(t)|\hat{H}\hat{L} - \hat{L}\hat{H}|s(t)\rangle,$$

or

$$\frac{d}{dt}\langle\lambda\rangle = \frac{i}{\hbar}\langle s|[\hat{H},\ \hat{L}]|s\rangle. \tag{19.8}$$

If the quantity l is an integral of motion, $\frac{d}{dt}\langle\lambda\rangle = 0$. It follows from (19.8) that the above-mentioned condition $[\hat{H}, \hat{L}] = 0$ is a condition for the conservation of he quantity l.

We introduce a new operator $\hat{\dot{L}}$, defining it by the relation

$$\langle s|\hat{\dot{L}}|s\rangle = \frac{d}{dt}\langle\lambda\rangle. \tag{19.9}$$

Comparing (19.9) with (19.8), we conclude that in the case when $\hat{L}$ is independent of time, the operator $\hat{\dot{L}}$

is of the form

$$\dot{\hat{L}} = \frac{i}{\hbar}[\hat{H}, \hat{L}]. \tag{19.10}$$

If $\hat{L}$ varies with time, we get instead of (19.10)

$$\dot{\hat{L}} = \frac{i}{\hbar}[\hat{H}, \hat{L}] + \frac{\partial}{\partial t}\hat{L}. \tag{19.11}$$

Unitary Invariance of Physical Results

The physical meaning of any result is obviously independent of the choice of a representation. In other words, the physical meaning of a result should not change upon a transition from one representation to another. Since these transitions are accomplished by means of unitary transformations, it means that *physical results must enter the mathematical apparatus as unitary invariants.* Thus, the requirement of unitary invariance of corresponding results may serve as an additional criterion of the correctness of the basic postulates formulated above and the consequences that follow from them. In this connection, we first mention the fact of unitary invariance of the property of hermiticity of an operator mentioned in Sec. 17, and also the unitary invariance of the spectrum of eigenvalues of a Hermitian operator. It is easy to see that the commutator $[\hat{H}, \hat{L}]$ is also a unitary invariant and, consequently, the condition of conservation of any physical quantity is, as expected, independent of the choice of a representation. We mention further that unitary invariance of the relation $\int \psi_n^* \psi_m \, dx$ now indicates the independence from the choice of representation of the condition of orthonormalization of eigenfunctions of a physical quantity. Finally, unitary invariance of the expression $\int \Phi^*(x) \hat{L}(x) \Phi(x) \, dx$ indicates the independence from the choice of representation of the mean values of physical quantities.

Note that the result (19.4) could have been obtained unambiguously from the requirement of the unitary invariance of the quantity $\langle \lambda \rangle$ using the expression (18.18) obtained for a special case. Indeed, from the requirement of unitary invariance it follows that $\langle \lambda \rangle$ must be represented by an expression of the type

$$\int \Phi^*(x) \hat{L}^n(x) \Phi(x) \, dx,$$

and a comparison with the particular result (18.18) indicates that in this case n must be put equal to 1.

Section 20 The Quantum-Mechanical Apparatus in Coordinate Representation

A further treatment of the apparatus of quantum mechanics requires a knowledge of the definite form of the operators of various physical quantities. For this it is essential to choose a definite representation. Let us choose the *coordinate representation* for this purpose.

Note the importance of finding the form of the two basic "physical operators", the coordinate and the momentum of a microparticle. Knowing these operators, we may obtain the energy operator [see (19.1)] and the angular momentum operator [see (19.2)].

Operators of Coordinate and Momentum

For simplicity we shall consider one-dimensional motion along the x-axis (the result so obtained can be easily generalized to a three-dimensional case). Taking into account the remarks made in Sec. 17 about the form of Hermitian operator in its eigen representation [see (17.26)], we conclude that the operator of a coordinate in the coordinate representation is the coordinate itself:

$$x(x) = x. \tag{20.1}$$

This result can be generalized to any coordinate function:

$$U(x) = U(x). \tag{20.2}$$

Let us now try to find the form of the momentum operator. First we shall prove the following *theorem*. Suppose an operator $\hat{O}$ somehow transforms a coordinate. If the Hamiltonian $\hat{H}$ remains invariant under this transformation, the operators $\hat{O}$ and H commute. *Proof*: Let $\hat{O}x = x'$; we act on $\hat{H}(x)\psi(x)$ with the operator $\hat{O}$ to get $\hat{O}\hat{H}(x)\psi(x) = \hat{H}(x')\psi(x') = \hat{H}(x)\psi(x') = \hat{H}(x)\,O\psi(x)$, which proves the theorem.

Suppose the operator $\hat{O}$ is the operator of infinitesimal translation along the x-axis: $\hat{O}\psi(x) = \psi(x + \Delta x)$. Making use of the smallness of the translation, we write

$$\psi(x+\Delta x) = \left[1 + \Delta x \frac{d}{dx}\right]\psi(x)$$

Thus

$$\hat{O} = 1 + \Delta x \frac{d}{dx}$$

Proceeding from the properties of homogeneity of space, we conclude that an operation by $\hat{O}$ must leave the Hamiltonian of a microparticle invariant. Hence, according to the theorem proved above, we obtain $[\hat{O}, \hat{H}] = 0$

or $\left[\frac{d}{dx}, \hat{H}\right] = 0$. But it was shown above in Sec. 19 that a commutation with the Hamiltonian expresses the law of conservation of a physical quantity. This means that d/dx is the operator of some physical quantity which is conserved. We know that momentum is a quantity whose conservation is a consequence of the homogeneity of space (see Sec. 1). Consequently, the operator d/dx must coincide with the momentum operator of a microparticle up to some constant factor:

$$\frac{d}{dx} = \gamma \hat{p}_x. \tag{20.3}$$

The factor γ is determined from a consideration of the limiting transition from quantum mechanics to classical mechanics (see Appendix B). It can be shown that $\gamma = i/\hbar$. Thus the operator of the x-component of a microparticle momentum in the coordinate representation has the form

$$\hat{p}_x = -i\hbar \frac{d}{dx} \tag{20.4}$$

The results (20.1) and (20.4) can be easily generalized to a three-dimensional case:

$$\hat{\vec{r}} = \vec{r}, \tag{20.5}$$

$$\hat{\vec{p}} = -i\hbar\nabla. \tag{20.6}$$

Eigenfunctions of Momentum

Using (20.4), we can write an equation for the eigenfunctions of the x-component of the momentum:

$$-i\hbar \frac{d}{dx} \psi_{p_x}(x) = p_x \psi_{p_x}(x). \tag{20.7}$$

It can be easily seen that (20.7) can be solved for any values of the parameter p_x. Consequently, the momentum of a microparticle is *not quantized* (the spectrum of the eigenvalues of the momentum is continuous).

From equation (20.7) it follows that the eigenfunctions of operator $\hat{p}_x$ have the form of *plane waves*:

$$\psi_{p_x}(x) = A \exp(ip_x x/\hbar). \tag{20.8}$$

To determine the factor A, we make use of the condition of orthonormalization (17.17):

$$\int \psi^*_{p'_x}(x)\, \psi_{p_x}(x)\, dx = \delta(p_x - p'_x).$$

Substituting (20.8) into this equation, we find

$$A^2 \int \exp[-ix(p'_x - p_x)/\hbar]\, dx = \delta(p_x - p'_x).$$

Further, taking into account (15.17), we obtain

$$\int \exp\left[ix(p_x - p'_x)/\hbar\right] dx = 2\pi\hbar\delta(p_x - p'_x).$$

Comparing the last two equations, we get $A^2 = (2\pi\hbar)^{-1}$. Consequently,

$$\psi_{p_x}(x) = (2\pi\hbar)^{-1/2} \exp(ip_x x/\hbar). \tag{20.9}$$

A generalization for the three-dimensional case gives

$$\psi_{\vec{p}}(\vec{r}) = (2\pi\hbar)^{-3/2} \exp(ipr/\hbar). \tag{20.10}$$

Note that the eigenfunction of the momentum (20.10) coincides with the wave function (15.15) derived in Sec. 15 for a freely moving microparticle.

Schrödinger Equation

Let us consider the equation (18.23) for eigenfunctions of a Hamiltonian:

$$\hat{H}\varphi_E(x) = E\varphi_E(x). \tag{20.11}$$

Using (19.1) for the Hamiltonian of a microparticle moving in an external field with potential $U(x)$, and taking into account (20.2) and (20.4), we get

$$\hat{H}(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x). \tag{20.12}$$

Substituting (20.12) into (20.11), we get

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi_E(x) + [U(x) - E]\varphi_E(x) = 0. \tag{20.13}$$

This is the one-dimensional *Schrödinger equation.* Generalizing it for the three-dimensional case, we write

$$-\frac{\hbar^2}{2m}\Delta\varphi_E(\vec{r}) + [U(\vec{r}) - E]\varphi_E(\vec{r}) = 0. \tag{20.14}$$

Knowing the functions $\varphi_E(x)$, we may write the expressions for amplitudes of stationary states $\Psi_E(x, t)$, since the time dependence in this case has the universal form discussed in Sec. 13. Using (13.4) and taking into account the fact that

$$\Psi_E(x, t) = \langle E \mid x, t\rangle = \langle x, t \mid E\rangle^* = C_E^*(t), \tag{20.15}$$

we get

$$\Psi_E(x, t) = \varphi_E(x)\exp(-iEt/\hbar). \tag{20.16}$$

It can be easily seen that the functions $\Psi_E^*(x, t)$ are the solutions of equation (18.22), where the Hamiltonian

(20.12) has been used in place of $\hat{H}$. In this case, the equation has the form

$$i\hbar \frac{\partial}{\partial t} \Psi = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi + U(x)\Psi. \tag{20.17}$$

It is also called the Schrödinger equation More precisely, equation (20.13) is called the *time-independent Schrödinger equation* and the equation (20.17) is called the *time-dependent Schrödinger equation.*

Schrödinger's contribution was that he guessed (yes, guessed!) how to write the Hamiltonian of a microparticle in the form (20.12). It is true that in our discussions (20.12) does not appear unexpectedly, it appears here as a consequence of results (19.1), (20.2) and (20.4). It should, however, be remembered that (19.1) has not been derived here, in fact it was postulated (more precisely, an analogy between classical and quantum-mechanical relations was postulated). When Schrödinger proposed his famous equation, this analogy was not yet apparent. Moreover, the result (20.12) itself, as we shall see below, served as the basis for this analogy. (For establishing the relation (20.17), we may make use of the transition from quantum to classical mechanics—see Appendix B.)

Operators of the Angular Momentum Projections and the Square of Angular Momentum

By using (19.2) and (20.4) we can easily get the expressions for the operators of projections of the angular momentum:

$$\left.\begin{aligned} \hat{M}_x &= -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right), \\ \hat{M}_y &= -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right), \\ \hat{M}_z &= -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \end{aligned}\right\} \tag{20.18}$$

The operator of the square of angular momentum is given by the expression

$$\hat{M}^2 = \hat{M}_x^2 + \hat{M}_y^2 + \hat{M}_z^2. \tag{20.19}$$

While considering the angular momentum operators, it is convenient to use spherical coordinates r, θ, φ instead of Cartesian coordinates x, y, z:

$$\left.\begin{aligned} x &= r\sin\theta\cos\varphi, \\ y &= r\sin\theta\sin\varphi, \\ z &= r\cos\theta. \end{aligned}\right\} \tag{20.20}$$

Using (20.20), we represent the derivative $\frac{\partial}{\partial\varphi}\psi$ in the form

$$\frac{\partial}{\partial\varphi}\psi=\frac{\partial\psi}{\partial x}\frac{\partial x}{\partial\varphi}+\frac{\partial\psi}{\partial y}\frac{\partial y}{\partial\varphi}+\frac{\partial\psi}{\partial z}\frac{\partial z}{\partial\varphi}$$

$$=-\frac{\partial\psi}{\partial x}r\sin\theta\sin\varphi+\frac{\partial\psi}{\partial y}r\sin\theta\cos\varphi$$

$$=\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)\psi.$$

From this, with the help of (20.18), we get

$$\hat{M}_z=-i\hbar\frac{\partial}{\partial\varphi}. \tag{20.21}$$

In a similar way from the derivative $\frac{\partial}{\partial\theta}\psi$ we find

$$\hat{M}_x\pm i\hat{M}_y=\hbar e^{\pm i\varphi}\left(\pm\frac{\partial}{\partial\theta}+i\cot\theta\frac{\partial}{\partial\varphi}\right) \tag{20.22}$$

from which, with the help of (20.19), we get

$$\hat{M}^2=-\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]. \tag{20.23}$$

Commutation Relations

These relations form the commutation rules for the operators of coordinate, momentum and angular momentum of a microparticle. Denoting the Cartesian components of these operators by subscripts *i*, *j*, *k*, we can write these commutation rules (it will be shown later on how they may be derived):

$$[\hat{r}_i,\hat{r}_j]=0, \tag{20.24}$$

$$[\hat{p}_i,\hat{p}_j]=0, \tag{20.25}$$

$$[\hat{p}_i,\hat{r}_j]=-i\hbar\delta_{ij}, \tag{20.26}$$

$$[\hat{p}_i,\hat{f}(\vec{r})]=-i\hbar\frac{\partial}{\partial r_i}\hat{f}(\vec{r}), \tag{20.27}$$

$$[\hat{M}_i,\hat{r}_j]=i\hbar\sum_k e_{ijk}\hat{r}_k, \tag{20.28}$$

$$[\hat{M}_i,\hat{p}_j]=i\hbar\sum_k e_{ijk}\hat{p}_k, \tag{20.29}$$

$$[\hat{M}_i,\hat{M}_j]=i\hbar\sum_k e_{ijk}\hat{M}_k. \tag{20.30}$$

Here e_{ijk} is a unit antisymmetric tensor of the 3rd rank, $e_{123}=e_{231}=e_{312}=1$, $e_{132}=e_{321}=e_{213}=-1$, and the remaining 21 components of this tensor are equal to zero (in these components at least two subscripts have the same value). It can be easily seen that in summations with respect to *k* not more than one term is present.

In the coordinate representation $\hat{r}_i = r_i$; therefore, the result (20.24) is obvious. It means that all three coordinates of a microparticle can be measured simultaneously (as was mentioned in Sec. 3, they occur in the same complete set of quantities).

From (20.4), we write

$$[\hat{p}_i, \hat{p}_j]\,\psi = -\hbar^2\left(\frac{\partial^2}{\partial r_i\,\partial r_j} - \frac{\partial^2}{\partial r_j\,\partial r_i}\right)\psi.$$

Since the value of the mixed derivative is independent of the order in which the differentiation is carried out, it follows that $[\hat{p}_i, \hat{p}_j] = 0$. This result means that all the three components of momentum can be measured simultaneously (they belong to the same complete set of quantities).

The result (20.26) is derived in the following way:

$$[\hat{p}_i, \hat{r}_j]\,\psi = -i\hbar\left\{\frac{\partial}{\partial r_i}(r_j\psi) - r_j\frac{\partial}{\partial r_i}\psi\right\}$$
$$= -i\hbar\frac{\partial r_j}{\partial r_i}\psi = -i\hbar\delta_{ij}\psi.$$

It means that components of momentum and coordinate which have different subscripts can be simultaneously measured, while components with like subscripts are unmeasurable, in complete accord with the uncertainty relations for coordinate and momentum of a microparticle described in Sec. 3. The result (20.26) also indicates that the three components of coordinate and the three components of momentum enter in different complete sets of quantities.

The result (20.27) is a generalization of (20.26). In fact,

$$[\hat{p}_i, \hat{f}]\,\psi = -i\hbar\left\{\frac{\partial}{\partial r_i}(f\psi) - f\frac{\partial}{\partial r_i}\psi\right\} = -i\hbar\frac{\partial f}{\partial r_i}\psi.$$

Results (20.28)-(20.30) can be obtained from (19.2) by using the preceding commutation relations (see Appendix C).

Results (20.28) and (20.29) mean that components of the angular momentum and coordinate (angular momentum and momentum) with like subscripts can be measured simultaneously, while those with different subscripts cannot be measured simultaneously. These results also mean that projections of the angular momentum cannot belong to complete sets which include coordinates or the momentum components.

The result (20.30) means that different components of angular momentum don't have a common closed system of eigenfunctions and cannot appear in the same complete set of quantities. Considering the examples discussed earlier, we can conclude that different components of angular momentum cannot be measured simultaneously. This conclusion is correct, but it should be slightly improved on the basis of the example of the components of angular momentum. As a matter of fact, there is one case when all the three components of angular momentum can be simultaneously measured—this is the particular case when all of them are equal to zero. This case, however, does not essentially change anything since, as has been remarked in Sec. 17, the presence of one common eigenfunction is in no way connected with the commutation of operators. By using relations (20.19) and (20.30), we can establish one more rule for commutation (see Appendix D):

$$[\hat{M}^2, \hat{M}_i] = 0 \qquad (20.31)$$

This means that we must include the square of the angular momentum and any one of the projections of the angular momentum in the same complete set of quantities.

Note that the simultaneous measurability of all the components of momentum and the impossibility of similar measurement for the angular momentum components have a very simple explanation. The fact is that the parallel translations associated with the momentum operator are commutative, while the rotations associated with the angular momentum operator are noncommutative. It is immaterial whether we move first along the x-axis and then along the y-axis, or in the reverse order.

However, the sequence of rotations is certainly not immaterial. Take, for example, a point on the z-axis and make two successive rotations through 90°—in one case first around the x-axis and then around the z-axis, in the other case first around the z-axis and then around the x-axis. It can be easily seen that the final positions of the point are different in these two cases.

The Inversion Operator; Parity

The inversion operator $\hat{P}$ is defined in the following way:

$$\hat{P}\psi(\vec{r}, t) = P\psi(-\vec{r}, t), \qquad (20.32)$$

where P is a constant. By applying the inversion operator twice, we obviously return to the initial function $\psi(\vec{r}, t)$. It follows from this that $P^2 = 1$, i.e.

$$P = \pm 1. \qquad (20.33)$$

The quantity P is called the *spatial parity*. If $P = 1$, and consequently, $\hat{P}\psi(\vec{r}, t) = \psi(-\vec{r}, t)$, the microparticle is said to possess even parity. If, however, $P = -1$

and, consequently, $\hat{P}\psi(\vec{r}, t) = -\psi(-\vec{r}, t)$, the microparticle is said to possess odd parity.

Suppose $[\hat{P}, \hat{H}] = 0$. In this case, according to (19.10), the parity is a conservable quantity. If at the initial moment of time the microparticle was, for example, in a state with even parity, it must have the same parity at subsequent moments of time (which, of course, imposes certain restrictions on the possible changes in the state of the microparticle).

It was mentioned in Sec. 1 that the laws of conservation of energy, momentum and angular momentum are the results of definite properties of the symmetry of space and time. The law of conservation of parity is no exception to this. It is a consequence of the symmetry with respect to inversion operation, which, as can be easily seen, reduces to a combination of the operation of rotation and reflection [in fact, the operation $(x, y, z) \to (-x, -y, -z)$ consists of rotation through 180°, say, arround the z-axis, and reflection in the plane perpendicular to the z-axis]. Taking into account that the conservation of angular momentum is linked with rotational symmetry, we conclude: the conservation of spatial parity is associated with the fact that physical processes take place identically in the "usual world" and the "mirror world" *

Eigenvalues and Eigenfunctions of the Operators $\hat{M}_z$ and $\hat{M}^2$

Let us write the equation for the eigenfunctions of the operator $\hat{M}_z$, defined by (20.21):

$$-i\hbar \frac{\partial}{\partial\varphi}\psi = M_z\psi. \tag{20.34}$$

The solutions of this equation are of the form

$$\psi(\varphi) = A \exp(iM_z\varphi/\hbar). \tag{20.35}$$

The function ψ is periodic: $\psi(\varphi + 2\pi) = \psi(\varphi)$. Consequently,

$$M_z = \hbar m, \quad m = 0, \pm 1, \pm 2, \tag{20.36}$$

The reader is already familiar with this results: the projection of angular momentum is quantized; it assumes values differing by multiples of Planck's constant (see Sec. 2). The factor A in (20.35) is determined from the normalization condition $\int_0^{2\pi} \psi_m^* \psi_m d\varphi = 1$. It is easy to

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* It must be noted that in some processes involving elementary particles, the symmetry of "usual world" and "mirror world" is violated. It was shown by Wu in 1957 that in experiments on the β-decay of nuclei, spatial parity is not conserved. This result was predicted in 1956 by Lee and Yang.

see that $A = (2\pi)^{-1/2}$. Thus

$$\psi_m(\varphi) = (2\pi)^{-1/2} \exp(im\varphi). \tag{20.37}$$

We now turn to the operator $\hat{M}^2$. Using (20.23), we write

$$-\hbar^2 \left[\frac{1}{\sin^2\theta} \frac{\partial^2\psi}{\partial\varphi^2} + \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial\psi}{\partial\theta} \right) \right] = M^2\psi. \tag{20.38}$$

This equation is known in mathematics as the *equation for spherical functions*. It has bounded solutions under the condition that

$$M^2 = \hbar^2 l\,(l + 1),\ l = 0,\ 1,\ 2, \tag{20.39}$$

Assuming that the condition (20.39) is satisfied, we write the solutions of (20.38) in the form of *spherical harmonics*:

$$\psi_{lm} = \sqrt{\frac{(l-|m|)!\,(2l+1)}{(l+|m|)!\,4\pi}}\, P_l^{|m|}(\cos\theta)\, e^{im\varphi}, \tag{20.40}$$

where $m = 0, \pm 1, \ldots, \pm l$. Taking (20.31) into consideration, we conclude that the eigenfunctions of $\hat{M}_z$ and $\hat{M}^2$ are common. Hence, m should be treated as a magnetic quantum number corresponding to the projection of the angular momentum of the z-axis. It assumes $2l + 1$ values (from $-l$ to l). The functions $P_l^{|m|}(\cos\theta)$ appearing in (20.40) are essentially the *associated Legendre functions*. We remind the reader that

$$P_l^m(x) = (1 - x^2)^{m/2} \frac{d^m}{dx^m} P_l(x) \tag{20.41}$$

where $P_l(x)$ are *Legendre polynomials**:

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} [(x^2 - 1)^l]. \tag{20.42}$$

The spherical functions $\psi_{lm}(\theta, \varphi)$ are orthonormalized:

$$\int_0^{2\pi}\int_0^{\pi} \psi_{lm}^*(\theta, \varphi)\, \psi_{l'm'}(\theta, \varphi) \sin\theta\, d\theta\, d\varphi = \delta_{ll'}\delta_{mm'}. \tag{20.43}$$

If the result (20.36) is known, we can derive the result (20.39) by assuming that

$$M^2 = 3\langle M_z^2 \rangle = 3\hbar^2 \langle m^2 \rangle.$$

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* Legendre polynomials and associated functions are considered in Appendix D.

The mean value $\langle m^2 \rangle$ is determined by the expression

$$\langle m^2 \rangle = \sum_{m=-l}^{l} \frac{m^2}{2l+1} = 2 \sum_{m=0}^{l} \frac{m^2}{2l+1} = \frac{1}{3} l(l+1).$$

This leads directly to (20.39).

Parity and Angular Momentum

It follows from (20.18) that the inversion operators commute with operators of any projection of the angular momentum. Moreover, the inversion operators and the operators of the square of the angular momentum commute:

$$[\hat{P}, \hat{M}_i] = 0, \quad [\hat{P}, \hat{M}^2] = 0. \tag{20.44}$$

This mean that the operators $\hat{P}$ and $\hat{M}_i$ have a common complete system of eigenfunctions. The same applies to the operators $\hat{P}$ and $\hat{M}^2$. From this it follows in particular that a state with a definite orbital quantum number l must also be characterized by a definite spatial parity. In spherical coordinates the inversion is of the form

$$r \to r, \quad \theta \to \pi - \theta, \quad \varphi \to \varphi + \pi. \tag{20.45}$$

Using (20.40)-(20.42) we find that for such a transformation the function $\psi_{lm}(\theta, \varphi)$ is multiplied by $(-1)^l$:

$$\psi_{lm} \to (-1)^l \psi_{lm}. \tag{20.46}$$

It follows hence that states with even l have an even parity while the states with odd l have an odd parity.

It is appropriate here to recall that the example given in Sec. 3 for the complete set of quantities describing the state of a photon includes M^2, M_z and P [see (3.7b)]. Note that the parity and the angular momentum occur in the same complete set of quantities. Formally, this is a consequence of relations (20.44). However, one can start from considerations based on direct physical intuition. In fact, the obvious "affinity" between the parity and the angular momentum is connected with the above-mentioned fact that the inversion operation includes rotation in addition to reflection. The order in which these operations are carried out is immaterial; rotation can follow reflection or, the other way round, it can precede reflection.

The Relations of Classical Mechanics in Operator Form

So far, we have several times used the fact that the apparatus of quantum mechanics is based on the well-known equations of classical mechanics written, however, in operator form. This fact is so important that it is appropriate to return to it once again.

We have mentioned above the brilliant guess by Schrödinger, who proposed the expression (20.12) for the Hamiltonian of a microparticle. If we use this guess and the fundamental result (19.10), we can easily see that the equations of classical mechanics can be actually transferred to quantum mechanics by replacing the physical quantities by the corresponding Hermitian operators. Substituting the operator $\hat{L} = x$ in (19.10), and using the expression (20.12) for the operator $\hat{H}$, we get

$$x = \hat{p}_x / m. \tag{20.47}$$

This is the well-known classical result: the velocity is equal to momentum divided by mass. In quantum-mechanical interpretation this result means that the velocity operator is equal to the momentum operator divided by the mass. Further, we substitute the operator $\hat{L} = \hat{p}_x$ in (19.10). Using the expression (20.12) for $\hat{H}$ as before, we get

$$p_x = -\frac{d}{dx} U(x). \tag{20.48}$$

It can be easily seen that this is just Newton's second law of motion, written in operator form.

Remember, that the operators of the type $\hat{\dot{x}}$ and $\hat{\dot{p}}_x$ are introduced in accordance with the definition (19.9). Hence, it follows that the results (20.47) and (20.48) indicate the validity of the classical relations for the mean values of physical quantities:

$$\frac{d}{dt} \langle x \rangle = \langle s \mid \hat{p}_x \mid s \rangle / m, \tag{20.47a}$$

$$\frac{d}{dt} \langle p_x \rangle = -\frac{d}{dx} U(x). \tag{20.48a}$$

Ehrenfest was the first to point out this and hence relations of the type (20.47a) or (20.48a) a[illegible]called *Ehrenfest theorems*. In short, Ehrenfest's theorems state that classical relations for physical quantities are transformed in quantum mechanics into relations for mean values of physical quantities.

It was noted in Sec. 19 that the mathematical analogy between classical mechanics and quantum mechanics considered here requires a certain amount of caution since operators don't always commute with each other. This leads to the conclusion that the information contained in the classical relations is insufficient for building up the quantum-mechanical apparatus. It is necessary to have additional information about the properties of commutation of the operators under consideration. In other words, the *classical relations must be supplemented by the commutation relations* of the type (20.26)-(20.30).

Thus, it is the commutation relations which carry the specific information essential to the apparatus of quantum mechanics. In this connection, we note that the right-hand sides of the commutation relations contain the specifically quantum-mechanical constant, i.e. the Planck's constant.

Section 21 Applications of the Schrödinger Equation

Some Characteristic Problems in Quantum Mechanics

We shall mention three types of problems involving the solution of the Schrödinger equation.

First type of problems. We consider the motion of a microparticle in a limited region of space or, in other words, in a potential well (for example, the motion of an electron in an atom). Such a motion is called *finite* and the microparticle is said to be in a *bound* state. In this case the time-independent Schrödinger equation is used [see (20.13) or (20.14)]. By solving the Schrödinger equation under certain boundary conditions imposed on the wave function and its first derivative*, the spectrum of the values of the energy of the microparticles and the wave functions of the stationary states can be found.

Second type of problems. The *infinite* motion (motion unbounded in space) of a microparticle in an external field is considered. For example, the microparticle passes through a potential barrier (we recall the tunneling effect mentioned in Sec. 4) or is scattered by some energy centre. Since the motion is infinite, the energy spectrum of the microparticle is continuous. By solving the time-independent Schrödinger equation, we can find the form of the wave functions of the microparticle far from the scattering centre (or barrier) from which, for example, the probability of scattering at a certain angle (or the probability of tunneling through the barrier as well as of reflection from it) can be calculated.

Third type of problems. In the two types of problems indicated above, we spoke of the stationary states of a microparticle. For those the time-independent Schrödinger equation was used. The third type of problems involves a *change in the state of a microparticle with time*, and for this the time-dependent Schrödinger equation is used [see

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* The boundary conditions are considered below during a discussion on specific problems.

(20.17)]. By solving this problem we can find the probability of any quantum transition taking place under the influence of a given external force.

Examples of problems of first two types are given in this section and in Sec. 24. The third type of problems can be found in Sec. 25. Naturally, we shall limit ourselves to just a few typical examples. But it should be mentioned here that the applied aspects of quantum mechanics are reflected quite comprehensively in the existing literature (in this connection, we recommend [34, 35] which give specially selected quantum-mechanical problems).

A Particle in a One-Dimensional Potential Well with Infinitely Hign "Walls"

Such a well is described by a potential U of the form

$$U(x)=\begin{cases}\infty, & x<0,\\ 0, & 0\leqslant x\leqslant a,\\ \infty, & x>a.\end{cases} \tag{21.1}$$

The parameter a is the width of the well. The energy is measured from the bottom of the well. Within the limits of the well ($0 \leqslant x \leqslant a$), the Schrödinger equation (20.13) is of the form

$$\frac{d^2\varphi}{dx^2}+k^2\varphi=0, \tag{21.2}$$

where

$$k^2 = 2mE/\hbar^2. \tag{21.3}$$

At the boundaries of the well (for $x = 0$ and $x = a$) the continuous wave function φ vanishes, since the infinitely high "walls" make it impossible for the particle to be found beyond the limits of the well* Thus in this case the boundary conditions are of the form

$$\varphi(0) = \varphi(a) = 0. \tag{21.4}$$

We can write the general solution of the differential equation (21.2) as follows:

$$\varphi(x) = A\sin(kx) + B\cos(kx). \tag{21.5}$$

Since $\varphi(0) = 0$, it follows that $B = 0$. Thus,

$$\varphi(x) = A\sin(kx). \tag{21.6}$$

From the condition $\varphi(a) = 0$, we conclude that

$$ka = \pi n, \text{ where } n \text{ is an integer.} \tag{21.7}$$

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* In the case of "walls" having a finite height, this possibility, as will be shown below, is not excluded.

Taking (21.3) into account, the last result can be rewritten in the following form:

$$E_n = n^2\pi^2\hbar^2/2ma^2. \qquad (21.8)$$

The expression (21.8) determines the spectrum of values of the energy (energy levels) of the particle in the potential well. It coincides with the expression (5.2) derived earlier.

According to (21.5) and (21.7), the wave function $\varphi_n(x)$ corresponding to the nth energy level, is of the form $\varphi_n(x) = A\sin(\pi nx/a)$. The integration constant A is determined from normalization condition [see (15.13) in this connection] $\int_0^a \varphi_n^2(x)dx = 1$. It can be easily seen that $A = \sqrt{2/a}$ and, consequently,

$$\varphi_n(x) = \sqrt{2/a}\sin(\pi nx/a). \qquad (21.9)$$

Thus, we have found the energy levels and the orthonormalized wave functions for the stationary states of a particle in a rectangular one-dimensional well with infinitely high "walls"

Rectangular Potential Well with "Walls" of Finite Height

Let us consider a rectangular potential well shown in Fig. 21.1 (a). Since the particle is inside the well, $E < U_1$ and $E < U_2$. The rectangularity of the potential enables us to clearly distinguish three spatial regions: region 1 ($x < 0$), region 2 ($0 \leqslant x \leqslant a$) and region 3 ($x > a$). We shall consider these regions separately and will then combine these results at the boundaries of the regions, i.e. at the points $x = 0$ and $x = a$. The Schrödinger equation (20.13) has the following form:
for region 1

$$\frac{d^2\varphi}{dx^2} - \varkappa_1^2\varphi = 0, \text{ where } \varkappa_1^2 = 2m(U_1 - E)/\hbar^2, \qquad (21.10a)$$

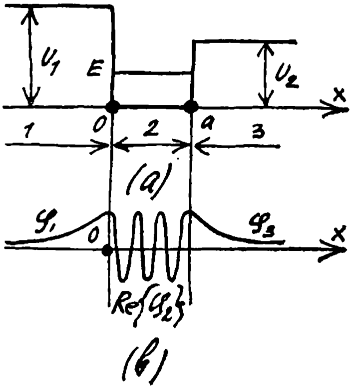
for region 2

$$\frac{d^2\varphi}{dx^2} + k^2\varphi = 0, \text{ where } k^2 = 2mE/\hbar^2, \qquad (21.10b)$$

and for region 3

$$\frac{d^2\varphi}{dx^2} - \varkappa_2^2\varphi = 0, \text{ where } \varkappa_2^2 = 2m(U_2 - E)/\hbar^2. \qquad (21.10c)$$

Fig. 21.1



The general solutions of these differential equations may be written in the following form:
for region 1

$$\varphi_1 = A_1\exp(\varkappa_1, x) + B_1\exp(-\varkappa_1 x), \qquad (21.11a)$$

for region 2

$$\varphi_2 = A_2 \exp(ikx) + B_2 \exp(-ikx), \tag{21.11b}$$

for region 3

$$\varphi_3 = A_3 \exp(\varkappa_2 x) + B_3 \exp(-\varkappa_2 x). \tag{21.11c}$$

[Note that the solution of equation (21.10b) may be written in the form (21.11b) or (21.5).] The boundedness of the wave function requires that B_1 and A_3 be put equal to zero. Thus,

$$\begin{aligned} &\varphi_1(x) = A_1 \exp(\varkappa_1 x), \\ &\varphi_2(x) = A_2 \exp(ikx) + B_2 \exp(-ikx), \\ &\varphi_3(x) = B_3 \exp(-\varkappa_2 x). \end{aligned} \tag{21.12}$$

The qualitative form of the functions φ_1, φ_3 and $\operatorname{Re}\{\varphi_2\}$ is shown in Fig. 21.1 (b). The reader should pay attention to the fact that in the case of a potential well with "walls" of finite height, there always exists a probability of finding the particle beyond the limits of the well; this probability decreases exponentially with the distance from the boundaries of the well.

In order to find the four coefficients (A_1, A_2, B_2, B_3), we make use of the fact that both the function and its first derivative must be continuous at the boundaries. The continuity of the wave function is obvious, while the continuity of the derivative can be easily shown. In order to do so, let us integrate Schrödinger's equation (20.13) over a certain interval ($a - \Delta$, $a + \Delta$) containing the potential jump. We get

$$\frac{d\varphi}{dx}(a+\Delta) - \frac{d\varphi}{dx}(a-\Delta) = \frac{2m}{\hbar^2} \int\limits_{a-\Delta}^{a+\Delta} [U(x) - E]\,\varphi\,dx.$$

Since the functions under the integral sign are bounded, in the limit of $\Delta \to 0$ this integral vanishes. As a result we get $\frac{d\varphi}{dx}(a+0) = \frac{d\varphi}{dx}(a-0)$, which wa[illegible] be proved.

Returning to our problem, we write the boundary conditions (conditions of 'piecing' together the solutions at the boundaries of the region):

$$\left.\begin{aligned} &\varphi_1(0) = \varphi_2(0), \\ &\varphi_2(a) = \varphi_3(a), \\ &\frac{d\varphi_1}{dx}(0) = \frac{d\varphi_2}{dx}(0), \\ &\frac{d\varphi_2}{dx}(a) = \frac{d\varphi_3}{dx}(a). \end{aligned}\right\} \tag{21.13}$$

Substituting the expressions (21.12) in these equations, we get the system of equations for the coefficients A_1, A_2, B_2, B_3:

$$\left.\begin{aligned} & A_1 = A_2 + B_2, \\ & A_2 \exp(ika) + B_2 \exp(-ika) = B_3 \exp(-\varkappa_2 a), \\ & \varkappa_1 A_1 = ik(A_2 - B_2), \\ & ikA_2 \exp(ika) - ikB_2 \exp(-ika) \\ & \qquad\qquad = -\varkappa_2 B_3 \exp(-\varkappa_2 a). \end{aligned}\right\} \quad (21.14)$$

The system (21.14) is a homogeneous system of linear equations. In order that such a system should have nontrivial solutions, it is necessary that its determinant should be equal to zero. Equating the determinant of the system to zero, we get an equation for the energy E (we recall that the quantities k, $\varkappa_1$, $\varkappa_2$ are expressed in terms of E). The solutions of this equation will give us the possible values of the energy of the particle.

We emphasize that from a mathematical point of view, the quantization of the energy in a well is a direct consequence of the homogeneity of the system (21.14). This is the crux of the problem of finding eigenvalues of physical quantities: the particle is left to its own devices, i.e. the external influences are eliminated thus eliminating inhomogeneities from the equation. As a result, the particle chooses its own course characterized by certain fundamental parameters (frequency, energy, etc.). The simplest example, taken from classical physics, is that of a pendulum. If a pendulum is not disturbed, it will oscillate with a difinite natural frequency, irrespective of the way the oscillation have been induced.

Thus, in order to determine the value of the energy of a particle, we should equate to zero the determinant of the system (21.14) and solve the equation so obtained. However, it is inconvenient in practice to consider a determinant of the 4th order. Hence we shall first simplify the system of equations. To do so, we rewrite the function φ_2 in the form $\varphi_2 = C \sin(kx + b)$ (this form is equivalent to the one used earlier; the reader may independently express the coefficients C and b in terms of the old coefficients A_2 and B_2). The system (21.14) will now have the following form:

$$\left.\begin{aligned} & A_1 = C \sin b, \\ & C \sin(ka + b) = B_3 \exp(-\varkappa_2 a), \\ & \varkappa_1 A_1 = kC \cos b, \\ & kC \cos(ka + b) = -\varkappa_2 B_3 \exp(-\varkappa_2 a). \end{aligned}\right\} \quad (21.15)$$

Dividing the third equation of this system by first and the fourth by second, we get

$$\left.\begin{aligned}\varkappa_1 &= k\cot b,\\ \varkappa_2 &= -k\cot(ka+b).\end{aligned}\right\} \qquad (21.16)$$

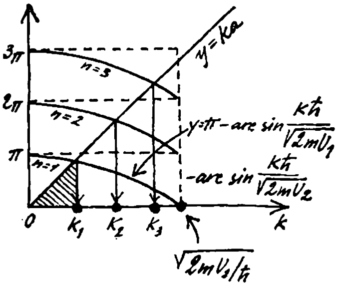
We now have a system of two equations in place of the system with four equations. From the first equation of the system (21.16) we find cot $b = \varkappa_1/k$, hence

$$\sin b = (1+\cot^2 b)^{-1/2} = \frac{k\hbar}{\sqrt{2mU_1}}.$$

Similarly, we get from the second equation of (21.16)

$$\sin(ka+b) = -\frac{k\hbar}{\sqrt{2mU_2}}.$$

Fig. 21.2



As a result, we get an equation that determines the value of k (and, consequently, the energy levels) in implicit form:

$$ka = n\pi - \arcsin\frac{k\hbar}{\sqrt{2mU_1}} - \arcsin\frac{k\hbar}{\sqrt{2mU_2}}, \qquad (21.17)$$

where n is an integer. Figure 21.2 shows the left- and right-hand sides of equation (21.17) as a function of k. In the situation shown in the figure, the particle has three energy levels corresponding to values of k equal to k_1, k_2, k_3. If we change the width of the well, the slope of the straight line $y = ka$ will change thus changing the the position and the number of possible energy levels. A decrease in the width of the well will decrease the slope of the straight line. The energy levels will "creep" out of the well, and their number will gradually decrease. An increase in the width of the well will raise the line $y = ka$; it will intersect a larger number of branches of the inverse sine graph, thus leading to a larger number of levels in the well. As $a \to \infty$, the numbes of levels in the well will rise indefinitely, and we finally get a continuous energy spectrum. It is easy to examine similarly the effect of a change in the depth of the well on the spectrum: the greater is the depth, the more levels there ar[illegible] the well. We should proceed further in the following way: find from (21.17) the possible values of k and the values E, $\varkappa_1$, and $\varkappa_2$ corresponding to them, then substitute these values in (21.15) and solve the system of equations containing the coefficients, and then substitute the final result in the expression (21.12) for the wave functions. However, on account of the mathematical complications involved, we shall not embark on this venture here.

In conclusion, we note that (21.17) may also be used for determining the minimum energy E_1 of a particle in a potential well. For this we just have to consider the hatched triangle in Fig. 21.2 and put $k_1 a \approx \pi$, whence we get $E_1 \approx \pi^2 \hbar^2 / 2ma^2$. This result is in good agreement with the estimate (4.11) obtained in Sec. 4 on the basis of the uncertainty relations (3.3).

A Particle in a Spherically Symmetrical Field

When considering the motion of a particle in a spherically symmetrical field, it is convenient to use spherical coordinates r, θ and φ. Spherical symmetry of the field means that $U(\vec{r}) = U(r)$. The Δ-operator in spherical coordinates has the form

$$\Delta = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \Delta_{\theta\varphi}, \tag{21.18}$$

where $$\Delta_{\theta\varphi} = \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \tag{21.19}$$

Taking this into account, we can rewrite the Schrödinger equation (20.14) in the form

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \psi \right) + \frac{1}{r^2} \Delta_{\theta\varphi} \psi (r, \theta, \varphi)$$
$$+ (2m/\hbar^2) [E - U(r)] \psi (r, \theta, \varphi) = 0. \tag{21.20}$$

Equation (21.20) allows the separation of variables. This means that its solution may be found in the form of a product of two functions, one of which depends only on r, and the other on the angular coordinates θ and φ:

$$\psi (r, \theta, \varphi) = R(r) \Phi (\theta, \varphi). \tag{21.21}$$

Substituting (21.21) into (21.20), we get the following result:

$$\frac{\frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + r^2 \frac{2m}{\hbar^2} [E - U(r)] R(r)}{R(r)} = - \frac{\Delta_{\theta\varphi} \Phi}{\Phi (\theta, \varphi)}. \tag{21.22}$$

Since the left- and right-hand sides of (21.22) depend on different independent variables (on r and on θ and φ, respectively), both sides must be equal to some constant, which we denote by λ. Introducing this constant, we write

$$- \Delta_{\theta\varphi} \Phi (\theta, \varphi) = \lambda \Phi (\theta, \varphi). \tag{21.23}$$

Comparing (21.19) with (20.23), we conclude that (21.23) is in fact the equation for the eigenvalues and eigenfunctions of the operator $\hat{M}^2$. This allows us to use (20.39) and (20.40) and write

$$\lambda = l(l+1), \quad l = 0, 1, 2, \tag{21.24}$$

$$\Phi (\theta, \varphi) = \sqrt{\frac{2l+1}{4\pi} \cdot \frac{(l - |m|)!}{(l + |m|)!}} P_l^{|m|} (\cos \theta) e^{im\varphi}$$
$$\equiv Y_{lm} (\theta, \varphi), \tag{21.25}$$

where $m = 0, \pm 1, \ldots, \pm l$. The functions $Y_{lm}(\theta, \varphi)$ are spherical harmonics (they were introduced in Sec. 20). It will be useful to write down the expressions for the first few spherical harmonics:

$$Y_{00} = \frac{1}{\sqrt{4\pi}}, \tag{21.26a}$$

$$Y_{10} = \sqrt{\frac{3}{4\pi}} \cos\theta; \quad Y_{1,\pm 1} = \sqrt{\frac{3}{8\pi}} \sin\theta e^{\pm i\varphi}, \tag{21.26b}$$

$$Y_{20} = \sqrt{\frac{5}{4\pi}} \left(\frac{2}{3}\cos^2\theta - \frac{1}{2}\right);$$

$$Y_{2,\pm 1} = \sqrt{\frac{15}{8\pi}} \sin\theta \cos\theta e^{\pm i\varphi};$$

$$Y_{2,\pm 2} = \sqrt{\frac{15}{32\pi}} \sin^2\theta e^{\pm 2i\varphi}. \tag{21.26c}$$

We emphasize that the "angular part" of the wave function is independent of the particular form of the potential $U(r)$; this is a direct and important consequence of the spherical symmetry of the potential.

We now turn to the "radial part" of the wave function, i.e. to the function $R(r)$. According to (21.22) and (21.24), this must be a solution of the equation

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) + \frac{2m}{\hbar^2}[E - U_l(r)] R(r) = 0, \tag{21.27}$$

where we have introduced the notation

$$U_l(r) = U(r) + \frac{\hbar^2 l(l+1)}{2mr^2}. \tag{21.28}$$

It should be noted that (21.27) may be reduced to the one-dimensional Schrödinger equation with a special boundary condition at $r = 0$. For this we must use the substitution

$$\varphi(r) = rR(r) \tag{21.29}$$

and in view of the boundedness of the function $R(r)$, require that the condition $\varphi(0) = 0$ be satisfied. It can be easily seen that the substitution (21.29) in fact converts (21.27) into the one-dimensional Schrödinger equation

$$\frac{d^2\varphi}{dr^2} + \frac{2m}{\hbar^2}[E - U_l(r)] \varphi(r) = 0. \tag{21.30}$$

In this case the boundary condition $\varphi(0) = 0$ corresponds to the one-dimensional potential well having an infinitely high vertical wall on the left (at $r = 0$).

Further study of (21.30) obviously requires a consideration of the particular form of the potential $U(\mathrm{r})$.
It should be noted that among the problems on the motion of a particle in a spherically symmetrical field are the problems of an electron in an atom and the scattering of particles by spherically symmetrical centres.

The Continuity Equation and the Schrödinger Equation

We shall establish a formal analogy between the time-dependent Schrödinger equation and the continuity equation, which is widely used in classical physics, especially in hydrodynamics. We assume that there is a certain medium (for example, a liquid) described by the functions $\rho(\vec{r})$ and $\vec{v}(\vec{r})$ [$\rho(\vec{r})$ is the density of the medium and $\vec{v}(\vec{r})$ is the velocity of the particles of the medium at the point $\vec{r}$; naturally, these functions may also depend on time]. Let us imagine a certain volume V in the medium to be isolated. The change in the quantity of liquid in this volume per unit time is equal to $\frac{\partial}{\partial t}\int_V \rho dV$

Let us isolate a certain element of surface area dS on the area S bounding the volume V, and associate with it a vector $\vec{dS}$ equal to dS in magnitude and directed along the outward normal to the surface. The amount of liquid passing per unit time from the volume V through an element of surface area $\vec{dS}$ is equal to $\rho\vec{v}\,\vec{dS}$. The amount of liquid passing through the entire surface per unit time is equal to $\oint_S \rho\vec{v}\,\vec{dS}$. The law of conservation of matter requires that $-\frac{\partial}{\partial t}\int_V \rho\, dV$ and $\oint_S \rho\vec{v}\,\vec{dS}$ be equal. Thus,

$$\frac{\partial}{\partial t}\int_V \rho\, dV+\oint_S \rho\vec{v}\,\vec{dS}=0.$$

By replacing the integral over the closed surface by a volume integral, we can rewrite the last equation in the following form:

$$\int_V\left(\frac{\partial\rho}{\partial t}+\operatorname{div}\vec{j}\right)dV=0, \tag{21.31}$$

where $\vec{j}=\rho\vec{v}$ is the vector of the density of flow of the liquid.
Equation (21.31) is independent of the choice of the volume V Using this fact, we can decrease the volume V to some particular point. In the limit as $V\rightarrow 0$, (21.31)

becomes a differential equation at this point:

$$\frac{\partial\rho}{\partial t}+\operatorname{div}\vec{j}=0. \tag{21.32}$$

This is the classical *continuity equation.*

Let us turn to the time-dependent Schrödinger equation. We shall generalize the one-dimensional equation (20.17) for the three-dimensional case:

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t)=-\frac{\hbar^2}{2m}\Delta\Psi(\vec{r},t)+U(\vec{r})\Psi(\vec{r},t). \tag{21.33}$$

We introduce purely formally a certain "medium" and define the density of this "medium" as $\Psi\Psi^*$ This density may be called the "probability density" In other words, the probability of finding a particle will be greater at those points of space, where the density of the "medium" is higher.

This "probability density" may be given a fairly simple physical meaning if we imagine that the space is filled with a large number of particles (the interaction of particles is to be neglected in this case). Obviously, the number of particles in some volume ΔV is proportional to the probability of finding a particle in this volume. With this approach, $\Psi\Psi^*$ may be considered simply as the density of the number of particles.

As in the classical case, we start by considering a certain finite volume V:

$$\frac{\partial}{\partial t}\int\limits_V \rho\,dV=\frac{\partial}{\partial t}\int\limits_V \Psi\Psi^*\,dV=\int\limits_V\left(\Psi^*\frac{\partial\Psi}{\partial t}+\Psi\frac{\partial\Psi^*}{\partial t}\right)dV$$

Substituting into this $\frac{\partial}{\partial t}\Psi$ and $\frac{\partial}{\partial t}\Psi^*$ from the Schrödinger equation (21.33), and from the complex conjugate of equation (21.33), we get

$$\begin{aligned}\frac{\partial}{\partial t}\int\limits_V \Psi\Psi^*\,dV&=\frac{i\hbar}{2m}\int\limits_V(\Psi^*\Delta\Psi-\Psi\Delta\Psi^*)\,dV\\&=\frac{i\hbar}{2m}\int\limits_V \operatorname{div}(\Psi^*\nabla\Psi-\Psi\nabla\Psi^*)\,dV.\end{aligned}$$

The last result can be written in the form

$$\int\limits_V\left[\frac{\partial}{\partial t}(\Psi\Psi^*)-\operatorname{div}\left\{\frac{i\hbar}{2m}(\Psi^*\nabla\Psi-\Psi\nabla\Psi^*)\right\}\right]dV=0, \tag{21.34}$$

or, after decreasing the volume V to a point,

$$\frac{\partial}{\partial t}(\Psi\Psi^*)-\operatorname{div}\left[\frac{i\hbar}{2m}(\Psi^*\nabla\Psi-\Psi\nabla\Psi^*)\right]=0. \tag{21.35}$$

By drawing an analogy between (21.34) and (21.31) [or between (21.35) and (21.32)], we come to the conclusion that the Schrödinger equation corresponds to some quantum-mechanical continuity equation, if in addition to the *probability density**

$$\rho = \Psi^* \Psi = \varphi^* \varphi \tag{21.36}$$

we also introduce the *vector of probability flow density*

$$\vec{j} = \frac{i\hbar}{2m} (\Psi \nabla \Psi^* - \Psi^* \nabla \Psi) = \frac{i\hbar}{2m} (\varphi \nabla \varphi^* - \varphi^* \nabla \varphi). \tag{21.37}$$

If we interpret (21.36) as the density of particles, then the vector (21.37) may be considered as the vector of density of the flow of particles. With such an interpretation the quantum-mechanical continuity equation (21.35) expresses the law of conservation of the number of particles.

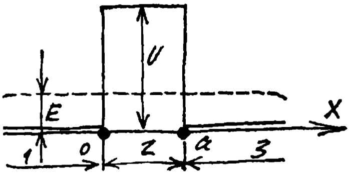
In the case of a one-dimensional motion along the x-axis, (21.37) assumes the form

$$j = \frac{i\hbar}{2m} \left(\varphi \frac{d\varphi^*}{dx} - \varphi^* \frac{d\varphi}{dx} \right) \tag{21.38}$$

In conclusion, let us note that we cannot assign the meaning of "flow" in the literal sense to the quantum-mechanical vector $\vec{j}$, since in order to determine the flow through any surface we must be able to measure the values of the velocity (momentum) at fixed points of the surface, which is obviously in contradiction to the uncertainty relations.

Passage of a Particle Under or Over a Potential Barrier

Fig. 21.3



Let us consider a one-dimensional rectangular potential barrier (Fig. 21.3) and assume that particles arrive at it from the left with an energy E which is less than the height U of the barrier. We can isolate three spatial regions and write the solutions of the Schrödinger equation (20.13) for these regions:

$$\begin{aligned} \varphi_1(x) &= A_1 \exp(ikx) + B_1 \exp(-ikx); \quad & k &= \sqrt{2mE}/\hbar, \\ \varphi_2(x) &= A_2 \exp(\varkappa x) + B_2 \exp(-\varkappa x); \quad & \varkappa &= \frac{\sqrt{2m(U-E)}}{\hbar}, \\ \varphi_3(x) &= A_3 \exp(ikx) + B_3 \exp(-ikx). \end{aligned} \tag{21.39}$$

The terms containing exp (ikx) describe the particles moving in the positive direction of the x-axis while the terms containing exp $(-ikx)$ indicate motion in the opposite direction. If we take into account that the par-

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* The functions $\Psi(\vec{r}, t)$ and $\varphi(\vec{r})$ are related to each other through a relation of the type (20.16).

ticles are moving in the positive direction, we must exclude the second term in the function φ_3: $B_3 = 0$. The other coefficients are non-zero. The term with A_1 describes particles falling on the barrier, the term with B_1 describes those reflected from the barrier, while the term with A_3 describes particles which have passed through the barrier.

The conditions of continuity of the wave function and its derivative at points $x = 0$ and $x = a$ give the following system of four equations:

$$\left.\begin{aligned} &A_1 + B_1 = A_2 + B_2, \\ &A_2 \exp(\varkappa a) + B_2 \exp(-\varkappa a) = A_3 \exp(ika), \\ &ik(A_1 - B_1) = \varkappa(A_2 - B_2), \\ &\varkappa[A_2 \exp(\varkappa a) - B_2 \exp(-\varkappa a)] \\ &= ikA_3 \exp(ika). \end{aligned}\right\} \tag{21.40}$$

It turns out that we have just four equations for five coefficients! But actually, only four and not five coefficients are known. The density of flow of particles incident on the barrier (j_{inc}) must be given. This density is given by (21.38), where we must substitute $\varphi = A_1 \exp(ikx)$. As a result of this, we get

$$j_{\text{inc}} = |A_1|^2 \hbar k/m. \tag{21.41}$$

Thus by knowing the quantity j_{inc} we can determine the coefficient A_1.

Similarly for the density of flow of the reflected particles we get

$$j_{\text{ref}} = |B_1|^2 \hbar k/m, \tag{21.42}$$

and for the density of flow of particles passing through the barrier we have

$$j_{\text{tr}} = |A_3|^2 \hbar k/m. \tag{21.43}$$

Usually in such problems the density j_{inc} is chosen in such a way that $A_1 = 1$. In this case the system (21.40) assumes the form

$$\left.\begin{aligned} &1 + B_1 = A_2 + B_2, \\ &A_2 \exp(\varkappa a) + B_2 \exp(-\varkappa a) = A_3 \exp(ika), \\ &k(1 - B_1) = \varkappa(A_2 - B_2), \\ &\varkappa[A_2 \exp(\varkappa a) - B_2 \exp(-\varkappa a)] = ikA_3 \exp(ika). \end{aligned}\right\} \tag{21.44}$$

The system (21.44) is the non-homogeneous system of four linear equations containing four unknown coefficients.

The inhomogeneous system has a solution for any values of k and $\varkappa$, i.e. for any values of the energy E of the particle. This is in agreement with the fact that for infinite motion of the particle its energy is not quantized.

We can determine the fraction of particles that has passed through the barrier:

$$D = j_{\mathrm{tr}}/j_{\mathrm{inc}}. \tag{21.45}$$

The quantity D is called the *transmission coefficient* of the barrier. Solving the system (21.44) (we shall omit the steps), we get

$$A_3 = -\frac{4ik}{\varkappa} e^{-ika}\left[e^{\varkappa a}\left(1-\frac{ik}{\varkappa}\right)^2 - e^{-\varkappa a}\left(1+\frac{ik}{\varkappa}\right)^2\right]^{-} \tag{21.46}$$

Further, using (21.43) and (21.45), we find

$$D = \frac{4k^2\varkappa^2}{4k^2\varkappa^2 + (k^2+\varkappa^2)^2 \sinh^2(\varkappa a)}. \tag{21.47}$$

In the particular case when $\varkappa a \geqslant 1$, (21.47) is simplified as

$$D = D_0 \exp\left[-\frac{2a}{\hbar}\sqrt{2m(U-E)}\right], \tag{21.48}$$

where

$$D_0 = 16\frac{E}{U}\left(1-\frac{E}{U}\right)$$

In addition to the transmission coefficient, we also have the *coefficient of reflection* at the barrier, defined as the fraction of the particles reflected by the barrier: $R = j_{\mathrm{ref}}/j_{\mathrm{inc}}$. It is clear from basic principles that $D + R = 1$ (all the particles not passing through the barrier must be reflected by it).

Finally we consider the case when a particle passes over the barrier ($E > U$). In this case, instead of (21.39) we get

$$\varphi_1(x) = \exp(ikx) + B_1 \exp(-ikx),$$
$$\varphi_2(x) = A_2 \exp(iKx) + B_2 \exp(-iKx),$$
$$\varphi_3(x) = A_3 \exp(ikx), \tag{21.49}$$

where

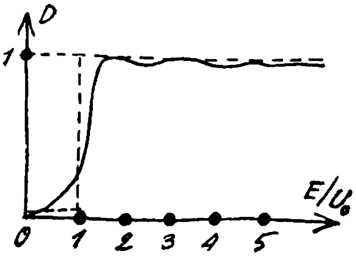
$$K = \sqrt{2m(E-U)}/\hbar.$$

Using (21.49), we write the boundary conditions for the points $x = 0$ and $x = a$. We then solve the system of equations so obtained and find the coefficient B_1. Further, from (21.42) we determine the coefficient of reflection

$R = j_{\text{ref}}/j_{\text{inc}}$. It turns out to be equal to

$$R = \frac{(k^2 - K^2)^2 \sin^2(Ka)}{4k^2K^2 + (k^2 - K^2)^2 \sin^2(Ka)}. \tag{21.50}$$

Fig. 21.4



Using (21.47) and (21.50) we can find the dependence of the transmission coefficient D on the ratio E/U. This dependence is shown graphically in Fig. 21.4. The same figure shows the dependence D (E/U) for a classical particle (dotted line). A comparison of the solid curve with the dotted line indicates the quantum-mechanical nature of microparticles. Note that for $E < U$ in classical mechanics all particles are reflected from the barrier and not a single particle passes through. In quantum mechanics, however, a part of the particles is reflected and a part passes through the barrier. For $E > U$, in classical mechanics all particles pass through and not a single particle is reflected, while in quantum mechanics a part of the particles passes through, and another is reflected. Both *sub-barrier transmission* and *above-barrier reflection* of microparticles are specifically quantum effects.

Section 22

The Hamiltonian in Some Specific Problems

Linear Harmonic Oscillator*

The Hamiltonian is of the form

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2 x^2}{2}. \tag{22.1}$$

It is obtained from (4.5) by taking (19.1) and (20.4) into account. The eigenvalues are

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \qquad n = 0,\ 1,\ 2, \tag{22.2}$$

[for $n = 0$ we get from (22.2) the energy of zero-point oscillations, which was determined in Sec. 4 on the basis of the uncertainty relations]. The eigenfunctions are

$$\varphi_n(x) = \sqrt[4]{m\omega/\hbar}\,\exp(-\xi^2/2)\,H_n(\xi), \tag{22.3}$$

where $\xi = x\sqrt{m\omega/\hbar}$, and $H_n(\xi)$ are called *Hermite polynomials*. Let us write down the expressions for the first few functions $\varphi_n(x)$:

$$\varphi_0(x) = \left(x_0\sqrt{\pi}\right)^{-1/2} \exp(-x^2/2x_0^2), \tag{22.4 a}$$

$$\varphi_1(x) = \left(2x_0\sqrt{\pi}\right)^{-1/2} \exp(-x^2/2x_0^2)\, 2x/x_0, \tag{22.4 b}$$

$$\varphi_2(x) = \left(8x_0\sqrt{\pi}\right)^{-1/2} \exp(-x^2/2x_0^2)\left(4\frac{x^2}{x_0^2} - 2\right) \tag{22.4 c}$$

(where $x_0 = \sqrt{\hbar/m\omega}$).

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* See Appendices E and F.

Note. Hermite polynomials, generalized Laguerre polynomials (mentioned below), harmonic functions and Legendre polynomials (introduced in Sec. 20) are called *special functions*. A considerable amount of mathematical literature has been devoted to special functions and their applications; for reference we mention [36, 37]. A basic account of polynomials and associated Legendre functions, special functions and Hermitian polynomials is given in Appendix E.

The Hydrogen Atom

The problem of the hydrogen atom is a well-known example of the motion of an electron in a spherically symmetrical Coulomb field. The Hamiltonian has the form

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta - \frac{e^2}{r} \qquad (22.5)$$

[it is obtained from (4.1) by using (19.1) and (20.6)]. The eigenvalues of this Hamiltonian are given by the following familiar expression [see (2.5)]:

$$E_n = -me^4/2\hbar^2 n^2; \quad n = 1,\ 2,\ 3, \qquad (22.6)$$

The eigenfunctions of the Hamiltonian (22.5) may be expressed in the form

$$\psi_{nlm} = R_{nl}(r)\, Y_{lm}(\theta, \varphi); \quad \begin{array}{l} l = 0,\ 1,\ \ldots,\ n-1; \\ m = 0,\ \pm 1, \quad \pm l. \end{array} \qquad (22.7)$$

Here $Y_{lm}(\theta, \varphi)$ are spherical functions. They define the "angular part" of the wave function irrespective of the particular form of the spherically symmetrical potential; $R_{nl}(r)$ is the "radial part" of the wave function, it is defined by (21.30) with the Coulomb potential $[U(r) = -e^2/r]$. The form of the function $R_{nl}(r)$ is described by the expression

$$R_{nl}(r) = \text{const}\, \exp(r/r_1 n)(2r/r_1 n)^l L_{n+l}^{2l+1}(2r/r_1 n), \qquad (22.8)$$

where $r_1 = \hbar^2/me^2$ (this quantity is already known to the reader as the radius of Bohr's first orbit) and L_{n+l}^{2l+1} are the so-called *generalized Laguerre functions* (see, for example, [36]).

Expressions for some of the first harmonic functions have been given in Sec. 21 [see (21.26)]. We shall now give the expressions for the first few functions $R_{nl}(r)$:

$$R_{10} = 2r_1^{-3/2} \exp(-r/r_1), \qquad (22.9a)$$

$$R_{20} = (2r_1^3)^{-1/2} \exp(-r/2r_1)\left(1 - \frac{r}{2r_1}\right), \qquad (22.9b)$$

$$R_{21} = \left(2\sqrt{6r_1^3}\right)^{-1} \exp(-r/2r_1)\, r/r_1. \qquad (22.9c)$$

In Sec. 5, when discussing the concept of an electron cloud we introduced the functions v_{nl} and Z_{lm}. Figure 5.2 (*a*) showed the form of some of the functions $w_{nl}(r) = r^2 v_{nl}(r)$, while Fig. 5.2 (*b*) showed some of the functions Z_{lm}. Returning to the functions considered in this section, we note that $v_{nl} = R^2_{nl}(r)$ and $Z_{lm} = |Y_{lm}(\theta,\varphi)|^2$. In particular, we note that (5.4) is in agreement with (22.9a).

By using (22.9) and (21.26), we can write the first few eigenfunctions of the Hamiltonian (22.5):

$$\psi_{100} = (\pi r_1^3)^{-1/2} \exp(-r/r_1), \tag{22.10a}$$

$$\psi_{200} = (8\pi r_1^3)^{-1/2} \exp(-r/2r_1)\left(1 - \frac{r}{2r_1}\right), \tag{22.10b}$$

$$\psi_{211} = \left(8\sqrt{\pi r_1^3}\right)^{-1} \exp(-r/2r_1) \sin\theta e^{i\varphi} r/r_1, \tag{22.10c}$$

$$\psi_{210} = \left(4\sqrt{2\pi r_1^3}\right)^{-1} \exp(-r/2r_1) \cos\theta r/r_1. \tag{22.10d}$$

The function (22.10a) describes the ground state of the hydrogen atom, while the functions (22.10b)-(22.10d) describe the excited states corresponding to the first excited energy level ($n = 2$).

On Degeneracy of Energy Levels

It follows from (22.6) that the energy of an electron in the hydrogen atom is determined only by the quantum number n, while the states (the functions ψ_{nlm}) are determined by three quantum numbers n, l and m. Besides, when considering electronic states we must take into account the quantum number σ which does not occur in these expressions. Since for a given value of the principal quantum number n the orbital quantum number l assumes integral values from 0 to $n - 1$, and for every l the magnetic quantum number acquires $2l + 1$ values, the following g_n states must correspond to an energy level E_n:

$$g_n = 2\sum_{l=0}^{n-1}(2l+1) = 2n^2 \tag{22.11}$$

(the factor 2 takes account of the two spin states of the electron). This means that the eigenvalue E_n of the Hamiltonian (22.5) (in other words, the nth energy level) is $2n^2$-fold *degenerate*.

Degeneracy of energy levels, as a rule, is associated with *symmetry* in the atomic system. Thus, for example, owing to the spherical symmetry of intra-atomic fields, there is degeneracy of the quantum numbers m and σ—the energy is independent of the orientation of the orbital momentum and the spin momentum of the electron. The degeneracy of the quantum number l is associated with the specific nature of the Coulomb potential; in non-Coulomb fields the energy of the electron depends not only on n but also on l.

Various fields, external as well as internal, may lower the degree of symmetry of the system. Thus, for example, "switching on" an external electric field leads to the appearance of a physically distinguished direction. As a result, the spherical symmetry disappears and is replaced by cylindrical symmetry. A decrease in symmetry leads to a removal of degeneracy (partial or total). This is exhibited in a splitting of energy levels, i.e. in their conversion into sets of new, less degenerate levels. Splitting of energy levels in an external electric field is known as *Stark's effect*, while the splitting in an external magnetic field is known as *Zeeman's effect*.

Crystal; the Adiabatic Approximation

The Hamiltonian of a crystal consisting of N nuclei and ZN electrons can be written in the form

$$\hat{H} = \frac{1}{2M}\sum_{i}^{N}\hat{P}_i^2 + \frac{1}{2m}\sum_{k}^{ZN}\hat{p}_k^2 + U_1(\{\vec{r}_k\}) + U_2(\{\vec{R}_i\}) + U_3(\{\vec{r}_k\},\ \{\vec{R}_i\}), \quad (22.12)$$

where M is the mass of the nucleus, $\hat{P}_i$ is the momentum operator for the ith nucleus, m is the mass of the electron, $\hat{p}_k$ is the momentum operator for the kth electron, $\{\vec{r}_k\}$ is the set of coordinates of the electrons, $\{\vec{R}_i\}$ is the set of coordinates of the nuclei. The function U_1 describes the interaction of electrons. It is of the form

$$U_1 = \frac{1}{2}\sum_{k\neq l}\sum e^2/r_{kl}, \quad (22.13)$$

where r_{kl} is the distance between the kth and lth electrons. The function U_2 describes the mutual interaction of the nuclei, while the function U_3 describes the interaction of the nuclei with the electrons.*

Since $M \gg m$, the nuclei move much more slowly than the electrons. This permits us to consider the motions of nuclei and electrons *separately*: when considering the motion of electrons, we assume that the nuclei are stationary, while when considering the motion of the nuclei, we assume that the electrons collectively create an average field which is independent of the coordinate of individual electrons. In this case the wave function of the

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* The functions U_1, U_2, U_3, describing the various interaction potentials, in fact correspond to operators in the coordinate representation.

crystal may be represented in the form of a product of "nuclear" and "electronic" functions:

$$\psi(\{\vec{r}_k\}, \{\vec{R}_i\}) = \Psi(\{\vec{R}_i\})\, \varphi_e(\{\vec{r}_k\}). \tag{22.14}$$

We also represent the Hamiltonian (22.12) as a sum of the "nuclear" Hamiltonian $\hat{H}_1$ and the "electronic" Hamiltonian $\hat{H}_2$:

$$\hat{H}_1 = \frac{1}{2M} \sum_i^N \hat{P}_i^2 + U_2(\{\vec{R}_i\}), \tag{22.15}$$

$$\hat{H}_2 = \frac{1}{2m} \sum_k \hat{p}_k^2 + \frac{1}{2} \sum_{k \neq l} \sum \frac{e^2}{r_{kl}} + U_3(\{\vec{r}_k\}). \tag{22.16}$$

The function U_3 describes the potential energy of the electrons in the field of the nuclei which are located at the lattice sites in the crystal.

Thus, instead of solving an extremely complicated Schrödinger equation for the entire crystal

$$\hat{H}\psi(\{\vec{r}_k\}, \{\vec{R}_i\}) = E^{\mathrm{cr}}\psi(\{\vec{r}_k\}, \{\vec{R}_i\}) \tag{22.17}$$

it is enough to solve two much simpler equations:

(a) for nuclei (for crystal lattice)

$$\hat{H}_1\Psi(\{\vec{R}_i\}) = E^{\mathrm{lat}}\Psi(\{\vec{R}_i\}), \tag{22.18}$$

(b) for electrons

$$\hat{H}_2\varphi_e(\{\vec{r}_k\}) = E^{\mathrm{e}}\varphi_e(\{\vec{r}_k\}), \tag{22.19}$$

where $E^{\mathrm{cr}} = E^{\mathrm{lat}} + E^{\mathrm{e}}$. This approximation is called *adiabatic*.

In conclusion, we make a fairly important clarification. When using the adiabatic approximation we consider, strictly speaking, not the bare nuclei, but nuclei together with those electrons which are tightly bound to them. Consequently, when we speak about a separate treatment of the electrons ensemble, we mean not all the electrons, but only those which have been "collectivized" by the crystal (in other words, the electrons moving over the crystal lattice, for example, the conduction electrons).

One-Electron Approximation

In accordance with the adiabatic approximation, we shall consider, without going into the dynamics of the crystal lattice, the motion of electrons which have been "collectivized" by the crystal. We use the expression (22.16) and consider that the function $U_3(\{\vec{r}_k\})$ may be represented as a summation over the "collectivized" electrons (since each electron interacts with the lattice field independently from other electrons): $U_3(\{\vec{r}_k\}) = \sum\limits_k U_4(\vec{r}_k)$. In this case the "electronic" Hamiltonian (22.16) assumes the form

$$\hat{H} = \frac{1}{2m}\sum_k \hat{p}_k^2 + \frac{1}{2}\sum_{k\neq l}\sum \frac{e^2}{r_{kl}} + \sum_k U_4(\vec{r}_k). \qquad (22.20)$$

Further simplification is based on the assumption that the term $\frac{1}{2}\sum\limits_k\sum\limits_l e^2/r_{kl}$ in (22.20) may be approximated by a summation over the electrons:

$$\frac{1}{2}\sum_{k\neq l}\sum \frac{e^2}{r_{kl}} \approx \sum_k U_5(\vec{r}_k). \qquad (22.21)$$

In other words, when considering electron-electron interaction, it is assumed that each electron moves in a certain field which is common for the whole ensemble (it is called the self-consistent field). As a result, the Hamiltonian of the electron ensemble can be represented as a sum of "one-electron" Hamiltonian. This allows us to represent the wave function of the ensemble in the form of a product of "one-electron" functions [we denote them by $\varphi(\vec{r}_k)$], after which the Schrödinger equation for the electron ensemble turns into set of "one-electron" equations of the form

$$\left[\frac{\hat{\vec{p}}^2}{2m} + U_4(\vec{r}) + U_5(\vec{r})\right]\varphi(\vec{r}) = E\varphi(\vec{r}). \qquad (22.22)$$

Here $\hat{\vec{p}}$ and $\vec{r}$ are the momentum operator and the coordinate of one of the "collectivized" electrons, E being the energy of the electron.

Thus, by using (22.21) we can go over from a consideration of the electron ensemble to consideration of a single electron moving in the field:

$$U(\vec{r}) = U_4(\vec{r}) + U_5(\vec{r}). \qquad (22.23)$$

This transition is called the *one-electron approximation.* The potential $U(\vec{r})$ is a *periodic* function with the period of the crystal lattice. It will be shown in Sec. 24 that the energy of an electron moving in a periodic field is broken up into alternate bands of allowed and forbidden values, i.e. has a *band structure*. An electron bound to an atom has energy levels, while a free electron is characterized by a continuous energy spectrum. An electron "collectivized" by the crystal occupies an "intermediate" position to a certain extent—it is "free", but only within the limits of the crystal. The band structure of the energy states of such an electron is obvious and is "intermediate" between the structure of discrete levels and that of a continuous spectrum.

The relative freedom of movement of a "collectivized" electron is reflected, in particular, in its wave function, which is represented in the form of what are called *Bloch functions:*

$$\varphi(\vec{r}) = u(\vec{r}) \exp(i\vec{p}\vec{r}/\hbar). \tag{22.24}$$

This is the wave function (15.15) of a free electron, modulated by the function $u(\vec{r})$, which has the period of the potential $U(\vec{r})$ (for more about Bloch functions, see Sec. 24).

The Hamiltonian of the Interaction of an Electron with Electromagnetic Radiation

We shall consider the system of a *bound electron plus radiation.* In the absence of interaction between the electron and the radiation, the system is described by the "unperturbed" Hamiltonian:

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + U + \hat{H}_\gamma, \tag{22.25}$$

where $\hat{p}^2/2m + U$ is the Hamiltonian of the electron, and $\hat{H}_\gamma$ is the Hamiltonian of the radiation. In the case of interaction between the electron and the radiation, the system is described by a "perturbed" Hamiltonian

$$\hat{H} = \left(\hat{\vec{p}} - \frac{e}{c}\vec{A}\right)^2 \Big/ 2m + U + \hat{H}_\gamma \tag{22.26}$$

where $\vec{A}$ is the operator of the vector potential of the radiation field [we recall that in the coordinate representation $\hat{\vec{A}}(\vec{r}) = \vec{A}(\vec{r})$]*. Note that the field potentials here have been chosen in such a way that the well-known calibration conditions div $\vec{A} = 0$ and $\varphi = 0$ (φ is the scalar potential of the field) are satisfied. Next, we represent the Hamiltonian in the following form:

$$\hat{H} = \hat{H}_0 + \hat{H}' \tag{22.27}$$

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* It is shown in classical field theory [38] that the interaction of a charge with an electromagnetic field may be considered by replacing $\vec{p}$ by $\vec{p} - \frac{e}{c}\vec{A}$. We use this classical result here, replacing the dynamic variables with the corresponding operators.

where $\hat{H}'$ is the interaction Hamiltonian, which plays the role of the perturbation. Comparing (22.25), (22.26) and (22.27), we find that

$$\hat{H}' = -\frac{e}{2mc}[\hat{\vec{p}}\vec{A}) + (\vec{A}\hat{\vec{p}})] + \frac{e^2}{2mc^2}A^2. \qquad (22.28)$$

This expression can be somewhat simplified if we put, in accordance with (20.27), $\hat{\vec{p}}\vec{A}(\vec{r}) - \vec{A}(\vec{r})\hat{\vec{p}} = -i\hbar\,\mathrm{div}\vec{A}(\vec{r})$. Using the fact that div $\vec{A} = 0$, we get

$$\hat{H}' = -\frac{e}{2mc}(\hat{\vec{p}}\vec{A}) + \frac{e^2}{2mc^2}A^2. \qquad (22.29)$$

It should be noted here that the Hamiltonian (22.29) is responsible for all processes of absorption and emission (spontaneous as well as induced) of photons by an electron.

Section 23 Transition to the Momentum Representation

We shall show how to go over from the coordinate to the momentum representation and shall give some results in the momentum representation.

Momentum and Coordinate Operators in the Momentum Representation

Obviously, the momentum operator in the momentum representation is the momentum itself:

$$\hat{p}_x = p_x; \quad \hat{\vec{p}} = \vec{p}. \qquad (23.1)$$

We shall, therefore, go over directly to a consideration of the x-coordinate.

Suppose that the amplitude of a state is given in the coordinate representation by the function $\varphi(x)$, and in the momentum representation by the function $\Phi(p_x)$. By using (17.33), we can write

$$\int \varphi^*(x)\,\hat{x}(x)\,\varphi(x)\,dx = \int \Phi^*(p_x)\,\hat{x}(p_x)\,\Phi(p_x)\,dp_x. \qquad (23.2)$$

The relation between the functions $\varphi(x)$ and $\Phi(p_x)$, according to (15.6), is of the form

$$\varphi(x) = \int \Phi(p_x)\,\psi_{p_x}(x)\,dp_x, \qquad (23.3)$$

where $\psi_{p_x}(x)$ are the eigenfunctions of the operator $\hat{p}_x$ in the coordinate representation. By using (20.9) we can rewrite the expression (23.3) in the following form:

$$\varphi(x) = (2\pi\hbar)^{-1/2}\int \Phi(p_x)\exp(ip_x x/\hbar)\,dp_x. \qquad (23.4)$$

By substituting (23.4) in the left-hand side of the equality (23.2), we get

$$\int \varphi^*(x)\, x\varphi(x)\, dx$$

$$=\frac{1}{2\pi\hbar}\int\int\int \Phi^*(p_x')\, e^{-ip_x'x/\hbar} x\Phi(p_x) e^{ip_x x/\hbar} dp_x' dp_x dx. \quad (23.5)$$

The factor $x\,\Phi(p_x)\exp\,(ip_x x/\hbar)$ under the integral sign in (23.5) may be expressed in the following form:

$$x\Phi(p_x)\exp(ip_x x/\hbar) = -i\hbar\frac{d}{dp_x}[\Phi\exp(ip_x x/\hbar)]$$

$$+i\hbar\frac{d\Phi}{dp_x}\exp(ip_x x/\hbar). \quad (23.6)$$

We substitute (23.6) into (23.5) and consider the integral with respect to p_x. In so doing, we take into account that

$$-i\hbar\int\limits_{-\infty}^{\infty}\frac{d}{dp_x}[\Phi\exp(ip_x x/\hbar)]\,dp_x$$

$$= -i\hbar\,\Phi(p_x)\exp(ip_x x/\hbar)\,\Big|_{-\infty}^{\infty}=0$$

[since it is physically impossible to attain an infinitely large momentum, we get $\Phi(\infty) = 0$ and $\Phi(-\infty) = 0$]. Thus in the integral with respect to p_x, only the second term on the right-hand side of (23.6), $i\hbar\frac{d\Phi}{dp_x}\exp\,(ip_x x/\hbar)$ should remain. As a result, (23.5) assumes the form

$$\int \varphi^*(x)\, x\varphi(x)\, dx$$

$$=\frac{1}{2\pi\hbar}\int\int\int \Phi^*(p_x')\, i\hbar\exp[i(p_x-p_x')x/\hbar]\frac{d\Phi(p_x)}{dp_x}dp_x' dp_x\, dx. \quad (23.7)$$

Integration with respect to x on the right-hand side of this equation gives, according to (15.17),

$$(2\pi\hbar)^{-1}\int\exp[i(p_x-p_x')x/\hbar]\,dx=\delta(p_x-p_x').$$

Further, using the property of the delta function, we perform an integration with respect to p_x':

$$\int \Phi^*(p_x')\,\delta(p_x-p_x')\,dp_x'=\Phi^*(p_x).$$

As a result, we are left with only the integral with respect to p_x, and (23.7) assumes the form

$$\int \varphi^*(x)\, x\varphi(x)\, dx=\int \Phi^*(p_x)\, i\hbar\frac{d}{dp_x}\Phi(p_x)\, dp_x. \quad (23.8)$$

Comparing the right-hand sides of (23.8) and (23.2), we find the expression for the x-coordinate operator in the momentum representation:

$$\hat{x}(p_x) = i\hbar \frac{d}{dp_x}. \tag{23.9}$$

A generalization to the three-dimensional case gives

$$\hat{\vec{r}}(\vec{p}) = i\hbar \nabla_{\vec{p}}, \tag{23.10}$$

where $\nabla_{\vec{p}}$ is the gradient in the momentum space.

Unitary Invariance of the Commutation Relations

By using (23.1) and (23.9) it is easy to see that the commutators of the operators of the coordinate and momentum components will be exactly the same in the momentum representation, as in the coordinate representation [we are speaking of the expressions (20.24)-(20.26)]. This conclusion may also be extended to the expressions (20.27)-(20.30). In other words, the commutation relations are independent of the choice of a representation, i.e. are *unitary invariants.* This is quite natural, if we recall that the mathematical fact of commutation of operators has a definite physical meaning which, obviously, cannot change while going over from one representation to another.

Schrödinger Equation in the Momentum Representation

Going over to the momentum representation, we can write (20.11) in the form

$$\hat{H}(p_x)\tau_E(p_x) = E\tau_F(p_x), \tag{23.11}$$

where $\tau_E(p_x)$ are the eigenfunctions of the Hamiltonian in the momentum representation. Note that the quantities E in (23.11) are exactly the same as in (20.11), since the spectrum of eigenvalues of a Hermitian operator is a unitary invariant. Since in the momentum representation $\hat{p}_x = p_x$ and $\hat{x} = i\hbar \frac{d}{dp_x}$, the Hamiltonian (20.12) will now have the form

$$\hat{H}(p_x) = \frac{p_x^2}{2m} + U\left(i\hbar \frac{d}{dp_x}\right). \tag{23.12}$$

As a result, we get the following equation in place of (20.13):

$$\left(\frac{p_x^2}{2m} - E\right)\tau_E(p_x) + U\left(i\hbar \frac{d\tau_E}{dp_x}\right) = 0. \tag{23.13}$$

This is the *time-independent Schrödinger equation in the momentum representation.*

As an example, let us write out the Hamiltonian of a linear harmonic oscillator:

$$\hat{H}(p_x) = \frac{p_x^2}{2m} - \frac{m\omega^2\hbar^2}{2}\frac{d^2}{dp_x^2}. \tag{23.14}$$

Compare this expression with (22.1), which describes the same Hamiltonian in the coordinate representation.

The momentum representation allows us to obtain fairly easily one result with which the reader is already familiar. If a microparticle moves freely, equation (23.13) is obviously simplified:

$$\left(\frac{p_x^2}{2m} - E\right) \tau_E(p_x) = 0, \tag{23.15}$$

from which it immediately follows that

$$E = p_x^2/2m. \tag{23.16}$$

The result (23.16) has been already mentioned in Sec. 1. It means that a freely moving particle simultaneously possesses a definite energy and a definite momentum; moreover, these quantities are related to each other by the classical relation (23.16). In the case of a freely moving microparticle, the stationary state is also an eigenfunction of the momentum operator. We emphasize that this can in no way be extended to bound microparticles (see the following example).

Probability of Momentum Values for a Particle in a Rectangular Well with Infinitely High Walls

In Sec. 21 we considered the problem of the motion of a particle in a one-dimensional rectangular potential well with infinitely high walls in the coordinate representation. The energy levels (21.8) and the orthonormalized amplitudes of stationary states (21.9) were determined.

When going over to the momentum representation, the result (21.8) obviously does not change, while the result (21.9) changes. By finding the amplitude of stationary states in the momentum representation, we can also find the probability of values of momentum of a particle in the n-th energy state. We denote these amplitudes by $\tau_n(p_x)$; the required probability will then be $|\tau_n(p_x)|^2$. The amplitude $\tau_n(p_x)$ are related to the amplitude of stationary states in the coordinate representation [to the amplitudes $\varphi_n(x)$] by superposition relations of the same type as (23.3):

$$\tau_n(p_x) = \int \varphi_n(x)\, \psi_x'^{*}(p_x)\, dx, \tag{23.17}$$

where $\psi_x'(p_x)$ are the eigenfunctions of the operator $\hat{x}$ in the momentum representation. By using the fact that $\psi_x'(p_x) = \psi^{*}_{p_x}(x)$, and (20.9), we can rewrite (23.17) in the following form:

$$\tau_n(p_x) = (2\pi\hbar)^{-1/2} \int_0^a \varphi_n(x) \exp(-ip_x x/\hbar)\, dx. \tag{23.18}$$

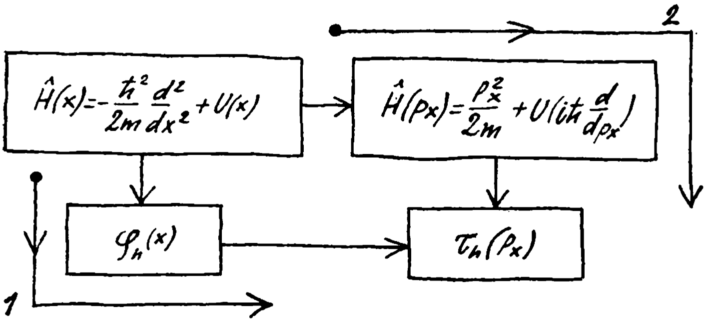
By substituting (21.9) into this equation and integration, we finally come to the following expressions for the probability:

$$|\tau_n(p_x)|^2 = \frac{4\pi a n^2}{\hbar\left(\pi^2 n^2 - \frac{p_x^2 a^2}{\hbar^2}\right)^2} \begin{cases} \cos^2\left(\frac{p_x a}{2\hbar}\right), & n \text{ is odd} \\ \sin^2\left(\frac{p_x a}{2\hbar}\right), & n \text{ is even} \end{cases} \tag{23.19}$$

Thus, it has been rigorously shown that the stationary states (energy levels) of a particle in the potential well are not characterized by a definite momentum but by a corresponding definite de Broglie wavelength. We remind the reader that this circumstance was qualitatively discussed in Sec. 5, when we solved futility of a graphical representation of a bound microparticle in the form of a classical wave in a resonator.

Summing up, we can compile a "scheme" for the transition from one representation to another as follows:

A Scheme for the Transition from the Coordinate to the Momentum Representation



This "scheme" assumes two methods of transition. The *first method*: the Schrödinger equation with the Hamiltonian $\hat{H}(x)$ is solved and the amplitudes of stationary states $\varphi_n(x)$ are found in the coordinate representation. Then with the help of the superposition relation (23.17) we perform a transition from the amplitudes $\varphi_n(x)$ to the amplitudes $\tau_n(p_x)$. This is the method that was adopted in the above example. However, it is also possible to follow a *second method*: the transition from $\hat{H}(x)$ to $\hat{H}(p_x)$ is made and the Schrödinger equation in the momentum representation (23.13) is solved. In this case, the derivation of the amplitudes $\tau_n(p_x)$ is reduced to the solution of the equation (23.13).

Section 24

An Electron in a Periodic Field

The quantum-mechanical problem of an electron in a periodic field plays an important role in the solid-state theory. We turn to this problem, using the one-electron approximation discussed in Sec. 22.

The Band Structure of the Energy Spectrum. Brillouin Zones

Let us consider a one-dimensional *periodic* potential $U(x)$ satisfying the condition

$$U(x+a) = U(x). \tag{24.1}$$

Following the second method in the scheme given at the end of the preceding section, we change over to the momentum representation. This means that the potential $U(x)$ should be expressed as an operator in the momentum representation, $\hat{U}(p_x)$. (In order to simplify the notation we shall write p for p_x here.)

We expand the periodic function (24.1) in a Fourier series:

$$U(x) = \sum_{n=-\infty}^{\infty} U_n \exp(-i2\pi nx/a)$$

and, changing to the momentum representation, we write

$$\hat{U}(p) = \sum_{n=-\infty}^{\infty} U_n \exp\left(\frac{2\pi n\hbar}{a}\frac{d}{dp}\right). \tag{24.2}$$

We shall now show that the operator $\exp\left(p_1 \frac{d}{dp}\right)$ is a displacement operator with a finite displacement in p-space by the amount $p = p_1$. This is so, as

$$\begin{aligned}\tau(p+p_1) &= \tau(p) + p_1 \frac{d\tau}{dp}(p) + \frac{1}{2!} p_1^2 \frac{d^2\tau}{dp^2}(p) + \dots \\ &= \left[1 + p_1\frac{d}{dp} + \frac{1}{2!} p_1^2 \frac{d^2}{dp^2} + \qquad \right]\tau(p) = \exp\left(p_1 \frac{d\tau}{dp}\right).\end{aligned}$$

Thus

$$\exp\left(p_1 \frac{d\tau}{dp}\right) = \tau(p+p_1). \tag{24.3}$$

From (24.2) and (24.3) it follows that

$$\hat{U}(p)\,\tau(p) = \sum_{n=-\infty}^{\infty} U_n \tau\left(p + \frac{2\pi\hbar}{a} n\right). \tag{24.4}$$

By using (24.4) we can write the Schrödinger equation (23.13) in the following form:

$$\left(\frac{p^2}{2m} - E\right)\tau(p) + \sum_{n=-\infty}^{\infty} U_n \tau\left(p + \frac{2\pi\hbar n}{a}\right) = 0. \tag{24.5}$$

In fact, (24.5) is a homogeneous system of linear equations containing the functions $\tau(p)$, $\tau(p-2\pi\hbar/a)$, $\tau(p+2\pi\hbar/a)$, etc. Generally speaking, this system consists of an infinite number of equations:

$$\left.\begin{array}{l}
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
\left[\frac{(p+2\pi\hbar/a)^2}{2m}-E\right]\tau\left(p+\frac{2\pi\hbar}{a}\right) \\
\qquad\qquad +\sum\limits_{n} U_n\tau\left(p+\frac{2\pi\hbar(n+1)}{a}\right)=0, \\
\left[\frac{p^2}{2m}-E\right]\tau(p)+\sum\limits_{n=-\infty}^{\infty} U_n\tau\left(p+\frac{2\pi\hbar n}{a}\right)=0, \\
\left[\frac{(p-2\pi\hbar/a)^2}{2m}-E\right]\tau\left(p-\frac{2\pi\hbar}{a}\right) \\
\qquad\qquad +\sum\limits_{n} U_n\tau\left(p+\frac{2\pi\hbar(n-1)}{a}\right)=0. \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots
\end{array}\right\} \qquad (24.6)$$

Nonzero solutions of this homogeneous system are possible only if its determinant is equal to zero. We denote this determinant by $D(E, p)$ and symbolically write

$$D(E, p) = 0. \qquad (24.7)$$

We fix p (let, say, $p = p_1$) and write the roots of equation (24.7) as $E_1(p_1)$, $E_2(p_1)$, $E_3(p_1)$, ... For a different value of p (say $p = p_2$) we get new roots: $E_1(p_2)$, $E_2(p_2)$, $E_3(p_2)$, By choosing different values of p, we finally get a set of functions defined by equation (24.7):

$$E_1(p),\ E_2(p),\ E_3(p), \quad ., E_j(p), \qquad (24.8)$$

For every index j, the energy is a continuous function of the momentum. By assuming that these functions are bounded we write for the index j

$$E_j^{\min} \leqslant E_j(p) \leqslant E_j^{\max}. \qquad (24.9)$$

The inequalities (24.9) include the energy values for the microparticle which constitute the jth energy band. If $E_{j-1}^{\max} < E_j^{\min}$, we get a region of unattainable energy values between the $(j-1)$th and jth energy bands. This region is usually called the forbidden band.

Thus, the energy spectrum of an electron in a periodic field must consist of a number of *energy bands*, some of which may be separated by forbidden bands. Within every energy band the energy varies continuously; it is described by some continuous function $E_j(p)$.

By replacing p by $p + 2\pi\hbar n/a$, the system (24.6) transforms into itself. It follows hence that

$$E_j\left(p + \frac{2\pi\hbar n}{a}\right) = E_j(p). \tag{24.10}$$

Since the above replacement does not change anything, we can say that the momentum p has physically different values within the limits of the band:

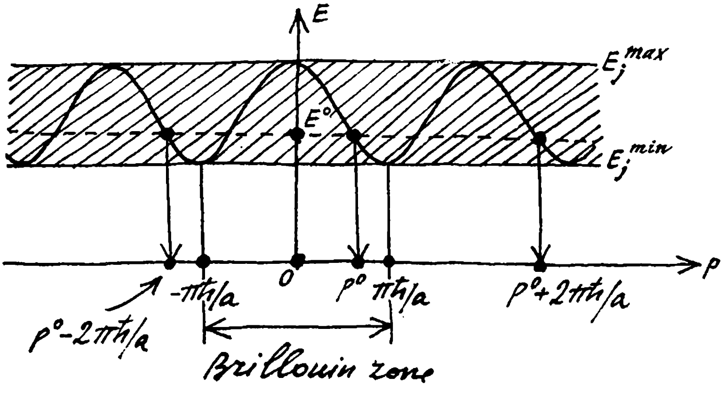
$$-\pi\hbar/a \leqslant p \leqslant \pi\hbar/a. \tag{24.11}$$

In other words, the p-space is split into intervals of length $2\pi\hbar/a$, and one has to consider p only within the limits of one individual interval. These intervals are called the *Brillouin zones*. In this case we are dealing with one-dimensional Brillouin zones. In general, the Brillouin zones are three-dimensional; they often have a very complex configuration, which reflects the specific nature of the periodic field under consideration.

The band structure of the energy spectrum is characteristic of an electron moving in the periodic field of a crystal lattice. The concepts of energy bands and Brillouin zones form the basis of the modern electronic theory of solids (see, for example, [39, 40]).

BLOCH FUNCTIONS. Let us consider the jth energy band. Figure (24.1) shows the dependence $E_j(p)$ for this band. We choose some value E^0 from this band and denote by p^0 the corresponding value

Fig. 24.1



of the momentum for motion to the right. The wave function of the chosen stationary state is denoted through $\tau_j^0(p)$. It can be easily seen that this function differs from zero only for $p = p^0 + 2\pi\hbar n/a$ [it can be seen from the figure that only at these points does the curve $E_j(p)$ intersect the straight line $E = E^0$]. Hence the function $\tau_j^0(p)$ may be written in the form

$$\tau_j^0(p) = \sum_n \Omega(p)\,\delta\left(p^0 + \frac{2\pi\hbar n}{a} - p\right). \tag{24.12}$$

Next, we go over to the coordinate representation by using the familiar rule (23.4):

$$\varphi_j^0(x) = (2\pi\hbar)^{-1/2} \int_{-\infty}^{\infty} \tau_j^0(p)\, \exp(ipx/\hbar)\, dp.$$

Substituting (24.12) into this, we get

$$\varphi_j^0(x) = (2\pi\hbar)^{-1/2} \sum_n \Omega\left(p^0 + \frac{2\pi\hbar n}{a}\right) \times \exp\left[i\left(p^0 + \frac{2\pi\hbar n}{a}\right) x/\hbar\right].$$

By introducing the notation

$$(2\pi\hbar)^{-1/2} \sum_n \Omega\left(p^0 + \frac{2\pi\hbar n}{a}\right) \exp\left(i\,\frac{2\pi n x}{a}\right) = u_j^0(x), \tag{24.13}$$

we can rewrite the above result in the following form:

$$\varphi_j^0(x) = u_j^0(x)\, \exp(ip^0x/\hbar).$$

The explicit form of the function $u_j^0(x)$ is not known [in order to know it, we should have known the explicit form of $U(x)$]. However, it can be seen from (24.13) that the function $u_j^0(x)$ is periodic with the period of the field:

$$u_j^0(x+a) = u_j^0(x). \tag{24.14}$$

Thus, the wave function of a stationary state given by the indices j and p has the following form in coordinate representation [cf. (22.24)]:

$$\varphi_{jp}(x) = u_{jp}(x)\, \exp(ipx/\hbar). \tag{24.15}$$

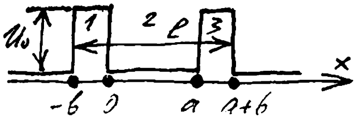
This is a plane wave [$\exp(ipx/\hbar)$] whose amplitude [$u_{jp}(x)$] is periodic with the period of the field. The functions (24.15) are referred to as *Bloch functions* in the literature.

The Kronig-Penney Potential

Let us consider the motion of a particle is a field whose potential is shown in Fig. 24.2 (the so-called Kronig-Penney potential). This is the simplest case of a periodic potential.

Figure 24.2 shows three spatial regions. Assuming first that $E > U_0$, we write the solution of the Schrödinger equation (20.13):

Fig. 24.2



for region *1*

$$\varphi_1(x)=A_1 \exp(ik_1x)+B_1 \exp(-ik_1x);$$

$$k_1=\sqrt{2m(E-U_0)}/\hbar;$$

for region *2*

$$\varphi_2(x)=A_2 \exp(ik_2x)+B_2 \exp(-ik_2x); \quad k_2=\sqrt{2mE}/\hbar.$$

The solution for region *3* may be expressed in terms of the solution for region *1* by using results obtained previously. Let us take a certain point x of region *3*. According to (24.15), we can write

$$\varphi_3(x) = u(x) \exp(ipx/\hbar). \tag{24.16}$$

The symmetric point $x - l$ in region *1* corresponds to the chosen point. At the point $x - l$ we have

$$\varphi_1(x - l) = u(x - l) \exp[ip(x - l)/\hbar].$$

In accordance with (24.14), we rewrite this equality in the form

$$\varphi_1(x - l) = u(x) \exp[ip(x - l)/\hbar]. \tag{24.17}$$

From (24.16) and (24.17) we find $\varphi_3(x) \exp(-ipx/\hbar) = \varphi_1(x - l) \exp(-ipx/\hbar) \exp(ipl/\hbar)$ or, finally,

$$\varphi_3(x)=\exp(ipl/\hbar)\{A_1 \exp[ik_1(x-l)] + B_1 \exp[-ik_1(x-l)]\} \tag{24.18}$$

By using (24.18) and the expression for φ_1 and φ_2, we can write the continuity conditions for the wave function and its first derivative at the points corresponding to the potential jump (the points $x = 0$ and $x = a$). These conditions form a homogeneous system of linear equations in terms of the coefficients A_1, B_1, A_2, B_2:

$$\left.\begin{aligned}
&A_1+B_1=A_2+B_2\\
&A_1 \exp(ik_2a)+B_1 \exp(-ik_2a)\\
&\qquad =\exp(ipl/\hbar)[A_1 \exp(-ik_1b)+B_1 \exp(ik_1b)],\\
&k_1A_1-k_1B_1=k_2A_2-k_2B_2,\\
&k_2[A_2 \exp(ik_2a)-B_2 \exp(-ik_2a)]\\
&\qquad =\exp(ipl/\hbar)[A_1 \exp(-ik_1b)-B_1 \exp(ik_1b)]\,k_1.
\end{aligned}\right\}$$

By equating the determinant of this system to zero, we get the following system (we omit the intermediate steps):

$$\cos(pl/\hbar)=\cos(k_2a)\cos(k_1b)\,\frac{k_1^2+k_2^2}{2k_1k_2}\sin(k_2a)\sin(k_1b). \tag{24.19}$$

Since the modulus of the cosine cannot be greater than unity, we get the following condition imposed on quantities k_1 and k_2 and, hence, on E:

$$-1 \leqslant \left[\cos(k_2a)\cos(k_1b) - \frac{k_1^2+k_2^2}{2k_1k_2}\sin(k_2a)\sin(k_1b)\right] \leqslant 1. \tag{24.20}$$

This condition defines the allowed energy bands.

We next consider the case when $E < U_0$.

Now k_1 is an imaginary quantity. Suppose $k_1 = ik_3$, where $k_3 = \sqrt{2m(U_0 - E)}/\hbar$. Since by replacing k_1 by ik_3 the cosine and the sine are converted into hyperbolic cosine and hyperbolic sine, respectively [$\cos(k_1b) \rightarrow \cosh(k_3b)$; $\sin(k_1b) \rightarrow i\sinh(k_3b)$], we can make use of the result (24.19), which in this case assumes the form

$$\cos\left(\frac{pl}{\hbar}\right) = \cos(k_2a)\cosh(k_3b) + \frac{k_3^2-k_2^2}{2k_2k_3}\sin(k_2a)\sinh(k_3b). \tag{24.21}$$

Accordingly, the condition (24.20) defining the energy bands is transformed into the following form:

$$-1 \leqslant \left[\cos(k_2a)\cosh(k_3b) + \frac{k_3^2-k_2^2}{2k_2k_3}\sin(k_2a)\sinh(k_3b)\right] \leqslant 1. \tag{24.22}$$

Let us consider a special case, when

$$b \ll a \ (a \approx l); \ E \ll U_0 \tag{24.23}$$

(the barriers are narrow and high). Since in this case the quantity b can become arbitrarily small, we can require that the following conditions be fulfilled:

$$b\sqrt{2mU_0}/\hbar \ll 1, \text{ or } k_3b \ll 1. \tag{24.24}$$

By taking (24.24) into account, we put $\cosh(k_3b) \cong 1$ and $\sinh(k_3b) \cong k_3b$, and besides, according to (24.23),

$$(k_3^2 - k_2^2)/2k_2k_3 \approx k_3/2k_2 \approx \frac{1}{2}\sqrt{U_0/E}.$$

As a result, (24.21) assumes the following form:

$$\cos(pa/\hbar) = F(k_2a), \tag{24.25}$$

where we have used the notation

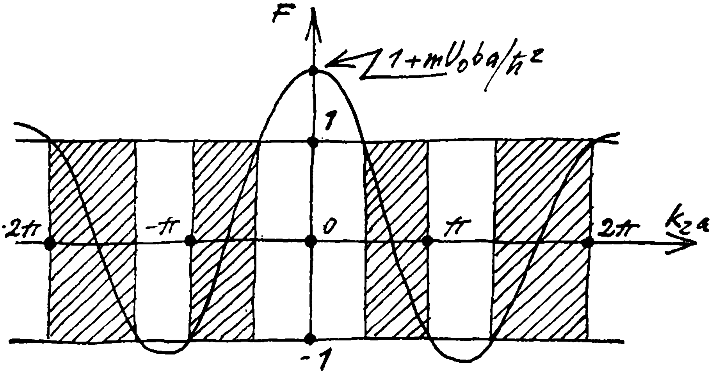
$$F(y) = \cos y + (mU_0b/k_2\hbar^2)\sin y. \tag{24.26}$$

The condition (24.22) assumes the form

$$-1 \leqslant F(k_2a) \leqslant 1. \tag{24.27}$$

The function $F(k_2a)$ is shown in Fig. 24.3. The parts of the k_2a axis, for which the condition (24.27) is satisfied, have been shaded in the diagram. They correspond to the allowed energy bands (remember that $k_2 = \sqrt{2mE}/\hbar$).

Fig. 24.3



Using (24.25)-(24.27), we shall make two remarks. Firstly, if $a \to \infty$ (transition to a free electron), $\cos(k_2a) \to \cos(pa/\hbar)$; this corresponds to a transition to the classical relation (23.16) for the energy and momentum of a particle. Secondly, it can be seen from Fig. 24.3 that a discontinuity in the energy of the electron occurs when $\cos(pa/\hbar) = \pm 1$, i.e. for $pa/\hbar = n\pi$, where n is an integer. According to (24.11), this means that the discontinuities in the energy of the electron occur at the boundary of the Brillouin zone.

Fig. 24.4

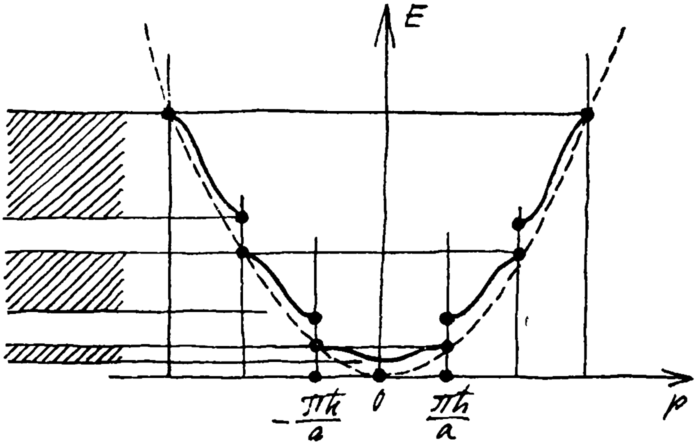


Figure (24.4) shows the dependence of the electron energy on momentum as determined by (24.25). The discontinuities in the energy mentioned above are clearly seen (the energy bands are shown on the left side by hatching). For comparison the classical dependence of energy on momentum is shown for a free electron: $E = p^2/2m$.

Formation of Energy Bands as an Effect of the Removal of Commutation Degeneracy

The conversion of energy levels of an electron in the atom into energy bands of an electron "collectivized" by the crystal may be seen as an effect of the removal of commutation degeneracy.

As was mentioned in Sec. 22, the electron energy in an atom in the general case of a non-Coulomb potential is determined by the quantum numbers n and l. This gives rise to a $2(2l + 1)$-fold degeneracy of this energy. By assuming that the atom is a part of some perfectly ordered ensemble of N similar atoms and that it remains isolated from its neighbours, the degeneracy in the electron energy must be taken as $2N(2l + 1)$-fold. The factor N is associated with the so-called *commutation degeneracy*: in an ordered ensemble, there are no physically isolated atoms, hence the energy of an electron cannot depend on any of the N atoms near which it is localized. However, in a real ensemble (i.e. a crystal), the atoms are not isolated—they interact with one another. This interaction leads to a "collectivization" of the electron and a partial removal of degeneracy of its levels. The level with a $2N(2l + 1)$-fold degeneracy is split up into a system consisting of $N(2l + 1)$ sublevels, each of which remains doubly degenerate (according to the spin quantum number σ). Thus a "collectivization" of the electron by the crystal leads to a removal of commutation degeneracy and degeneracy with respect to the quantum number m.

It is significant that a system of $N(2l + 1)$ sublevels is in reality not discrete, but forms a band of allowed values of the electron energy. Indeed, let ΔE be the width of this system of sublevels, and $\Delta\varepsilon$ be the distance between the neighbouring sublevels: $\Delta\varepsilon = \Delta E/N(2l + 1)$. For the system of sublevels to be discrete, it is essential that $\Delta\varepsilon > \hbar/\tau$, where τ is the lifetime of an electron in a crystal. In other words, the distance between sublevels must be greater than the uncertainty in the energy of the sublevel described by the relation (3.2). This means that the condition

$$\hbar(2l + 1)N/\Delta E < \tau \tag{24.28}$$

must be satisfied. Assuming that $N(2l + 1) \approx 10^{23}$, $\Delta E \approx 1$ eV, we find that τ should be more than 10^8 s, i.e. more than 10 years. Since the real lifetime of a "collectivized" electron in the crystal may only be less than this, the relation (24.28) is obviously not satisfied. This enables us to consider the system of $N(2l+1)$ sublevels as an energy band. Naturally the number of electron states in the band remains finite—the band may "accommodate" up to $2N(2l+1)$ electrons. In this connection we speak of the degree of filling in of a band, of completely filled bands, etc.

Section 25 The Probability of Quantum Transitions

Quantum Transitions and the Principle of Superposition of States

We assume that a microparticle undergoes a transition from one stationary state to another under the action of some external factor. How to find the probability of such a transition?

The initial and the final states of the microparticle are described by functions of the type (20.16). For example, let the initial state be given by $\Psi_n(x, t) = \varphi_n(x) \exp(-iE_nt/\hbar)$. For simplicity, the set of spatial coordinates is denoted by x. The functions Ψ_n satisfy the Schrödinger equation (20.17):

$$i\hbar \frac{\partial}{\partial t} \Psi_n = \hat{H}\Psi_n \tag{25.1}$$

(we shall call it the "unperturbed" equation). The physical nature of external factor, which causes the quantum transition of the microparticle, is arbitrary. In particular, it may be the interaction of the microparticle with electromagnetic radiation. In the quantum theory apparatus such a factor appears in the form of an interaction potential which must be added to the "unperturbed" Hamiltonian $\hat{H}$. In Sec. 22 in the example of the interaction of an electron with radiation, this "addition" to the Hamiltonian was interpreted as some perturbation and was denoted by $\hat{H}'$ We shall use the same notation here. By taking into account the perturbation $\hat{H}'$, we can rewrite the Schrödinger equation in the form

$$i\hbar \frac{\partial}{\partial t} \Phi_n = (\hat{H} + \hat{H}')\,\Phi_n. \tag{25.2}$$

This equation is called the "perturbed" equation. Its solutions Φ_n are no longer stationary states. Hence the index n here does not fix the energy level, but merely indicates the past history: the given "perturbed" state has "emerged" from nth "unperturbed" state.

Essentially, the state Φ_n is a *superposition* state:

$$\Phi_n(x, t) = \sum_n \chi_{nk}(t)\Psi_k(x, t). \tag{25.3}$$

If at a certain time t we "switch on" the corresponding *detector*, the superposition (25.3) is destroyed and the microparticle will be observed in one of the stationary states, for example, in the state Ψ_m. This means that the microparticle has undergone a quantum transition from the state Ψ_n to the state Ψ_m. It is well known that the probability of such a transition is $|\chi_{nm}(t)|^2$.

The reader is in fact familiar with all this. The remarks made above are in agreement with those made in Sec. 10, regarding the relation (10.3), which is essentially equivalent to the relation (25.3).

Thus, the transition probability is, as expected, the square of the modulus of the corresponding transition amplitude:

$$w_{nm} = |\chi_{nm}(t)|^2. \tag{25.4}$$

This amplitude is one of the coefficients in the superposition (25.3), which is just an expansion of the "perturbed" state Φ_n in terms of "unperturbed" states.

Transition to the Energy Representation

In order to find the probability w_{nm}, we should first solve equation (25.2) and then find the expansion coefficients of the solutions obtained for states of the type (20.16). As can be easily seen, such an approach corresponds to the first method in the "scheme" of transition from one representation to another, considered in Sec. 23. The other approach corresponding to the second method in this scheme, however, is more rational. We shall follow the second method here.

According to (15.5), the coefficients χ_{nk} of the superposition (25.3) may be treated as a wave function describing the "perturbed" state, though not in the coordinate representation (in the coordinate representation this is done by the function Φ_n), but in the representation of a set of those physical quantities with respect to which the functions Ψ_k are eigenfunctions. Since the functions Ψ_k are eigenfunctions of the Hamiltonian, we call this representation the *energy* representation. Thus, following the second method in the "scheme" in Sec. 23, we must "translate" the "perturbed" equation (25.2) given in the coordinate representation into the energy representation. This will give us a new equation—the "perturbed" Schrödinger equation in the energy representation. The solutions of this equation will be the required transition amplitudes. Performing the operations indicated above, we substitute (25.3) into (25.2), and take into account (25.1). We get

$$i\hbar \sum_k \frac{d\chi_{nk}}{dt} \Psi_k = \sum_k \chi_{nk} \hat{H}'(t) \Psi_k. \qquad (25.5)$$

Premultiplying both sides of (25.5) by Ψ_m^* and integrating with respect to the spatial coordinates, we obtain

$$i\hbar \sum_k \frac{d\chi_{nk}}{dt} \int \Psi_m^* \Psi_k \, dx = \sum_k \chi_{nk} \int \Psi_m^* \hat{H}'(t) \Psi_k \, dx.$$

Taking into account the orthonormalization of stationary states, we can rewrite the last expression in the following form:

$$i\hbar \frac{d\chi_{nm}}{dt} = \sum_k \chi_{nk} \int \Psi_m^* \hat{H}' \Psi_k \, dx. \qquad (25.6)$$

Next, we introduce the expression

$$\int \Psi_m^* \hat{H}' \Psi_k \, dx = \exp(i\omega_{mk} t) \int \varphi_m^* \hat{H}' \varphi_k \, dx$$
$$= \exp(i\omega_{mk} t) \langle m | \hat{H}' | k \rangle, \qquad (25.7)$$

where

$$\omega_{mk} = (E_m - E_k)/\hbar. \qquad (25.8)$$

Taking into account (25.7) we may rewrite (25.6) in the following final form:

$$\frac{d}{dt} \chi_{nm} = -\frac{i}{\hbar} \sum_k \chi_{nk} \langle m | \hat{H}'(t) | k \rangle \exp(i\omega_{mk} t). \qquad (25.9)$$

Thus, we have obtained the "perturbed" Schrödinger equation in the energy representation. In fact (25.9) is not one equation, but a system of equations. We emphasize that the system (25.9) is more convenient than (25.2), since by solving this system we can at once determine the transition amplitudes χ_{nm}. It is also quite significant that when solving the system (25.9), the perturbation method can usually be applied.

Application of the Method of Perturbations to Computation of the Transition Probabilities

The perturbation is usually very small, which enables us to obtain an approximate solution of the system (25.9) by using the *method of perturbations*. A small perturbation means that the function Φ_n may be represented in the form

$$\Phi_n = \Psi_n + \Lambda_n, \qquad (25.10)$$

where Λ_n is a small addition to the unperturbed function Ψ_n. In accordance with (25.10), we can write

$$\chi_{nk} = \delta_{nk} + \chi_{nk}^{(1)} + \chi_{nk}^{(2)} + \chi_{nk}^{(3)} + \dots . \tag{25.11}$$

It can be easily seen that $\Lambda = \sum\limits_k [\chi_{nk}^{(1)} + \chi_{nk}^{(2)} + \chi_{nk}^{(3)} + \dots] \Psi_k$. According to (25.11), the small addition Λ is in turn split into additions differing in the order of smallness: the functions $\chi_{nk}^{(1)}$ are of the same order as the perturbation, $\chi_{nk}^{(2)}$ are of the order of the square of perturbation, etc. Substituting (25.11) into (25.9), we get

$$\frac{d}{dt}\chi_{nm}^{(1)} + \frac{d}{dt}\chi_{nm}^{(2)} + \frac{d}{dt}\chi_{nm}^{(3)} + \dots$$
$$= -\frac{i}{\hbar}\sum_k (\delta_{nk} + \chi_{nk}^{(1)} + \chi_{nk}^{(2)} + \dots)\langle m | \hat{H}' | k \rangle \exp(i\omega_{mk}t). \tag{25.12}$$

We rewrite (25.12), retaining terms of only first order in the perturbation:

$$\frac{d}{dt}\chi_{nm}^{(1)} = -\frac{i}{\hbar}\langle m | \hat{H}' | n \rangle \exp(i\omega_{nm}t). \tag{25.13}$$

This is the approximate expression for the amplitudes χ_{nm}, obtained in the *first-order approximation in the method of perturbations.*

If it turns out that $\langle m \mid \hat{H}' \mid n \rangle = 0$, we must use the approximate expression for the amplitudes in the *second-order approximation in the method of perturbations.* It is obtained from (25.12) by retaining terms of the second order in the perturbation:

$$\frac{d}{dt}\chi_{nm}^{(2)} = -\frac{i}{\hbar}\sum_k \chi_{nk}^{(1)}\langle m | \hat{H}' | k \rangle \exp(i\omega_{mk}t). \tag{25.14}$$

Similarly, for the *third-order approximation in the method of perturbations* we get

$$\frac{d}{dt}\chi_{nm}^{(3)} = -\frac{i}{\hbar}\sum_k \chi_{nk}^{(2)}\langle m | \hat{H}' | k \rangle \exp(i\omega_{mk}t) \tag{25.15}$$

etc.

Knowing the transition amplitudes for any order in the method of perturbations, we may obtain the transition probabilities in the corresponding approximation. In the first approximation, we get, from (25.13),

$$w_{nm}^{(1)} = |\chi_{nm}^{(1)}(t)|^2$$
$$= \frac{1}{\hbar^2}\left| \int_{-\infty}^{t} \langle m | \hat{H}'(t) | n \rangle \exp(i\omega_{mn}t)\, dt \right|^2 \tag{25.16}$$

For the second-order approximation in the method of perturbations we get, from (25.14),

$$w^{(2)}_{nm} = \frac{1}{\hbar^2}\left|\sum_{k}\int_{-\infty}^{t}\chi^{(1)}_{nk}(t)\langle m|H'(t)|k\rangle \times \exp(i\omega_{mk}t)\,dt\right|^2 \qquad (25.17)$$

etc.

Note that the result (25.17) describes the interference of amplitudes. The resulting transition amplitude here is the sum of the transition amplitudes through various intermediate states. The impossibility of finding the microparticle in any intermediate state leads to the indistinguishability of alternatives and permits us to speak of intermediate states as virtual states.

The further course of action envisages a substitution of definite operators $\hat{H}'$ in expressions of the type (25.16) and (25.17). In quantum electronics, for example, the operator (22.29) is used. A detailed consideration of such questions is beyond the scope of this book. The reader is advised to refer, for example, to [12, 41], in this connection.

Feynman's Diagrams and the Calculation of Transition Probabilities

In conclusion, we return to the Feynman's diagrams considered in Sec. 6 (see the diagrams 6.1, relating to the scattering of one electron by another). Note that all the diagrams shown in Fig. 6.1 are associated with the same quantum transition—the transition of two electrons from particular initial states to particular final states. Strictly speaking, each particular transition must be described by an infinite number of diagrams, with an ever increasing number of vertices. In this connection, we recall the remark expressed in Sec. 6: "In order to calculate the probability of scattering of an electron by an electron, it is necessary, in principle, to take into account the contribution (to this transition) of various processes described by different diagrams."

Returning to Feynman's diagrams, we can now clarify the meaning of the remark quoted above. We can now explain the meaning of "taking into account" of the contribution from different diagrams. What happens is that to each diagram there corresponds a definite transition amplitude. The resulting amplitude is the sum of these amplitudes. Consequently, in order to compute the probability of a particular quantum transition, it is necessary *firstly* to form all the possible Feynman's diagrams of the transition and write the amplitudes corresponding to the various diagrams, and, *secondly*, sum all these amplitudes and find the square of the modulus of the sum.

In Sec. 6 we had the sentence: "Fortunately, the contribution of different processes (different diagrams) is different." This means that in practice the method of perturbations is used, which allows us to restrict the summation of amplitudes to just the first few terms. The dimensionless quantity $(e^2/\hbar c)^{n/2}$, mentioned in Sec. 6, is the factor which in the above-mentioned sum of amplitudes contains the amplitudes corresponding to the diagrams with n vertices. The smallness of this quantity explains the applicability of the method of perturbations in quantum electrodynamics.

It may be said that the quantum-mechanical idea of interference of transition amplitudes along with the method of perturbations forms, from a most general point of view, the foundation of quantum electrodynamics as a quantum theory.

Section 26

Ways of Describing Evolution of Microsystems with Time

To conclude the book, let us discuss in very general terms the very important problem of the methods of describing the evolution of microsystems with time. The quantum-mechanical apparatus so far developed uses three different methods. Three different forms of the equations of motion in quantum mechanics correspond to these methods. We shall discuss these methods below. Usually we refer to them as three different representations: the *Schrödinger representation*, the *Heisenberg representation* and the *interaction representation (Dirac representation)*. The term "representation" is used here in a different, wider sense than in the previous sections. We may also speak of Schrödinger's coordinate representation or Schrödinger's momentum representation. In the previous sections we restricted ourselves to the Schrödinger representation but considered various representations, understood in a more restricted sense—the coordinate, the momentum and the energy representations. We shall now consider Schrödinger, Heisenberg and Dirac representations, restricting ourselves to the coordinate representation.

Schrödinger Representation

Here, the evolution of a microsystem with time is described as an *evolution of the amplitudes of states* of the given microsystem:

$$\psi(x, t) = \hat{U}(t, t_0)\,\psi(x, t_0). \qquad (26.1)$$

The operator $\hat{U}(t, t_0)$ satisfies the conditions

$$\hat{U}(t_0, t_0) = 1, \tag{26.2}$$

$$\hat{U}\hat{U}^+ = \hat{U}^+\hat{U} = 1. \tag{26.3}$$

The condition (26.2) is obvious. The condition (26.3) of unitarity is a direct consequence of the independence of the normalization of amplitudes of state from the choice of the instant of time:

$$\int \psi^*(x, t)\, \psi(x, t)\, dx = \int \psi^*(x, t_0)\, \psi(x, t_0)\, dx.$$

The quantum-mechanical equation of motion in the Schrödinger representation (corresponding to Schrödinger's equation) is of the form

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = \hat{H}(x)\, \psi(x, t), \tag{26.4}$$

where the operator $\hat{H}$ does not depend on time. By using (26.4) and (26.2), we can easily find the form of the operator $\hat{U}(t, t_0)$:

$$\hat{U}(t, t_0) = \exp\left[-\frac{i}{\hbar}(t - t_0)\, \hat{H}(x)\right]. \tag{26.5}$$

The exponent should be treated here as an expansion into a power series.

Heisenberg Representation

The evolution of a microsystem with time is described as an *evolution of Hermitian operators* describing a given microsystem. The amplitudes of states are treated as time-independent:

$$\varphi(x, t) = \varphi(x, t_0). \tag{26.6}$$

The transition from amplitudes in the Schrödinger representation to amplitudes in the Heisenberg representation is carried out, as can be seen from (26.1), with the help of the operator $\hat{U}^+(t, t_0)$:

$$\varphi(x, t) = \hat{U}^+(t, t_0)\, \psi(x, t_0). \tag{26.7}$$

For, substituting (26.1) into (26.7), we get

$$\varphi(x, t) = \hat{U}^+\hat{U}\psi(x, t_0) = \psi(x, t_0)$$
$$= \hat{U}(t_0, t_0)\, \varphi(x, t_0) = \varphi(x, t_0)$$

Let $\hat{L}(x)$ be the operator of some physical quantity in Schrödinger's representation. According to (17.32) and (26.7), this operator in the Heisenberg representation will have the form

$$\hat{L}(x, t) = \hat{U}^+(t, t_0)\, \hat{L}(x)\, \hat{U}(t, t_0). \tag{26.8}$$

Substituting (26.5) into (26.8), we find

$$\hat{L}(x,\ t)=\exp\left[\frac{i}{\hbar}(t-t_0)\,\hat{H}(x)\right]\hat{L}(x)$$
$$\times\exp\left[-\frac{i}{\hbar}(t-t_0)\,\hat{H}(x)\right]. \qquad (26.9)$$

Differentiating (26.9) with respect to time, we get

$$i\hbar\frac{\partial}{\partial t}\hat{L}(x,\ t)=\exp\left[\frac{i}{\hbar}(t-t_0)\,\hat{H}(x)\right]\hat{L}(x)\,\hat{H}(x)$$
$$\times\exp\left[-\frac{i}{\hbar}(t-t_0)\,\hat{H}(x)\right]-\exp\left[\frac{i}{\hbar}(t-t_0)\,\hat{H}(x)\right]$$
$$\times\hat{H}(x)\,\hat{L}(x)\,\exp\left[-\frac{i}{\hbar}(t-t_0)\,\hat{H}(x)\right]. \qquad (26.10)$$

This may be written in the form

$$i\hbar\frac{\partial}{\partial t}\hat{L}(x,\ t)=\hat{U}^{+}\hat{L}(x)\,\hat{H}(x)\,\hat{U}-\hat{U}^{+}\hat{H}(x)\,\hat{L}(x)\,\hat{U} \qquad (26.11)$$

or, by taking into account (26.3), in the form

$$i\hbar\frac{\partial}{\partial t}\hat{L}(x,\ t)=\hat{U}^{+}\hat{L}(x)\,\hat{U}\hat{U}^{+}\hat{H}(x)\,\hat{U}-\hat{U}^{+}\hat{H}(x)\,\hat{U}\hat{U}^{+}\hat{L}(x)\,\hat{U}. \qquad (26.12)$$

Using (26.8) with respect to the operator $\hat{L}(x)$ as well as the operator $\hat{H}(x)$, we get the quantum-mechanical equation of motion in the Heisenberg representation [cf. (19.10)]:

$$i\hbar\frac{\partial}{\partial t}\hat{L}(x,\ t)=[\hat{L}(x,\ t),\ \hat{H}(x,\ t)]. \qquad (26.13)$$

Comparison of Schrödinger and Heisenberg Representations

We note that at the time t_0 we have $\varphi(x,\ t_0)=\psi(x,\ t_0)$ and $\hat{L}(x,\ t_0)=\hat{L}(x)$, i.e. both the amplitudes of states and the operators coincide in these two representations. However, at subsequent moments of time, we encounter two different situations. In the Schrödinger representation the amplitude of state changes, while the operator remains the same as it was at the moment t_0; in the Heisenberg representation, on the contrary, the operator changes, while the amplitude of state remains the same as it was at the moment t_0. It could be said that in the Schrödinger representation the dependence on time is shifted to the amplitudes of states, and in the Heisenberg representation, to the operators.

For practical calculations, it is usually more convenient to use the Schrödinger representation. However, the Heisenberg representation has the advantage that it permits us to draw a mathematical analogy between quantum mechanics and classical mechanics. In Heisenberg's representation the quantum-mechanical relations have the form of classical relations, in which the physical quantities are replaced by operators (in this connection, we recall the last item of Sec. 20).

Schrödinger, when he introduced in 1926 the representation now named after him, considered the time-dependent amplitudes of states as the amplitudes of certain waves, and thus gave birth to the subject of "wave mechanics". A year earlier, Heisenberg proposed his method of describing the evolution of microsystems with time, thus introducing for the first time equation (26.13) in matrix form. This gave rise to the subject of "matrix mechanics". The difference between both these subjects is reduced to the above-mentioned difference between the Schrödinger and the Heisenberg representations, i.e. it is of a strictly formal, mathematical nature.

Interaction Representation (Dirac Representation)

Suppose that the Hamiltonian of a microsystem can be broken into two components, one of which ($\hat{H}_0$) represents the Hamiltonian of the microsystem itself, and the other ($\hat{H}_1$) describes the interaction of the initial microsystem with external fields or other systems (in other words, is "responsible" for the effect of perturbation of the initial microsystem):

$$\hat{H}(x, t) = \hat{H}_0(x) + \hat{H}_1(x, t). \tag{26.14}$$

In this case, it is convenient to use the *interaction representation* introduced by Dirac.

The amplitude of state $\Psi(x, t)$ in the interaction representation is expressed through the amplitude of state $\psi(x, t)$ in the Schrödinger representation in the following way:

$$\Psi(x, t) = \exp\left[\frac{i}{\hbar}\hat{H}_0(x)(t-t_0)\right]\psi(x, t). \tag{26.15}$$

In accordance with (17.32) we find from here the form of the operator $\hat{L}_B(x, t)$ in the interaction representation:

$$\hat{L}_B(x, t) = \exp\left[\frac{i}{\hbar}(t-t_0)\hat{H}_0(x)\right]\hat{L}(x) \times \exp\left[-\frac{i}{\hbar}(t-t_0)H_0(x)\right]. \tag{26.16}$$

We emphasize that in (26.15) and (26.16) we have used not the entire Hamiltonian, but just its "unperturbed" component $\hat{H}_0(x)$. Differentiating (26.15) with respect to time, we get

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = -\hat{H}_0(x)\Psi(x, t)$$
$$+ i\hbar \exp\left[\frac{i}{\hbar}(t-t_0)\hat{H}_0(x)\right]\frac{\partial}{\partial t}\psi(x, t).$$

Since

$$i\hbar \frac{\partial}{\partial t}\psi(x, t) = [\hat{H}_0(x) + \hat{H}_1(x, t)]\psi(x, t),$$

the last result can be written in the following form:

$$i\hbar \frac{\partial}{\partial t}\Psi(x, t) = \exp\left[\frac{i}{\hbar}(t-t_0)\hat{H}_0(x)\right]\hat{H}_1(x, t)\psi(x, t)$$
$$= \exp\left[\frac{i}{\hbar}(t-t_0)\hat{H}_0(x)\right]\hat{H}_1 \exp\left[-\frac{i}{\hbar}(t-t_0)\hat{H}_0(x)\right]$$
$$\times \Psi(x, t) = \hat{H}_1^B(x, t)\Psi(x, t). \quad (26.17)$$

Combining the results obtained above, we write the quantum-mechanical equations of motion in the interaction representation as

$$i\hbar \frac{\partial}{\partial t}\hat{L}_B(x, t) = [\hat{L}_B(x, t), \hat{H}_0(x, t)], \quad (26.18)$$

$$i\hbar \frac{\partial}{\partial t}\Psi(x, t) = \hat{H}_1^B(x, t)\Psi(x, t) \quad (26.19)$$

[note that (26.18) is obtained as a result of differentiation of (26.16) with respect to time].

Thus, in the interaction representation, the dependence of the amplitude of state on time is determined by the interaction (perturbation) Hamiltonian $\hat{H}_1^B$, while the time dependence of the operator is determined by the "unperturbed" Hamiltonian $\hat{H}_0$. In this sense the interaction representation lies in between the Schrödinger and the Heisenberg representations.

On the Vector Analogy Again

The vector analogy enables us to compare quite clearly all the three representations considered above. We correlate the system of basic states of the microparticle with the system of mutually orthogonal basic vectors in some arbitrary space. We shall consider all operators in matrix form defined by the system of basic vectors. The states of the microparticle are described by vectors considered in the coordinate system defined by the basic vectors. Thus we have a system of basic vectors and a set of vector states to be considered relative to this system.

We now turn to various representations. In Schrödinger's representation the evolution of a microparticle with time assumes a rotation of the vector state relative to the stationary system of basic vectors. In the Heisenberg representation the evolution of a microparticle with time assumes, on the contrary, a rotation of the system of basic vectors relative to the stationary vector state. Finally, in the interaction representation we assume a rotation of both the system of basic vectors and the vector state. Moreover, the rotation of the vector state is caused exclusively by the interaction of the microparticle with the external fields (perturbation) and is therefore dynamic in nature. The rotation of its system of basic vectors, however, is not related to the external factors, and is kinematic in nature.

One Additional Remark

The methods of describing the evolution of microsystems with time considered above are based on the use of the quantum-mechanical equations of motion. They assume a continuous evolution in time of either amplitudes of states or of certain Hermitian operators, or simultaneously of the amplitudes of states and the operators both. However, there are other qualitatively different processes. Thus, it is well known that a destruction of the superposition of states caused by the detector in the act of measurement leads to an *abrupt* change in the amplitude of state. It is obvious that this change in the amplitude does not follow any equation of motion and obeys only probabilistic predictions.

In this connection two types of process are distinguished in quantum mechanics: processes associated with a continuous change in the amplitude of state in accordance with the equation of motion, and those connected with abrupt, unpredictable, unambiguous changes in the amplitude of state in the act of measurement. In the existing quantum-mechanical apparatus processes of the *first* kind are mainly involved. A considerable increase in recent times in the interest in quantum-mechanical problems of measurement indicates the starting point of serious research into processes of the *second* type (in this connection see the remarks about the problem of measurement in quantum mechanics in [42]).

It is often believed that the probabilistic interpretation of quantum mechanics is limited by the introduction of probability amplitudes, since the latter can be predicted unambiguously from a solution of the Schrödinger equation. Such a belief, as can be easily seen, is associated with a fact that the above-mentioned processes of the second type are not taken into account. Undoubtedly, these processes intensify and complicate the probability aspect of quantum mechanics since they point to the necessity of considering a sort of "secondary probability"—the probability of the realization of the amplitude of probability.

It must be admitted that the theory of quantum-mechanical measurement is still far from complete; processes of the second type have not been sufficiently incorporated into the apparatus of quantum mechanics. This means that modern quantum mechanics, in spite of its strictness and indisputable mathematical beauty, "conceals" unsolved problems, which predetermine its further development as a physical theory.

On the History of Origin and Growth of Quantum Mechanics

(A Brief Historical Survey)

"*The Crisis in Physics*". 19th century was an era of rapid growth in physics. It is enough to mention just a few areas: the achievements in electricity and magnetism which led to Maxwell's electromagnetic field theory and permitted the inclusion of optics into the framework of electromagnetic phenomena; the significant progress in the development of classical mechanics which came close to perfection as the result of a number of brilliant mathematical works; the enunciation of many universal principles in physics, of prime importance among them being the law of conservation and transformation of energy. It is not astonishing that towards the end of the 19th century it was generally believed that the description of the laws of nature was in a final stage. In this respect the famous remarks of Planck are worth noting. After defending his Ph.D. thesis, Planck wrote to his teacher and mentor Philip Jolly asking his advice as to whether he should seek a career in theoretical physics. *Young man*, replied Jolly, *Why do you want to ruin your life? The theoretical physics is practically finished, the differential equations have all been solved. All that is left now is to consider individual special cases involving variations of initial boundary conditions. Is it worthwhile taking up a job which does not hold any prospects for the future?*

In the August of 1900, the celebrated mathematician Hilbert presented his famous 23 problems before the Second International Congress of Mathematicians. One of these problems (the sixth one) pertained to axiomation in physics. Hilbert proposed that a finite number of initial axioms should be formulated so that all the results needed for a *complete* description of the physical picture of the world could be obtained from them by purely logical means. The very fact that such a problem was stated speaks in most convincing manner of the belief held by scientists at the time that a final description of physical phenomena was at hand.

Events which followed dispelled such illusions very soon. At the turn of the 20th century a number of fundamental discoveries which could not be contained within the framework of the existing theories in physics were reported. The list of these discoveries was quite imposing: X-rays, the dependence of the mass of an electron on its velocity, the incomprehensible laws of the photoelectric effect, radioactivity, etc. It appeared that nature had decided to "laugh" at the self-confidence of people who thought they had uncovered all its secrets.

Such an unexpected turn of events forced many physicists and philosophers to speak of a *collapse* of the earlier foundations, of the impossibility of knowing everything about matter, of the absence of objective laws of nature, of the "disappearance of mass", etc. The earlier unanimity was replaced by sharp differences of opinion about fundamental ideas.

In his book "Materialism and Empiriocriticism" published in 1908, V I. Lenin called this period in the development of physics a period of "crisis in physics": *The essence of the crisis in modern physics consists in the break-down of the old laws and basic principles, in the rejection of an objective reality existing outside the mind, that is, in the replacement of materialism by idealism and agnosticism. 'Matter has disappeared'—one may thus express the fundamental and characteristic difficulty in relation to many particular questions which has created this crisis.*

Analysing the causes that led to this crisis, Lenin wrote: *It is mainly because the physicists did not know dialectics that the new physics strayed into idealism.*

Defending the dialectical point of view, Lenin emphasized that *'Matter disappears' means that the limit within which we have hitherto known matter disappears and that our knowledge is penetrating deeper.*

Lenin pointed out that the period of crisis will culminate in a new leap in the development of physics and that its further development will occur on the lines of materialistic dialectics. He wrote: *Modern physics is in travail; it is giving birth to dialectical materialism. The process of child-birth is painful.*

Looking back, we can now say that this "travail" led also to the birth of quantum mechanics. As Lenin envisaged, the overcoming of this "crisis in physics" resulted in a *deepening* of our knowledge of matter, and demanded a decisive turn from metaphysical to dialectical ideas. This was reflected most clearly in the quantum-mechanical concepts. We have every reason to associate quantum mechanics with a *qualitative leap* in our knowledge about nature (see Sec. 16).

Considering the history of the initial period of quantum mechanics, we can isolate three distinct stages. The *first stage*: end of 19th century-1912 (first experiments and first attempts to explain them). The *second stage*: 1913-1922 (Bohr's quantum theory). The *third stage*: 1923-1927 (establishment of quantum mechanics). We shall now proceed to study these three stages in detail.

First Experiments and First Attempts to Explain Them (end of 19th century-1912). The foundations of quantum mechanics were laid by experiments conducted at the end of the 19th century and the beginning of the 20th century in various branches of physics which at that time were not connected with one another, e.g. atomic spectroscopy, study of black body radiation and the photoelectric effect, solid state physics, study of the structure of atom. By the end of the 19th century a lot of experimental material on the *radiation spectra of atoms* was accumulated. It turned out that atomic spectra are ordered sets of discrete lines (series). In 1885, Balmer discovered a series of lines of atomic hydrogen, later named after him, that could be described by a simple formula. In 1889, Rydberg found a series of lines for thallium and mercury. Extensive studies of the spectra of different atoms were conducted during this period by Kaiser and Runge who used photographic methods. In 1904, Lyman discovered a series of hydrogen lines falling in the ultraviolet region of the spectrum and in 1909, Paschen found a hydrogen series in the infrared region of the spectrum. Remarkably, the Lyman and Paschen series could be described by a formula which was very close to the one established earlier by Balmer. Noticing the regularities among various series of an atom, Ritz in 1908 formulated his famous *combination principle* (see Sec. 2). However, right until 1913, this formula could not be explained, the nature of the spectral lines remained unclear.

Wien in 1896, studying *black body radiation*, derived a formula which accounted for the experimental results obtained for high radiation frequencies quite accurately (*Wien's law*). This formula, however, was not applicable for lower frequencies. In 1900, Rayleigh proposed a formula which agreed fairly well with experiments for low frequencies (the *Rayleigh-Jeans law*) but led to absurd results for higher frequencies (this situation was known as 'ultraviolet catastrophe'). In the same year Lummer and

Pringsheim conducted detailed experimental studies over a wide frequency range. In order to explain the results obtained by Lummer and Pringsheim, Planck proposed his famous empirical formula which transformed into Wien's and Rayleigh's formulae in the corresponding limiting cases.

The formula proposed by Planck contained a certain constant, which he called an *elementary quantum of action* (i.e., the Planck's constant $\hbar$). According to Planck (see [44]), *Either the quantum of action was a fictitious quantity, in which case all the deductions from the radiation theory were largely illusory and were nothing more than mathematical juggling. Or the radiation theory is founded on actual physical ideas, and then the quantum of action must play a fundamental role in physics, and proclaim itself as something quite new and hitherto unheard of, forcing us to recast our physical ideas, which, since the foundation of the infinitesimal calculus by Leibniz and Newton, were built on the assumption of continuity of all causal relations.*

After a careful consideration of his formula, Planck arrived at a brilliant conclusion: it must be assumed that every radiating atom in a solid emits energy only *discretely, in quanta*, the energy of an individual quantum being equal to $\hbar\omega$. This resulted in the historic paper by Planck *Theory of the Law of Distribution of Energy in a Normal Spectrum*, which he presented before the Berlin Academy of Sciences on 14th December, 1900. This day may, in fact, be considered as the birthday of quantum mechanics.

Planck's discovery was in sharp contradiction with the classical theory. It must be admitted that this was at first disturbing for Planck himself. In an attempt to reconcile his discovery with classical concepts, Planck proposed in 1911 a hybrid conception. According to this conception, only the emission process in radiation is discrete while the processes of propagation and absorption of radiation are continuous ones.

Planck's hybrid hypothesis got no recognition. Earlier, in 1905, Einstein gave a brilliant explanation of all the laws of the *photoelectric effect* known at that time by assuming that light is emitted as well as absorbed discretely. Later, in 1917, Einstein came to the conclusion that a light quantum possesses not only a definite *energy* but also a definite *momentum* equal to $\hbar\omega/c$.

In 1907, Einstein successfully applied the idea of quantization to solve an important problem in solid-state physics which had baffled scientists for many years. Physicists in the 19th century had faced a violation of the classical law by Dulong and Petit. It was observed that the specific heat of solids is not constant but decreases upon a considerable lowering of temperature. As an example, let us consider the experiments conducted by Weber in 1875. He discovered a temperature dependence of the specific heat of boron, carbon and silicon. The fact that specific heats of solids depend on temperature could not be explained within the framework of classical theory until the appearance in 1907 of Einstein's paper *Correlating Planck's Radiation Theory and the Specific Heat Theory*. Applying Planck's idea of quantization of energy to atomic vibrations in crystals, Einstein deduced a formula which, in agreement with experiment, described the temperature dependence of the specific heat of solids. Einstein's work laid the foundation of the modern theory of the specific heat of solids.

Finally, we must mention *studies of the atomic structure* whose origin can be tracted to the year 1904 when Thomson proposed a model for the hydrogen atom in the form of a uniformly positively charged sphere with one electron at the centre. Later, Thomson came to the conclusion that the number of electrons in an atom must be proportional to the atomic weight and that the stability of the atom is impossible without the motion of the electrons. In 1908 Geiger and Marsden began studies on the scattering of α-particles passing through thin foils of different metals. They discovered that most of the α-particles pass through the foil without being scattered while some α-particles, roughly one in ten thousand, are strongly deflected (by an angle greater than 90°). In 1911, Rutherford came to the conclusion that the strong deflection of an α-particle occurs not as a result of many collisions, but in a single act of collision with an atom and, consequently, there must be a small positively charged nucleus at the centre of the atom, containing almost the entire mass of the atom. This was a decisive step towards the creation of the *planetary model of the atom* which Rutherford finally formulated in 1913.

Thus, from the end of the 19th century to the year 1913 a large number of experimental facts, which could not be explained on the basis of existing theory, were accumulated: the discovery of ordered series in atomic spectra, the discovery of the quantization of energy in black body radiation, the photoelectric effect, and the specific heat of solids; also the planetary model of the atom was created. However, until 1913, all these discoveries were considered separately. It was Bohr's genius that understood the common character of these facts and created a fairly harmonious quantum theory on the atom based on these facts.

Bohr's Quantum Theory (1913-1922). Bohr's famous paper *On the Constitution of Atoms and Molecules* appeared in 1913. It considered the theory of the planetary model of the hydrogen atom based on the idea of quantization (the energy and the angular momentum of an electron in an atom were quantized). Resolutely departing from accepted concepts, Bohr's theory ruled out a direct link between the frequency of the radiation emitted by an atom and the frequency of the rotation of the electron in the atom. Having acquainted himself with Bohr's theory, Einstein remarked: *Then the frequency of light does not depend at all on the frequency of the electron.... This is an enormous achievement!* In fact, Bohr's frequency rule provided a convincing explanation for Ritz' combination principle and permitted calculations of the Rydberg constant. Later, in 1945, referring to Bohr's theory, Einstein wrote: *This insecure and contradictory foundation sufficient to enable a man of Bohr's unique instinct and tact to discover the major laws of spectral lines and of the electron-shells of the atoms together with their significance for chemistry appeared to me like a miracle and appears to me as a miracle even today. This is the highest form of musicality in the sphere of thought.*

Experiments conducted in 1914 gave *direct* experimental evidence for the fact that an atom may change its energy only discretely. These were the famous experiments by Franck and Hertz on the measurement of the electron energy spent on exciting mercury atoms.

In 1915-1916, Sommerfeld developed Bohr's theory. In particular, he generalized the method of quantization for the case of systems having more than one degree of freedom, by changing from circular orbits to elliptical ones, and studied the precession of an elliptical orbit in its own plane. In 1916 Debye and Sommerfeld came to the conclusion that the angular momentum components in the direction of a magnetic field are quantized, thus introducing the concept of *quantization in space.* This received excellent confirmation later in the experiments of Stern and Gerlach (1921) on the splitting of atomic beams in nonuniform magnetic fields.

Continuing his researches in the field of quantum theory of atoms, Bohr in 1918 introduced the famous *correspondence principle* (in his article *On the Quantum Theory of Line Spectra*) which he had been using in fact since 1913. According to this principle, the laws of quantum physics must turn into the laws of classical physics for large values of quantum numbers of a system, i.e. if the relative values of the quantum of action are negligibly small. It follows from this that classical physics is of great importance in the discovery of laws of quantum mechanics. The period from 1913 to the early twenties can be considered as the period of the creation and development of Bohr's quantum theory. The achievements of this theory are beyond a shadow of doubt. It served as the most important step towards the creation of quantum mechanics. However, in the course of the development of Bohr's theory, its internal contradictions associated to a considerable extent with contradictions in the very idea of quantization and of "quantum jumps" (see Sec. 2) became more and more apparent. The theory clearly betrayed a stage of crisis. A further development of quantum mechanics demanded an overcoming of this crisis and the introduction of new ideas. As was mentioned in Sec. 2, these contradictions were overcome by introducing the idea of wave-particle duality. By eliminating the contradictions of the "old quantum theory" the idea of duality marked the beginning of a new stage in the establishment of quantum mechanics as a genuine theory in physics, culminating in the creation of its apparatus, and, consequently, in the solution of a number of problems of atomic and nuclear physics.

The Growth of Quantum Mechanics (1923-1927). In 1923, Compton discovered the effect, later named after him, of a decrease in the wavelength of X-rays upon scattering by matter. This effect clearly indicated the existence of wave as well as corpuscular properties of radiation. Light quanta were introduced into physics as elementary particles once and for all under the name of *photons.*

In 1923-1924, de Broglie suggested in his doctoral thesis that the idea of wave-particle duality should be extended to all microparticles, associating both wave and corpuscular characteristics with every particle (see Sec. 2). Later (in 1927), the idea of duality received a convincing confirmation by experiments on electron diffraction conducted simultaneously in several different laboratories. In 1925 de Broglie introduced the concept of "matter waves" described by the so-called *wave function.*

The combination of the idea of quantization with the idea of wave-particle duality proved to be very fruitful for the development of quantum mechanics. The whole *apparatus* of quantum mechanics was, in fact, built in 1925-1926. Heisenberg in 1925 took the first step in this direction. He suggested that every quantized dynamic variable should be represented in the form of some *matrix* whose diagonal elements are essentially the experimentally observed values of the variable (the reader is familiar with this approach for the case of the Hamiltonian, or energy, matrix which has been discussed in detail in the book). Using the correspondence principle, Heisenberg converted the matrix relations into classical relations for corresponding variables. In doing so, however, Heisenberg took into account the possibility of the commutativity of the product of the matrices involved. In 1926, Schrödinger in his paper *On Quantization as an Eigenvalue Problem* used the wave concepts to introduce his well-known differential equation for a wave function (this equation is now termed the *Schrödinger equation*). The problem of calculating the energy levels of a bound microparticle was reduced by Schrödinger to the problem of finding eigenvalues.

After the appearance of Schrödinger's work, it was at first believed that we now had two independent theories, Schrödinger's *wave mechanics* and Heisenberg's *matrix mechanics.* However, already in 1926, Schrödinger showed that both these theories are, in fact, equivalent and are just two different ways of looking at the same problem. It should be mentioned that the wave formalism of Schrödinger's theory was very well received, since it enabled a solution of quantum-mechanical problem with the help of established methods of *mathematical physics.* Planck's opinion [46] of Schrödinger equation is worth noting. According to him, the fundamental importance of this differential equation lies not only in the way it has been derived, but also in its physical interpretation, whose details are still not clear. But most important is the fact that owing to the introduction of the quantum law into the well-known system of usual differential equations, we get an entirely new method which, with the help of mathematics, can solve the complicated quantum-mechanical problem. This is the first case when a quantum of action, which thus far was impervious to all attempts to look at it from the point of view of classical physics, can be included in a differential equation.

While the formalism of Schrödinger's theory was readily accepted, the problem of the interpretation of wave mechanics and the physical description of the concept of the "wave function" remained the subject of heated discussion for a long time. In 1926, Born proposed a *probability* interpretation of the wave function; "matter waves" were replaced by "probability waves" The impossibility of interpreting the wave function as the amplitude of a certain material field (like the electromagnetic or the gravitational fields) was recognized even at that time. Planck in 1928, commenting on the nature of the wave function, wrote (see [46]) that the impossibility of a physically intuitive representation of this quantity, which only has an indirect symbolic meaning, is a direct consequence of the fact that the wave motion takes place not in the ordinary three-dimensional space, but in the so-called configurational space, where the dimensionality is determined by the number of degrees of freedom of the system being considered.

This meant that de Broglie waves could not be interpreted as classical waves of some sort.

The next important step towards the development of quantum mechanics, which revealed its physical and philosophical aspects, was made in 1927 by Heisenberg who introduced his famous *uncertainty relation*. Through these relations Heisenberg showed how the concepts of energy, momentum, coordinate, etc. should be applied to the case of microparticles (see Sec. 3). The appearance of the uncertainty relations marked a final break of quantum mechanics from classical determinism, thus establishing quantum mechanics as a statistical theory. Starting from the uncertainty relations, Bohr formulated in the same year one of the leading discoveries of 20th century, i.e. the *complementarity principle* (see Sec. 16).

The twenties was undoubtedly a period of most intensive development of quantum mechanics. It is impossible to describe here all the important researches conducted during this period. We shall simply mention a few points below to supplement the above picture.

In 1924, Pauli proposed that an electron could be assigned an additional (fourth) degree of freedom which can have two values. Uhlenbeck and Goudsmit, using Pauli's idea, introduced in 1925 the concept of a "spinning electron" (in other words, the *spin* concept).

In 1924, Bose carried out fundamental studies, which were extended by Einstein in the form of a statistical theory for photons which came to be known as *Bose-Einstein statistics*. In the framework of this theory, Planck's formula for black-body radiation at last found a complete explanation.

In 1925, Pauli formulated his famous *exclusion principle* for electrons.

In 1925, Born and Jordan formulated Heisenberg's theory in matrix form.

In 1925, Dirac developed the *relativistic* theory of electron and hydrogen-like atoms.

In 1926, Fermi and Dirac carried out fundamental studies on the statistical theory of electrons, later called the *Fermi-Dirac statistics.*

Naturally, the history of the development of quantum mechanics did not terminate in 1927. In the following years, quantum mechanics was enriched by many new methods, applications, and most importantly by further studies of its physical and philosophical aspects. Some problems of quantum mechanics (above all, the problem of measurement) are still being investigated. However, we shall end our brief historical discussion with the year 1927, assuming that further developments in quantum mechanics form the subject of a special study.

Readers who want to go further into details concerning the origin and development of quantum mechanics are advised to refer to [47-50].

Appendix A

Eigenvalues and Eigenfunctions of a Hermitian Operator

Theorem: An operator has real values if and only if it is Hermitian.
Proof: From (17.13) we get

$$\int \psi^*(x)\,\hat{L}\psi(x)\,dx=\lambda\int \psi^*(x)\,\psi(x)\,dx,$$

or

$$\int \psi(x)\,\hat{L}^*\psi^*(x)\,dx=\lambda^*\int \psi(x)\,\psi^*(x)\,dx.$$

It follows hence that

$$\int \psi^*\hat{L}\psi\,dx-\int \psi\hat{L}^*\psi^*\,dx=(\lambda-\lambda^*)\int \psi^*\psi\,dx.$$

Thus

$$\int \psi^*(\hat{L}-\hat{L}^+)\,\psi\,dx=(\lambda-\lambda^*)\int \psi^*\psi\,dx.$$

It can be seen from here that the equality $\lambda = \lambda^*$ (denoting the real positive eigenvalues) is satisfied if and only if the operator $\hat{L}$ is Hermitian (i.e. if and only if $\hat{L} = \hat{L}^+$).
Theorem: The eigenfunctions of a Hermitian operator which correspond to different eigenvalues are mutually orthogonal.
Proof: Using (17.13), we write

$$\hat{L}\psi_n=\lambda_n\psi_n;\qquad \hat{L}^*\psi_m^*=\lambda_m^*\psi_m^*,$$

or

$$\int \psi_m^*\hat{L}\psi_n\,dx=\lambda_n\int \psi_m^*\psi_n\,dx;$$

$$\int \psi_n\hat{L}^*\psi_m^*\,dx=\lambda_m^*\int \psi_n\psi_m^*\,dx.$$

It follows from here that

$$\int \psi_m^*(\hat{L}-\hat{L}^+)\,\psi_n\,dx=(\lambda_n-\lambda_m^*)\int \psi_m^*\psi_n\,dx.$$

If the operator $\hat{L}$ is Hermitian, then $\hat{L} = \hat{L}^+$ (and also $\lambda_m^* = \lambda_m$). In this case the last equality acquires the form

$$(\lambda_n-\lambda_m)\int \psi_m^*\psi_n\,dx=0.$$

Since $\lambda_n \neq \lambda_m$, we get

$$\int \psi_m^*\psi_n\,dx=0.$$

Appendix B

Transition from Quantum Mechanics to Classical Mechanics

There is a formal analogy between the transition from quantum mechanics to classical mechanics and the transition from wave optics to geometrical optics (i.e. the optico-mechanical analogy); see, for example, [10, 11]. A transition to geometrical optics means that the optical field is described by nearly plane waves of the type

$$e^{i\Phi} = e^{i(\vec{k}\vec{r} - \omega t)}. \tag{B.1}$$

It can be seen from (B.1) that

$$\vec{k} = \nabla\Phi; \qquad \omega = -\frac{\partial\Phi}{}. \tag{B.2}$$

The vector $\vec{k}$ is directed along the light beam. At every point in space the light beam is perpendicular to the surface of constant phase (i.e. perpendicular to the surface $\Phi = \text{const}$).

When going over to classical mechanics, the quantum-mechanical wave function must acquire a form analogous to (B.1); moreover, the phase of the wave function will be proportional to the mechanical action S:

$\Phi = AS.$

The momentum $\vec{p}$ and energy E of a particle are expressed through the action S in the following way:

$$\vec{p} = \nabla S; \qquad E = -\frac{\partial S}{\partial t} \tag{B.3}$$

The trajectories are lines perpendicular to the surface of constant action (in the same way as the light rays are perpendicular to the urface of constant phase). Comparing (B.2) and (B.3) and taking into account that $\vec{p} = \hbar\vec{k}$, we find that

$\Phi = S/\hbar.$

Thus the quasiclassical wave function is of the form

$$\psi = ae^{iS/\hbar}. \tag{B.4}$$

By using (B.4) it is easy to determine the coefficient γ in the expression for the momentum operator

$\hat{\vec{p}} = \gamma\nabla.$

Let us consider the equation for the eigenfunctions of the momentum operator (the equation $\hat{\vec{p}}\psi = \vec{p}\psi$) in the quasiclassical case. In this case we get $\vec{p} = \nabla S$, $\psi = ae^{iS/\hbar}$. Thus the above equation assumes the form

$\gamma\nabla e^{iS/\hbar} = \nabla S e^{iS/\hbar}$

or

$$\gamma e^{iS/\hbar}\nabla S\,\frac{i}{\hbar}=\nabla S\cdot e^{iS/\hbar}.$$

It can be easily seen that $i\gamma/\hbar = 1$, and, consequently, $\gamma = -i\hbar$. The quasiclassical case may be used to substantiate the Schrödinger equation. It can be easily seen that the well-known classical Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t}+\frac{1}{2m}(\nabla S)^2+U=0$$

s a limiting case of the Schrödinger equation (20.17). By putting $\Psi = e^{iS/\hbar}$, we get in this case

$$i\hbar\frac{\partial}{\partial t}\Psi=-\frac{\partial S}{\partial t}e^{iS/\hbar};$$

$$-\frac{\hbar^2}{2m}\Delta\Psi=-\frac{\hbar^2}{2m}\nabla(\nabla\Psi)=-\frac{\hbar^2}{2m}$$

$$\times\nabla\left(\frac{i}{\hbar}\nabla S\cdot e^{iS/\hbar}\right)=-i\frac{\hbar}{2m}\Delta S\cdot e^{iS/\hbar}+\frac{1}{2m}(\nabla S)^2e^{iS/\hbar}.$$

Substituting these results into (20.17) and neglecting terms containing Planck's constant in the expression for $\Delta\Psi$, we get the equation

$$-\frac{\partial S}{\partial t}e^{iS/\hbar}=\frac{1}{2m}(\nabla S)^2e^{iS/\hbar}+Ue^{iS/\hbar}.$$

By cancelling out the factor $e^{iS/\hbar}$, this equation becomes the Hamilton-Jacobi equation.

Appendix C

Commutation Relations

We shall show how the commutation relations (20.28)-(20.30) can be derived. To start with we remark that the equality $\hat{\vec{M}} = (\hat{\vec{r}}\times\hat{\vec{p}})$ may be written in the form

$$\hat{M}_i=\sum_{k=1}^{3}\sum_{n=1}^{3}e_{ikn}\hat{r}_k\hat{p}_n, \qquad \text{(C.1)}$$

where e_{ikn} is a unit antisymmetric tensor of the 3rd rank ($e_{123} = e_{231} = e_{312} = 1$, $e_{132} = e_{321} = e_{213} = -1$, all the other components of the tensor are equal to zero).

Let us consider the commutator $[\hat{M}_i, \hat{r}_j]$. By using (C.1), we can write this commutator in the following form:

$$\hat{M}_i,\ \hat{r}_j]=\hat{M}_i\hat{r}_j-\hat{r}_j\hat{M}_i=\sum_k\sum_n e_{ikn}(\hat{r}_k\hat{p}_n\hat{r}_j-\hat{r}_j\hat{r}_k\hat{p}_n).$$

Taking into account that $\hat{r}_j\hat{r}_k = \hat{r}_k\hat{r}_j$, we get

$$[\hat{M}_i,\ \hat{r}_j] = \sum_k \sum_n e_{ikn}\hat{r}_k\,[\hat{p}_n,\ \hat{r}_j].$$

According to (20.26), $[\hat{p}_n,\ \hat{r}_j] = -i\hbar\delta_{nj}$. This leads to the required relation (20.28):

$$[\hat{M}_i,\ \hat{r}_j] = -i\hbar\sum_k e_{ikj}\hat{r}_k = i\hbar\sum_k e_{ijk}\hat{r}_k.$$

This relation means that

$$[\hat{M}_1,\ \hat{r}_2] = i\hbar\hat{r}_3,$$

$$[\hat{M}_2,\ \hat{r}_3] = i\hbar\hat{r}_1,$$

$$[\hat{M}_3,\ \hat{r}_1] = i\hbar\hat{r}_2,$$

$$[\hat{M}_1,\ \hat{r}_1] = [\hat{M}_2,\ \hat{r}_2] = [\hat{M}_3,\ \hat{r}_3] = 0.$$

Next let us consider the commutator $[\hat{M}_i,\ \hat{p}_j]$. By using (C.1), we can write it in the form

$$[\hat{M}_i,\ \hat{p}_j] = \sum_k \sum_n e_{ikn}(\hat{r}_k\hat{p}_n\hat{p}_j - \hat{p}_j\hat{r}_k\hat{p}_n).$$

Taking into account that $\hat{p}_n\hat{p}_j = \hat{p}_j\hat{p}_n$, we get

$$[\hat{M}_i,\ \hat{p}_j] = \sum_k \sum_n e_{ikn}\,[\hat{r}_k,\ \hat{p}_j]\,\hat{p}_n.$$

According to (20.26), $[\hat{r}_k,\ \hat{p}_j] = i\hbar\delta_{kj}$. As a result, we get the required relation (20.29):

$$[\hat{M}_i,\ \hat{p}_j] = i\hbar\sum_n e_{ijn}\hat{p}_n.$$

Thus

$$[\hat{M}_1,\ \hat{p}_2] = i\hbar\hat{p}_3,$$

$$[\hat{M}_2,\ \hat{p}_3] = i\hbar\hat{p}_1,$$

$$[\hat{M}_3,\ \hat{p}_1] = i\hbar\hat{p}_2,$$

$$[\hat{M}_1,\ \hat{p}_1] = [\hat{M}_2,\ \hat{p}_2] = [\hat{M}_3,\ \hat{p}_3] = 0.$$

Going over to the commutator $[\hat{M}_i,\ \hat{M}_j]$, we shall restrict ourselves for simplicity to the case when $i = 1$, $j = 2$. Using

$$\hat{M}_1 = \hat{r}_2\hat{p}_3 - \hat{r}_3\hat{p}_2, \qquad \hat{M}_2 = \hat{r}_3\hat{p}_1 - \hat{r}_1\hat{p}_3,$$

we can write

$$[\hat{M}_1,\ \hat{M}_2] = (\hat{r}_2\hat{p}_3 - \hat{r}_3\hat{p}_2)(\hat{r}_3\hat{p}_1 - \hat{r}_1\hat{p}_3) - (\hat{r}_3\hat{p}_1 - \hat{r}_1\hat{p}_3)$$
$$\times(\hat{r}_2\hat{p}_3 - \hat{r}_3\hat{p}_2) = \hat{r}_2\hat{p}_3\hat{r}_3\hat{p}_1 - \hat{r}_2\hat{p}_3\hat{r}_1\hat{p}_3 - \hat{r}_3\hat{p}_2\hat{r}_3\hat{p}_1$$
$$+\hat{r}_3\hat{p}_2\hat{r}_1\hat{p}_3 - \hat{r}_3\hat{p}_1\hat{r}_2\hat{p}_3 + \hat{r}_3\hat{p}_1\hat{r}_3\hat{p}_2 + \hat{r}_1\hat{p}_3\hat{r}_2\hat{p}_3 - \hat{r}_1\hat{p}_3\hat{r}_3\hat{p}_2.$$

Note that $\hat{r}_2\hat{p}_3\hat{r}_1\hat{p}_3 = \hat{r}_1\hat{p}_3\hat{r}_2\hat{p}_3$ and $\hat{r}_3\hat{p}_2\hat{r}_3\hat{p}_1 = \hat{r}_3\hat{p}_1\hat{r}_3\hat{p}_2$.

By taking this into account, we write the expression for $[\hat{M}_1 \hat{M}_2]$:

$$[\hat{M}_1, \hat{M}_2] = (\hat{r}_2\hat{p}_3\hat{r}_3\hat{p}_1 - \hat{r}_3\hat{p}_1\hat{r}_2\hat{p}_3) + (\hat{r}_3\hat{p}_2\hat{r}_1\hat{p}_3 - \hat{r}_1\hat{p}_3\hat{r}_3\hat{p}_2)$$

$$= \hat{r}_2\hat{p}_1(\hat{p}_3\hat{r}_3 - \hat{r}_3\hat{p}_3) + \hat{r}_1\hat{p}_2(\hat{r}_3\hat{p}_3 - \hat{p}_3\hat{r}_3).$$

Since $\hat{r}_3\hat{p}_3 - \hat{p}_3\hat{r}_3 = i\hbar$, we finally obtain

$$[\hat{M}_1, \hat{M}_2] = i\hbar(\hat{r}_1\hat{p}_2 - \hat{r}_2\hat{p}_1) = i\hbar\hat{M}_3 .$$

Proceeding in the same way, it can be easily seen that

$$[\hat{M}_2, \hat{M}_3] = i\hbar\hat{M}_1,$$

$$[\hat{M}_3, \hat{M}_1] = i\hbar\hat{M}_2.$$

All these results can be combined in the relation (20.30).

Appendix D

Commutation of Operators $\hat{M}^2$ and $\hat{M}_i$

Let us consider the case when $i = 1$:

$$[\hat{M}^2, \hat{M}_1] = (\hat{M}_1^2 + \hat{M}_2^2 + M_3^2)\hat{M}_1 - \hat{M}_1(\hat{M}_1^2 + \hat{M}_2^2 + \hat{M}_3^2)$$

$$= (\hat{M}_2^2 + \hat{M}_3^2)\hat{M}_1 - \hat{M}_1(M_2^2 + \hat{M}_3^2)$$

$$= \hat{M}_2\hat{M}_2\hat{M}_1 + \hat{M}_3\hat{M}_3\hat{M}_1 - \hat{M}_1\hat{M}_2\hat{M}_2 - \hat{M}_1\hat{M}_3\hat{M}_3$$

$$= (\hat{M}_2\hat{M}_1\hat{M}_2 - i\hbar\hat{M}_2\hat{M}_3) + (\hat{M}_3\hat{M}_1\hat{M}_3 + i\hbar\hat{M}_3\hat{M}_2)$$

$$-(\hat{M}_2\hat{M}_1\hat{M}_2 + i\hbar\hat{M}_3\hat{M}_2) - (\hat{M}_3\hat{M}_1\hat{M}_3 - i\hbar\hat{M}_2\hat{M}_3) = 0.$$

Similarly, we get $[\hat{M}^2, \hat{M}_2] = 0$ and $[\hat{M}^2, \hat{M}_3] = 0$. This proves the relation (20.31).

Appendix E

Some Special Functions

Legendre Polynomials: The Legendre polynomials $P_l(x)$ may be defined as the coefficients in the expansion of the function

$$H(x, t) = (1 + t^2 - 2tx)^{-1/2}, \quad |t| < 1$$

as a power series in t:

$$(1 + t^2 - 2tx)^{-1/2} = \sum_{l=0}^{\infty} P_l(x)\, t^n \tag{E.1}$$

($-1 \leqslant x \leqslant 1$, l is a non-negative integer).

The polynomials $P_l(x)$ are the solutions of the differential equation

$$(1 - x^2)y'' - 2xy' + l(l+1)y = 0, \quad (l = 0, 1, 2, \ldots) \tag{E.2}$$

and satisfy the condition $y(1) = 1$. They can be written in the form

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} [(x^2 - 1)^l]. \tag{E.3}$$

We note that

$$P_l(1)=1, \qquad P_l(-x)=(-1)^l P_l(x),$$
$$P_0(x)=1,$$
$$P_1(x)=x,$$
$$P_2(x)=\frac{1}{2}(3x^2-1),$$
$$P_3(x)=\frac{1}{2}(5x^3-3x),$$

The Legendre polynomials are orthonormalized:

$$\int_{-1}^{1} P_l(x)\,P_{l'}(x)\,dx=\frac{2}{2l+1}\,\delta_{ll'}. \tag{E.4}$$

The basic recurrence relations are

$$(l+1)\,P_{l+1}+lP_{l-1}-x\,(2l+1)\,P_l=0,$$
$$P_l-P'_{l+1}-P'_{l-1}+2xP'_l=0,$$
$$P'_{l+1}-P'_{l-1}=(2l+1)\,P_l.$$

Associated Legendre Functions: The associated Legendre functions $P_l^m(x)$ are defined through the Legendre polynomials $P_l(x)$ in the following way:

$$P_l^m(x)=(1-x^2)^{m/2}\,\frac{d^m}{dx^m}\,P_l(x) \tag{E.5}$$

(m and l are positive integers, $m \leqslant l$),

$$P_l^0(x)=P_l(x); \quad P_l^l(x)=3\times 5\times 7\,\ldots\,(2l-1)\,(1-x^2)^{l/2}.$$
$$P_1^1(x)=(1-x^2)^{1/2},$$
$$P_2^1(x)=3x\,(1-x^2)^{1/2},$$
$$P_2^2(x)=3\,(1-x^2),$$
. . . .

The functions $P_l^m(x)$ satisfy the differential equation

$$(1-x^2)\,y''-2xy'+\left[l\,(l+1)-\frac{m^2}{1-x^2}\right]y=0. \tag{E.6}$$

They are orthonormalized:

$$\int_{-1}^{1} P_l^m(x)\,P_{l'}^m(x)\,dx=\frac{2}{2l+1}\,\frac{(l+m)!}{(l-m)!}\,\delta_{ll'}. \tag{E.7}$$

The basic recurrence relations are

$$(2l+1)\,xP_l^m(x)=(l-m+1)\,P_{l+1}^m(x)+(l+m)\,P_{l-1}^m(x),$$
$$P_{l+1}^{m+1}(x)-P_{l-1}^{m+1}(x)=(2l+1)\,\sqrt{1-x^2}\,P_l^m(x).$$

Harmonic Functions. The harmonic function $Y_{lm}(\theta, \varphi)$ is defined as the product of the Legendre associated function $P_l^{|m|}(\cos\theta)$ and the function $\exp(im\varphi)$:

$$Y_{lm}(\theta, \varphi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}\, P_l^{|m|}(\cos\theta)\, e^{im\varphi} \tag{E.8}$$

(l is a non-negative integer, $m = 0, \pm1, \pm2, \ldots, \pm l$, θ and φ are angular coordinates, $0 \leqslant \theta \leqslant \pi$, $0 \leqslant \varphi \leqslant 2\pi$). Expressions for the first few harmonic functions are given in Sec. 21 (see (21.26)). The harmonic functions satisfy the differential equation

$$\Delta_{\theta\varphi} y + l(l+1)\, y = 0, \tag{E.9}$$

where

$$\Delta_{\theta\varphi} = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right).$$

The spherical functions are orthonormalized:

$$\int_0^{2\pi}\int_0^{\pi} Y_{lm}^*(\theta, \varphi)\, Y_{l'm'}(\theta, \varphi) \sin\theta\, d\theta\, d\varphi = \delta_{ll'}\,\delta_{mm'}. \tag{E.10}$$

Hermite Polynomials. The Hermite polynomials $H_n(x)$ may be defined as expansion coefficients of the function $\exp(2xt - t^2)$:

$$\exp(2xt - t^2) = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!} \tag{E.11}$$

($-\infty < x < \infty$, n is a non-negative integer).
Hermite polynomials are described by the expression:

$$H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}. \tag{E.12}$$

$$H_n(-x) = (-1)^n H_n(x).$$

$$H_0(x) = 1,$$

$$H_1(x) = 2x,$$

$$H_2(x) = 4x^2 - 2,$$

$$H_3(x) = 8x^3 - 12x,$$

The polynomials $H_n(x)$ satisfy the differential equation

$$y'' - 2xy' + 2ny = 0 \quad (n = 0, 1, 2, \ldots). \tag{E.13}$$

They are orthonormalized:

$$\int_{-\infty}^{\infty} H_n(x)\, H_{n'}(x)\, e^{-x^2}\, dx = \sqrt{\pi}\cdot 2^n n!\; \delta_{nn'}. \tag{E.14}$$

The basic recurrence relations are

$$2xH_n - 2nH_{n-1} = H_{n+1},$$

$$2nH_{n-1} = H_n'.$$

Modified Hermite Polynomials. (*Hermite-Gauss Polynomials*). The Hermite-Gauss polynomials $h_n(x)$ are defined in terms of the Hermite polynomials $H_n(x)$ by the formula

$$h_n(x) = (2^n n! \sqrt{\pi})^{-1/2} H_n(x)\, e^{-x^2/2} \qquad \text{(E.15)}$$

The condition of orthonormalization for them has the form

$$\int_{-\infty}^{\infty} h_n(x)\, h_{n'}(x)\, dx = \delta_{nn'}. \qquad \text{(E.16)}$$

These polynomials satisfy the differential equation

$$y'' + (2n+1-x^2)\, y = 0. \qquad \text{(E.17)}$$

Appendix F

Linear Harmonic Oscillators

By taking (22.1) into account, we can write Schrödinger's equation for the oscillator:

$$\varphi''(x) + \frac{2m}{\hbar^2} E\varphi(x) - \frac{m^2\omega^2}{\hbar^2} x^2 \varphi(x) = 0. \qquad \text{(F.1)}$$

We introduce the notation

$$\xi = x\sqrt{m\omega/\hbar}, \qquad \lambda = 2E/\hbar\omega.$$

In the new notation, (F1) acquires the form

$$\varphi''(\xi) + (\lambda - \xi^2)\,\varphi(\xi) = 0. \qquad \text{(F.2)}$$

The differential equation for Hermite-Gauss polynomials is of the same form (see (E.17)). Moreover, $\lambda = 2n + 1$ and, consequently,

$$E = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2,$$

The wave function $\varphi_n(\xi)$ is apart from a constant factor a Hermite-Gauss polynomial:

$$\varphi_n(\xi) = C h_n(\xi).$$

The factor C is determined from the normalization condition for the wave function $\varphi_n(x)$:

$$\int_{-\infty}^{\infty} \varphi_n^2(x)\, dx = 1.$$

Thus

$$1=\int_{-\infty}^{\infty}\varphi_n^2(x)\,dx=\int_{-\infty}^{\infty}\varphi_n^2(\xi)\,\frac{dx}{d\xi}\,d\xi$$

$$=\sqrt{\frac{\hbar}{m\omega}}\int_{-\infty}^{\infty}\varphi_n^2(\xi)\,d\xi=\sqrt{\frac{\hbar}{m\omega}}\;C^2\int_{-\infty}^{\infty}h_n^2(\xi)\,d\xi$$

Taking (E.16) into account we conclude that $\sqrt{\frac{\hbar}{m\omega}}\,C^2=1$ and, consequently, $C=\sqrt[4]{m\omega/\hbar}$. Thus we arrive at the relation (22.3)

$$\varphi_n=\sqrt[4]{m\omega/\hbar}\,h_n(\xi)$$

$$=\sqrt[4]{\frac{m\omega}{\hbar}}\,e^{-\xi^2/2}\,H_n(\xi)\,\frac{1}{\sqrt{2^n\cdot n!\,\sqrt{\pi}}}$$

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