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BASICS OF NANOELECTRONICS

Course of lectures
for students of the first (bachelor's) level of higher education
of the educational program "Electronics"
of the field of knowledge G Engineering, manufacturing and construction
of the specialty G5 Electronics, electronic communications, instrumentation and radio engineering
of the full-time and part-time forms of study

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F 50 **Basics of nanoelectronics** [Text]: Course of lectures for students of the first (bachelor's) level of higher education of the educational program "Electronics" of the field of knowledge G Engineering, manufacturing and construction of the specialty G5 Electronics, electronic communications, instrumentation and radio engineering of the full-time and part-time forms of study / compiled by S.V. Luniov, Yu.V. Koval. – Lutsk: LNTU, 2026. – 61 p.

The publication contains educational materials on the basics of quantum mechanics, which explain quantum-dimensional effects in nanostructures, and presents the characteristics and classification of the basic elements of nanoelectronics.

1. Introduction

Scientific knowledge from the natural sciences is now beginning to represent a basic resource of the economy, surpassing material resources in significance. This kind of knowledge, together with modern technologies, forms a new lifestyle, and a highly qualified person cannot distance themselves from it. The lion's share of this knowledge comes from subjects such as physics. Physics is not only the science of nature, but is also becoming a direct productive force in human society. The close connection between physics and technology, and their interdependence, is immediately evident. It is difficult to find a branch of technology now that would not have grown out of physics. The entire history of the development of technology is an example of brilliantly implemented theoretical and experimental physical discoveries in engineering designs and technologies: the laws of thermodynamics used in heat engines; the scientific physical ideas of K.E. Tsiolkovsky, embodied in rocket technology; Maxwell and Faraday's electrodynamics became the basis of modern radio electronics; A. Einstein's theory of relativity and the discovery of uranium nuclear fission are the basis of nuclear power engineering, etc.

In connection with the above, it is now necessary to restructure the teaching of both fundamental disciplines in general and physics in particular. In the concepts of physics, the student must see not only separate bodies of knowledge but also a holistic picture of the world. This means that fundamental knowledge should be acquired not in separate clusters, but in a single, comprehensive system. A major obstacle on this path is the tendency to divide the physics course into "necessary" and "unnecessary" parts. The result is that the student, studying the individual laws, does not see a holistic physical picture of the world. We also have to deal with students who believe that physics will never be useful to them in their professional activities, despite the fact that they will be pursuing an engineering specialty. All this reduces educational motivation and lowers the quality of knowledge. A student can get a full-fledged modern idea of the world around him only by studying a complete, logically closed, holistic course of physics. According to the concept of fundamental education, formulated at the beginning of the 19th century by the philologist and philosopher Wilhelm Humboldt, the subject of study should be that fundamental knowledge emerging at the forefront of science. The beginning of the 21st century was marked by the rapid study of nanostructures and the rapid development of nanotechnologies. The theoretical basis of this area of science is solid-state physics and quantum mechanics. These sections have long been included in the physics curriculum not only for students of engineering and technical specialties, but also in the curricula of courses on the concepts of modern natural science for economists, lawyers, and a wide range of other specialties, even in the humanitarian field.

Quantum mechanics is the science of the motion of microparticles, taking into account their dual nature as particles, which originated at the beginning of the 20th century. thanks to the pioneering works of Planck, Bohr, Schrödinger, Heisenberg, Dirac, etc. If, at first, quantum mechanics had purely academic interest and was used by physicists to explain phenomena that could not be explained from the standpoint of classical physics, then, as science developed, it began to occupy an ever broader range of positions. It completely conquered spectroscopy, atomic and nuclear physics, and became an integral part of solid-state physics, chemistry, modern biophysics, and other areas of science. At present, none of the phenomena in solid-state physics can be explained without recourse to quantum mechanics. However, in microelectronics, along with quantum mechanics, classical physics is used to describe many processes; in nanoelectronics, by contrast, it is based entirely on quantum-mechanical phenomena. However, the transition from classical mechanics and electrodynamics to quantum physics poses many difficulties, primarily methodological. It is not easy to convey to students in a fairly short time the three fundamental ideas of quantum mechanics, which show its essential difference from classical mechanics:

- discreteness or quantization of energy,
- corpuscular-wave dualism or the dual nature of an electron or any other microparticle,
- the probabilistic nature of the laws of the microworld, although at the same time, the laws of conservation of energy, mass, charge, and momentum are common to both quantum and classical mechanics. Therefore, the proposed lecture texts explain in detail the foundations of quantum-mechanical concepts in various ways, including the method of primitive analogies. That is why the lecture texts are almost not mathematized. The main attention is paid to the physical essence of the phenomena of the microworld under consideration.

Currently, there are two independent, inconsistent descriptions of nature: classical mechanics and quantum mechanics. In general, this is strange and illogical, because if nature is one, then physics, the science that studies natural phenomena, must also be one.

Modern physics has influenced almost all aspects of social life. It is the basis for all natural sciences, and the combination of natural and technical sciences has radically changed the conditions of our life on Earth, with both positive and negative consequences. It is reflected in the entire culture and, in particular, in the way of thinking, in the revision of our views on the Universe and our attitude towards it.

Physicists and philosophers have discussed these changes introduced by modern physics over the past decades. However, it has rarely been noted that all these changes bring us closer to a perception of the world akin to that of Eastern mystics. The concepts of modern physics very often show a striking similarity to the ideas embodied in the religious philosophies of the Far East. Although these parallels have not been considered in detail until now, they were noticed by some of the outstanding physicists of our century who became acquainted with the cultures of India, China, and Japan during visits to these countries to give lectures. As Heisenberg noted, quantum mechanics, which is the avant-garde of modern physics, gave hope for the reunion of two different parts - the objective world, which classical mechanics describes, and the world of man. There is some connection between these worlds. Therefore, the gap between subject and object in quantum theory is no longer possible. The general laws of human cognition, which also emerged in the discoveries of atomic physics, are not unprecedented or completely new. They also existed in our culture, but occupied a much more significant place in Buddhist and Hindu philosophies. What is happening now is the confirmation, continuation and renewal of ancient wisdom." (Robert Oppenheimer). The conceptual structure of modern physics increasingly resembles the philosophy of Hinduism" (A. Salam, Nobel laureate) "We can find a parallel to the lessons of atomic theory in the epistemological problems that such thinkers as Lao-tzu and Buddha have already encountered, trying to comprehend our role in the grand spectacle of being - the role of spectators and participants at the same time" (Niels Bohr). Quantum theory and the theory of relativity - as two cornerstones of twentieth-century physics - lie at the heart of a worldview very similar to the worldview of a Hindu, Buddhist, or Taoist. This similarity is enhanced when we try to combine these theories to describe the phenomena of the microworld: the properties and interactions of elementary particles. Here, the parallels between modern physics and Eastern mysticism are most noticeable, so it is impossible to say who was the first to express certain ideas: physicists or Eastern mystics. The word "quantum" comes from the Latin quantum ("how much, how much") and the English quantum ("quantum, portion"). "Mechanics" has long been the name given to the science of the motion of matter. Accordingly, the term "quantum mechanics" means the science of the motion of matter in portions (or, in modern scientific language, the science of the motion of matter that is canted. The term "quantum" was first introduced by the German physicist Max Planck to describe the interaction of light with atoms.

2. Comparative characteristics of "old" and "new" physics

The birth of modern science was preceded by the recognition of the complete separation of matter and spirit, thanks to the work of René Descartes, whose worldview was based on the fundamental division of nature into two independent spheres: the sphere of consciousness and the sphere of matter. As a result of the "Cartesian" division, scientists were able to consider matter as something inanimate and completely separate from themselves, and the material world as a large, complex aggregate. This mechanistic worldview was also adopted by Newton, who based it on his mechanics, which became the foundation of classical physics. From the second half of the 17th century to the end of the 19th century, the Newtonian model of the Universe was the most influential.

The worldview that was rejected by modern physics was based on the Newtonian mechanistic model of the Universe. This model was a powerful framework of classical physics and the basis of all sciences and natural philosophy.

According to Newton, all physical phenomena occur in a three-dimensional space described by Euclidean geometry. This is an absolutely unchanging space. All changes in the physical world were described in terms of absolute time - a special dimension that distinguished between the past, present, and future. "Absolute, truly mathematical time, by its very nature, flows at a constant speed, not subject to the influence of external factors," Newton argued.

According to Newton's ideas, material particles moved in this space - small, solid, indivisible objects, of which all matter consists - "point mass". According to Newton, all physical phenomena are reduced to the movement of material points in space, caused by their mutual attraction - the force of gravity. For a strictly mathematical description of force, Newton used completely new concepts and mathematical operations of differential calculus.

The basis of classical mechanics is Newton's equation of motion. It was believed to reflect the absolute law governing the motion of material points. According to Newton, particles, forces between them, and the fundamental laws of motion are interconnected. Thus, the entire Universe was set in motion and continues to move.

The mechanistic view of nature was closely related to determinism. The great cosmic mechanism was subject to certain laws. Everything had its cause and led to a certain result, or, knowing the system's state perfectly today, it was possible to predict its future accurately. The philosophical basis of strict determinism was the fundamental distinction between the world and man, introduced by Descartes. Moreover, as a result of the distinction, confidence arose in the possibility of an objective description of the world, without mentioning the personality of the observer. Moreover, in such an objective description of the world, science saw its ideal.

Newtonian mechanics reached its heyday in the 18th-19th centuries. On this basis, Laplace successfully and in detail described the motion of planets, satellites, and comets. Inspired by the brilliant success of Newtonian mechanics in astronomy, physicists used it to describe the continuous flow of fluids and the oscillations of elastic bodies, and achieved success once more. Even the theory of heat received a mechanistic justification. The triumph of Newtonian mechanics convinced physicists that its laws govern the motion of the entire Universe and are the fundamental laws of nature.

It all began with the discovery and study of the phenomena of electricity and magnetism, which did not allow for mechanistic interpretations. Faraday and Maxwell introduced the concept of a field, which changed the idea of physical reality. The simultaneous emergence of the theory of relativity and the theory of the atom called into question the basic concepts of Newtonian mechanics. The old concepts did not apply to new areas of physics.

At the origins of modern physics are the great achievements of one man, Albert Einstein. His two papers, published in 1905, contained two radically new ideas. The first became the basis of the special theory of relativity (STR); the second forced us to look at electromagnetic radiation in a new way and formed the basis of the theory of the atom - quantum theory. Einstein was convinced that nature was inherently harmonious and sought a common basis for all of physics. The first step was to unify electrodynamics and mechanics within the framework of the special theory of relativity.

According to the theory of relativity, it is correct that space has three dimensions and that time exists separately from them. One is closely connected with the other, and together they create a four-dimensional "space-time" continuum. Space and time do not exist by themselves; there is no single flow of time. All dimensions in space and time become relative, lose their absolute character. Both time and space are only elements of the language that a certain observer uses to describe phenomena. The concepts of time and space are so fundamental that altering them requires a fundamental shift in the approach to describing natural phenomena. The most important consequence of this change is the realization that mass is one form of energy. Even a stationary object has energy

$$E=mc^2.$$

In 1915, Einstein put forward the general theory of relativity, which, unlike the special theory, accounted for gravity. According to the theory, gravity can distort space and time. This means that in a curved space, the laws of Euclidean geometry do not apply.

Thus, the general theory of relativity completely denies the concept of absolute space and time. Not only are all dimensions in space and time relative, but the very structure of space-time also depends on the distribution of matter in the Universe, and the concept of "space" loses its meaning.

Classical mechanics considered the motion of rigid bodies in space. This approach remains appropriate today, but in relation to the so-called "zone of intermediate dimensions", that is, the area of our everyday experience. The expression "space" has lost its meaning in astrophysics and cosmology - the sciences of the Universe as a whole, and the concept of a rigid body has been called into question by atomic physics - the science of the infinitely small.

Instead of the solid and continuous particles described by the ancients, scientists were faced with incredibly small particles - electrons, which move around the nucleus at a huge distance. Later, quantum mechanics emerged, proving the fallacy of ideas about solid bodies and the strict determinism of natural laws. At the subatomic level, instead of solid material objects, some wave-like probabilistic models reflect the probability of the existence of not things, but relationships.

In studying the subatomic world, it became clear that elementary particles needed to be abandoned.

Dirac laid the beginning of a new approach to particles. Dirac's theory revealed the fundamental symmetry of matter and antimatter. Pairs of particles and antiparticles arise if there is sufficient energy and are converted into pure energy during the reverse process of annihilation.

Experiments over the past few decades have revealed the dynamic nature of particle physics. Any particle can be transformed into another, energy can be transformed into particles, and vice versa. The Universe is a moving network of inextricably linked energy processes. A universal theory to describe the subatomic world has not yet been found. However, several models, sometimes contradictory, show that particles' properties can be understood only in terms of their activity and that particles should be considered an integral part of the whole, not separately.

Thus, according to modern physics, the Universe is a dynamic, indivisible whole that includes the observer. Here, the traditional concepts of space and time, isolated objects, and cause and effect lose their meaning. At the same time, similar ideas took place in Eastern mystical traditions. This parallel becomes even more obvious when considering the quantum-relativistic model of subatomic physics.

The construction of quantum mechanics (or rather, the creation of a quantum worldview) meant a break, the destruction of classical ideas. To understand what was destroyed, it is necessary to outline the basic ideas of classical mechanics briefly. The initial image of classical mechanics is that of a material point moving along a given trajectory. The latter is given by the initial conditions and the force acting on the material point. The discovery of the atomic structure of matter has materialized this basic image of classical mechanics.

Material points are atoms, electrons, protons - in a word, those particles that should be considered elementary when considering a particular movement. Based on this concept, the properties of macroscopic bodies should be understood as those of collections of particles (material points) that interact with one another and move along certain trajectories. The mechanics of material points cannot be constructed if the forces of interaction between them are unknown. Note that quantum mechanics does not subject the idea of forces to revision.

So, the basis of the classical mechanical worldview is a material point, a particle, about which it is possible to say exactly where it is at a given moment in time and with what speed it moves in the medium.

However, the discovery of radio waves and the clarification of the wave nature of light showed that matter exists not only in the form of particles of matter (corpuscles) but also in the form of waves. However, nothing (if by "something" we mean only particles) oscillates. A wave in this sense is a primary, such image that cannot be reduced to any analogy. An electromagnetic wave, or rather, its simplest form - a plane wave of a certain frequency - is an elementary form of existence of a special type of matter, which is called an electromagnetic field. It is interesting to note that the elementary form, that is, the form from which all possible electromagnetic fields are constructed, is an infinitely long wave in space and time.

Not only at first glance, but also with any in-depth approach, a wave and a particle are incompatible concepts, such that they mutually exclude each other. Before us is either a particle - something very small, which is at each moment in a certain place and moves with a certain speed, or a wave - something widespread, widespread, such that it fills the entire space. True, a wave is also associated with a certain speed. Even two. First, the speed of movement of the wave phase - phase speed

$$V_{ф} = \omega/k,$$

where ω is the circular frequency of the wave, and k is the wave number related to the wavelength by the relation

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

The phase velocity characterizes the wave's structure but does not directly determine its rate of energy transfer.

The second velocity is the rate of energy transfer. It is called the group velocity because the wave packet (a group of waves) propagates at this speed. Group velocity

$$Vgr=\frac{d\varpi}{dk}.$$

If $V_f=V_{gr}$, then we speak of the absence of dispersion. For electromagnetic waves in a vacuum, $V_f=Vgr=C=3\cdot10^8$ m/sec.

The difference between a particle and a wave is especially clearly manifested when studying two particles or two waves. A characteristic property of waves is interference - the possibility of a decrease in intensity when two (or more) waves are superimposed. A similar result is completely impossible for corpuscles. Two particles are always more than one. In other words, if two particles fall into one point, then the reaction must be doubled (for simplicity, we assume that the particles are absolutely identical).

It should be noted that sometimes the difference between particles and corpuscles is not entirely obvious. Observing a beam of light, it is quite difficult to imagine that a thin, “razor-like” beam is a collection of infinitely long waves. Rather, one wants to agree that it is a stream of particles flying along a straight trajectory. It is known that wave optics easily coped with this difficulty and reconciled the rectilinear propagation of light with its wave nature by taking into account the interference of waves.

Summing up, the classical picture of the world is built from two entities: particles and waves.

However, one can also stop at such a point of view. According to classical physics, the world is built of particles. They interact with one another and move along specific trajectories. Some of them are charged. These particles, moving with acceleration, emit electromagnetic waves. Since this movement occurs always and everywhere, the world, which consists of particles, is filled with electromagnetic waves. Some of these waves we can feel (visible light), but most penetrate the surrounding environment, remaining inaccessible to our sense organs. Certain waves are easily recorded by radio receivers or other devices that enable a person to expand the range of his sense organs.

Without going into details, the above is a complete classical picture of the world around us. Is it correct?

The answer is obvious. If the classical picture were correct, there would be no need to talk about a revolution in natural science; there would be no need for the revolution itself.

Then it is logical to ask the following question: to what extent does the classical picture of the world depict true nature, to what extent?

As long as we are interested in macroscopic movements (simply put, the movements of things and objects), classical mechanics accurately describes experimental results. There is no reason to doubt its correctness. As long as we have not gone beyond the scope of its applicability, there is no reason to revise anything in its foundations.

However, when we enter the world of atomic particles, well-being becomes illusory. The very existence of stable atoms and molecules cannot be understood without remaining in the positions of classical mechanics. Thus, we are not talking about a quantitative disagreement, but about the fundamental impossibility of explaining the most fundamental facts.

For example, if we take the position of the structure of the atom according to Bohr's theory, then the rotation of the electron around the nucleus occurs at such a centripetal acceleration, and, consequently, the radiation of energy (any electric charge that moves with acceleration radiates), that the electron will give this energy to the surrounding space in a time of 10-10 seconds. Therefore, the atom as a stable object will exist no longer than the given value. This number is the best demonstration of the powerlessness of classical physics. Using obvious conclusions (the impossibility of the existence of a stationary structure of charged particles without motion and the fact that a particle that moves with acceleration radiates), we have obtained that atoms cannot exist at all! In fact, this is the main contradiction between the conclusions of classical physics and experiments. It was in order to eliminate this contradiction that a new mechanics was created - quantum (or wave), based on completely new ideas, the development of which required a radical change in our old visual representations. For example, everyone who has at least become acquainted with the elements of quantum mechanics will not deny that a particle is a wave enclosed in a ring, and particle mechanics is a part of wave mechanics.

Quantum mechanics (unlike classical - Newtonian and relativistic - Einsteinian) was created not by one person, but by a whole galaxy of famous physicists of the 20th century: Max Planck, Niels Bohr, Louis de Broglie, Werner Heisenberg, Erwin Schrödinger, Wolfgang Pauli, Paul Dirac, Max Born, etc. The founders of quantum mechanics built a beautiful structure. However, they started building this structure from the second floor, with descriptions of the probability distributions and average values of the measured quantities. Therefore, for the stability of this structure, a large number of “supports” were needed in the form of various principles: the uncertainty principle, the superposition principle, the complementarity principle, the principle of unrecognizability, etc. All these principles appear largely artificial and are difficult to interpret physically.

3. Fundamental ideas of quantum mechanics

Before considering the basic principles of quantum mechanics in detail, let us recall that it describes the motion of particles that exhibit wave properties. In addition, the main issue in quantum mechanics is the discreteness of the quantities being studied. Note that the concept of discreteness was introduced into physics a long time ago. In particular, it reflects the idea of the atomic-molecular structure of matter. Quantum physics has significantly expanded the idea of discreteness and its role in physics. The essence of the idea of quantization is as follows: some physical quantities that describe a microobject, under certain conditions, take only discrete values. Initially, discreteness was extended to electromagnetic waves.

1. Light is emitted in portions (quanta), the energy of which is determined by the formula $\Delta E = h\nu$, $h = 6.62 \cdot 10^{-34}$ J·s. This idea was put forward by M. Planck in 1900, but he considered that radiation is discrete, and absorption is continuous.

2. In 1905, A. Einstein extended the idea of discreteness to absorption processes in order to explain the mysteries of the photoelectric effect: the existence of a red limit of the photoelectric effect and the dependence of the energy of a photoelectron on frequency, not on intensity. According to Einstein's assumption, electrons in matter absorb light in portions $h\nu$ as well as during radiation. Later, a quantum of light with energy $h\nu$ was called a photon.

3. The energy of any microobject located in a limited space is quantized, for example, an electron in an atom. Quantization means that an electron in an atom can have only a certain discrete set of values. Each energy value is called an energy level or a stationary state. Being in these stationary states, electrons do not emit photons. However, the transitions between levels are called quantum transitions or quantum jumps.

N. Bohr introduced the idea of quantizing the energy of an electron in an atom to explain the mysterious stability of atoms. The quantization rules introduced by Bohr are considered one of the unique phenomena in the history of science. Discreteness is not the result of some mechanism of interaction of light with matter - it is an inherent property of the radiation itself. The frequency of radiation does not depend on the electron's orbital rotation frequency. However, it is determined by the energy difference between the corresponding energy levels, reflecting the atom's discrete emission and absorption of light. Instead of a continuous process requiring a certain time for emission or absorption of an electromagnetic wave, an instantaneous act of creation or destruction of a photon occurs, while the state of the atom changes in a jump-like manner. This frequency rule explains not only the linear nature of atomic spectra but also the observed regularities in their structure. Discreteness is the main feature of phenomena at the microworld level. Here, it makes no sense to act on a quantum system (microobject) arbitrarily weakly, since, up to a certain point, it does not feel it. However, if the system is ready to perceive it, it jumps into a new quantum state. Like any other physical theory, quantum mechanics is based on certain postulates. The correctness of these postulates can be confirmed by comparing the predictions of quantum mechanics with the results of experiments in which the wave properties of particles cannot be neglected. One of the postulates of quantum mechanics states that the state of a particle is completely described by a wave function, which has a probabilistic meaning and determines the probability of finding a particle in different regions of space. This moment is decisive in the need to introduce the uncertainty principle.

4. Heisenberg's uncertainty principle and the principles of quantum mechanics

Let us answer the question posed by the second point of the instructions in an explicit form. When describing the microworld, one has to abandon the most obvious representation of classical mechanics. The motion of a microparticle cannot be imagined as moving along a certain trajectory. The fact is that the concept of "trajectory" is inextricably linked with the need to accurately specify the coordinates of a particle and its velocity at the same time. However, one of the basic principles of quantum mechanics states. A particle cannot have a certain coordinate and velocity or coordinate and momentum at the same time (in quantum mechanics, it is customary to use not the concept of velocity V, but the concept of momentum p). This statement can be written in the form of an inequality - the famous Heisenberg relation:

$$\Delta x \cdot \Delta px \geq \hbar,$$

where $\hbar = h/2\pi$, $h = 6.62 \cdot 10^{-34}$ J·s,
discovered in 1927.

How should we understand this relation, which is often elevated to the rank of a principle? The symbol Δx (or $\Delta \rho\chi$) means the uncertainty of the coordinate x (or the projection of the momentum $\rho\chi$). The term “uncertainty of a physical quantity” means the following. Let an atomic particle be in a certain state (the words "a particle is in a certain state” should be understood as follows: "a particle performs a certain motion"). So, the particle is in a certain state. We measure the particle's coordinate. We record the result obtained. Then we repeat the experiment. We record it again and again. To each value of the coordinate x, we assign the number N(x), which shows how many times the value x was obtained, and we construct a graph (Fig. 1), from which it is clearly visible what is usually denoted by the symbol Δx. The uncertainty relation contains a new parameter, a new letter - a hook called Planck's constant. Planck's constant is a new universal constant. It entered physics only with quantum mechanics, when classical ideas were abandoned. Formally, the transition to classical mechanics can always be made by setting $h=0$. Indeed, according to the Heisenberg uncertainty principle, the uncertainties in coordinate and momentum (Δx and $\Delta\rho_x$) can simultaneously be zero; the particle is therefore allowed to move along a trajectory.

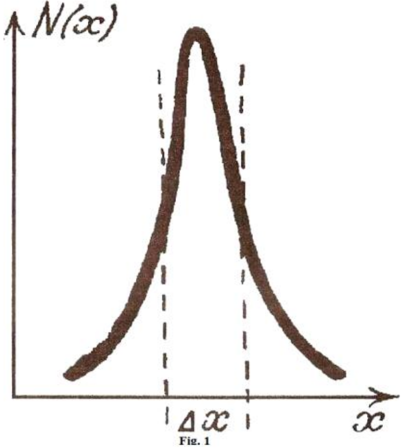

Fig. 1

Without going into the discussion of the uncertainty principle, let us find out whether it imposes restrictions on the motion of macroscopic bodies. Suppose a ball with a mass m = 1 g is moving, the trajectory of which we can measure with an accuracy of Δx = 10-4 cm. Then the uncertainty of the ball's velocity will be « 10-24 m/s. This example convincingly shows that there is no reason to be "afraid" of quantum uncertainty when considering the motion of a steam locomotive, or a car, or even the smallest part in these machines. The change in the velocity of a body with a mass of 1 g caused by the impact of an air molecule is many times greater: $\Delta v \approx$ 3-10-19 cm/s.

The uncertainty relation has been subjected to countless attacks from the most diverse positions for many years. Few people know that the creator of the theory of relativity, A. Einstein, is one of the founders of quantum theory and, at the same time, one of its greatest opponents (paradoxically, Einstein received the Nobel Prize for his work on quantum theory). So, the existence of the uncertainty principle means that an atomic particle, by its nature, requires a statistical (probabilistic) approach to describe its behavior. It was precisely the rejection of strict definiteness characteristic of classical mechanics that was most difficult for physicists (even Einstein).

Indeed, it is very difficult to imagine (for a layperson even today) that the behavior of a single electron moving under the action of a strictly defined force cannot be fully described without using such concepts as probability, uncertainty, and average value, which would seem to be inextricably linked with a large number of particles. But it is so. The most rigorous analysis shows that the description of microobjects adopted in quantum mechanics is logically perfect and, in principle, cannot contradict experiment. More precisely, it is impossible, using any phenomena, devices, means, calculations, to determine the momentum and coordinate of a particle exactly simultaneously. At first glance, the uncertainty principle sets a limit on human capabilities: we cannot learn more precisely about a particle's momentum and position simultaneously. However, this is correct! A particle does not have both momentum and coordinates at the same time. Various attempts to attribute to a particle specifying, as they say, internal parameters fail. Moreover, it has been strictly shown that such attempts are incompatible with modern quantum mechanics - a science that describes the world of atoms and molecules without any contradictions. This is surprising, of course, especially if we consider that attempts to attribute dimensions to an electron, to introduce an electron radius, are also unsuccessful. We emphasize that the uncertainty of the coordinate is the uncertainty in the spatial position of the particle, and is in no way connected with the dimensions of the particle. (In some cases, they talk about the radius of the electron. It turns out to be equal to $\approx 10^{-13}$ cm, that is, 105 times smaller than the uncertainty of the position of the electron in the atom. In other words, the electron should be considered a point located somewhere in the atom.

The uncertainty relation has an unexpected consequence, especially in solid-state physics: the motion of a quantum particle (electron, ion, atom), localized in a limited region of space, cannot be slowed down - stopping ($p_x=0$, and therefore $\Delta p_x=0$) contradicts the Heisenberg inequality, since it requires complete delocalization of the particle ($\Delta x \rightarrow \infty$). This indestructible motion is often called zero.

So, there is a pair of quantities (coordinate – momentum) that cannot be measured accurately at the same time for the phenomena of the microworld:

$$\Delta x \Delta p_x \geq \hbar. \qquad (1)$$

Energy and time uncertainties were also identified:

$$\Delta E \cdot \Delta t \geq \hbar. \qquad (2)$$

(1) differs from (2) in that (2) deals with the uncertainties of energy and time at a given coordinate value, and (1) deals with the uncertainties of momentum and coordinate at a given time.

Reflecting on the uncertainty relation, we can conclude that it has a wave origin. Indeed, a relation of this type occurs in wave optics. Here, it is proved that a plane wave fills the entire space. However, it is well known: it is possible to concentrate the electromagnetic field in a limited (and if desired, in a sufficiently small) region of space. However, for this, a large number of waves is required. Some of them reinforce each other, while others, when they interfere, cancel each other out. Such a “construction” of waves is called a wave packet. A wave packet is characterized by an interval Δkx of wave numbers, which are necessary for the concentration of the electromagnetic field in a region of space Δx. The more diverse the set of wave vectors, the smaller the spatial dimensions Δx of the packet. There is a purely wave relation

$$\Delta x \Delta k_x \geq 1.$$

Comparing the last relation with the Heisenberg uncertainty relation, we see that they are equivalent as long as

$$p = \hbar k .$$

This equality was first written by the French physicist Louis de Broglie in 1925. It bears his name. The uncertainty principle recognizes that particles exhibit wave-like properties.

As already mentioned, the uncertainty relation is a strict consequence of quantum mechanics. No less strictly, quantum mechanics showed that waves have corpuscular properties, and particles - wave ones. The corpuscular properties of wave motion are manifested in the fact that the energy E of waves with a frequency ω is equal to the whole number of energy quanta $\hbar\omega$ ($E = n \hbar\omega$, where n is 1,2,3,...), and the momentum p of the wave is equal to $n\hbar k$.

The contradiction between a wave and a particle (more precisely, the alternation of the concepts of “wave” and “particle”: either a wave or a particle!) was destroyed on both sides. Both on the part of particles - they acquired wave properties, and on the part of waves - they acquired corpuscular properties. Both the wave properties of particles and the corpuscular properties of waves have been repeatedly confirmed experimentally. In some cases, for example, the same electron behaves as a particle, and in others - as a wave. The same is true of electromagnetic waves: in some phenomena, they are typical waves, in others, without a doubt, particles.

The corpuscular-wave dualism, or corpuscular-wave duality of atomic particles, is such an important property for understanding the world around us that it is necessary to dwell in detail on the direct experimental evidence of this amazing feature of microscopic objects.

The proof of the dual nature of atomic particles and light is, in fact, simple and requires an understanding of only the basic concepts of physics, and to some extent, a feeling for how a wave should behave in the appropriate conditions, not as a particle.

In 1955, A. Einstein in the preface to L. de Broglie's book "Physics and Microphysics" said: "It was de Broglie who was the first to realize the close physical and formal relationship between the quantized states of matter and the phenomena of resonance, even at a time when the wave nature of matter had not been discovered experimentally" (A. Einstein. Collected Scientific Works. - M.: Nauka, 1967, vol. IV, p. 340). Fortunately, physicist Davisson was aware of Louis de Broglie's work, who, together with Germer, studied the scattering of electrons by a metal surface. Moreover, as often happens, a random incident prompted the experimenters to make a major discovery. The vessel in which the nickel plate was stored broke (the nickel plate was used to study electron reflections). The plate oxidized, and in order to continue the study, it had to be calcined for a long time. After calcining, the results turned out to be sharply different from those before calcining (many authors like to emphasize the randomness of the discoveries made, but the fact that random events happen to those who can understand their meaning is not at all a coincidence): the dependence of the number of scattered electrons on the angle turned out to be sharply anisotropic. The experimenters lost several years trying to understand what was happening. Moreover, they understood that applying de Broglie's idea to the explanation. The point is this: during calcining, the plate underwent recrystallization - large crystallites formed in it. They were responsible for the anisotropy of scattering. However, the anisotropy of the scattering itself allowed us to determine only if we assume that the electrons are reflected from the crystal in a manner characteristic of waves. In this case, it should be assumed that the wavelength of the electron satisfies the de Broglie relation:

$$\lambda=h/p.$$

Electrons undergo diffraction as a result of the reflection of electron waves from crystal planes, just like X-rays. Electron diffraction (an unnatural phrase, if you consider that an electron is a particle) is one of the main methods of studying the structure of crystals, along with X-ray structural analysis and neutron diffraction. The discovery of electron diffraction did not cancel the corpuscular properties of electrons. They cannot be canceled. They exist. However, there are also wave properties. An electron is both a particle and a wave. Such is the nature of microscopic particles. Sometimes the dual nature of microscopic particles manifests in a single experiment (more strictly, this means that two experiments are taking place simultaneously). For example, a neutron is scattered by a crystal. In this case, one of two events can occur. Either the neutron will not change its energy at all, or it will slow down slightly. (At a temperature of the crystal other than absolute zero, the neutron may even accelerate slightly - take energy from the crystal). Scattering without a change in energy (elastic scattering) clearly exhibits diffraction features. It serves as a reliable method for studying the structure of crystals (especially magnetic ones, in neutron elastic scattering). When describing inelastic scattering, it is necessary to consider the neutron as a particle. Therefore, the main feature of quantum phenomena is their discreteness. In the quantum world, nothing happens a little bit — interactions there occur only quantum: either everything or nothing. We cannot arbitrarily weakly influence a quantum system – until a certain point, it will not feel this influence at all. However, when the action has grown so much that the system is ready to perceive it, it suddenly passes into a new (also quantum) state or dies. The transition of the system to a new state is a phenomenon. If we observe it, then, from the point of view of quantum-mechanical concepts, this means that we simultaneously influence it. Therefore, in atomic physics, “phenomenon" and “observation” are inseparable from each other. In fact, “observation” is also a phenomenon, and far from the simplest one. This was first pointed out by the same W. Heisenberg. He said that any measurement is the interaction of the device and the object that we are studying. Moreover, any interaction violates the initial state of both the device and the object, so that, as a result of measurements, we obtain information about the phenomenon distorted by the device's intervention. Based on this, we can say that the process of observation in quantum mechanics resembles taste more than vision. "In order to learn about the properties of pudding, it is necessary to eat it," the creators of quantum mechanics liked to repeat. Moreover, just as we cannot re-evaluate our impressions of pudding after having eaten it once, we cannot infinitely refine our information about a quantum system: it will be destroyed, as a rule, by the first measurements. Heisenberg not only grasped this harsh fact for the first time but also wrote it down in the strict language of formulas. The defining one among them was the uncertainty relation formula, one of the most important in quantum mechanics. Immediately after this, it became clear to N. Bohr that the uncertainty relation and the corpuscular-wave dualism are only partial manifestations of one general principle - the principle of complementarity (Proclaimed in 1927 at the International Physical Congress by N. Bohr), according to which, when studying microobjects (elementary particles), different methods of observation give different results. These results should not be considered as contradictory, but as complementary. The truth is that, under some conditions of observation, one result is obtained; under others, another. The description of the phenomenon will be complete only when both observations are made, which complement each other. This principle can be formulated in another way: simultaneous observation of wave and corpuscular properties is impossible. It can be said with absolute certainty that the principle of complementarity is one of the most profound philosophical and natural science ideas of our time, with which only such ideas as the principle of relativity or the idea of a physical field can be compared. Its universality prevents it from being reduced to any single statement; it must be mastered gradually, using specific examples. The simplest approach (as N. Bohr did in his time) is to start with an analysis of the process of measuring the momentum p and the coordinate x of a microparticle. It turned out that the coordinate and momentum of an atomic particle cannot be measured not only simultaneously, but also using the same device. Indeed, to measure the momentum p of an atomic particle without changing it very much, it is necessary to have a light, mobile "device.” However, it is this mobility that makes its position quite uncertain. When we speak into a microphone, the sound waves of our voice are converted into vibrations of the membrane there. The lighter and more mobile the membrane, the more precisely it follows the air's vibrations. However, it is more difficult to determine its position at any given moment. To measure the x coordinate, we must therefore take another, very massive device that will not move when a particle hits it. However, no matter how much its momentum changes in this case, we will not even notice it. This is the simplest experimental illustration of the Heisenberg uncertainty relation: it is impossible to determine both the x coordinate and the momentum p of an atomic object in the same experiment. This requires two measurements and two fundamentally different devices, whose properties complement each other. Similarly to this example, we cannot observe electrons as particles and as waves at the same time, not because it is too difficult, but because the state of the world depends on the instruments we use for observation. If we come to a laboratory where the corpuscular properties of electrons are studied, then the world is in a state in which electrons do not have wave properties; if we come to a laboratory where wave properties are studied, then the world is in a state in which electrons do not have corpuscular properties. We can try to measure these properties simultaneously. However, then, as a result, we will have very rough, approximate “measurement data" that are subject to the Heisenberg uncertainty relation. Following N. Bohr, we can call the relationship between these two laboratories a relation of newness. It should be noted that Bohr put forward a hypothesis according to which the principle of complementarity is universal for human cognition and manifests itself, in particular, when people try to connect physiological and mental phenomena. Complementarity - this is the word and that turn of thought that became accessible to everyone thanks to Bohr. Before him, everyone agreed that the incompatibility of two types of devices necessarily entails a contradiction in the properties that are determined with their help. Bohr denied such straightforwardness of judgments and explained: yes, these properties are indeed incompatible, but for a complete description of a quantum object, both of them are equally necessary and therefore do not contradict, but complement each other. We encounter such a situation at every step. For example, if we use a lens and sunlight to set fire to paper, then we are dealing with one characteristic of the sun's beam: it carries energy in the form of photons. But if the same sun's beam is passed not through a lens, but through a prism, then we will see a spectrum. This is a second, additional characteristic of the same beam: it consists of waves of different lengths. A lens and a prism are different devices that allow us to observe various physical phenomena that characterize different complementary properties of a single quantum object. These properties cannot be observed simultaneously, in the same experiment, with the same instrument, but they are equally necessary to imagine the essence of the sun's ray in all its completeness. Physical science does not study objects in themselves, but specific implementations of the experimental situation, which we call "phenomena". From the point of view of the experiment, any phenomenon is an ordered set of numbers, which are the results of measurements of the object's reaction to the action of a device of the chosen type. By choosing different, complementary devices, we change the experimental situation; by implementing it, we influence different characteristics of the object; finally, by observing the consequences of this influence, we obtain different sets of numbers, that is, we study different phenomena. Moreover, although complementary phenomena cannot be studied simultaneously in a single experiment, they nevertheless characterize a single quantum object and are equally necessary for its complete characterization. It has always been important what questions we ask nature. When asking questions about quantum nature, we must be especially careful, because the way in which the single nature is divided into two parts depends on the choice: object + observer. Therefore, in quantum mechanics, not only concepts but also the very formulation of questions about the essence of phenomena are of particular importance. Pauli once even proposed calling quantum mechanics the “complementarity theory.”) However, the significance of the complementarity principle goes far beyond quantum mechanics, where it originally arose. Only later, during attempts to extend it to other areas of science, did its true significance for the entire system of human knowledge become clear. Bohr himself liked to give an example from biology, related to the life of a cell, whose role is completely analogous to the significance of an atom in physics. If an atom is the smallest particle of matter that still retains its properties, then a cell is the smallest particle of any organism that still represents life in its complexity and uniqueness. To penetrate the details of the mechanism of the cell's life, we examine it under a microscope - first a regular one, then an electronic one - we heat the cell, pass an electric current through it, irradiate it, decompose it into its constituent particles... However, the more we study the life of a cell, the more we will interfere with its functions and the natural processes that occur within it. In the end, we will destroy it and therefore learn nothing about it as a whole living organism. Nevertheless, the answer to the question "What is life?" requires both analysis and synthesis. These processes are incompatible but not contradictory; they are complementary, and the need to take them into account simultaneously is only one of the reasons why there is still no answer to the question of the essence of life. As in a living organism, the integrity of an atom's "wave-particle" properties is important. The finite divisibility of matter gave rise not only to the finite divisibility of atomic phenomena but also led to the limit of the divisibility of the concepts with which we describe these phenomena. N. Bohr showed that the question “wave or particle?” when applied to an atomic object is incorrectly posed. There are no such separated properties of atoms. Therefore, it does not have an unambiguous answer of “yes” or “no,” just as there is no answer to the question “Which is larger: a meter or a kilogram?” and similar questions. A quantum object is neither a particle nor a wave, nor even one or the other at the same time. A quantum object is something third, not equal to the simple sum of the properties of a wave and a particle, just as a melody is more than the sum of the sounds of which it consists, and a centaur is not a simple sum of a horse and a man, but something qualitatively new. This quantum “nothing” is not given to us in sensations, and nevertheless, it is certainly real. We do not have the images and senses to imagine the properties of this reality fully. Two complementary properties of quantum reality cannot be separated, destroying the completeness and unity of the natural phenomenon we call, for example, an atom, just as it is impossible to cut a centaur in two, keeping both a horse and a man alive. Therefore, when Heisenberg rejected the idealization of classical physics - the concept of “a state of a physical system independent of observation”- he thereby anticipated one of the consequences of the principle of complementarity, since "state" and "observation" are complementary concepts. Taken separately, they are incomplete and therefore can only be defined together, one through the other. Strictly speaking, they do not exist separately at all: we always observe not something in general, but necessarily some state. 1 On the contrary, any state is a thing in itself until we find a way to observe it. The very concepts of "wave" and "particle", "state" and "observation of the system" are certain idealizations, equally necessary for understanding the quantum world. In this regard, in general, N. Bohr came to a general conclusion: any truly profound phenomenon of nature cannot be defined unambiguously using the words of our language and requires at least two mutually exclusive complementary concepts for its definition. Not everyone knows that N. Bohr came to his principle of complementarity not “from physics”, but “from philosophy”. The idea of complementarity matured in him in his youth under the influence of Kierkegaard's philosophy. Later, it was strengthened and refined until it finally acquired a worthy application in quantum physics. The principle of complementarity itself, taken outside the boundaries of physics, is an ancient invention. In fact, it is a fairly well-known category of dialectical logic and has been repeatedly expressed in various forms by various philosophers throughout history. Aristotle, for example, said that “harmony is the mixing and compatible manifestation of opposites”. In Ancient China, the Tao philosophy arose, based entirely on the principle of complementarity symbolized by the “yin-yang” symbol, etc. Therefore, in the generalizations of scientific achievements of the 20th century. The named principle occupies a special place: “In order to adequately describe any object of reality, it must be described in two opposite systems of description. This is the principle of complementarity, formulated in quantum mechanics by Niels Bohr, and then transferred to any scientific description." And further: "It is impossible to describe two interconnected objects simultaneously accurately. This is an expanded understanding of the so-called Heisenberg uncertainty relation, which demonstrates the impossibility of simultaneously measuring the coordinate and momentum of an elementary particle with arbitrary accuracy. The last statement shows that the uncertainty relation has no less philosophical genesis than the principle of complementarity. Thus, the uncertainty relation is a particular case and a specific expression of the general principle of complementarity. It is this principle that allows us to reconcile the seemingly irreconcilable: after all, a microparticle manifests itself in different experiments as either a particle or a wave. Quantum mechanics synthesizes these concepts and enables the prediction of the outcome of any experiment in which both corpuscular and wave properties of particles are manifested. We note once again that the most famous examples of possible complementary pairs are momentum and coordinate, energy and time, and, from a more general point of view, continuity and discreteness. When considering the behavior of a particle in an infinitely deep potential well, discrete values of possible energies are obtained.

$$E_n = \frac{h^2}{8ml^2} n^2 \ ,$$

where l is the width of the well, n = 1,2,3…

These energy values are commonly called energy levels. The reason that causes energy quantization is the stitching of the wave function at the boundaries of the regions. There is a general theorem in quantum mechanics stating that energy cannot be conserved in systems that cannot extend to infinity, but it can be conserved in systems that can extend to infinity. Thus, if a particle in the well has a total energy E greater than the potential energy U, energy quantization does not occur. We also note that the minimum value of the energy of a particle in the well will be at n=1

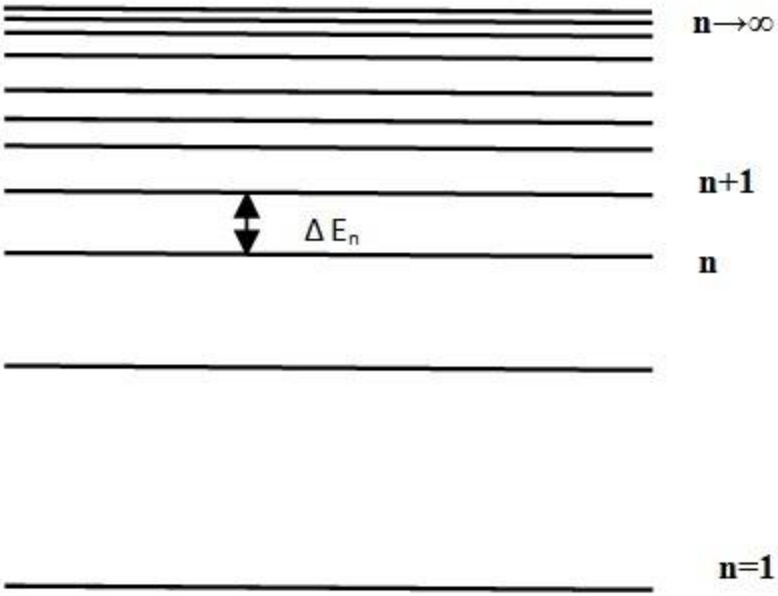

Fig. 2

and is not equal to zero. In classical physics, a particle can "lie" at the bottom of a well. In quantum physics, this is not possible. We can estimate the relative distance between the energy levels, i.e.

$$\frac{\Delta E_n}{E_n} = \frac{E_{n+1} - E_n}{E_n} = \frac{2}{n} + \frac{1}{n^2} \approx \frac{2}{n}.$$

From the obtained relation, it is clear that the distance between the energy levels, divided by the energy value, decreases with increasing n. For very large n, it is so small that the distribution of allowed energy values is practically continuous (Fig. 1). This means that at large quantum numbers, particles behave “classically”. Similarly, with increasing system size (increasing the width of the potential well), a "quantum-mechanical particle” at lower and lower energy turns into a "classical particle". Thus, under certain conditions (at large n), quantum physics passes into classical physics; the behavior of particles under this condition increasingly loses the features characteristic of microparticles. This result is a special case of a more general physical principle introduced in 1923 by N. Bohr – the correspondence principle. This principle states that the laws of quantum physics must be formulated so that, in the classical limit, when many quanta are involved in a process, they reduce to classical equations for averaged quantities. Alternatively, more generally, any new theory that claims greater generality than the generally accepted theory must necessarily pass into the old, classical theory under the conditions in which the "old physics" was built and tested experimentally. Quantum mechanics, as we see, satisfies the correspondence principle. In other words, the correspondence principle requires that there be a regular connection between any theory that is a development of the classical one and the original classical theory - in certain limiting cases, the new theory must pass into the old one. We have previously been convinced of the validity of this principle. For example, the formulas of kinematics and dynamics of the theory of relativity pass into the formulas of classical mechanics at such speeds that v2/c2→0. Moreover, in quantum and classical mechanics, the boundary between the two is associated with the possibility of neglecting the finite value of ħ and treating ħ→0. To illustrate a better understanding of the correspondence principle, let us turn to a simplified model of the atom first presented by N. Bohr. In Bohr's atom, electrons can only be in "allowed" orbits. Orbits are arranged according to the principal quantum numbers. The orbit closest to the nucleus has a principal quantum number equal to 1; the next one, 2, etc. The larger the quantum number of an electron orbit, the further it is from the nucleus. In contrast, in the classical case described by Newtonian mechanics, electrons could revolve around the nucleus in arbitrary orbits at any distance from the nucleus (this could actually occur if quantum effects were not taken into account). Now, although the physical radius of the orbits increases steadily as the principal quantum number increases, the kinetic energy of the electrons in these orbits does not increase at all in proportion to the expansion of the orbits. However, at a decreasing rate, there is an upper limit to the energy required to hold electrons in orbit around the nucleus, usually called the ionization energy. Accelerating to such an energy, the electron theoretically finds itself in an orbit of infinite radius; in other words, it becomes a free electron and leaves the boundaries of the already ionized atom. Between this extreme limit of the energy of the electron's release and the other extreme limit of the energy of the electron's presence in the first orbit to the nucleus, there is a certain (but infinite) number of permissible discrete energy states in which an electron held by the nucleus can be, and, according to the laws of quantum mechanics, at sufficiently large distances from the nucleus, the permissible orbits of electrons begin to overlap. This happens because the allowable energy of an electron in a certain orbit (and the radius of this orbit as a consequence) is not determined by an exact quantum number, but, in accordance with the Heisenberg uncertainty principle, is fuzzy - that is, we only have a probability distribution of the electron being in one of the neighboring orbits. This is where the "erasure of the difference" begins between the quantum-mechanical model of the atom, where the electron can be in only fixed energy states, absorb and emit energy in fixed portions (quanta), and, accordingly, be in strictly defined orbits, and the classical model of the atom, where the electron can have arbitrary energy and move in arbitrary orbits.

In other words, at large distances from the nucleus, the atom behaves like a classical system obeying Newtonian mechanics. The correspondence principle applies at the blurred boundary between quantum and classical mechanics. It once again demonstrates to us that in nature there are no clear boundaries between phenomena, just as there is no clear demarcation between theoretical descriptions of natural phenomena. Moreover, it demonstrates that quantum mechanics, for example, does not at all cancel or replace Newtonian classical mechanics, but only represents a limiting case as phenomena move to the scale of the microworld. In general, natural science theories grow out of one another as our previously accumulated knowledge expands, like new branches on the tree of knowledge of the surrounding world. One of the conclusions that follows from the Heisenberg uncertainty principle is the false statement that there is no place for the principle of causality in the phenomena of the microworld. Let us recall: the principle of causality means the ability to accurately predict the state of a system at any subsequent time based on its state at a given point in time. Thus, classical Newtonian mechanics, based on the coordinates x_0, y_0, z_0 and the projections of the velocities vx_0, vy_0, vz_0 known at a time t_0, makes it possible to determine the coordinates and projections of the velocities of the system at a time t. This position is called mechanical determinism. Since the coordinates and velocities of microobjects can simultaneously be found only within the framework of the uncertainty relation, the state of the system cannot be accurately determined at the initial time t_0. Therefore, the system's state is unpredictable at subsequent times; i.e., the principle of causality is violated. However, it should be emphasized that in quantum mechanics, the very concept of the state of the system is different from that in classical physics. The most accurate specification of the state of a microobject in quantum mechanics is the specification of its Ψ–function (we will talk about this function in more detail below). Moreover, the Ψ–function has the property that its specification at the time instant t0 determines its value at all time instants $t>t_0$. In other words, in quantum mechanics, in accordance with the causality principle, the state of a microobject at some time instant t0 unambiguously predicts its subsequent states. The causality principle in the form of the classical approach cannot be applied to microobjects. Thus, at a general philosophical level, the causality principle establishes the temporal sequence of the flow and the mutual connections among events in a given system. According to this principle, the state of a physical system at any given time instant determines its state for any subsequent time instant. Despite the probabilistic nature of the description of the microworld's objects, quantum processes are also causally interconnected (deterministic). They can be described by equations of motion that unambiguously define wave functions or other quantities equivalent to them. In this case, the system's initial state completely determines its subsequent evolution. If the system has identical particles (same mass, electric charge, spin, etc.), then they are called identical particles. The unusual properties of a system of identical particles are manifested in the fundamental principle of quantum mechanics - the principle of indistinguishability of identical particles, according to which it is impossible to distinguish these particles experimentally. In classical mechanics, identical particles can be distinguished by their location in space and by their momentum. In quantum mechanics, it is different. From the uncertainty relation (again, this relation), it follows that for microparticles, it is impossible to apply the concept of trajectory at all. One can only look for the probability $|\Psi|^2$ (Ψ is a wave function, which is discussed in detail below) of the location of a particle in the vicinity of a particular point in space. If the wave functions of two identical particles overlap in space, then it makes no sense to talk about the location of any individual particle in a given region of space; one can only talk about the probability of finding one of the identical particles in a given region. So, in the quantum mechanical sense, identical particles completely lose their individuality and become unrecognizable. This means that $|\Psi(x_1,x_2)|^2= |\Psi(x_2,x_1)|^2$. Hence $\Psi(x_1,x_2)=\pm\Psi(x_2,x_1)|$. So, if the wave function does not change sign when the particles are swapped, it is called symmetric; if it does, it is called antisymmetric. It has been established that particle spin determines whether wave functions are symmetric or antisymmetric.

Depending on the nature of symmetry, all elementary particles and systems built from them are divided into two classes. Particles with half-integer spin (electrons, protons, neutrons, etc.) are described by antisymmetric wave functions and obey Fermi-Dirac statistics. Therefore, they are called fermions. Particles with zero or integer spin (π-mesons, photons, etc.) are described by symmetric wave functions and obey Bose-Einstein statistics; these particles are called bosons. Complex particles (for example, atomic nuclei), which consist of an odd number of fermions, are fermions (total spin is half-integer), and those with an even number are bosons (total spin is integer). If identical particles have the same quantum numbers, then their wave function is symmetric with respect to the permutation of the particles. It follows that two identical fermions that are part of the same system cannot be in the same states, since for fermions the wave function must be antisymmetric. Moreover, this conclusion fully corresponds to the Pauli principle. The Austrian physicist Wolfgang Pauli (1900-1958) formulated the principle according to which fermion systems occur in nature only in states described by antisymmetric wave functions. Alternatively, in a system of identical fermions, no two of them can be in the same state at the same time. This principle is fundamental in quantum mechanics and is also often called the prohibition principle. The easiest way to imagine the essence of the principle is to compare electrons with cars in a multi-story parking lot. Only one car is placed in each box, and after all the boxes on the lower floor of the parking lot are occupied, the cars have to drive to the next floor to find free spaces. The same is true of electrons in atoms – in each orbit around the nucleus, no more of them are placed than there are “parking spots”, and after all the places in the orbit are occupied, the next electron looks for a place in a higher orbit. Further, electrons behave, conditionally speaking, as if they were rotating around their own axis (i.e., they have their own angular momentum, called spin, which can take only two values: +1/2 and 1/2). Two electrons with opposite spins can occupy the same orbital. It is as if a right-hand-drive car and a left-hand-drive car could fit into one box at the same time, but two cars with the same steering wheel placement would not. That is why in the first row of Mendeleev's periodic table, we see two atoms (hydrogen and helium): in the lower orbit, only one double place is allocated for electrons with opposite spins. The next orbit already accommodates eight electrons (four with spin -1/2 and four with spin +1/2), so in the second row of the periodic table, we already see eight elements. And so on. The state of an electron in an atom is uniquely determined by a set of four quantum numbers:

principal n (n=1, 2, 3, …..);
orbital l (l= 0, 1, 2, ….., n – 1);
magnetic ml (m_l=-l, -l+1, -l+2,…..,0, 1, 2,…,+l);
spin m_s (m_s=+1/2, -1/2)

and satisfies the Pauli exclusion principle: in the same atom, there cannot be more than one electron with the same set of four quantum numbers, i.e. Z(n, l, ml, ms) = 0 or 1.

From the Pauli exclusion principle, it follows that two electrons bound in the same atom differ by at most one quantum number.

In classical physics, the superposition principle is one of the most common principles. In its simplest formulation, it states that the effect of external forces on an object is the sum of the effects of each force. The superposition principle for quantum mechanics is that if a quantum-mechanical system can be in states described by wave functions Ψ_1, Ψ_2, Ψ_3,….. Ψn, then the superposition of these states will also be physically permissible, that is, the state $\Psi=c_1\Psi_1+c_2\Psi_2+\ldots+c_n\Psi_n$, where c_1, c_2 …c_n are arbitrary complex numbers. That is, in quantum mechanics, wave functions are added. It is known that the square of the modulus of the wave function determines the probabilities of processes. From this, it is clear that quantum mechanics is not reduced to the classical theory of probability: a characteristic effect of interference of states Ψ_1, Ψ_2, Ψ_3,….. Ψ_n arises, which has no analog in classical physics. Quantum superposition is one of the most mysterious concepts of quantum mechanics. Indeed, if a quantum system can exist in states Ψ1 and Ψ_2, then it can exist in states of their superposition $\Psi=c_1\Psi_1+c_2\Psi_2$. This means that along with any two states Ψ_1 and Ψ_2, their linear combination (superposition) is also a possible state. For example, if a point particle can be in one of two points, then it can be "simultaneously in both points”. Here, the mysterious, counterintuitive quality of quantum superposition is clearly visible: the ability of a quantum system to be in two mutually exclusive states at the same time. Thus, we can say more specifically that quantum superposition means the system can be in several mutually exclusive states at the same time. Namely, taking them simultaneously, not sequentially. This circumstance is as incontrovertible from a mathematical and formal point of view as it is unacceptable from a logical, common sense, and even philosophical and worldview point of view. Therefore, the explanation of the principle of superposition is impossible without the use of extra-logical concepts - miracle, magic, the most possible supernatural entities, and extra-temporal, extra-spatial models.

5. Wave function (Ψ-function) and its physical meaning

The principle of superposition discussed above can be understood in depth only when the physical essence of the wave function is also understood in depth. When we talk about photons, it is clear to us that we are talking about portions of light (electromagnetic) energy. At the same time, it does not occur to us to ask the question: "What does a photon consist of?" It is also impossible to ask such a question about an electron (at least today). This contradicts the concept of an electron's elementary nature. Moreover, what is the wave process that accompanies the motion of microscopic particles according to the de Broglie relation? It has been stated and proven many times that particles have wave properties. So, an electron is a wave. However, a wave is something extended in space and time. What is the difference between a point in space in which a wave is present at a given moment in time and a point in which there is no wave? It is better even in the last sentence to replace the word “wave” with the word “something”: what is the difference between a point in space where “something” is at a given moment in time and a point where there is nothing? The quantity that oscillates in a wave is usually denoted by the letter Ψ. If at some point it is equal to zero, then there is nothing at this point; if Ψ is different from zero, then there is something.

Simply put, we need to answer the question: what physical meaning does Ψ have? First, let us propose a negative judgment: the

Ψ function is not a field. Then this should be understood as follows: if the Ψ function is nonzero at some point, it does not mean that a force acts on another particle at that point. The Ψ function has no simple direct meaning. The fact that the Ψ function is not a field is evident from the fact that, in the mathematical sense, Ψ is a complex quantity, and all physical quantities, of course, are real quantities. (Physics uses complex quantities, but their real part always has physical meaning.) The Ψ-function is information. An electron in an atom is described using the Ψ-function. What meaning it has in this case is one of the most difficult questions in quantum mechanics. Most agree that an electron in an atom does not exist as a particle. It diffuses there into a kind of cloud. The shape and density of this cloud are determined by the wave function Ψ(x), and at a distance x from the nucleus, the density ρ(x) of the electron cloud is equal to the square of this function:

$$\rho(x)=|\Psi(x)|^2.$$

To explain this idea, let us imagine a watermelon and depict its density ρ(x) as a function of the distance x from its center in the figure. It is obvious that the function ρ(x) for a watermelon is approximately constant everywhere; it only decreases slightly towards the surface (the skin is lighter than the flesh) and, finally, abruptly breaks off at the edge of the watermelon. Looking at the figure, a person who has never seen a watermelon in his life can schematically imagine how it is built inside. True, at the same time, a person will not have the slightest idea about its taste, color, and aroma, as well as about the thousands of small features that distinguish one watermelon from another. Trying to penetrate the inside of an atom, we all find ourselves in the place of a person who has never seen a watermelon in his life, but wants to imagine it in terms of the function ρ(x). For an atom, the function ρ(x) can be found from the Schrödinger equation and then, with its help, draw the distribution of the electron cloud in the atom. These pictures replace the visual image of the atom, to which everything unconsciously strives. These pictures appear in almost all textbooks on both general physics and quantum mechanics.

The physical meaning of the Ψ-function was understood by M. Born (1926). It turned out that the square of the modulus of the Ψ-function determines the probability of detecting a particle at a particular point in space. Thus, the wave process we have discussed extensively describes a probability wave. More precisely, a wave from which, by a known method, the probability of detecting a particle can be constructed.

The probabilistic meaning of the wave function (Ψ-function) has completely radically changed the manner of describing events in mechanics. It was necessary to reconsider the concept of causality.

In classical mechanics, specifying the initial conditions and the forces acting between particles allows the system's evolution to be accurately calculated. In quantum mechanics, knowledge of the system's initial state also allows us to trace its evolution unambiguously. However, the state of the system is described in terms completely different from those. Due to the uncertainty relation, or, which is the same thing, due to the wave properties of particles, the state of the system cannot be described with the same degree of detail as adopted in classical mechanics. The maximum detail of the description of a mechanical system is the specification of the wave function. Knowing this, we can conclude the results of a physical experiment. However, these results are formulated in probabilistic terms. We cannot say that something will happen, but we can only say that the probability of this event is such and such. This means that verifying quantum laws is possible only when the experiment is repeated (in practice, this is always the case). This does not mean that quantum mechanics does not make unambiguous predictions. This is not the case. For example, an electron in an atom has a completely defined energy. Measuring the energy of an electron, say, by measuring the ionization potential, gives a completely unambiguous result, no matter how many times the experiment is repeated. However, if we want to measure the coordinate or momentum of an electron in an atom, we will get different results, the probability of which is determined by the wave function.

In classical physics, knowing the initial conditions and the forces acting on the bodies at a given moment, we can use Newton's equations - at least in principle - to determine the position of particles at any subsequent moment. Everything that we said earlier (about the uncertainty relation, about the wave properties of particles) serves as a convincing argument that this cannot be done when studying the motion of atomic particles. A fundamentally new approach is needed.

The formulation of the fundamental equations always bears the features of phenomenology (description). The fundamental equations cannot be derived (at least not yet, until a more general theory emerges). They are the most compact formulation of experimental data. Of course, when creating them, the authors had suggestive theoretical ideas, but they were suggestive, and not some random, strict logical scheme...

Quantum mechanics has its own rigorously developed, logically consistent mathematical scheme for calculating physical quantities, which allows it to predict the results of the most diverse experiments. The motion of atomic particles with velocities small compared to the speed of light is described by the famous Schrödinger equation, which plays the role of Newton's equations of classical mechanics; the Ψ-function is the solution of this equation. W. Heisenberg created another (not at all similar in form) mathematical apparatus. Later, it was shown that both methods yield identical physical results.

6. Schrödinger's equation

The name of the outstanding physicist Erwin Schrödinger is inextricably linked with the formation and development of quantum theory. His wave equation occupies a central place in this theory, elevating Schrödinger among the great scientists of our time.

Schrödinger developed wave mechanics in his own way, treating the atom as an oscillatory system and identifying its possible natural oscillations with stable energy states in the atom. He proposed that the equation of motion of an electron in an atom should be a wave-type equation with boundary conditions that determine the possible values of energy. This bold decision was the birth of quantum mechanics.

The classical equation of motion was consistent with this description. The total energy of an object is the sum of its kinetic and potential energies.

$$T+U=E. \qquad (1)$$

The kinetic energy T is equal to $mv^2/2$. The potential energy of an electron in an atom at a distance r from the nucleus is equal to $-e^2/r$. Therefore, equation (1) can be rewritten as

$$mv^2/2-e^2/r=E. \qquad (2)$$

To obtain the equation in impulse form, as used by Niels Bohr, we replace the product mv with p:

$$\frac{1}{2}\frac{p^2}{m}-\frac{e^2}{r}=E\,. \qquad (3)$$

Schrödinger considered that this was not yet a wave equation. Nevertheless, he found a way to obtain a real wave equation from equation (3). Schrödinger replaced the classical momentum p with a mathematical operator (an instruction to perform a mathematical operation on a mathematical quantity). It is clear that an operator was chosen that would transform (3) into a wave equation. To do this, it was necessary to invent a new function; Schrödinger called it a wave function and denoted it by the Greek letter Ψ (psi). Such a wave function had to be introduced into the equation so that the operator had something to act on. Now the Schrödinger equation looks like this:

$$(\frac{1}{2}\frac{p^2}{m}-\frac{e^2}{r})\psi=E\psi, \qquad (4)$$

It should be remembered that in this new wave mechanics, p is no longer the product of mass and velocity, but an “order to act by the operator” on the function Ψ. It turned out that all the data about an electron's behavior in an atom are encoded in the function Ψ. Now we need to find the boundary conditions - after all, the line spectrum of an atom is obtained through them. Here, we will have to rely only on the physical content. If information about the location of an electron in a hydrogen atom is hidden in the Ψ-function, the boundary conditions should be constructed based on the limiting cases that make sense for this problem. One of the boundary conditions is obvious: if the electron in a hydrogen atom were infinitely far from the proton, the attraction between them would disappear. Therefore, the following mathematical restriction is imposed on the function Ψ: it must be equal to zero at infinity. In addition, this function must not allow jumps, that is, be continuous and, of course, be finite. The latter physically means that the electron cannot move at an infinite speed. These conditions cause the appearance in the solutions of equation (4) of a line spectrum that completely coincides with the spectrum of the hydrogen atom.

This achievement was only the beginning of a series of unprecedented successes of the new quantum mechanics. Without going into their details and chronology, it can be convincingly argued that quantum mechanics can explain all of chemistry. In principle, if the mathematical difficulties of each new, more complex problem did not increase, it would be possible to foresee any chemical changes.

But let us return to the Schrödinger equation. When solving this wave equation, we immediately obtain two quantities that interest us: E is the allowed energy levels of the atom or molecule, and for each allowed energy value, Ψ is the function of the spatial coordinates of the electron. What data can be obtained from Ψ?

We have two possible models. The energy conservation equation (1) $T+U=E$ is related to the classical description of the motion of particles in a system. The Schrödinger equation (4) is a wave-type equation; it is related to the oscillatory motion of, for example, guitar strings or drum heads. In classical mechanics, particles move along certain trajectories, while wave motion is described by a displacement function that gives a picture of nodes, displacement amplitudes, and phase signs. When studying Ψ, it turns out to be closer to the second-wave model. The function Ψ is characterized by nodal surfaces, at the intersection of which the phase sign changes. If two wave functions interact with each other, then, like waves, they either add when the phases coincide or mutually cancel each other when the phases are opposite. However, Ψ contains absolutely no information about the trajectory of the electron. In fact, in the microworld, the very concept of the “electron trajectory” in an atom or molecule has lost its meaning. Instead, the function Ψ or its square Ψ_2 allows us to determine only the probability of an electron being in a given volume. Where the value of Ψ_2 is large, the probability of an electron being found is also large. Where Ψ_2 is small, the electron is rare. On a nodal surface, the value of Ψ is zero – there the electron never is.

7. Classification of nanostructures and their characteristics

Humans have been using nanoparticles in their activities for a long time. For example, two thousand years ago in ancient Rome, concrete made from volcanic dust nanoparticles was used, and about a thousand years ago in Europe, art glass was created, the color of which was determined by the presence of nanoparticles of silver and gold. The significance of research and development in the field of nanoobjects was first scientifically substantiated by the American physicist and Nobel laureate R. Feynman (hence he is called the “father of nanotechnology”). Feynman noted that the laws of physics do not prohibit manipulating individual atoms, arranging them one by one in the desired order, and creating atomic structures with specified properties. However, the level of scientific and technological development in the 1950s did not allow for the implementation of such technologies. Nanotechnology began to be introduced into electronics and other fields of technology only in the late 80s. Nanotechnology is a scientific and technical field for the creation of materials, functional structures, and devices at the nanoscale. It is precisely due to the small size of the blocks (particles, granules, phases) from which they are built that nanomaterials demonstrate unique mechanical, optical, electrical, and magnetic properties. Research and application of nanostructured materials are among the most dynamic areas of materials and device development, with important applications in technology and medicine. Nanostructured materials exhibit unique properties compared to their conventional bulk counterparts. Nanostructured materials include modern and future technologies for manufacturing semiconductors, catalysts, environmental-cleaning materials, and biological materials. This is the future of electrical engineering, high-strength materials technology, microelectronics, optics, biomedicine, food science, and pharmaceuticals. A special branch of science is developing to describe the properties of nanomaterials - nanophysics. It has long been discovered that reducing the size of blocks – crystals in a substance (primarily in metals and ferroelectrics) can lead to a significant change in their properties. Such changes occur when the average crystal grain size does not exceed 100 nm and are most noticeable when the grain size is less than 10 nm. Polycrystalline fine-grained materials with an average grain size of 40 – 150 nm are sometimes called submicrocrystalline, and if the average grain size is less than 40 nm, then nanocrystalline. In these cases, the concept of "long-range order of the arrangement of atoms of a substance" can no longer be used. The term "nano" comes from the Greek word "nannos" – dwarf. The main types of nanocrystalline structures are shown in Fig. 1. Their characteristic sizes are 5 – 300 nm. The properties of the surface of a solid differ significantly from its bulk properties. The point is that on the surface of the crystal, the regular electronic bonds of atoms are "broken", as a result of which the equilibrium structure of the surface is arranged differently than the structure of the volume. Studies have shown that at the crystal surface, the number of atoms in the unit cell changes, a different symmetry appears, and the vibration frequencies of the atoms in the crystal lattice (phonon frequencies) also change. As a result, the Debye temperature of the crystal changes (usually decreases) on the surface of the crystal and, accordingly, its melting point decreases.

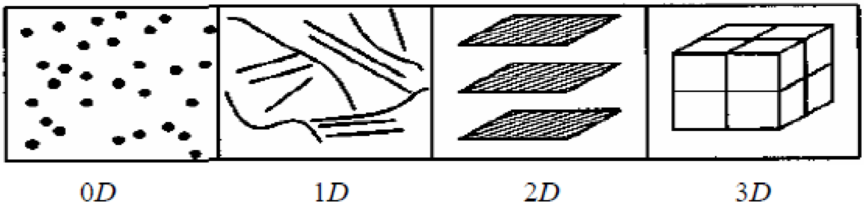

Fig. 1. Types of nanocrystalline materials: 0D – “zero-dimensional” clusters (quantum dots); 1D – one-dimensional clusters (nanotubes, fibers and wires); 2D – two-dimensional nanomaterials (films and layers); 3D – three-dimensional (nanocomposites and polycrystals)

These properties are fundamental, since they are determined by the peculiarity of bonds in solids. Lowering the melting point of the near-surface layer is widely used in epitaxial layer manufacturing. Lowering the melting point of nanomaterials can be quite large. The experimental dependence of the melting point of micro and nanoparticles of two different substances – gold (metallic bond) and the semiconductor cadmium sulfide (ionic-covalent bond) is shown in Fig. 2.

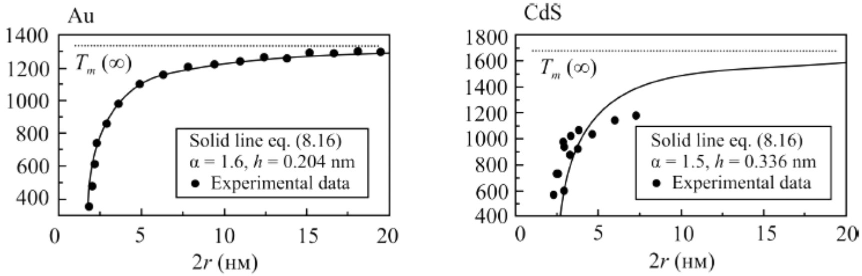

Fig. 2. Dependence of the melting point of gold and cadmium sulfide nanoparticles on their size

As shown in Fig. 2, the decrease in the melting point of nanoparticles can reach 1000 K, which is used in nanotechnology. The main reason why nanomaterials differ from conventional materials is that in such substances, the surface area to volume ratio coefficient is very large, that is, the ratio of the number of atoms on the surface of the nanocluster and in the volume of the cluster. Moreover, the smaller the nanocluster, the more surface properties affect its volume properties. In a certain sense, nanostructures allow you to “transform” the properties of the crystal surface into volume properties. At the same time, depending on the ratio of the surface of the clusters to their volume, the properties of a particular substance in a nanostructured form are quite different. Therefore, by changing the size and shape of the clusters, these properties can be purposefully changed. In addition, the structural state of the nanocluster grain itself also changes significantly. Defects in the crystal structure, typical of single crystals and large (over 10–50 μm) polycrystals, such as dislocations (which usually have a density of about 10^4 cm^{-2}), as well as vacancies and packing defects (10^6–10^{10} cm^{-3}) in a nanomaterial often cannot be contained inside the grain and emerge to the surface, transforming the grain structure into an almost defect-free one. The intergranular boundary is structurally unstable, and therefore, nanocrystalline materials exhibit atom diffusion mobility 5–6 orders of magnitude higher than in conventional polycrystalline materials. The theoretical model of nanocluster formation of various sizes is shown in Fig. 3. It is assumed that interatomic bonds are spherically symmetric (a model of densely packed elastic balls). In the first cluster, 1 atom is surrounded by 12 atoms, since 12 is the maximum coordination number. The first cluster contains 13 atoms. In this simplest case, the percentage ratio of the number of atoms on the surface (12) to the number of atoms contained in the volume (1) is 92%. In the second cluster, another layer of atoms is added to the surface, bringing the total to 55, and the volume ratio is 76%. As the number of atoms in the clusters increases, only about half of them are contained inside the volume.

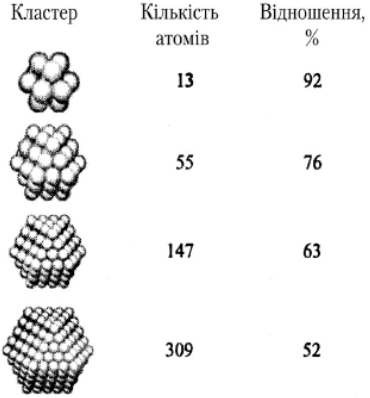

Fig. 3. Percentage ratio of the number of atoms inside the cluster to the number of atoms located on the surface.

Generalized data on the surface part of atoms in nanostructures, depending on the size of the cluster, are shown in Fig. 4.

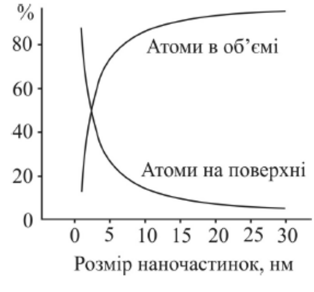

Fig. 4. Percentage ratio of the number of atoms that reach the surface of a nanograin to the atoms contained in the volume, depending on the particle size in nanometers: at a particle size of 4 nm, about 50% of them are on the surface.

The "size" effect described above affects not only the properties of crystal lattices, but also the energy spectrum of electrons in the cluster (for example, the width of the forbidden band of semiconductors changes).

Reducing the size of grain clusters is considered an effective method of controlling many properties of solids. There are good reasons for such predictions. The small grain size leads to significant changes in the solid's structure. If we assume, in a rough approximation, that the grain shape is spherical, with a diameter of d and a boundary thickness of t, then the fraction of intergranular boundaries in the total grain volume is

$$\Delta V/V = [\pi d^3/6 - \pi/6(d - 2\,t)^3]/[\pi d^3/6] \approx 6\,t/d. \qquad (1)$$

At a boundary thickness t of three to four atomic monolayers (0.5 to 1.5 nm), the surface layer accounts for up to 50% of the entire substance. Let us recall that in ordinary crystals and polycrystalline substances, this ratio is 10^{-9} to 10^{-6}, respectively. The intergranular boundary of the nanocomposite itself is characterized by structural instability. Therefore, nanocrystalline materials are characterized by high diffusion mobility of atoms, which is 5 to 6 orders of magnitude higher than in ordinary polycrystalline materials. The development of diffusion in nanocrystalline materials can be caused by:

– a lower concentration of impurities in intergranular boundaries compared to boundaries of the usual type characteristic of polycrystals;

– the presence of porosity in nanocrystalline materials.

A rather important achievement in nanoelectronics is the discovery of special molecules composed of carbon atoms: fullerenes and nanotubes.

A fullerene combines 60 (C_{60}) or more (C_{70}, C_{76}, C_{120}, etc.) carbon atoms. The C60 fullerene is composed of 12 pentagonal (five-sided) and 20 hexagonal (six-sided) faces, arranged symmetrically, forming a shape close to a sphere with a diameter of about 1 nm (Fig. 5).

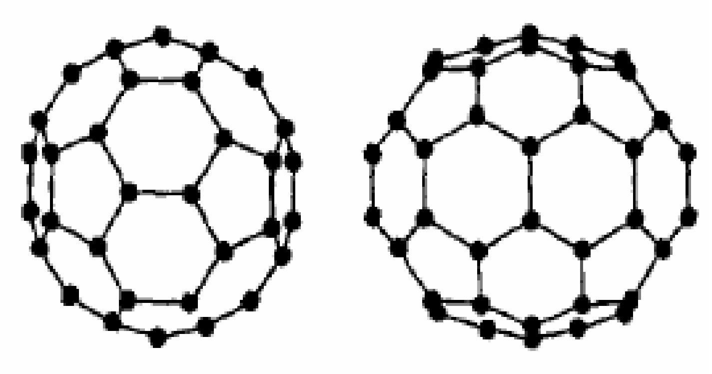

Fig. 5. Structure of C60 and C70 molecules

A soccer ball made of hexagons and pentagons has the same shape. The discovery of fullerenes was the result of studies of the nature of the interstellar medium. Scientists recreated the conditions in which carbon pairs in the outer layers of special stars (“red giants”) and, as a result, recorded the formation of C_{60} fullerenes under similar conditions. The high binding energy of carbon atoms in fullerene clusters (~7 eV per atom) and the symmetry of the molecules determine their anomalously high thermal stability. Experimental data show that the C_{60} molecule retains its thermal stability up to 1700 K. Carbon molecules – C_{60} clusters (as well as C_{70})- can form solid crystals – fullerites. In them, clusters of fullerenes are combined into a crystal by Van der Waals forces with large voids between the fullerenes. The placement of alkali element atoms in these voids initially transforms the dielectric properties of fullerene crystals into semiconductor properties, and at low temperatures into superconducting ones. After the discovery (1984) of fullerenes, an intensive search for other forms of carbon nanoparticles began. In 1991, tubular structures made of carbon atoms were discovered - carbon nanotubes (Fig. 6).

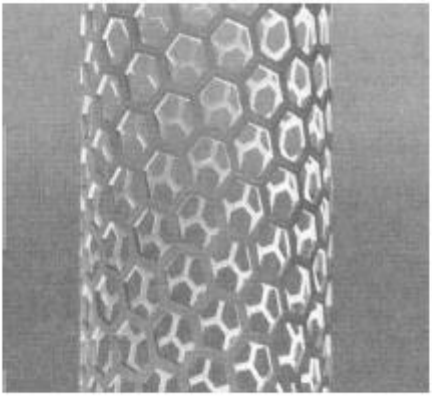

Fig. 6. Schematic representation of a single-walled carbon nanotube with a cylindrical structure

They are formed by folding the hexagonal plane of the graphite lattice, consisting of hexagonal cells, at the vertices of which carbon atoms are located. Nanotubes are quasi-one-dimensional carbon filamentary crystals characterized by a tubular structure, the properties of which are comparable to the properties of an ideal graphite fiber. The diameter of such tubes usually does not exceed several nanometers (~0.4 nm for single-layer and up to 100 nm for multilayer), and the length ranges from tenths of a micron to several microns. In a longitudinal section, it turns out that each thread consists of one or more layers, each of which is a hexagonal graphite grid (Fig. 6). The basis of such a grid is hexagons, at the vertices of the corners of which carbon atoms are located. In all cases, the distance between the layers is 0.34 nm, i.e., the same as between the layers in crystalline graphite. The upper ends of the tubes are closed with single- or multilayer hemispherical caps, each layer of which is composed of hexagons and pentagons, resembling the structure of half a fullerene molecule. Carbon nanotubes can be single- and multilayered (Fig. 7).

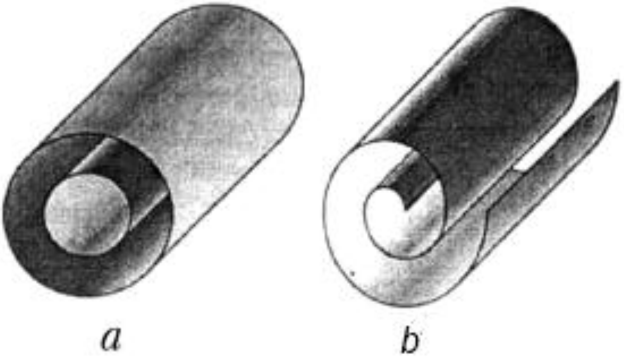

Fig. 7. Cross-sectional models of multilayer nanotubes:

a – “Russian Motriyka”; b – scroll.

The uniqueness of the nanotube structure lies in the spiral arrangement of carbon hexagons on the surface of the layer, which represents a lattice. The spiral structure, characterized by the symmetry of the configuration and the diameter of the tube (each of these parameters determines the size of the repeating structural element), introduces significant changes in the electron density of states, and, therefore, determines the unique electrical properties of nanotubes. Another influencing factor is topology, that is, the geometric configuration of individual layers in each tube, oriented in a specific way, which greatly affects the physical properties. The combination of size, structure, and topology gives nanotubes unusual mechanical properties (stability, strength, hardness, or flexibility during deformation), as well as features of electrical charge transfer (coherent movement of electrons). By nature, nanotubes can be semiconducting or metallic, depending on their structural organization, which is controlled technologically. Moreover, carbon tubes can be filled with "monatomic threads" of various metals or compounds. The inner surface of nanotubes can be so large that it is possible to create structures with a specific surface area of 500 m^2/m - promising for hydrogen accumulation. Thus, carbon nanotubes have extraordinary electrical, mechanical, magnetic and electronic properties, and technological influences can modify these properties. Carbon nanotubes are widely used in practice. Nowadays, nanotubes are made not only from carbon but also from other materials.

8. Quantum-scale effects in nanostructures. Basic elements of nanoelectronics

In electronic structures, quantum-scale effects are observed when the critical length lcr is played by the de Broglie wavelength λ for electrons, that is, when the size of the structure in at least one dimension is of the order of λ. Thus, quantum-scale effects arise from the wave nature of electrons. In nanoscale areas, the behavior of electrons is determined by the reflection of electron waves from the boundaries of the separation of such areas, as well as by the interference of electron waves or the passage of waves through potential barriers, the quantization of the energy of electrons spatially limited in their movements, the passage of electrons through nanometer dielectric layers, the quantization of the electrical resistance of nanowires, etc. The de Broglie wavelength for an electron with an effective mass m* and moving in a crystal with a velocity υ has the following value: $\lambda=\hbar/p=\hbar/m^*\upsilon$, where $p=m^*\upsilon$ is the momentum. Thus, the de Broglie wavelength is larger when the electron's effective mass is smaller. In most metals, it is almost the same as in vacuum $m^* \sim m_e$, therefore, the de Broglie wavelength is relatively small. However, in semiconductor materials, the electron's effective mass can vary widely. At room temperatures (~ 300 K) for silicon $m^*=1.1me$ and $\lambda=8$ nm, for gallium arsenide $m^*=0.07m_e$ and $\lambda=30$ nm. Therefore, in semiconductors, the de Broglie wavelength is nanoscale, and, in this regard, quantum-scale effects are easier to create. The energy spectrum characterizes the dependence of the energy of a particle on its momentum E(p) or, which is the same, the dependence of the energy on the wave vector E(k), since the momentum and the wave vector are related by a simple relation (the modulus of the wave vector is determined by the inverse of the wavelength: $k=2\pi/\lambda$). The energy spectrum is a set of possible values of the energy of a particle under certain conditions. If the energy is quantized, then the energy spectrum is called discrete (quantum). If the energy can take on a continuous series of values, then the spectrum is called continuous. The density of states g(E) determines the number of quantum states of electrons that fall per unit volume, area, or length (depending on the dimensionality of the object) in a unit energy interval. According to this definition, the density of states is equal to the number of possible states dn(E) in the energy interval from E to E + dE. Knowledge of the density of states g(E) and the probability of their filling by electrons w(E) allows us to establish the distribution of electrons by quantum states and describe the electrical, optical, and some other properties of a solid. Electrons have a half-integer spin. Therefore, the probability of their filling quantum states is determined by Fermi-Dirac statistics, which is based on the Pauli exclusion principle.

"Infinite" crystal. Characterized by a three-dimensional (3D) long-range arrangement of atoms. From the point of view of nanophysics, even a micron-sized crystal already looks "infinite" because in all directions its regular crystal lattice consists of thousands of atoms, which is many times the de Broglie wavelength. In metals and semiconductors, the crystal is filled with a volumetric (three-dimensional) 3D electron gas in which electrons can move freely in any direction. Electron energy in a 3D gas

$$E = \frac{m^* v^2}{2} = \frac{(p_x^2 + p_y^2 + p_z^2)}{2m^*} = \hbar^2 \frac{(k_x^2 + k_y^2 + k_z^2)}{2m^*}, \qquad (2)$$

where p and k are the quasi-momentum and quasi-wave vector of the electron, respectively, and m* is its effective mass (for simplicity, it is assumed to be isotropic). The spectral dependence of E(k) looks like a quasi-continuous one, since there are as many energy levels as electrons are contained in the 3D crystal (10^{14} – 10^{22} cm^{-3}). The dependence of the energy on the components of the electron wave vector near the bottom of the conduction band is shown in Fig. 8, b. The density of quantum states of electrons g(E) for an unlimited size (3D) crystal, which is also depicted by the parabola g(E) ~ $E^{1/2}$, is shown in Fig. 8, c. The density of states is small near the bottom of the conduction band (where the count begins), but gradually increases with increasing E, reaching saturation.

From Fig. 8, it is seen that within the same zone, the functions E(k) and g(E) are quasi-continuous, and therefore, the properties of 3D crystals under the influence of fields change continuously.

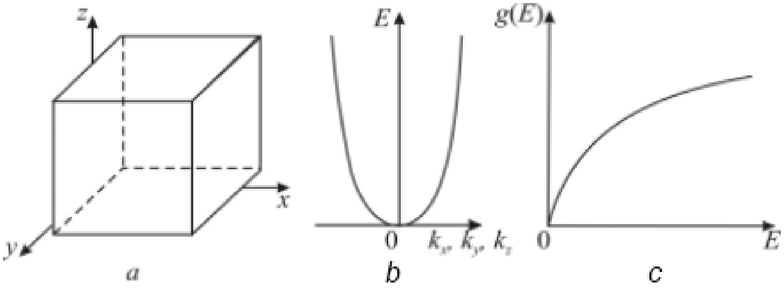

Fig. 8. Electronic spectrum of an unlimited crystal:
a – crystal sample; b – dependence of electron energy on the components of the quasiwave vector; c – dependence of the density of quantum states (g(E)) on the electron energy (E)

Quantum well. A quantum well corresponds to a two-dimensional (2D) object. Usually, it is a thin layer of a crystal, the thickness of which d is proportional to the de Broglie wavelength (d ~ λ). The system of electrons in such a layer is called a two-dimensional (or 2D) electron gas. A fragment of such a layer is shown in Fig. 9, a. The motion of electrons in this layer is limited by a segment dx in the x direction and is not limited in the y and z directions. Moving in the x direction, the electron is unable to leave a thin layer, since its work function (equal, for example, in aluminum arsenide, about 4.5 eV) is much greater than the energy of thermal motion (~ 0.026 eV at room temperature). Therefore, the motion in the x direction can be rightly considered as the motion in a one-dimensional, sufficiently deep rectangular potential well with a width of dx (Fig. 9, a). The energy of such a motion is quantized and characterized by the quantum number n = 1, 2, 3, ... If the well were infinitely deep, then its width dx would fit an integer number of half-waves λn/2, i.e. dx = pλn/2. This means that only those states of electron motion would be stationary, which would correspond to a standing wave formed by the de Broglie waves incident and reflected from the walls of the well. The quantities En are called quantum-dimensional levels. The energy of motions along the y and z axes is not quantized and is defined by the same expressions as that of a free particle or its volume. Therefore, the total energy of an electron, provided that the effective mass of the electron m* is the same for motions in all directions, can be given by:

$$E = \hbar^2 (k_y^2 + k_z^2)/2m^* + \hbar^2 \pi^2 n^2 / 2m^* d_x^2, \qquad (3)$$

where the quantum number n = 1, 2, 3, ...

Therefore, the energy spectrum of an electron in a quantum well of a two-dimensional nanoobject will be discretely continuous. Each dimensional level En corresponds to a set of possible energy values due to the free motion of the electron along the y and z axes. This set of energies E is called a two-dimensional subband of dimensional quantization. The dependencies E(ky,kz) and g(E) are shown in Fig. 9, b, c. The graph of the dependence E(ky,kz) is a system of paraboloids; the bottom of the n-th paraboloid corresponds to the level E = En. The dependence of g(E) is stepped. Each dimensional subband makes the same contribution m*/πħ2 to the density of states. Strictly speaking, the model of an infinitely deep rectangular potential well is valid only for the motion of an electron in an "isolated" thin film with a nanoscale thickness d. Such a separate, extended, plane-parallel film of nanometer thickness is difficult to realize. In practice, in nanoscale structures, such nanolayers are created within the crystal so that carrier motion is limited to one dimension; therefore, these carriers can be considered to be in a one-dimensional potential well. For example, electrons in a nanometer-thick layer of a narrow-gap semiconductor sandwiched between two layers of a wide-gap semiconductor can be cited. Practical examples of quantum wells with 2D electron gas can be conductive channels in unipolar transistors (metal-oxide-semiconductor structures on silicon).

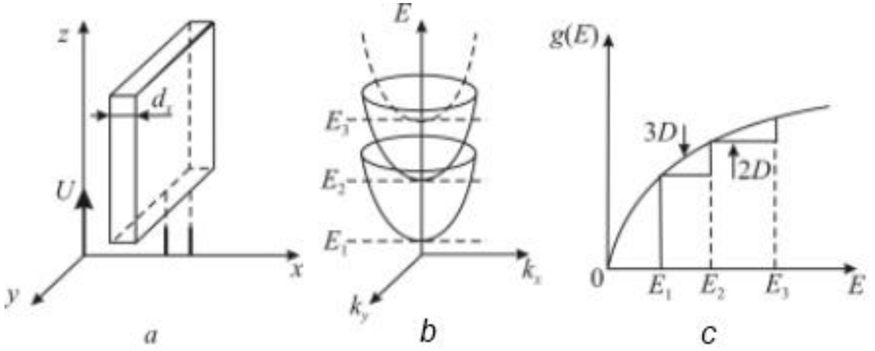

Fig. 9. Two-dimensional (2D) nanoobject (thin layer):
a – schematic representation of a thin layer limited along the x-axis;
b – potential wells for electrons in this layer;
c – dependence of the density of states on energy in the case of an infinitely deep quantum well

Quantum wire (quantum filament). This is a one-dimensional (1D) object. The motion of electrons is limited along the x- and z-axes by the dimensions dx and dz, respectively, but is not limited along the y-axis (Fig. 10). The square cross-section of the quantum wire is a model for calculation; it may be different from that shown in the model drawing. The only important thing is that the potential well for free electrons in the quantum wire (filament) is two-dimensional. The electron energy associated with motion along the y and z axes should be quantized in the same way as in one-dimensional potential wells of widths dy and dz.

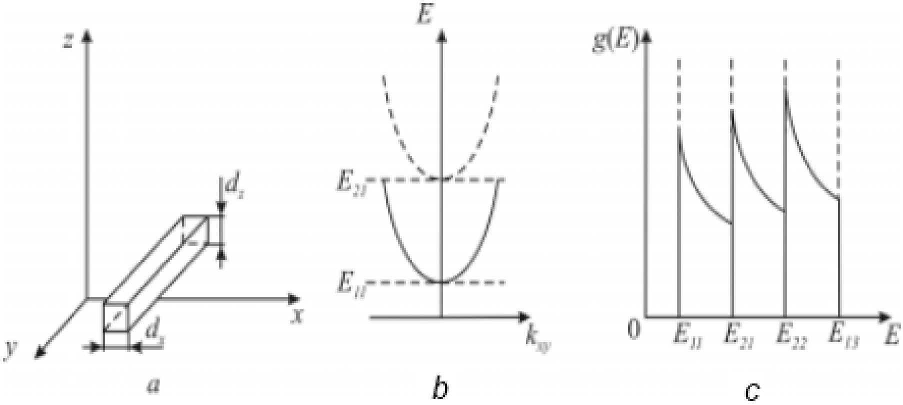

Fig. 10. One-dimensional (1D) nanoobject – quantum wire:
a – model image; b – dependence of energy on the value of the wave vector; c – dependence of the density of states on energy

Total energy of an electron:

$$E = \hbar^2 k_y^2 / 2m^* + E_{mn} = \hbar^2 k_y^2 / 2m^* + \hbar^2 \pi^2 n^2 / 2m^* d_x^2 + \hbar^2 \pi^2 m^2 / 2m^* d_z^2,$$

where m, n= 1, 2, 3, ... and E_{mn} is the energy of the dimensional levels. The position of each of them depends on two quantum numbers, т and н, as well as on the values dx, dz, and in the direction of wire stretching (y), the spectrum is continuous. The conduction band in a quantum wire contains one-dimensional subbands (Fig. 10, b). The density of states per unit length, g(E), has several sharp peaks (Fig. 10c), corresponding to the dimensional levels. This means that most of the electrons in the subband have an energy close to the corresponding dimensional level. Most methods of manufacturing quantum wires rely on the fact that, in a two-dimensional electron gas (usually a heterostructure), electron motion in one direction is limited by a specific technological method. The conductivity of quantum wires can have important features. The most interesting of them is inherent in short filaments, the length of which is less than the free flow length of electrons (it is determined by scattering on impurities and defects of the filament). In this case, an electron, having flown from one contact of a quantum wire, reaches the other contact without collisions, like a projectile fired from a cannon. By analogy, structures with no electron collisions, often called ballistic, are considered.

Quantum dot as a zero-dimensional (0D) object (Fig. 11, a). The motion of electrons for the dot is limited in all three dimensions: x, y, and z. Fig. 11 shows a convenient model for calculations; in reality, the shape of a quantum dot is usually not cubic.

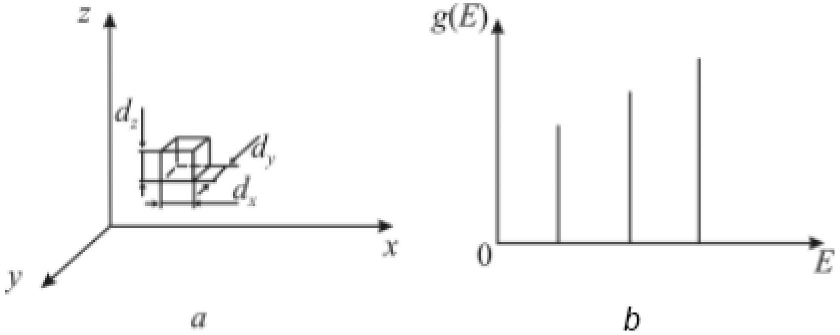

Fig. 11. Zero-dimensional (0D) nanoobject – quantum dot:
a – model image of a quantum dot, b – dependence of the density of states on energy.

The potential well for a quantum dot is three-dimensional. The energy of free electrons must be quantized for motions in all three dimensions. The energy spectrum of electrons in a quantum dot is completely discrete, as in an individual atom. The expression defines the energy

$$E = \hbar^2\pi^2 l^2 / 2m^* d_x^2 + \hbar^2\pi^2 n^2 / 2m^* d_y^2 + \hbar^2\pi^2 m^2 / 2m^* d_z^2 , \quad (4)$$

where l, m, n = 1, 2, 3,...; dx, dy, dz are the dimensions of the area in three dimensions (Fig. 11, a). The energy spectrum of electrons consists of discrete energy levels Elmn, which resemble the spectrum of an isolated atom. The magnitude of the energy Elmn depends on the three quantum numbers l, m, n, and the dimensions dx, dy, and dz. The density of states graph g(E) in a quantum dot has a δ-like form: g(E)=∞, if $E=El_{mn}$ (E coincides with the dimensional level) and g(E)=0, if E ≠ Elmn (i.e. E is in the gap between the dimensional levels). An example of quantum dots is nanocrystals of one material on the surface of a growing epitaxial layer of another material. Fig. 12 shows an atomic force microscopy image of an island of Ge atoms grown on the Si surface.

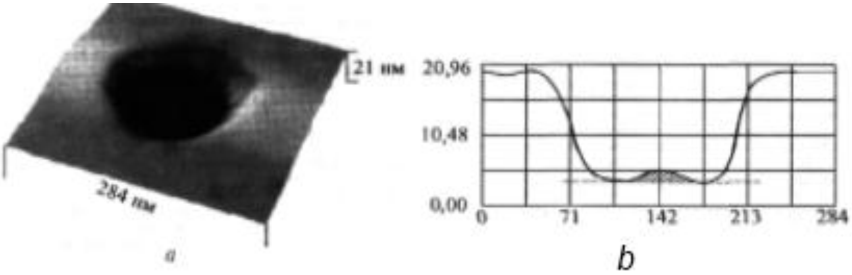

Fig. 12. A section of the silicon surface with a well with a diameter of about 100 nm and a depth of about 16 nm, at the bottom of which a quantum dot of Ge atoms, obtained by deposition from the gas phase, is placed: a – image obtained using an atomic force microscope; b – cross-sectional profile of the well with a quantum dot with a diameter of ~ 3.3 nm.

Historically, the first quantum dots were microcrystals of cadmium selenide CdSe. An electron in such a microcrystal is confined to a three-dimensional potential well, so it has several stationary energy levels with characteristic spacings between them (the exact energy-level equation depends on the shape of the quantum dot). During a transition between the energy levels of a quantum dot, a photon can be emitted, similar to an electron's transition between the energy levels of an atom. It is also possible to excite ("throw") an electron to a higher energy level and obtain radiation from the transition between lower levels (luminescence). In this case, unlike real atoms, the transition frequencies are easily controlled by changing the dimensions of the microcrystal. The observation of luminescence in cadmium selenide crystals, with the luminescence frequency determined by crystal size, marked the first observation of quantum dots.

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