

Quantum mechanics.

Quantum mechanics (QM) is the science about the motion of microscopic physical objects. QM takes into account wave-particle duality and uncertainty principles. The waves discussed in QM are de Broglie waves also known as matter waves. The quantity oscillating in this wave is the probability to find a physical object in the certain part of the space. Square of the amplitude A of the matter wave is equal to probability density that we get if we divide probability to find particle in certain part of the space ΔP by the volume of this space ΔV : So we have $A^2 = \Delta P / \Delta V$ or more precisely $A^2 = dP / dV$. If the object can move only along the x -axis, then $A^2 = dP / dx$, we are talking about the linear density of the probability.

Uncertainty relation between the coordinate and momentum $\Delta x \cdot \Delta p_x \sim \hbar$ says that we are not able to determine simultaneously the coordinate (x) and the momentum along the same axis (p_x). The more accurately we know one of these values, the less accurately we know the other. The sign “ \sim ” should be read “*is in the same order of magnitude*”. The constant $\hbar = h / (2\pi) = 1.054 \cdot 10^{-34}$ J · s (called *h-bar*) is the reduced Planck constant. The principal difference between classical and quantum mechanics is lying in the uncertainty relation. According to the classical mechanics $\Delta x \cdot \Delta p_x = 0$, there are no uncertainties. All the values of coordinate and momentum are predictable. So the classical mechanics is a special case of QM, considering the Planck constant being negligibly small (equal to zero).

In the case of certain energy values of physical objects, generated by strong spatial restriction, the coordinate-momentum uncertainty relation is written in the form $\Delta x \cdot \Delta p_x \geq \hbar/2$. In particular, this relation states that the complete stopping of thermal motion of the matter particles is impossible. If the particle is completely at rest, then its coordinate and momentum are both equal to zero. The zero values are certain values. According to the uncertainty relation $\Delta x \cdot \Delta p_x \geq \hbar/2$, this situation is not possible.

The coordinate-momentum uncertainty relation represents the intercourse between wave and particle nature of physical objects. If we know the momentum of the particle and hence its wavelength ($\Delta p_x = 0$), then we cannot talk about particle nature ($\Delta x = \infty$, the whole space is “full” of wave). If we know the exact position of the particle ($\Delta x = 0$), then physical object behaves only as a particle. We cannot find its wavelength and momentum. The future of the object is completely unpredictable.

Uncertainty relation between the energy and time $\Delta E \cdot \Delta t \sim \hbar$ states that energy and lifetime of quantum state cannot be simultaneously determined. This represents the finite distance between energy levels. The energy of emitted photon is fully determined ($\Delta E = 0$) only when the emission process lasts for eternity ($t = \infty$). The law of energy conservation can be violated by the amount $\Delta E \sim \hbar / \Delta t$ during the time interval Δt .

Wave function is a function describing completely in QM the condition of a physical object. For the particle moving along x -axis: $\Psi = A \cos(\omega t - kx)$ or in complex form $\Psi = A \exp[i(\omega t - kx)]$. Wave function is a solution of the Schrödinger equation. In the QM textbooks, the wave function is obviously presented in the form $\Psi = A \exp[i(kx - \omega t)]$, using at first the spatial part of the phase (kx) and then the temporal one (ωt).

Schrödinger equation is describing the motion of the physical object in the QM like the Newton's laws do it in the classical mechanics. Schrödinger equation is the energy conservation law: $E = E_k + E_p$ or according to quantum mechanical notation $\hbar\omega = \hbar^2 k^2 / (2m) + U$. The kinetic energy of the object is represented in the QM through the momentum p and wave number k in the form of $E_k = m^2 v^2 / (2m) = p^2 / (2m) = \hbar^2 k^2 / (2m)$. The momentum of the physical object is proportional to its wave number according to de Broglie formula: $p = h / \lambda = (h / 2\pi) (2\pi / \lambda) = \hbar k$.

The Schrödinger equation for the particle moving along the x -axis: $i\hbar (\partial \Psi / \partial t) = (-\hbar^2 / 2m) (\partial^2 \Psi / \partial x^2) + U \Psi$. For an electron located in atom, the Schrödinger equation and the wave functions do not depend on time: $\{(-\hbar^2 / 2m) \Delta + U\} \psi = E \psi$, where $\psi = A \exp(ikx)$ and $\Delta = \partial^2 / \partial x^2 + \partial^2 / \partial y^2 + \partial^2 / \partial z^2$ is called Laplace operator. Expression $\{(-\hbar^2 / 2m) \Delta + U\}$ is called Hamilton operator or hamiltonian (notation \hat{H}). The hamiltonian is the operator of the total energy of the QM system. It means that the eigenvalues of the hamiltonian are the values of the net energy of the system.

The operator is a prescription or manual that describes what kind of manipulations one should perform with the function written after operator. These manipulations are called the implementation of the operator. For example, if we implement time derivative operator $(\partial./\partial t)$ on wave function $\Psi = A \exp [i(kx - \omega t)]$, we get relation $(\partial./\partial t) \Psi = -i\omega \Psi$, that is called **eigenvalue equation**. The quantity $(-i\omega)$ on the right side of equation is called eigenvalue. The functions that satisfy the certain eigenvalue equation are called eigenfunctions. Therefore, the Schrödinger equation for the atom $\hat{H}\psi = E\psi$ is an eigenvalue equation. Eigenvalues of Hamilton operator are the energies of the atom. The operator is like a camera used for taking photograph of some QM object. All the information about the object is included in the wave function but we cannot obtain it all at once. The eigenvalue is like a photograph. It includes the information, which has been reachable with this camera at the given moment.

Potential well is the region surrounding a local minimum of potential energy. Potential well has the walls or potential barriers restricting the motion of the physical object inside the well. The walls are considered to be perpendicular to the coordinate axis x , along which the object can move. The potential well is described by the Schrödinger equation: $\{(-\hbar^2/2m)(\partial^2/\partial x^2) + U\}\psi = E\psi$. This equation can be transformed to the form $(\partial^2/\partial x^2)\psi + \{2m(E - U)/\hbar^2\}\psi = 0$. In case $U = 0$ (within the potential well), this equation describes standing wave with wave number $k = (2mE)^{1/2}/\hbar$. In the area outside of the well, the energy of the object E is lower than the height of the potential barrier U . So the quantity $\{2m(E - U)/\hbar^2\}$ is negative there and the Schrödinger equation describes the decrease of the matter wave amplitude A in the potential barrier area according to the exponential decay law $A(x) = A_0 e^{-\kappa x}$, where x is distance from barrier edge and the absorption coefficient $\kappa = \{2m(U - E)\}^{1/2}/\hbar$.

Tunnelling is the QM phenomenon where an object is going through a barrier not penetrable according to the classical mechanics. Usually the walls of the potential well are impenetrable for physical objects because the probability wave amplitude A decreases very quickly. However, if the height of the potential barrier is moderate ($U - E \neq \infty$) and the barrier is thin enough, then the amplitude A of the probability wave at the other side of the barrier is different from zero. This means that the object can go through the barrier with some probability. The tunnelling plays an essential role in several physical phenomena, such as the nuclear fusion that occurs in the Sun. It has important applications to modern devices such as the tunnel diode, quantum computing, and the scanning tunnelling microscope.

Electron microscope is a microscope that uses a beam of high-energy electrons as a source of illumination. As the wavelength of an electron can be up to 10^5 times shorter than the wavelength of visible light photons, electron microscopes have a higher resolving power than light microscopes and can reveal the structure of smaller objects. A transmission electron microscope (TEM) can achieve a resolution better than 50 pm and magnifications of up to about 10^7 times whereas most of light microscopes are diffractionally limited by resolution about 200 nm and useful magnifications below 2000 times. The wavelength of electrons λ can be easily controlled by adjustment of the acceleration voltage U , because $\lambda = h/(2meU)^{1/2}$.

Scanning electron microscope (SEM) is a type of electron microscope that produces images of a sample by scanning it with a focused beam of electrons. The electrons interact with atoms in the sample, producing various signals that contain information about the surface topography of sample and its composition. The electron beam is generally scanned in a raster scan pattern, and the information considering the beam's position is combined with the detected signal to produce an image. SEM can achieve resolution better than 1 nanometer.

Scanning tunnelling microscope (STM) is an instrument for imaging surfaces at the atomic level. The STM is based on the concept of quantum tunnelling. When a conducting tip is brought very near to the surface to be examined, a voltage applied between the tip and the surface can allow electrons to tunnel through the vacuum between them. The resulting tunneling current is a function of tip position, applied voltage, and the local density of electronic states of the sample.

Interpretations of quantum mechanics are different answers to the question: *At which moment something that can occur with quantum probability becomes real?* There are two main groups of interpretations. Einstein concept states that there is no randomness at all. QM is just a bad theory, not able to predict the future. Bohr concept or the Copenhagen interpretation of QM states that the observer himself takes part in the formation of physical reality. The new reality is created when the observation or experiment is done. If something has happened, then all the contrary possibilities have become impossible.

Quantum computers are different from the binary digital electronic computers based on transistors. Common digital computing requires that the data be encoded into binary digits (bits), each of which is always in one of the two definite states (0 or 1). Quantum computer uses quantum bits called qubits, which are normally in entangled state. This state can be a superposition of infinite number (not only 0 or 1!) of elementary states. Quantum computer does not search for exact correct answer, it is searching for the most probable answer.

Quantum cryptography is a secure method of information transfer based on the laws of quantum mechanics. Information is coded within the states of electromagnetic photons (polarization, for example). Information is sent in packages that contain certain number of photons. Because a single photon can be absorbed only once, the complete arrival of the package at destination secures that it was not disturbed on the way. Hence, there is no information leakage.