

First, I want to remind you of the relation between classical mechanics and quantum theory.

Within the framework of classical mechanics, the coordinates and velocity of any particle can be calculated exactly as a solution of Newton's second law. The second Newton's law show the relation between the body acceleration and acting force. This law looks like a second order differential equation that can be solved analytically or numerically by classical mathematics methods . As a result, we obtain the dependence of the three coordinates of the particle on time $x(t)$, $y(t)$ and $z(t)$. This three functions allow to determine the exact position of particle at **certain** time moment. All this three functions are continuous (important note). The time derivative of coordinates give us the velocity and second derivative give acceleration. It is very important to note that all these parameters can be calculated with any accuracy.

What about quantum theory?

In quantum mechanics, any classical quantity is associated with the operator of the same name.

Instead of coordinates, we need to use the coordinate operator.

The classical impulse must be replaced by the impulse operator, and the energy by the Hamilton operator.

The value of physical quantities, such as coordinate, momentum, energy, etc., can be represented as a **solution to the eigenvalue problem** for the corresponding differential equations.

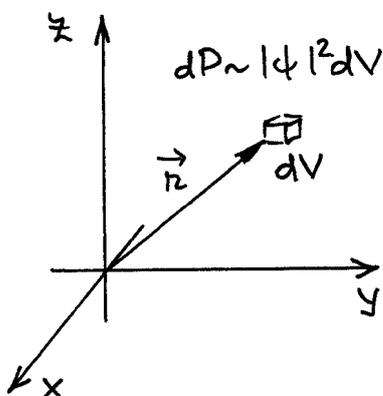
For example for a stationary systems to find the value of the energies, we need to solve the Schrodinger equation $\hat{H} \cdot \varphi = E \cdot \varphi$, here H is a Hamilton operator, E-calculated energies of system and φ - so called wave function. Wave function can be used to calculate the probability to find particle in certain point of space and for calculating the average values of physical quantities.

II. Basis principles of quantum mechanics.

1. Schrödinger equation

II.1.1 Wave function. We start with single microparticle. Its state is described by the wave function

$$\Psi = \Psi(r, t),$$



which is determined in finite region of space or infinite space, depends on time and has in general complex values ($\Psi \in \mathbb{C}$). In our course we use mainly the old fashioned name – wave function, but Ψ is also called state function, or probability amplitude.

The physical meaning of the wave function is the following: its square of modulus $|\Psi(r,t)|^2$ is proportional to the probability to find our particle at certain moment of time t in the small element of volume dV

$$dP \sim |\Psi|^2 \cdot dV$$

Therefore the wave function itself is not directly measurable quantity, but its square of module is.

II.1.2 Normalization of the wave function. For Ψ there are two possibilities – integral over the square of modulus (we integrate over the whole space or region where the wave function is nonzero) is finite or it is infinite.

1. In the first case we can normalize the integral to unit. In other words we consider only these wave functions, which satisfy

$$\int |\Psi(\vec{r}, t)|^2 dV = 1$$

(We simplify our notations and write space integrals as $\int dV$ not $\iiint dx dy dz$ and also omit the boundaries, if these are not necessary.)

Now the wave function gives us the probability of finding particle in certain volume element dV

$$dP = |\Psi(\vec{r}, t)|^2 dV$$

since the sum over the whole space is equal to 1, condition is means that particle is exist somewhere in universe.

$$\int dP = 1 = \int |\Psi(\vec{r}, t)|^2 dV$$

The square of modulus of wave function gives us probability density

$$\rho(\vec{r}, t) = \frac{dP}{dV} = |\Psi(\vec{r}, t)|^2$$

Problem 1.1 Prove, that if the integral $\int |\Psi(\vec{r}, t)|^2 dV = a$ is finite the wave function can be normalised to unit.

2. In the second case we have

$$\int |\Psi(\vec{r}, t)|^2 dV \rightarrow \infty$$

(example: free particle, described by the de Broglie wave). One can compare probabilities in different places, but not directly calculate them. In that case wave functions usually are normalized to Dirac δ -function (see next paragraph).

II.1.3 Schrödinger equation

The basic equation in quantum mechanics is the Schrodinger equation. Its general form is the following:

$$i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = -\frac{\hbar^2}{2M} \Delta \Psi(\vec{r}, t) + U(\vec{r}, t) \Psi(\vec{r}, t),$$

where i -imaginary unit, $U(\vec{r}, t)$ is the potential function of a given particle (potential energy), M is a mass of particle and Δ is the Laplace operator (in rectangular coordinates $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$). It is also called time dependent Schrödinger equation. How this equation was obtained? As a result of mathematical derive? No, this equation was invented () by Erwin Schrodinger.

II.1.4 Continuity equation. From the Schrodinger equation it follows the **continuity equation** for probability density $\rho = |\Psi(\vec{r}, t)|^2$

$$\frac{\partial \rho}{\partial t} + \text{div } \vec{j} = 0, \quad ,$$

where the vector quantity

$$\vec{j} = \frac{i\hbar}{2M} (\Psi \cdot \text{grad } \Psi^* - \Psi^* \cdot \text{grad } \Psi)$$

is called the **probability current density**. This vector is directly related to the electric current in the conductors and semiconductors. And can be used to calculate one.

Problem 1.2. Derive the continuity equation.

In the case of electrically charged particles we can obtain charge density and current density. If the electrical charge, carried by particle, is q then the charge density is (electric current carrier)

$$\rho_l = q\rho$$

and current density is

$$j_v = q j.$$

Example. The wave function for free particle moving in 1d space is follows:

$$\Psi(x,t) = A e^{-\frac{i}{\hbar}(Et - px)}$$

Now $\rho = |A|^2$ (probability density is constant) and probability current density is

$$j = \frac{i\hbar}{2M} \left(\frac{d\Psi^*}{dx} \Psi - \Psi^* \frac{d\Psi}{dx} \right) = \frac{p}{M} |\Psi|^2 = \frac{p}{M} |A|^2$$

Since $p = Mv$, we get

$$j = v |A|^2,$$

which describes the particle, moving with the velocity v , or **flux of moving particles**.

II.1.5 Schrödinger equation for stationary states.

Have a very important application in quantum mechanics. If $U = U(r)$, the Schrödinger equation simplifies, since the time dependence may be eliminated.

Indeed, in

$$i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = -\frac{\hbar^2}{2M} \Delta \Psi(\vec{r}, t) + U(\vec{r}) \Psi(\vec{r}, t)$$

it is possible to separate the variables. Writing

$$\Psi(\vec{r}, t) = f(t) \psi(\vec{r}),$$

we have

$$i\hbar \frac{df(t)}{dt} \psi(\vec{r}) = -\frac{\hbar^2}{2M} f(t) \Delta \psi(\vec{r}) + U(\vec{r}) f(t) \psi(\vec{r}).$$

Dividing both sides by $f\psi$ we get the equation where the variables (time and coordinates) are separated

$$i\hbar \frac{1}{f(t)} \frac{df(t)}{dt} = -\frac{\hbar^2}{2M} \frac{1}{\psi(\vec{r})} \Delta \psi(\vec{r}) + U(\vec{r}).$$

If we equalize both sides to some constant E , the left side gives

$$i\hbar \frac{1}{f(t)} \frac{df(t)}{dt} = E,$$

which after simple integration gives

$$f(t) = e^{-\frac{i}{\hbar} E t} .$$

The right side gives us the Schrödinger equation for stationary states (also known as time independent Schrödinger equation)

$$-\frac{\hbar^2}{2M} \Delta \psi(\vec{r}) + U(\vec{r}) \psi(\vec{r}) = E \psi(\vec{r}) .$$

Constant E is the total energy of a given particle. On the other hand the latter equation is the eigenvalue problem

$$\hat{H} \psi(\vec{r}) = E \psi(\vec{r}) .$$

of the Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2M} \Delta + U(\vec{r}) .$$

For each solution for stationary states there is the following solution for the general Schrödinger equation

$$\Psi(\vec{r}, t) = e^{-\frac{i}{\hbar} E t} \psi(\vec{r}) .$$

The function $\psi(r)$ is also called wave function and it has the same probability interpretation as $\Psi(\vec{r}, t)$

$$\rho = |\Psi(\vec{r}, t)|^2 = |\psi(\vec{r})|^2 \quad \text{otherwise} \quad \rho = |\Psi(\vec{r}, t)|^2 = |\Psi(\vec{r}, 0)|^2 .$$

The probability density does not depend on time, therefore the probability is time independent – stationary.

II.1.6 Superposition principle. The general Schrödinger equation is linear concerning the wave equation Ψ

$$i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = -\frac{\hbar^2}{2M} \Delta \Psi(\vec{r}, t) + U(\vec{r}, t) \Psi(\vec{r}, t) .$$

We can write it symbolically as

$$\hat{A} \Psi = 0 .$$

The superposition principle means that if Ψ_1 and Ψ_2 are two arbitrary solutions, then their arbitrary linear combination

$$\Psi = a_1 \Psi_1 + a_2 \Psi_2$$

is also a solution of a given Schrödinger equation.

However, it is a common property of linear equations, but in quantum mechanics it has a totally different meaning compared with classical physics. If for example Ψ_1 and Ψ_2 are two stationary states corresponding to different energies

$$\Psi_1(\vec{r}, t) = e^{-\frac{i}{\hbar} E_1 t} \psi_1(\vec{r}), \quad \Psi_2(\vec{r}, t) = e^{-\frac{i}{\hbar} E_2 t} \psi_2(\vec{r}),$$

where $\hat{H} \psi_1(\vec{r}) = E_1 \psi_1(\vec{r})$ ja $\hat{H} \psi_2(\vec{r}) = E_2 \psi_2(\vec{r})$, then the possible physical state is also their linear combination

$$\Psi(\vec{r}, t) = c_1 \Psi_1(\vec{r}, t) + c_2 \Psi_2(\vec{r}, t) .$$

The physical meaning of a given solution (see next paragraph) is the following: in the state $\Psi(\vec{r}, t)$ the energy is not uniquely fixed, if we measure energy, we get both values, sometimes E_1 , sometimes E_2 , probabilities of both results depend on c_1 ja c_2 .

Comments:

1. In the stationary case the general solution of the time dependent Schrödinger equation is the arbitrary linear combination

$$\Psi(\vec{r}, t) = \sum_n c_n e^{-\frac{i}{\hbar} E_n t} \psi_n(\vec{r}) .$$

2. In paragraph 13 the above given Schrödinger equation is generalized to the case where an external electromagnetic field is present.

3. Phase transformations. The wave equation is not determined uniquely. Even if normed, the functions

$$\Psi(r, t) \quad \text{and} \quad e^{i\alpha} \Psi(r, t)$$

(where $\alpha \in \mathbb{R}$) give the same probability density. Here is no physical contradictions. Therefore these transformations in ordinary quantum mechanics are not physically interesting, but as we see later, analogical phase transformations where the phase factor $\alpha = \alpha(\vec{r}, t)$ is a function of space and time are very important in modern particle physics.

4. Microparticles have dualistic properties – they are at the same time both – particles and waves. Free particle is described with the help of de’Broglie wave (one dimensional case), which one can represent in two equivalent forms

$$\Psi(x, t) = e^{-\frac{i}{\hbar}(Et - px)} \equiv e^{-i(\omega t - kx)},$$

(particle side is characterized by energy and momentum, wave side by frequency and wave number). It satisfies the free particle equation

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\hbar^2}{2M} \frac{\partial^2 \Psi(x, t)}{\partial x^2}.$$

De’Broglie wave cannot be interpreted as a classical wave: it has complex values and is not a solution of classical wave equation.

Classical wave equation is

$$\frac{1}{v^2} \frac{\partial^2 \Psi(x, t)}{\partial t^2} = \frac{\partial^2 \Psi(x, t)}{\partial x^2},$$

where v is a velocity of a given wave.

There are different interpretations of the wave function. Is the wave function a real physical object or is it just a mathematical method of describing the properties of microparticles? It doesn't matter if quantum mechanics works well. Do not ask just use.

Problem. Prove that 1) de’Broglie wave is not a solution of classical wave equation; 2) de’Broglie wave must be complex valued function, since its real part $\phi(x, t) = \text{Re} \Psi(x, t) = \cos(\omega t - kx)$ does not satisfy the Schrödinger equation.