

Lecture 4. The Uncertainty Principle . The Schrodinger equation

time-dependent equation- нестационарное уравнение

partial differential equation - дифференциальное уравнение в частных производных

one-dimensional, three- dimensional - одномерное, трехмерное

imaginary unit - мнимая единица

temporal and spatial parts - временная и пространственная часть

an infinite rigid box - твердый ящик (бесконечно глубокая потенциальная яма)

Goal. To give definition to the uncertainty principle and to use the Schrodinger equation

Let the particle moves in free space with constant velocity. De Broglie has assumed that plain monochromatic wave is connected with such particle, extending in a direction of the velocity

$$\Psi = Ae^{i(\vec{k}\vec{r}-\omega t)} = Ae^{i\left(\frac{\vec{k}\vec{r}}{h}-\frac{Et}{h}\right)}$$

About the nature of this wave, i.e. physical sense of function, de Broglie couldn't tell anything. These waves have received the name of phase waves, waves of substance or de Broglie waves.

According M.Born square of absolute value of psi-function denotes the probability dP that the particle will be found in element dV :

$$dP = |\Psi|^2 dV$$

$|\Psi(x, y, z)|^2$ is probability density of particle to be found at the point x, y, z

$$\int dP = \int |\Psi|^2 dV = 1$$

is normalization condition for three-dimensional case, for one-dimensional case $|\Psi(x)|^2$ is the probability density for finding the particle at x . This means that in the case of a one-dimensional system, that $|\Psi(x)|^2 dx$ is the probability P of finding the particle between x and $x + dx$.

$$P(\text{between } x \text{ and } x + dx) = |\Psi(x)|^2 dx$$

Since the total probability of finding the particle anywhere must be 1, it follows that

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 dx = 1$$

This relation is called the normalization condition and a wave function that satisfies it is said to be normalized. The normalization condition defines the value of the constant A, which is therefore called the normalization constant.

The Uncertainty Principle

One important consequence of the wave-particle duality of nature was discovered by Heisenberg, and is called the uncertainty principle. To formulate it, let us imagine that we want to measure the position and the momentum of a particular particle. To do so we must "see" the particle, and so we shine some light of

wavelength λ on it. You know that there is a limit to the resolving power of the light used to see the particle given by the wavelength of light used. This gives an uncertainty in the particle's position:

$$\Delta x \sim \lambda \quad (4.1)$$

This results from considering the light as a wave. However, viewed as a photon, the light, when it strikes the particle, could transfer some or all of its momentum to the particle. Since we don't know how much it transfers, as we don't measure the photon's properties, there is an uncertainty in the momentum of the particle; using $p = k\hbar$, we find

$$\Delta p \sim h / \lambda \quad (4.2)$$

Combining equations (4.1), (4.2), we find

$$\Delta x \Delta p \sim h \quad (4.3)$$

Note that this is independent on the used wavelength, and there is a limit in principle as to how accurately one can simultaneously measure the position and momentum of a particle - if one tries to measure the position more accurately by using light of a shorter wavelength, then the uncertainty in momentum grows, whereas if one uses light of a longer wavelength in order to reduce the uncertainty in momentum, then the uncertainty in position grows. One cannot reduce both down to zero simultaneously - this is a direct consequence of the wave-particle duality of nature.

The arguments used in deriving Eq.(4.3) are somewhat rough. A more refined treatment, developed by Heisenberg, results in the following relation:

$$\Delta x \Delta p_x \geq \hbar / 2 \quad (4.4)$$

As with de Broglie waves, for everyday macroscopic objects such as bowling balls the uncertainty principle plays a negligible role in limiting the accuracy of measurements, as we shall see in some examples. However, for microscopic objects such as electrons in atoms the uncertainty principle does become a very important consideration. Another uncertainty relations:

$$\Delta E \Delta t \geq \hbar / 2$$

$$\Delta y \Delta p_y \geq \hbar / 2$$

$$\Delta z \Delta p_z \geq \hbar / 2$$

The Schrodinger equation

In physics, specifically quantum mechanics, the Schrodinger equation, formulated by Austrian physicist Erwin Schrodinger, is an equation that describes how the quantum state of a physical system changes in time. It is as central to quantum mechanics as Newton's laws are to classical mechanics. In the standard interpretation of quantum mechanics, the quantum state, also called a wave function or state vector, is the most complete description that can be given to a physical system. Solutions of Schrodinger's equation describe not only molecular, atomic and subatomic systems, but also macroscopic systems, possibly even the whole universe. The equation is named after Erwin Schrodinger, who constructed it in 1926.

The most general form is the time-dependent Schrodinger equation, which gives a description of a system evolving with time. For systems in a stationary state, the time-independent Schrodinger equation is sufficient. Approximate solutions to the time-independent Schrodinger equation are commonly used to calculate the energy levels and other properties of atoms and molecules. Time-dependent equation for a single particle with potential energy U , the Schrodinger equation takes the form:

$$-\frac{\hbar^2}{2m} \Delta \psi + U \psi = i\hbar \frac{\partial \psi}{\partial t} \quad (4.5)$$

where $-\frac{\hbar^2}{2m}\Delta = -\frac{\hbar^2}{2m}\nabla^2$ is the kinetic energy operator, where m is the mass of the particle.

$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is the Laplace operator, $\Psi(r, t)$ is the wave function.

Time independent or stationary equation

The time independent equation, again for a single particle with potential energy U takes the form:

$$\Delta \psi + \frac{2m}{\hbar^2}(E - U)\psi = 0 \quad (4.6)$$

This equation describes the solutions of the time-dependent equation, which are the states with definite energy.

The Schrodinger equation has solutions not for any values of parameter E , but only for some selected values. These selected values are called as own values. The functions $\Psi(r)$ which are the solutions of the Schrodinger equation at own values of E are called as own functions. In case of the discrete spectra the own values and own functions can be enumerated:

$$E_1, E_2, \dots, E_n, \dots; \Psi_1, \Psi_2, \dots, \Psi_n, \dots$$

Particle in an infinite Rigid Box

Assume the potential $U(x)$ to be zero inside in one-dimensional box of length l and infinite outside the box (figure 4.1).

The Schrodinger equation for particle in box is:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0 \quad (4.7)$$

Since the probability of finding of particle outside the box is zero, the wave function must go to zero at the walls

$$\Psi(0) = \Psi(l) = 0 \quad (4.8)$$

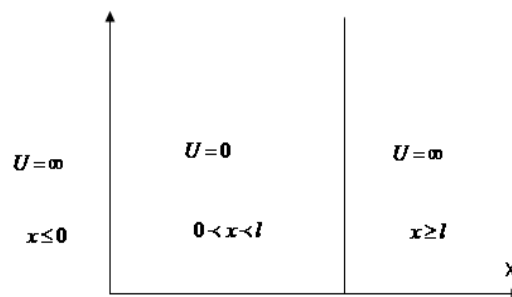


Figure 4.1. Rigid Box

Solution of eq.(4.7) is:

$$\psi(x) = A \sin(kx + \alpha)$$

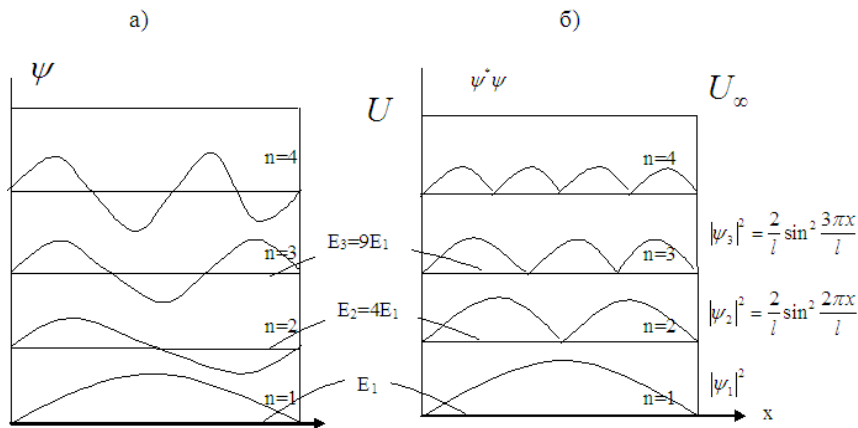
here $k^2 = \frac{2m}{\hbar^2} E$

At taking into account (4.8) wave function at the wall is:

$$\begin{aligned}\psi(0) &= a \sin \alpha = 0 \\ \psi(l) &= A \sin kl = 0\end{aligned}\quad (4.9)$$

Form (4.9) one can find $\alpha = 0$ and $kl = \pm\pi \cdot n$. It is following

$$\begin{aligned}E_n &= \frac{\pi^2 \hbar^2}{2ml^2} n^2, \quad (n = 1, 2, 3, \dots) \\ \psi_n(x) &= A \sin\left(\frac{n\pi x}{l}\right) \\ A^2 \int_0^l \sin^2\left(\frac{n\pi x}{l}\right) dx &= 1 \rightarrow A = \sqrt{\frac{2}{l}} \\ \psi_n(x) &= \sqrt{\frac{2}{l}} \sin\left(\frac{n\pi x}{l}\right)\end{aligned}$$



- a) Diagrams of own functions of particle in the rigid box.
- b) Density of the probability of particle finding in points of different values of x .

Figure 4.2.

Normalization and orthogonal conditions can be written in one expression as

$$\int \psi_m^* \psi_n dx dy dz = \delta_{nm} = \begin{cases} 1 (n = m) \\ 0 (n \neq m) \end{cases}$$

The checklist of lection 4

CONCEPT	DETAILS
Superposition principle	If Ψ_1 and Ψ_2 are possible waves, so is $A\Psi_1 + B\Psi_2$
Time-independent Schrödinger equation	$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}[U(x) - E]\psi$
Particle in a one-dimensional rigid box $0 \leq x \leq a$	Moves freely inside $0 \leq x \leq a$ but cannot escape outside
Boundary conditions	$\psi(0) = \psi(a) = 0$
Allowed energies	$E_n = n^2(\pi^2\hbar^2/2ma^2)$
Wave functions	$\psi(x) = \sqrt{2/a} \sin(n\pi x/a)$
Normalization condition	$\int \psi(x) ^2 dx = 1$
Behavior of wave functions	
In classically forbidden zone ($E < U$)	$\psi = 0$
In classically allowed zone ($E > U$)	Curves toward the axis and oscillates sinusoidally
Simple harmonic oscillator *	$U = \frac{1}{2}kx^2$
Allowed energies	$E_n = \left(n + \frac{1}{2}\right)\hbar\omega_c$
Tunneling *	Ability of a quantum particle to penetrate into a classically forbidden zone
Probability of tunneling	$P = e^{-2aL}$
Time-dependent Schrödinger equation *	$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x) \right) \Psi(x, t)$

Problems.

1. Estimate uncertainty of the electron velocity in the hydrogen atom, taking into consideration its size of the order of 10^{-8} cm. Compare the obtained value with the electron velocity on the first Bohr orbit.
2. Assess the smallest error in determination of the velocities of the electron, proton, and uranium atom trapped in a region with size of 1 micron.
2. Assess for an electron localized in a region of size l : a) the lowest possible kinetic energy, if $l = 10^{-8}$ cm; b) the relative speed uncertainty $\Delta v/v$, if its kinetic energy $T \approx 10$ eV and $l = 1 \mu m$.
3. Based on the uncertainty relation evaluate the electron coupling energy in the ground state of the hydrogen atom and the corresponding distance of the electron from the nucleus.
4. Evaluate the lowest possible energy of the electrons in the He atom, and the corresponding distance of the electron from the nucleus.

Literatures

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