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Physics for Computer Scientist I.

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Quantum Mechanics

Plank constant

Plank constant h is defined by

$$h = 6.6260755 \times 10^{-34}[J \cdot s]. \tag{1}$$

Sometimes $\hbar = h/2\pi$ is used.

Equation of Motion of Electron Beam

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = i\hbar\frac{\partial \psi}{\partial t} \tag{2}$$

This equation is called the Schrödinger equation.

Energy and Solution

We assume that the Energy relation holds:

$$E = \frac{p^2}{2m}. \tag{3}$$

Then, we have a solution of (2) as

$$\psi(x,t) = Ae^{i(px-Et)/\hbar}. \tag{4}$$

In fact,

$$\begin{aligned} i\hbar\frac{\partial\psi}{\partial t} &= E\psi, \\ -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} &= \left(\frac{p^2}{2m}\right)\psi. \end{aligned} \tag{5}$$

Phase velocity vs group velocity

Phase velocity

The phase velocity is determined from the condition

$$px - Et = \text{const} \tag{6}$$

as

$$v_p = \frac{E}{p} = \frac{p}{2m} = \frac{v}{2}. \tag{7}$$

This does not coincide with the classical view of electron being a particle moving with the velocity v. In fact, by the quantum mechanics the probability of detecting electron is given by

$$|\psi(x,t)|^2 = |A|^2. \tag{8}$$

Group velocity

Dispersion relation

Put

$$k = \frac{p}{\hbar}, \quad \omega = \frac{E}{\hbar}. \tag{9}$$

Then, the wave function of electron beam becomes

$$\psi(x,t) = Ae^{i(kx-\omega t)}. \tag{10}$$

Here,

$$\hbar\omega = \frac{\hbar^2 k^2}{2m}. \tag{11}$$

Wave Packet

Let

$$\begin{aligned} \psi_1(x,t) &= Ae^{i(kx-\omega t)}, \\ \psi_2(x,t) &= Ae^{i[(k+\Delta k)x-(\omega+\Delta\omega)t]}. \end{aligned} \tag{12}$$

Consider $\psi = \psi_1 + \psi_2$. Then,

$$|\psi(x,t)|^2 = 2|A|\{1+\cos[(\Delta k)x-(\Delta\omega)t]\}. \tag{13}$$

In this case, we can see the wave packet moves with the group velocity

$$\frac{d\omega}{dk} = v. \tag{14}$$

Schrödinger equation in potential

If electron is in a potential $V(x, y, z)$, then the following Schrödinger equation holds:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)+V(x,y,z)\psi = i\hbar\frac{\partial\psi}{\partial t}. \qquad (15)$$

If we use

$$\nabla^2 = \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}, \qquad (16)$$

we can rewrite eq.(15) as

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(x,y,z)\psi = i\hbar\frac{\partial\psi}{\partial t}. \qquad (17)$$

Hamitonian form

If we put

$$\mathcal{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(x, y, z), \tag{18}$$

the Schrödinger equation becomes

$$\mathcal{H}\psi = i\hbar\frac{\partial\psi}{\partial t}. \tag{19}$$

Time independent Schrödinger equation

Let us assume that a wave function has a form

$$\psi(x, y, z, t) = u(x, y, z)(Ae^{-iEt/\hbar}). \tag{20}$$

Then, eq.(19) becomes

$$\mathcal{H}u = Eu. \tag{21}$$

This is called a time-independent Schrödinger equation.

One-dimensional Problem

We consider a simple case of $V(x,y,z) = V(x)$. In this case, the Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t} \tag{22}$$

Its time independent one is

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} + V(x)u(x) = Eu(x). \tag{23}$$

We put normalization conditions

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = 1, \quad \text{or} \quad \int_{-\infty}^{\infty} |u(x)|^2 dx = 1. \tag{24}$$

Infinite Wall

Consider an infinite wall:

$$V(x) = \begin{cases} \infty & (x < 0) \\ 0 & (0 \leq x \leq L) \\ \infty & (L < x) \end{cases} \tag{25}$$

The time independent Schrödinger equation becomes

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} &= Eu(x) & (0 \leq x \leq L), \\ -\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} + V_0(x)u(x) &= Eu(x) & (x < 0,\ L < x). \end{aligned} \tag{26}$$

Here, $V_0 = \infty$.

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Solution

It is easily seen that

$$u(x) = 0 \quad (x < 0, L < x). \tag{27}$$

Moreover, from the continuity of the wave function, we have

$$u(0) = u(L) = 0. \tag{28}$$

We solve

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} = Eu(x) \quad (0 \le x \le L) \tag{29}$$

under the boundary condition (28). If we put $k^2 = 2mE/\hbar^2$, eq.(29) becomes

$$\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} = -k^2u(x). \tag{30}$$

Eigenvalue Problem

The general solution of eq.(30) is given by

$$u(x) = A \sin kx + B \cos kx. \tag{31}$$

Here, $k = \sqrt{2mE}/\hbar$. From the boundary condition (28), we have

$$0 = u(0) = A \sin 0 + B \cos 0 = B = 0. \tag{32}$$

Moreover, from

$$u(L) = 0 \tag{33}$$

we have

$$k = \frac{n\pi}{L}, \quad (n = 1, 2, \cdots). \tag{34}$$

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Discrete Eigenvalues

Therefore, we have

$$u_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}, \quad (n = 1, 2, \cdots ; 0 \leq x \leq L) \tag{35}$$

for

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL}. \tag{36}$$