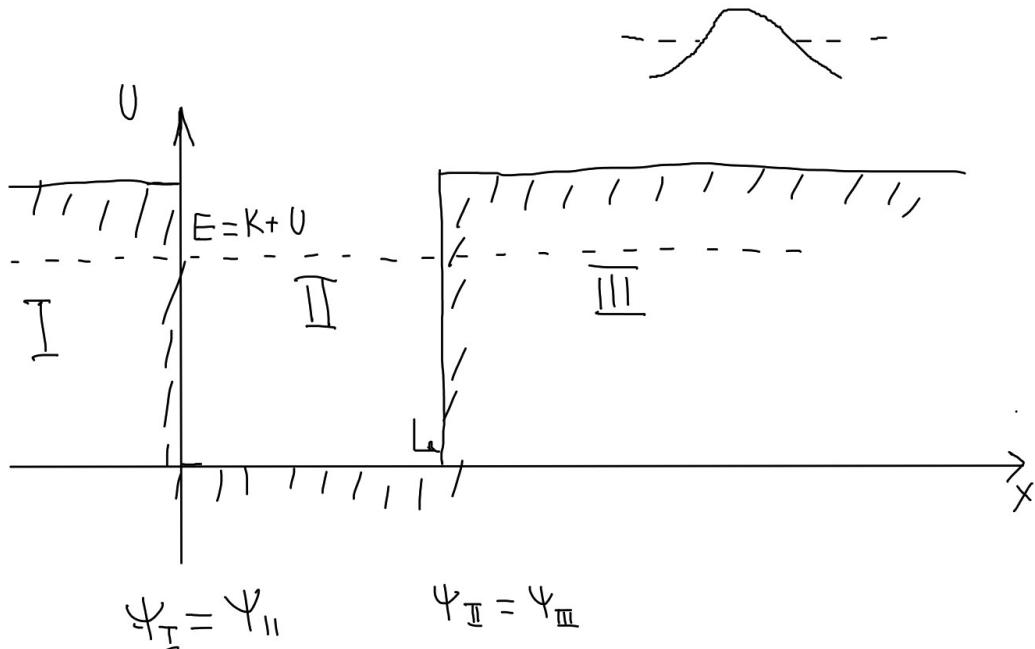


Рівняння Шрьодінгера

$$\begin{aligned}\hat{H}\psi &= E\psi \\ (\hat{K} + \hat{U})\psi &= E\psi \\ \left(\frac{\hat{p}^2}{2m} + U\right)\psi &= E\psi \\ \left(-\frac{\hbar^2}{2m}\Delta + U(x, y, z)\right)\psi &= E\psi\end{aligned}\tag{1.1}$$

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$$\frac{\partial \Psi_I}{\partial x} = \frac{\partial \Psi_{II}}{\partial x} \quad \frac{\partial \Psi_{II}}{\partial x} = \frac{\partial \Psi_{III}}{\partial x}$$

$$\left(-\frac{\hbar^2}{2m}\Delta + U\right)\psi = E\psi\tag{1.2}$$

В області II:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = E\psi\tag{1.3}$$

$$\begin{aligned}\frac{d^2}{dx^2}\psi + \frac{2mE}{\hbar^2}\psi &= 0 \\ \frac{d^2}{dx^2}\psi + \omega^2\psi &= 0\end{aligned}\tag{1.4}$$

Розв'язки:

$$\psi_{II} = A \cos \omega x + B \sin \omega x\tag{1.5}$$

В області I, III:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi = -(U - E) \psi \quad (1.6)$$

$$\frac{d^2\psi}{dx^2} - \frac{2m(U-E)}{\hbar^2} \psi = 0$$

$$\frac{d^2\psi}{dx^2} - \lambda^2 \psi = 0 \quad (1.7)$$

Розв'язки:

$$\psi = A e^{-\lambda x} + B e^{\lambda x} \quad (1.8)$$

В області III ($B=0$):

$$\psi_{III} = A e^{-\lambda x} \quad (1.9)$$

В області I ($A=0$):

$$\psi_I = B e^{\lambda x} \quad (1.10)$$

Границі умови при $U \rightarrow \infty$:

$$\psi_{II}(0) = 0$$

$$A \cos \omega \cdot 0 + B \sin \omega \cdot 0 = 0 \quad (1.11)$$

$$A = 0$$

$$\psi_{II}(L) = 0$$

$$B \sin \omega L = 0$$

$$\omega L = \pi n$$

$$\omega_n = \frac{\pi n}{L} \quad (1.12)$$

$$\sqrt{\frac{2mE_n}{\hbar^2}} = \frac{\pi n}{L}$$

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

Середній імпульс:

$$\begin{aligned} \langle \psi_1 \hat{p} \psi_1 \rangle &= \int_0^L \psi_1^* \left(-i\hbar \frac{d\psi_1}{dx} \right) dx = -i\hbar B^2 \int_0^L \sin(\omega x) \cdot \omega \cos(\omega x) dx = \\ &= -i\hbar B^2 \int_0^L \sin(\omega x) \cdot d(\sin(\omega x)) = -i\hbar B^2 \frac{\sin^2 \omega x}{2} \Big|_0^L = 0 \end{aligned} \quad (1.13)$$

Матричний елемент імпульса

$$\begin{aligned} \langle \psi_2 \hat{p} \psi_1 \rangle &= \int_0^L \psi_2^* \left(-i\hbar \frac{d\psi_1}{dx} \right) dx = \\ &= -i\hbar B^2 \int_0^L \sin\left(\frac{2\pi}{L}x\right) \cdot \frac{\pi}{L} \cos\left(\frac{\pi}{L}x\right) dx = -i\hbar B^2 \int_0^L 2 \sin\left(\frac{\pi}{L}x\right) \cdot \frac{\pi}{L} \cos^2\left(\frac{\pi}{L}x\right) dx = \\ &= i\hbar B^2 2 \left(\frac{\cos^3 \frac{\pi L}{3}}{3} - \frac{1}{3} \right) = \frac{-4i\hbar B^2}{3} = \frac{4i\hbar}{3L} \end{aligned} \quad (1.14)$$

Середній квадрат імпульса:

$$\begin{aligned}
 & \langle \hat{p}^2 \rangle = \int_0^L \psi^* \left(-\hbar^2 \frac{d^2 \psi}{dx^2} \right) dx = \\
 & = -\hbar^2 \int_0^L B \sin \omega x \frac{d^2 B \sin \omega x}{dx^2} dx = \\
 & = -\hbar^2 B^2 \int_0^L -\omega^2 \sin^2 \omega x \cdot dx \\
 & = \hbar^2 B^2 \omega^2 \int_0^L \frac{1 - \cos 2\omega x}{2} dx = \hbar^2 B^2 \omega^2 \left(\frac{L}{2} - \frac{\sin 2\omega x}{4\omega} \Big|_0^L \right) = \frac{\hbar^2 B^2 \omega^2 L}{2} = \hbar^2 \omega^2 = \frac{\hbar^2 \pi^2}{L^2}
 \end{aligned} \tag{1.15}$$

Нормування:

$$\begin{aligned}
 & \int_0^L |\psi_H|^2 dx = 1 \\
 & \int_0^L B^2 \sin^2 \omega x \cdot dx = 1 \\
 & B^2 \int_0^L \frac{1 - \cos 2\omega x}{2} dx = B^2 \left(\frac{L}{2} - \frac{\sin 2\omega x}{4\omega} \Big|_0^L \right) = 1 \\
 & \sin 2\omega L = 2 \sin \omega L \cdot \cos \omega L \\
 & B = \sqrt{\frac{2}{L}}
 \end{aligned} \tag{1.16}$$

Хвильова функція:

$$\psi_H = B \sin \omega x = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n}{L} x\right) \tag{1.17}$$

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$$\begin{aligned}
 & \langle r \rangle = \int \psi^* r \psi dV = \int \int \int \psi^* r \psi \sin \theta r^2 dr d\varphi d\theta = \int_0^\infty A^2 e^{-2r/r_1} 4\pi r^3 dr = \\
 & = A^2 4\pi \int_0^\infty \left(\frac{2r}{r_1} \right)^n \left(\frac{r_1}{2} \right)^n e^{-2r/r_1} d\left(\frac{2r}{r_1} \right) \frac{r_1}{2} = A^2 4\pi \cdot \Gamma(n+1) \left(\frac{r_1}{2} \right)^{n+1} = A^2 4\pi \cdot 3! \left(\frac{r_1}{2} \right)^4 = \frac{3r_1}{2} \\
 & A^2 4\pi \cdot 2! \left(\frac{r_1}{2} \right)^3 = 1
 \end{aligned} \tag{1.18}$$

$$dP = f(r) 4\pi r^2 dr = |\psi|^2 4\pi r^2 dr$$

$$\frac{dP}{dr} = |\psi|^2 4\pi r^2$$

Дз
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