

23.12.21 рівняння Шрьодингера, квантово-механічні задачі

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1 \quad (1.1)$$

Метод обрахунку інтегралу Гаяса

$$Y(\alpha) = \int_{-\infty}^{\infty} e^{-\alpha x^2} dx \quad (1.2)$$

$$Y_x(\alpha) = Y_y(\alpha) = Y_z(\alpha) \Rightarrow$$

$$Y^3 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\alpha(x^2+y^2+z^2)} dx dy dz = \int_0^{\infty} e^{-\alpha R^2} 4\pi R^2 dR = 4\pi \int_0^{\infty} e^{-\alpha R^2} R^2 dR = \\ = 2\pi \int_{-\infty}^{\infty} e^{-\alpha R^2} R^2 dR \quad (1.3)$$

$$\frac{dY}{d\alpha} = \frac{d}{d\alpha} \int_{-\infty}^{\infty} e^{-\alpha R^2} dR = - \int_{-\infty}^{\infty} e^{-\alpha R^2} R^2 dR \quad (1.4)$$

$$Y^3 = 2\pi \left(-\frac{dY}{d\alpha} \right)$$

$$d\alpha = -2\pi \frac{dY}{Y^3} \quad (1.5)$$

$$\alpha = \pi \frac{1}{Y^2}$$

$$Y = \sqrt{\frac{\pi}{\alpha}}$$

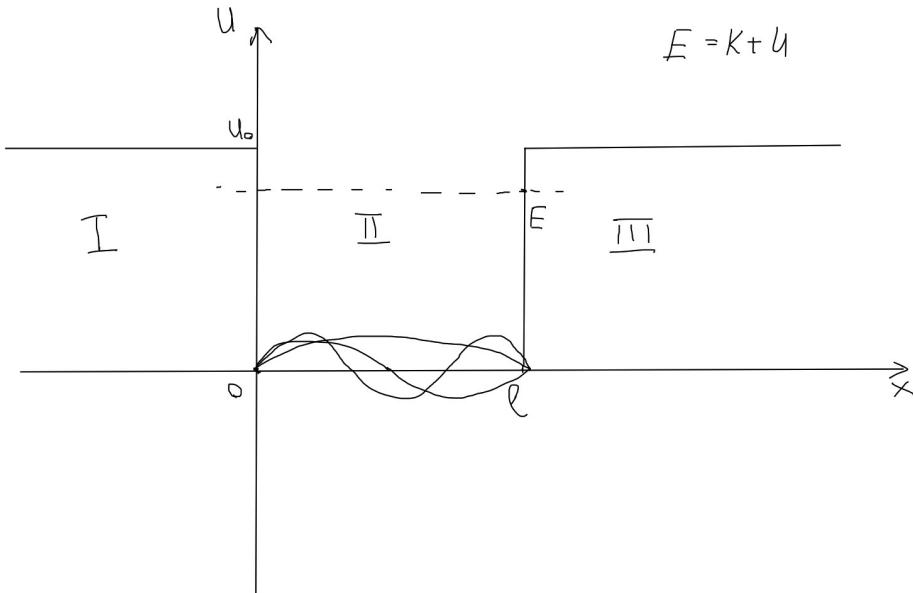
$$\int_{-\infty}^{\infty} e^{-\frac{x^2}{\sigma^2}} dx = \sigma \sqrt{\pi} \quad (1.6)$$

$$\int_{-\infty}^{\infty} x^n e^{-\frac{x^2}{\sigma^2}} dx = \frac{x^{n+1}}{n+1} e^{-\frac{x^2}{\sigma^2}} \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \left(e^{-\frac{x^2}{\sigma^2}} \right)' \frac{x^{n+1}}{n+1} dx = - \int_{-\infty}^{\infty} \left(e^{-\frac{x^2}{\sigma^2}} \right)' \frac{x^{n+1}}{n+1} dx = \\ = - \int_{-\infty}^{\infty} e^{-\frac{x^2}{\sigma^2}} \left(\frac{-2x}{\sigma^2} \right) \frac{x^{n+1}}{n+1} dx = \frac{2}{\sigma^2(n+1)} \int_{-\infty}^{\infty} x^{n+2} e^{-\frac{x^2}{\sigma^2}} dx \quad (1.7)$$

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Рівняння Шрьодингера:

$$\begin{aligned} \hat{H}\psi &= E\psi \\ \hat{K}\psi + U\psi &= E\psi \\ \frac{p^2}{2m}\psi + U(x)\psi &= E\psi \end{aligned} \quad (1.8)$$



В нескінченно глибокій ямі

$$\begin{aligned} \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi &= E\psi \\ \psi'' + \frac{2mE}{\hbar^2} \psi &= 0 \end{aligned} \quad (1.9)$$

Власні функції (розв'язки)

$$\psi = A \cos(kx) + B \sin(kx) \quad (1.10)$$

Границі умови

$$\psi(0) = \psi(l) = 0 \quad (1.11)$$

$$\psi(0) = 0 \quad (1.12)$$

$$A = 0$$

$$\psi(l) = 0$$

$$B \sin(kl) = 0$$

$$kl = \pi n \quad (1.13)$$

$$k = \frac{\pi n}{l}$$

$$\psi_n = B \sin\left(\frac{\pi n}{l} x\right) = \sqrt{\frac{2}{l}} \sin\left(\frac{\pi n}{l} x\right) \quad (1.14)$$

Нормування:

$$\int_0^l \psi^2 dx = 1$$

$$\int_0^l B^2 \sin^2\left(\frac{\pi n}{l} x\right) dx = B^2 \int_0^l \frac{1 - \cos\left(\frac{2\pi n}{l} x\right)}{2} dx = B^2 \left[\frac{x}{2} - \frac{l}{4\pi n} \sin\left(\frac{2\pi n}{l} x\right) \right]_0^l = \quad (1.15)$$

$$= B^2 \frac{l}{2} = 1$$

$$B = \sqrt{\frac{2}{l}}$$

Енергія

$$\frac{2mE}{\hbar^2} = k^2 = \left(\frac{\pi n}{l}\right)^2$$

$$E_n = \frac{\hbar^2}{2m} \left(\frac{\pi n}{l}\right)^2$$
(1.16)

$$\begin{aligned} <\hat{p}^2> &= \int_0^l \psi^* \hat{p}^2 \psi dx = \int_0^l B \sin\left(\frac{\pi nx}{l}\right) \left(-\hbar^2 \frac{d^2}{dx^2} B \sin\left(\frac{\pi nx}{l}\right)\right) dx = \\ &= \hbar^2 B^2 \frac{\pi^2 n^2}{l^2} \int_0^l \sin\left(\frac{\pi nx}{l}\right) \sin\left(\frac{\pi nx}{l}\right) dx = \hbar^2 \frac{\pi^2 n^2}{l^2} B^2 \int_0^l \sin^2\left(\frac{\pi nx}{l}\right) dx = \hbar^2 \frac{\pi^2 n^2}{l^2} = \hbar^2 k^2 \end{aligned}$$
(1.17)

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