Kvantmehaanika, loengud 6-9



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1. How is looks like Schrodinger equation for tunnel effect (topic 4.3) for regions I, II, and III? Derive equations.

$$-\frac{\hbar^2}{2M}\frac{d^2\psi}{dx^2} + U\psi = E\psi \implies \psi'' + \frac{2M}{\hbar^2}(E-U)\psi = 0$$

Region I (x < 0):

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$$U = 0 \implies \psi'' + \frac{2M}{\hbar^2} E\psi = 0 \implies \psi'' + k^2\psi = 0, \quad k^2 = 2ME/\hbar^2$$

$$\psi(x) = e^{rx} \implies (e^{rx})'' + k^2e^{rx} = (r^2 + k^2)e^{rx} = 0 \implies r^2 + k^2 = 0 \implies r = \pm ik \implies$$

$$\implies \psi(x) = Ay_1(x) + By_2(x), \quad y_1 = e^{ikx}, \quad y_2 = e^{-ikx} \implies \psi_I(x) = Ae^{ikx} + Be^{-ikx}$$

$$\boxed{\text{Kui } A = 1} \quad \psi_I(x) = e^{ikx} + Be^{-ikx}$$

Region II $(0 \le x \le a)$:
$$\boxed{\text{miks ?}}$$

$$U = U_0 \implies \psi'' + \frac{2M}{\hbar^2} (E - U_0) \psi = 0 \implies \psi'' - \frac{2M(U_0 - E)}{\hbar^2} \psi = 0 \implies \psi'' - \kappa^2 \psi = 0, \quad \kappa^2 = 2M(U_0 - E)/\hbar^2$$

$$\psi(x) = e^{rx} \implies (e^{rx})'' - \kappa^2 e^{rx} = (r^2 - \kappa^2) e^{rx} = 0 \implies r^2 - \kappa^2 = 0 \implies r = \pm \kappa \implies$$

$$\implies \psi(x) = Cy_1(x) + Dy_2(x), \quad y_1 = e^{\kappa x}, \quad y_2 = e^{-\kappa x} \implies \psi_{II}(x) = Ce^{\kappa x} + De^{-\kappa x}$$

Region III (x > a):

$$U = 0 \implies \psi'' + k^2 \psi = 0$$
 (same as region I), $k^2 = 2ME/\hbar^2$

The process of deriving equation is the same as for region I: $\psi_{III} = Fe^{ikx} + Ge^{-ikx} \implies$

A wave comes in from the left $(x \to -\infty)$ and reaches the barrier. Part of it is reflected, and part of it goes through the barrier to the right. Since there are no wave sources for $x \to +\infty$, there must be no left-going wave in region III. Meaning:

$$\implies \psi_{III}(x) = Fe^{ikx}, \quad G = 0$$

excluding any e^{-ikx} part of equation.

10. Calculate the average of the coordinate $\langle x \rangle$, the square of the coordinate $\langle x^2 \rangle$, and the square of the velocity $\langle v^2 \rangle$ for quantum numbers n = 1 and n = 2.

$$\begin{aligned} \text{Wave function} : \varphi_n(x) &= \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \\ \langle x \rangle_n &= \int_0^a \varphi_n^* x \varphi_n dx = \int_0^a x |\varphi|^2 dx = \frac{2}{a} \int_0^a x \sin^2\left(\frac{n\pi x}{a}\right) = \frac{a}{2} \\ \langle x^2 \rangle_n &= \int_0^a \varphi_n^* x^2 \varphi_n dx = \int_0^a x^2 |\varphi|^2 dx = \frac{2}{a} \int_0^a x^2 \sin^2\left(\frac{n\pi x}{a}\right) = \frac{a^2}{3} - \frac{a^2}{2n^2 \pi^2} \begin{cases} n = 1 : a^2\left(\frac{1}{3} - \frac{1}{2\pi^2}\right) \approx 0.2827a^2 \\ n = 2 : a^2\left(\frac{1}{3} - \frac{1}{8\pi^2}\right) \approx 0.3207a^2 \end{cases} \\ \langle v^2 \rangle_n &= \frac{\langle p^2 \rangle}{M^2} = \frac{2E_n}{M} = \frac{\pi^2 \hbar^2 n^2}{M^2 a^2} = \begin{cases} n = 1 : \frac{\pi^2 \hbar^2}{M^2 a^2} \\ n = 2 : \frac{4\pi^2 \hbar^2}{M^2 a^2} \end{cases} \end{aligned}$$

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16. Why zero energy solution (E = 0) of equation $\tan\left(\frac{a\sqrt{2mE}}{\hbar}\right) = \frac{2\sqrt{E(U_0 - E)}}{2E - U_0}$ should be imposed?

ignored?

For finite potential well:

$$U = \begin{cases} U_0, & x < 0 \implies \psi'' = \kappa^2 \psi \\ 0, & 0 \le x \le a \implies \psi'' = 0 \\ U_0, & x > a \implies \psi'' = \kappa^2 \psi \end{cases} \implies \begin{cases} \psi_I(x) = Ce^{\kappa x} \\ \psi'' = 0 \implies \psi' = A \implies \psi_{II}(x) = Ax + B \\ \psi_{III}(x) = De^{-\kappa x} \end{cases}$$

where $\kappa^2 = \frac{2M(U_0 - 0)}{\hbar^2} = \frac{2MU_0}{\hbar^2}$

Continuity property + boundary conditions:

$$\begin{aligned} x &= 0: \begin{cases} \psi_{I}(0) = \psi_{II}(0) \implies Ce^{\kappa \cdot 0} = A \cdot 0 + B \implies C = B\\ \psi'_{I}(0) = \psi'_{II}(0) \implies C\kappa = A \end{cases} \\ \psi_{II}(x) &= Ax + B = C\kappa x + C = C(\kappa x + 1) \end{cases} \\ x &= a: \begin{cases} \psi_{II}(a) = \psi_{III}(a) \implies C(\kappa a + 1) = De^{-\kappa a}\\ \psi'_{II}(a) = \psi'_{III}(a) \implies C\kappa = -D\kappa e^{-\kappa a} \implies C = -De^{-\kappa a}\\ \implies C(\kappa a + 1) = -C \implies \kappa a + 1 = -1 \implies \kappa a = -2 \end{cases} \end{aligned}$$

The conditions $\kappa > 0$ and a > 0 are both not satisfied, hence E = 0 does not have nontrivial solutions.

24. Calculate the next matrix element for *x*-coordinate for harmonic oscillator $\int_{-\infty}^{+\infty} \psi_1^* \hat{x} \psi_3 dx$. Tabular integrals from lectures can be used.

$$\int_{-\infty}^{+\infty} \psi_1^* \hat{x} \psi_3 dx = \int_{-\infty}^{+\infty} \psi_n^* \hat{x} \psi_m dx, \quad [m = 3, n = 1] =$$

$$= \frac{\hbar A_n A_m}{M\omega} \left[\frac{1}{2} \int_{-\infty}^{+\infty} H_n(\xi) H_{m+1}(\xi) e^{-\xi^2} d\xi + m \int_{-\infty}^{+\infty} H_n(\xi) H_{m-1}(\xi) e^{-\xi^2} d\xi \right] =$$

$$= \begin{cases} \sqrt{\frac{\hbar}{M\omega}} \sqrt{\frac{n+1}{2}}, & \text{if } m = n+1; \\ \sqrt{\frac{\hbar}{M\omega}} \sqrt{\frac{n}{2}}, & \text{if } m = n-1; \end{cases} = [3 \neq 1 \pm 1 \implies m \neq n \pm 1] = 0$$

$$0, \quad \text{if } m \neq n \pm 1.$$

20 36. Why does the heat capacity tend to zero at low temperatures? Physical explanation.

• First explanation: Quantum freezing of degrees of freedom.

At low temperatures the thermal energy of the system $k_B T$ is much smaller than $\hbar\omega$ ($k_B T \ll \Delta E$), so transitions to excited quantum states are suppressed. As a result, the degrees of freedom remain in their ground states, and adding heat does not significantly change the system's energy distribution.

• Second explanation: Third law of thermodynamics

$$T \to 0 \implies \lim_{T \to 0} \left(\frac{\partial S}{\partial T}\right)_x = 0 \implies S \to \text{const} \implies C_x = T\left(\frac{\partial S}{\partial T}\right)_x \to 0$$

where x is any thermodynamic parameter as a constant.

At low temperatures, the system's entropy approaches a constant value and no longer changes as the temperature varies. Since the heat capacity is proportional to the rate of change of entropy with respect to temperature, it therefore tends to zero.