Kvantmehaanika ja spektroskoopia

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5. What does the transparency window mean (in case $E > U_0$) for a rectangular barrier and the conditions for its appearance?

We have $E > U_0$ and rectangular barrier with width of a and height of U_0. We can split coordinate-area into three regions: before-, after-barrier and barrier regions. From Schrodinger equations for different regions we get solution for particle in each region:

$$\varphi_1 = Ae^{ik_1x} + Be^{-ik_1x}, \varphi_2 = Ce^{ik_2x} + De^{-ik_2x}, \varphi_3 = Fe^{ik_1x},$$

where $k_1 = \frac{\sqrt{2mE}}{\hbar}$, $k_2 = \frac{\sqrt{2m(E-U_0)}}{\hbar}$ both parameters are real numbers. The unknown parameters A, B, C, D and F can be calculated from continuity property of wavefunction (at the border of regions).

$\varphi_1(0) = \varphi_2(0)$, $\varphi_2(a) = \varphi_3(a)$, $\frac{d\varphi_1}{dx}|_{x=0} = \frac{d\varphi_2}{dx}|_{x=0}$, $\frac{d\varphi_2}{dx}|_{x=a} = \frac{d\varphi_3}{dx}|_{x=a}$.

Taking $A = 1$ we get system of linear equations

$$1 + B = C + D$$

$$(1 - B) \cdot k_1 = (C - D) \cdot k_2$$

$$Ce^{ik_2a} + De^{-ik_2a} = Fe^{ik_1a}$$

$$Ck_2e^{ik_2a} - Dk_2e^{-ik_2a} = k_1Fe^{ik_1a}$$

From this system we can get the unknown parameters. We are interested in transmission coefficient $T = \frac{j_t}{j_i}$ where $j_t = \frac{\hbar k_1}{m}F^2$ is particles that pass throught the barrier and $j_i = \frac{\hbar k_1}{m}$ is particles going towards the barries. From this we get T:

$$T = \frac{4k_1^2k_2^2}{4k_1^2k_2^2\cos^2(k_2a) + (k_1^2 + k_2^2)^2\sin^2(k_2a)} \text{ for } E > U_0.$$

From this we can see thet in cases where $k_2a = \pi n$, we get $T = 1$. Solving for energy we get $E_n = \frac{\pi^2\hbar^2n^2}{2ma^2} + U_0$.

From this we get transparancy window where particles with energy E_n bass through the barrier with coefficient $T = 1$.

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8. Show that the probability current density (or wavefunction) inside of the walls (areas 1 and 3) should be zero? Why?

Infinite potential well. $U_0 \to \infty$ in areas 1 and 3, in area 2, $U = 0$.
In regions where $U_0 = \infty$, the Schrödinger equation becomes:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \infty\right)\psi(x) = E\psi(x).$$

The only way this equation can hold is if $\psi(x) = 0$ in these regions.

The wavefunction must be continuous everywhere. Since $\psi(x) = 0$ in the walls, it must also be zero at the boundaries $x = 0$ and $x = a$, which matches the condition $\psi(0) = \psi(a) = 0$.

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15. Can you show that equation for calculating energy of particle inside of finite potential well

$$\tan\left(a\sqrt{\frac{2mE}{\hbar}}\right) = \frac{2\sqrt{E(U_0 - E)}}{2E - U_0}$$

give the correct values for energy for infinite potential well (topic 5.1)

$$E_n = \frac{(\pi\hbar)^2}{2Ma^2} \cdot n^2, \quad n = 1, 2, \ldots$$

in limit $U_0 \to \infty$?

Lets take $k_1 = \frac{\sqrt{2mE}}{\hbar}$, $k_2 = \frac{\sqrt{2m(E-U_0)}}{\hbar}$ and $k_1^2 = \frac{2mE}{\hbar^2}, k_2^2 = \frac{2mU_0}{\hbar^2} - k^2$ from which we get

$$\tan(k_1 a) = \frac{2k_1k_2}{k_2^2 - k_1^2}$$

Form right side we get $\frac{2k_1k_2}{k_2^2-k_1^2} = \frac{2\frac{k_1}{k_2}}{1-(\frac{k_1}{k_2})^2}$. As $U_0 \to \infty$, $k_2 \to \infty$, so $\frac{k_1}{k_2} \to 0$.

$$\frac{2\frac{k_1}{k_2}}{1-(\frac{k_1}{k_2})^2} \approx 2\frac{k_1}{k_2} \to 0$$

From this we finnaly get

$$\tan(k_1 a) = 0, \text{ solving it we get } k_1 a = n\pi, n = 1, 2, 3, \ldots$$

Substituting back we get

$$\frac{\sqrt{2mE}}{\hbar}a = n\pi, \text{ solving for E we get: } E = \frac{n^2\pi^2\hbar^2}{2ma^2}, n = 1, 2, 3, \ldots$$

Which gives us energy for infinite potential well.

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19. Why asymptotical solution of Schrodinger equation for harmonic oscillator is looks like so

$$\psi(\xi) = e^{-\frac{\xi^2}{2}}$$

? Why the option

$$\psi(\xi) = e^{\frac{\xi^2}{2}}$$

should be ignored?

From classical physics parabolic potential energy $U = kx^2/2$ we get harmonic oscillator, whit frequency $\omega = \sqrt{k/M}$,

Considering potential energy as

$$U(x) = \frac{M\omega^2 x^2}{2}$$

we get following Schrödinger equation

$$-\frac{\hbar^2}{2M}\frac{d^2\psi(x)}{dx^2} + \frac{M\omega^2 x^2}{2}\psi(x) = E\psi(x).$$

case we define

$$\xi = \sqrt{\frac{M\omega}{\hbar}}, \quad \lambda = \frac{2E}{\hbar\omega}$$

and write our equation as

$$-\frac{d^2\psi(\xi)}{d\xi^2} + \xi^2\psi(\xi) = \lambda\psi(\xi)$$

For finding a solution If $|\xi| \to \infty$, we demand that $\psi(\xi) \to 0$.

If $|\xi| \gg \lambda$ we get $-\frac{d^2\psi(\xi)}{d\xi^2} + \xi^2\psi(\xi) = 0$ from which we get approximate solution

$$\psi(\xi) = e^{\pm\frac{\xi^2}{2}}$$

$\psi(\xi) = e^{\frac{\xi^2}{2}}$ should be ignored because as ξ increases, $\psi(\xi)$ increases exponentialy and at large values it tends to infinity, which is unphysical.

We finnaly get asymptotical solution of Schrodinger equation for harmonic oscillator

$$\psi(\xi) = e^{-\frac{\xi^2}{2}}$$

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

Total thermal kinetic energy of whole crystal is equal to $\frac{kTN}{2}$, where N is number of atoms in the chain. The average kinetic and potential energies associated with thermal motion are equal. Meaning total internal energy of crystal is kTN. At low temperatures thermal enegy becomes smaller than energy spaceing between quantum states. Vibrations are quantized as phonons with specific energy levels. When the temperature is very low, there isn't enough thermal energy available to excite these vibrational modes. At very low temperatures (when $kT \ll \hbar\omega$), the probability of exciting even the lowest energy phonon becomes exponentially small ($\sim e^{-\hbar\omega/kT}$).