Kvantmehaanika ja spektroskoopia

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Küsimused loeng 6-9

20 6. Show that as U_0 tends to zero, the transfer coefficient T(E) tends to 1 for both cases $E>U_0$ and $E<U_0$.

In case $E>U_0$ the transfer coefficient is $T = \frac{4k_1^2k_2^2}{4k_1^2k_2^2 cos^2(k_2a)+(k_1^2+k_2^2)^2 sin^2(k_2a)}$ where $k_1 = \frac{\sqrt{2mE}}{\hbar}$ and $k_2 = \frac{\sqrt{2m(E-U_0)}}{\hbar}$ and a is the width of the barrier. When $U_0 \rightarrow 0$ then $k_2 \rightarrow k_1$ therefore the coefficient will become as follows:

$$T = \frac{4k_1^2k_1^2}{4k_1^2k_1^2\cos^2(k_1a)+(k_1^2+k_1^2)\sin^2(k_1a)} = \frac{4k_1^4}{4k_1^4\cos^2(k_1a)+4k_1^4\sin^2(k_1a)}$$

$$= \frac{\cancel{4k_1^4}\,1}{\cancel{4k_1^4}\,1\,\underbrace{(\sin^2(k_1a)+\cos^2(k_1a))}_{=1}} = 1$$

Similarly, in the case of $E<U_0$, the transfer coefficient is $T = \frac{4k_1^2k_2^2}{4k_1^2k_2^2 cosh^2(k_2a)+(k_1^2-k_2^2)^2 sinh^2(k_2a)}$. In the case where U_0 tends to zero, it is visible, that T will tend to 1. When considering that E needs to be smaller than U_0 it would make k_1 also tend to 0. Then $cosh^2(k_1a)$ will tend to 1 and T will also tend to 1.

$$T = \frac{4k_1^2k_1^2}{4k_1^2k_1^2\cosh^2(ak_1)+\underbrace{\underbrace{(k_1^2-k_1^2)^2}_{\to 0}\sinh^2(k_1a)}_{=0}} = \frac{1}{\cosh^2(k_1a)} = 1$$

$$k_1 \to 0 \Rightarrow \cosh^2(k_1a) \to 1$$

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

In the case of a finite barrier, the Schrödinger's equation for inside the barrier would be

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi_1}{\partial x^2} + U_0\varphi_1 = E\varphi_1$$

But when $U_0 \rightarrow \infty$ the $U_0\varphi_1$ can only be finite, when $\varphi_1 = 0$. Same goes for the other wall too, which means that $\varphi_3 = 0$ as well. There cannot be an exponential decay, like in the case of a finite barrier, so the probability is forced to be exactly zero on the barrier limit.

10 15. Can you show that equation for calculating energy of particle inside of finite potential well $tan\left(\frac{a\sqrt{2mE}}{\hbar}\right) = \frac{2\sqrt{E(U_0 - E)}}{2E - U_0}$ gives the correct values for energy for infinite potential well (topic 5.1) $E_n = \frac{(\pi\hbar)^2}{2Ma^2}n^2,\ n = 1, 2, \ldots$ in limit $U_0 \to \infty$?

Kust te selle said?

We can show that the equation for the finite well gives the correct values for energy because as $U_0 \to \infty$ then $\lim\limits_{U_0 \to \infty} \frac{2\sqrt{E(U_0 - E)}}{2E - U_0} = 0$. That would mean that $tan\left(\frac{a\sqrt{2mE}}{\hbar}\right) = 0$ as well. Tangent can be zero if $\frac{a\sqrt{2mE}}{\hbar} = n\pi$. Rearranging:

$$\frac{a\sqrt{2mE}}{\hbar} = n\pi$$

$$\sqrt{E} = \frac{n\pi\hbar}{a\sqrt{2m}}$$

$E = \frac{(\pi\hbar)^2}{2ma^2}n^2,\ n = 1, 2, \ldots$ which is the same as the energy values for the infinite potential well. n cannot be zero, because the energy ground state is nonzero.

5 28. How can the energy of a harmonic oscillator be calculated at a non-zero temperature? (Don't forget that thermal motion is fully chaotic and can be described by a random force acting on an oscillating point mass). NB! Some ideas from calculation of heat capacity for 1d crystal lattice can be used (next topic V).

In quantum oscillator the ground energy is nonzero: $E_0 = \frac{\hbar\omega}{2}$, the energy is discrete. Energy values are given as $E_n = \hbar\omega(n + \frac{1}{2}),\ n = 1, 2, \ldots$

Kuidas saab arvutada kvantarvu n, kui T ei ole null?

If the temperature of the crystal is not zero, then the average thermal kinetic energy associated with one degree of freedom is equal to $\frac{kT}{2}$ and the total thermal kinetic energy for the whole crystal is $\frac{kTN}{2}$. The average kinetic and potential energies for the thermal motion are equal, so the total internal energy of the crystal is equal to kTN.

For 1d crystal lattice:

$$E_{tot} = \frac{2N}{\pi}\int_0^{\omega_0} \frac{\hbar\omega}{\sqrt{(\omega_0^2 - \omega^2)}(e^{\frac{\hbar\omega}{kT}} - 1)}d\omega,\ where\ \omega_0 = \sqrt{\frac{4g}{m}}$$

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37. Can you show that (for 1d crystal) phase and group velocities of harmonic waves are equal in limit of very long waves (λ→∞).

1d crystal phase velocity $v_p = v_0 \left| \frac{sin\frac{aq}{2}}{\frac{aq}{2}} \right|$ and group velocity $v_g = v_0 \left| cos\frac{aq}{2} \right|$, where a is the distance between the closest atoms, and q is the wave vector. The length of the wave vector is $q = \frac{2\pi}{\lambda}$. In case of $\lambda \to \infty$ it is visible that $q \to 0$. Therefore both $v_p and\ v_g \to v_0$ because the sine and cosine functions tend to 1. So we can say that $v_0 = v_p = v_g$ in very long wavelengths.