Quantum mechanics III

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The electron falling on the barrier. The kinetic energy of particle is 8 eV and height of barrier 10 eV. How large the probability of transmission of electron through barrier. The width of barrier is 0.5 A.(7)

Since  $E < V_0$ , the electron may tunnel through the barrier.

$$\begin{split} T &\approx e^{-2\kappa a} \\ \kappa &= \frac{\sqrt{2m(V_0 - E)}}{\hbar} \\ V_0 - E &= 2eV = 2 \times 1.602e - 19J = 3.204e - 19J \\ \kappa: \\ \kappa &= \frac{\sqrt{2 \times 9.11 \times 10^{-31} \times 3.204 \times 10^{-19}}}{1.055 \times 10^{-34}} = \frac{\sqrt{5.835 \times 10^{-49}}}{1.055 \times 10^{-34}} \approx \frac{7.64 \times 10^{-25}}{1.055 \times 10^{-34}} \approx 7.24 \times 10^9 \,\mathrm{m^{-1}} \\ T: \\ T &\approx e^{-2 \times \kappa \times a} = e^{-2 \times 7.24 \times 10^9 \times 0.5 \times 10^{-10}} = e^{-0.724} \approx 0.485 \end{split}$$

 $T \approx 0.485$  (or 48.5%)

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 $\mathbf{2}$ 

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 (10)

$$\begin{split} \varphi_n(x) &= \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \\ \langle x \rangle_n &= \int_0^a \varphi_n^* x \varphi_n dx = \int_0^a x \varphi^2 dx \\ &= \frac{2}{a} \int_0^a x \sin^2\left(\frac{n\pi x}{a}\right) dx = a \left(\frac{1}{2} - \frac{1}{2n\pi} \sin\left(2n\pi\right)\right) = \frac{a}{2} \\ \langle x^2 \rangle_n &= \int_0^a \varphi_n^* x^2 \varphi_n dx = \int_0^a x^2 \varphi^2 dx \\ &= \frac{2}{a} \int_0^a x^2 \sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{a^2}{2} \left(\frac{1}{3} - \frac{1}{2n^2\pi^2}\right) \\ &\Rightarrow \begin{cases} n = 1 : a^2 \left(\frac{1}{3} - \frac{1}{2\pi^2}\right) \approx 0.28a^2 \\ n = 2 : a^2 \left(\frac{1}{3} - \frac{1}{8\pi^2}\right) \approx 0.32a^2 \end{cases} \\ \langle v^2 \rangle_n &= \frac{\langle p^2 \rangle}{M^2} = \frac{2E_n}{M} = \frac{\pi^2 \hbar^2 n^2}{M^2 a^2} \Rightarrow \begin{cases} n = 1 : \frac{\pi^2 \hbar^2}{M^2 a^2} \\ n = 2 : \frac{4\pi^2 \hbar^2}{M^2 a^2} \end{cases} \end{split}$$

## 5

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## The wavefunction inside of finite potential well should be real on complex? Why?(17)

In a finite potential well with real and time-independent potential V(x), the time-independent Schrödinger equation: See ei ole seletus küsimusele MIKS?

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

has solutions  $\psi(x)$  that can be complex. However, because the equation has real coefficients, if  $\psi(x)$  is a solution, so is  $\psi^*(x)$ . Therefore, one can construct a real solution:

$$\psi_r(x) = rac{1}{2}(\psi(x) + \psi^*(x))$$

This means that for **bound states**, the wavefunction can always be chosen to be real, including inside the well.

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4

Why should the power series  $\nu(\xi) = \sum_{r=0}^{\infty} a_r \xi^r$  (where  $a_{r+2} = \frac{2r+1-\lambda}{(r+2)(r+1)}a_r$  for the wave function of a harmonic oscillator be limited? Why is it necessary to take into account only a limited number of terms in the series? (26)

As  $r \to \infty$ , unless the series terminates, the wave function  $\nu(\xi)$  will behave like  $e^{\xi^2}$  for large  $\xi$  due to the asymptotic behavior of the Hermite differential equation. This causes the overall wave function

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

to diverge as  $\xi \to \infty$ , making it non-normalizable — which is unphysical for a quantum mechanical wave function.

To ensure that  $\psi(\xi)$  remains normalizable and physically meaningful, the series should be able to terminate after a finite number of terms. This occurs only when  $\lambda = 2n + 1$  for some non-negative integer n, which leads to polynomial solutions for  $\nu(\xi)$ . This condition would quantize the energy levels.

mmm? miks?

\* pidin otsima lisainformatsiooni, et õige vastuseni jõuda: http://physics.gmu.edu/ dmaria/590

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## 5 Give a classical estimate of the heat capacity of a threedimensional crystal (as was done for a one-dimensional lattice). Remember that atoms in a 3D crystal vibrate in all three dimensions it means that number of degrees of freedom must be increased (in compare with 1d lattice).(34)

Classical physics says that each quadratic degree of freedom contributes an average energy of  $\frac{1}{2}kT$ , where k is the Boltzmann const. and T is the absolute temperature measured in Kelvins. For 1 - D crystals, each atom is vibrating along a single direction. Therefore the total internal energy for N atoms is:

 $E_{1D} = NkT$ 

For a 3 - D crystal, each atom vibrates independently in the directions of each axes (x, y and z), which gives us 3kT per atom. Leading the total energy to become:

$$E_{3D} = 3NkT$$

Moving to heat capacity, the heat capacity at constant volume is the derivative of internal energy with respect to energy and we obtain:

$$C_V = \left(\frac{dE}{dT}\right)_V = \frac{d}{dT}(3kNT) = 3Nk$$

If  $N = N_A$  then:

$$C_V = 3N_A k = 3R$$

Therefore we have obtained the classical estimate of heat capacity for 3D crystals:

$$C_V = 3N_A k = 3R$$

which is the form per mole and is also known as the classical Dulong-Petite law.