Loengud 6-9

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Question 3

How looks like dependence of R(E) and T(E) on energy for rectangle barrier in classical physics? What does it mean the tunnel effect for rectangle barrier?

Answer

For a particle encountering a rectangular barrier of height V_0:

$$T(E) = \begin{cases} 1 & \text{if } E > V_0 \\ 0 & \text{if } E < V_0 \end{cases} \qquad R(E) = 1 - T(E)$$

Quantum case (Tunnel Effect):
For $E < V_0$, due to wave-like behavior of particles:

$$T(E) > 0 \quad \text{(tunneling possible)}$$

This is known as the *quantum tunnel effect.*

Question 10

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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 $n = 2$.

Answer

Wavefunction:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \quad 0 < x < L$$

Average position:

$$\langle x \rangle = \int_0^L x|\psi_n(x)|^2 dx = \frac{L}{2}$$

Mean square position:

$$\langle x^2 \rangle = \int_0^L x^2|\psi_n(x)|^2 dx = \frac{L^2}{3} - \frac{L^2}{2n^2\pi^2}$$

Mean square velocity:
Using total energy $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$ and kinetic energy $E_k = \frac{1}{2}m\langle v^2 \rangle$, we get:

$$\langle v^2 \rangle = \frac{2E_n}{m} = \frac{n^2\pi^2\hbar^2}{m^2L^2}$$

Results for quantum numbers $n = 1$ and $n = 2$:

Quantity	$n = 1$	$n = 2$
$\langle x \rangle$	$\frac{L}{2}$	$\frac{L}{2}$
$\langle x^2 \rangle$	$\frac{L^2}{3} - \frac{L^2}{2\pi^2}$	$\frac{L^2}{3} - \frac{L^2}{8\pi^2}$
$\langle v^2 \rangle$	$\frac{\pi^2\hbar^2}{m^2L^2}$	$\frac{4\pi^2\hbar^2}{m^2L^2}$

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Question 14

What does the Schrödinger equation and the continuity conditions looks like for finite potential well (for E¡U0)? Derive equations.

Answer

Potential:

$$U(x) = \begin{cases} 0, & 0 < x < a \\ U_0, & x < 0 \text{ or } x > a \end{cases}$$

Regions and Solutions:

- Region I ($x < 0$): $\psi_I(x) = Be^{\kappa x}$
- Region II ($0 < x < a$): $\psi_{II}(x) = C\sin(kx) + D\cos(kx)$
- Region III ($x > a$): $\psi_{III}(x) = Fe^{-\kappa x}$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}}, \quad \kappa = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$$

Continuity Conditions:

$$\psi_I(0) = \psi_{II}(0), \qquad \psi_I'(0) = \psi_{II}'(0)$$
$$\psi_{II}(a) = \psi_{III}(a), \qquad \psi_{II}'(a) = \psi_{III}'(a)$$

Quantization Condition:

$$\kappa = k\tan(ka) \quad \text{or} \quad \tan(ka) = \frac{\kappa}{k}$$

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Question 25

Calculate matrix element for the dipole transition from the ground state to the first excited state for the harmonic oscillator:

$$\int_{-\infty}^{+\infty} \psi_0(x)\, x\, \psi_1(x)\, dx$$

Answer

We want to evaluate the integral:

$$\int_{-\infty}^{+\infty} \psi_0(x)\, x\, \psi_1(x)\, dx$$

The harmonic oscillator wavefunctions are:

$$\psi_n(x) = N_n H_n(\xi) e^{-\xi^2/2}, \quad \xi = \sqrt{\frac{m\omega}{\hbar}}x$$

For $n = 0$ and $n = 1$:

$$\psi_0(x) = N_0 e^{-\xi^2/2}, \quad \psi_1(x) = N_1 \cdot 2\xi\, e^{-\xi^2/2}$$

Substituting into the integral:

$$\int_{-\infty}^{+\infty} \psi_0(x)\, x\, \psi_1(x)\, dx = 2N_0N_1 \int_{-\infty}^{+\infty} x\xi e^{-\xi^2}\, dx$$

Change variable: $\xi = \sqrt{\frac{m\omega}{\hbar}}x \Rightarrow dx = \sqrt{\frac{\hbar}{m\omega}}d\xi$, so:

$$x = \sqrt{\frac{\hbar}{m\omega}}\xi \quad \Rightarrow x\xi = \sqrt{\frac{\hbar}{m\omega}}\xi^2$$

$$\Rightarrow \int_{-\infty}^{+\infty} x\xi e^{-\xi^2}\, dx = \sqrt{\frac{\hbar}{m\omega}} \int_{-\infty}^{+\infty} \xi^2 e^{-\xi^2}\, dx = \frac{\hbar}{m\omega} \int_{-\infty}^{+\infty} \xi^2 e^{-\xi^2}\, d\xi$$

Use tabular integral:

$$\int_{-\infty}^{+\infty} \xi^2 e^{-\xi^2} d\xi = \frac{\sqrt{\pi}}{2}$$

Normalization constants:

$$N_n = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} \Rightarrow N_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}, \quad N_1 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \cdot \frac{1}{\sqrt{2}}$$

$$N_0 N_1 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \cdot \frac{1}{\sqrt{2}}$$

Combining everything:

$$\int_{-\infty}^{+\infty} \psi_0(x)\, x\, \psi_1(x)\, dx = 2 \cdot N_0 N_1 \cdot \frac{\hbar}{m\omega} \cdot \frac{\sqrt{\pi}}{2} = \frac{1}{\sqrt{2}} \cdot \sqrt{\frac{\hbar}{m\omega}} = \sqrt{\frac{\hbar}{2m\omega}}$$

Final result:

$$\boxed{\int_{-\infty}^{+\infty} \psi_0(x)\, x\, \psi_1(x)\, dx = \sqrt{\frac{\hbar}{2m\omega}}}$$

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Question 34

.Give a classical estimate of the heat capacity of a three-dimensional 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).

Answer

In classical physics, the equipartition theorem states that each quadratic degree of freedom contributes an average energy of $\frac{1}{2}kT$, where k is the Boltzmann constant and T is the absolute temperature.

1D Crystal

In a one-dimensional crystal, each atom vibrates along a single direction. Each vibrational mode contributes:

$$\text{Kinetic energy: } \frac{1}{2}kT, \quad \text{Potential energy: } \frac{1}{2}kT \quad \Rightarrow \quad \text{Total: } kT$$

Therefore, the total internal energy for N atoms is:

$$E_{\text{1D}} = N \cdot kT$$

3D Crystal

In a three-dimensional crystal, each atom vibrates independently along the x, y, and z directions. This gives:

$$3 \text{ directions} \times \left(\frac{1}{2}kT + \frac{1}{2}kT\right) = 3kT \text{ per atom}$$

Hence, the total internal energy is:

$$E_{\text{3D}} = N \cdot 3kT = 3NkT$$

Heat Capacity

The heat capacity at constant volume is the derivative of internal energy with respect to temperature:

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

Per Mole Result

If $N = N_A$ (Avogadro's number), and using the relation $R = N_A k$, the molar heat capacity becomes:

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

Conclusion

The classical estimate of heat capacity for a 3D crystal is:

$$\boxed{C_V = 3Nk = 3R \text{ (per mole)}}$$

This is the classical Dulong–Petit law, which agrees well with experiment at high temperatures, but deviates at low temperatures where quantum effects become significant.