

Control Questions of Lectures 6 to 9

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1 Question 3 20

Consider a rectangular potential barrier of height V_0 .

In classical physics, particles either have enough energy to go over the barrier or they don't.

Thus:

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

In quantum mechanics, even when $E < V_0$, the particle has a non-zero probability of appearing on the other side of the barrier. The transmission coefficient in the quantum case for $E < V_0$ is approximately:

$$T(E) \propto e^{-2\kappa a} \quad (2)$$

where a is the width of the barrier and

$$\kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}. \quad (3)$$

This shows that the probability of tunneling decreases exponentially with both the barrier width a and the energy difference $V_0 - E$.

2 Question 10 huvitavad detailid 10

$$\begin{aligned} n = 1 : \quad \langle x \rangle &= 0, \quad \langle x^2 \rangle = \frac{3}{2} \cdot \frac{\hbar}{m\omega}, \quad \langle v^2 \rangle = \frac{3}{2} \cdot \frac{\hbar\omega}{m} \\ n = 2 : \quad \langle x \rangle &= 0, \quad \langle x^2 \rangle = \frac{5}{2} \cdot \frac{\hbar}{m\omega}, \quad \langle v^2 \rangle = \frac{5}{2} \cdot \frac{\hbar\omega}{m} \end{aligned} \quad (4)$$

3 Question 18 15

The wavefunction can be either real or complex inside the walls of a finite potential well. Both are mathematically valid:

$$\psi(x) = A \sin(kx) + B \cos(kx) \quad (\text{real form}) \quad (5)$$

Vastus on lihtsam.

1

Osakes ei saa tekitada osakeste voogu (elektrivoolu) seinä sees, mille voolu tõenäosustihedus ei ole null. Kuid reaalse lainefunktsiooni korral on voolu tõenäosustihedus alati null.

or

$$\psi(x) = Ce^{ikx} + De^{-ikx} \quad (\text{complex form}) \quad (6)$$

where

$$k = \frac{\sqrt{2mE}}{\hbar}. \quad (7)$$

In quantum mechanics, the full wavefunction is typically written as:

$$\Psi(x, t) = \psi(x)e^{-iEt/\hbar}. \quad (8)$$

Even if $\psi(x)$ is real, the total wavefunction is complex due to time evolution. Complex exponentials correspond to definite momentum states $p = \hbar k$, while real combinations are superpositions of momenta. Complex wavefunctions simplify calculations in quantum phenomena like tunneling.

Inside the walls of a finite potential well, I would prefer real-valued wavefunctions for bound states, because they are easier to interpret, directly reflect the standing wave nature of the bound state, and are mathematically simpler for normalization and boundary conditions.

However, if dealing with time-dependent problems, complex wavefunctions are necessary.

4 Question 27

20

The ground state wavefunction of the quantum harmonic oscillator is:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right). \quad (9)$$

We wish to compute the following integral:

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi_0(x)|^2 dx. \quad (10)$$

Substituting the wavefunction:

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \exp\left(-\frac{m\omega x^2}{\hbar}\right) dx. \quad (11)$$

Recall the integral:

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{\sqrt{\pi}}{2a^{3/2}}, \quad \text{for } a > 0. \quad (12)$$

Let $a = \frac{m\omega}{\hbar}$, then:

$$\langle x^2 \rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \times \frac{\sqrt{\pi}}{2 \left(\frac{m\omega}{\hbar}\right)^{3/2}} = \frac{\hbar}{2m\omega}. \quad (13)$$

5 Question 33

20

The density of states (DOS), $g(\omega)$, describes the number of vibrational modes per unit frequency at a given angular frequency ω . It tells us how the vibrational energy is distributed across different frequencies in the system.

The function $g(\omega)$ quantifies the number of vibrational states that a system can occupy at a certain frequency. For example, in a solid, $g(\omega)$ represents how phonons¹ are distributed across different frequencies.

The density of vibrational states, $g(\omega)$, is defined such that

$$g(\omega) d\omega \quad (14)$$

gives the number of vibrational modes with frequencies between ω and $\omega + d\omega$.

For a one-dimensional chain of N atoms with a mass m connected by springs with a spring constant g , the phonon dispersion relation is

$$\omega(k) = 2\sqrt{\frac{g}{m}} \left| \sin\left(\frac{ka}{2}\right) \right|, \quad (15)$$

where a is the lattice spacing.

The maximum angular frequency is

$$\omega_0 = 2\sqrt{\frac{g}{m}} = \sqrt{\frac{4g}{m}}. \quad (16)$$

The corresponding density of states is

$$g(\omega) = \frac{N}{\pi} \frac{1}{\sqrt{\omega_0^2 - \omega^2}}, \quad 0 \leq \omega \leq \omega_0. \quad (17)$$

We wish to compute:

$$\int_0^{\omega_0} g(\omega) d\omega = \int_0^{\omega_0} \frac{N}{\pi} \frac{1}{\sqrt{\omega_0^2 - \omega^2}} d\omega = \frac{N}{\pi} \int_0^{\omega_0} \frac{d\omega}{\sqrt{\omega_0^2 - \omega^2}}. \quad (18)$$

Using the standard integral:

$$\int_0^u \frac{dx}{\sqrt{u^2 - x^2}} = \frac{\pi}{2}, \quad (19)$$

where $u = \omega_0$, we get:

$$\int_0^{\omega_0} \frac{d\omega}{\sqrt{\omega_0^2 - \omega^2}} = \frac{\pi}{2}. \quad (20)$$

¹A phonon is a collective excitation in condensed matter that quantizes vibration modes in elastic structures. Phonons can be thought of as quanta of lattice vibrations and are an essential concept in understanding thermal and mechanical properties of solids. In mathematical notation, phonons are often represented by the symbol $\mathbf{q}$ or $\mathbf{k}$, where $\mathbf{q}$ represents the wavevector and $\mathbf{k}$ is the crystal momentum.

Thus:

$$\int_0^{\omega_0} g(\omega) d\omega = \frac{N}{\pi} \times \frac{\pi}{2} = \frac{N}{2}. \quad (21)$$

Since each vibrational mode in 1D corresponds to one degree of freedom per atom, and we have two modes, left-moving and right-moving, per k -point, the total number of modes is N .

Thus, the result $\frac{N}{2}$ corresponds to half the vibrational modes. When taking into account both k and $-k$ directions, we would recover exactly N modes total.