Loengu 6-9

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1.

Potential Barrier Setup

Assume a potential barrier $V(x)$ as follows:

- Region I: $x < 0, V(x) = 0$
- Region II: $0 \leq x \leq a, V(x) = V_0$
- Region III: $x > a, V(x) = 0$

Schrödinger Equation

The time-independent Schrödinger equation is given by: $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$

Region I: $x < 0$

In this region, the potential $V(x) = 0$, so the Schrödinger equation simplifies to: $-\frac{\hbar^2}{2m}\frac{d^2\psi_I(x)}{dx^2} = E\psi_I(x)$ The general solution is: $\psi_I(x) = Ae^{ikx} + Be^{-ikx}$ where $k = \sqrt{\frac{2mE}{\hbar^2}}$.

Region II: $0 \leq x \leq a$

In this region, the potential $V(x) = V_0$, so the Schrödinger equation becomes: $-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}(x)}{dx^2} + V_0\psi_{II}(x) = E\psi_{II}(x)$ Rewriting, we get: $\frac{d^2\psi_{II}(x)}{dx^2} = \frac{2m(V_0-E)}{\hbar^2}\psi_{II}(x)$ Let $\kappa = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$, then the general solution is: $\psi_{II}(x) = Ce^{\kappa x} + De^{-\kappa x}$

Region III: $x > a$

In this region, the potential $V(x) = 0$, so the Schrödinger equation simplifies again to: $-\frac{\hbar^2}{2m}\frac{d^2\psi_{III}(x)}{dx^2} = E\psi_{III}(x)$ The general solution is: $\psi_{III}(x) = Fe^{ikx} + Ge^{-ikx}$

8.

Infinite Potential Well Setup

Consider an infinite potential well with walls at $x = 0$ and $x = L$. The potential $V(x)$ is defined as:

- $V(x) = 0$ for $0 < x < L$
- $V(x) = \infty$ for $x \leq 0$ and $x \geq L$

Wavefunction Inside the Well

Inside the well ($0 < x < L$), the Schrödinger equation is: $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$

The solutions to this equation are sinusoidal functions: $\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$ where n is a positive integer.

Probability Current Density

The probability current density $J(x)$ is given by: $J(x) = \frac{\hbar}{2mi}\left(\psi^*(x)\frac{d\psi(x)}{dx} - \psi(x)\frac{d\psi^*(x)}{dx}\right)$

For the wavefunctions inside the well, we have: $\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$

Since $\psi_n(x)$ is real, $\psi^*(x) = \psi(x)$. Therefore, the probability current density simplifies to: $J(x) = \frac{\hbar}{2mi}\left(\psi(x)\frac{d\psi(x)}{dx} - \psi(x)\frac{d\psi(x)}{dx}\right) = 0$

Inside the Walls (Areas 1 and 3)

In areas 1 ($x \leq 0$) and 3 ($x \geq L$), the potential is infinite. This means the wavefunction $\psi(x)$ must be zero in these regions because the probability of finding the particle in an area with infinite potential is zero. Therefore: $\psi(x) = 0 \quad \text{for} \quad x \leq 0 \quad \text{and} \quad x \geq L$

Since $\psi(x) = 0$ in these regions, the probability current density $J(x)$ is also zero: $J(x) = 0 \quad \text{for} \quad x \leq 0 \quad \text{and} \quad x \geq L$

Why is $J(x)$ Zero?

The probability current density represents the flow of probability. In regions with infinite potential, the wavefunction is zero, indicating no probability of finding the particle there. Consequently, there is no flow of probability, and thus the probability current density is zero.

16.

Finite Potential Well Setup

Consider a finite potential well with potential $V(x)$ defined as:

- $V(x) = 0$ for $x < 0$ and $x > a$
- $V(x) = V_0$ for $0 \leq x \leq a$

Schrödinger Equation

The time-independent Schrödinger equation for a particle in a potential well is: $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$

Regions

- **Region I** ($x < 0$): $V(x) = 0$
- **Region II** ($0 \leq x \leq a$): $V(x) = V_0$
- **Region III** ($x > a$): $V(x) = 0$

Zero Energy Solution

The equation given is: $\tan\left(\frac{\alpha a}{2}\right) = \frac{2\sqrt{E(U_0 - E)}}{2E - U_0}$

For $E = 0$:

- The left-hand side becomes $\tan(0) = 0$.
- The right-hand side becomes $\frac{2\sqrt{0(U_0 - 0)}}{2\cdot 0 - U_0} = 0$.

Why Ignore $E = 0$?

1. **Physical Interpretation**: A zero energy solution implies that the particle has no kinetic energy. In quantum mechanics, a particle in a potential well must have some kinetic energy to exist within the well. Zero energy would mean the particle is stationary, which contradicts the principles of quantum mechanics where particles exhibit wave-like behavior.
2. **Wavefunction Behavior**: For $E = 0$, the wavefunction $\psi(x)$ would not exhibit the oscillatory or exponential decay behavior expected in a potential well. Instead, it would be a constant or zero, which does not satisfy the boundary conditions of the well.
3. **Normalization**: The wavefunction must be normalizable, meaning the total probability of finding the particle within the well must be 1. A zero energy solution would not yield a normalizable wavefunction.

Conclusion

The zero energy solution is ignored because it does not align with the physical and mathematical requirements of a particle in a finite potential well. The particle must have some non-zero energy to exhibit the expected quantum behavior and satisfy the boundary conditions.

26.

Harmonic Oscillator Setup

The Schrödinger equation for a one-dimensional harmonic oscillator is: $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi(x) = E\psi(x)$

Power Series Solution

The wave function $\psi(x)$ can be expressed as a power series: $\psi(\xi) = \sum_{r=0}^{\infty} a_r \xi^r$ where $\xi = \sqrt{\frac{m\omega}{\hbar}}x$.

The recurrence relation for the coefficients a_r is given by: $a_{r+2} = \frac{2r+1-\lambda}{(r+2)(r+1)}a_r$ where $\lambda = \frac{2E}{\hbar\omega}$.

Limiting the Power Series

The power series solution should be limited for the following reasons:

1. **Normalization**: The wave function must be normalizable, meaning the total probability of finding the particle must be finite. If the series is not limited, the wave function may diverge, leading to an infinite probability, which is physically meaningless.
2. **Physical Boundaries**: The harmonic oscillator potential grows infinitely as x increases. The wave function must decay to zero at large x to ensure the particle is confined within the potential well. Limiting the series ensures the wave function exhibits this decay.
3. **Eigenvalues and Eigenfunctions**: The harmonic oscillator has discrete energy levels. The power series solution corresponds to these quantized energy levels. Limiting the series ensures that the wave function corresponds to a specific eigenvalue E_n.

Conclusion

It is necessary to take into account only a limited number of terms in the series to ensure the wave function is normalizable, decays appropriately at large x, and corresponds to the discrete energy levels of the harmonic oscillator.

31.

Harmonic Wave Function

The function given is: $\alpha(q) = \alpha_0 \sin\left(qa\frac{\alpha}{2}\right)$

We need to show that this function and the condition $q + q' = \frac{2\pi}{a}$ describe the same harmonic wave: $u_{k_n}(t) = A_{k_n} e^{i(\omega t - k_n x)}$

Wave Function Equivalence

To show that $u_{k_n}(t) = u_{k_{\pi-2a/q}}(t)$, we need to demonstrate that the wave functions are equivalent under the given conditions.

1. **Wave Vector Relationship**: Given $q + q' = \frac{2\pi}{a}$, we can write: $q' = \frac{2\pi}{a} - q$
2. **Substitute q' into $\alpha(q)$**: $\alpha(q') = \alpha_0 \sin\left(\left(\frac{2\pi}{a} - q\right) a\frac{\alpha}{2}\right)$ Simplifying: $\alpha(q') = \alpha_0 \sin\left(\pi\alpha - qa\frac{\alpha}{2}\right)$
3. **Using Trigonometric Identity**: Using the identity $\sin(\pi - x) = \sin(x)$, we get: $\alpha(q') = \alpha_0 \sin\left(qa\frac{\alpha}{2}\right)$ Therefore: $\alpha(q') = \alpha(q)$

Harmonic Wave Function Equivalence

Since $\alpha(q)$ and $\alpha(q')$ describe the same function, the harmonic wave functions $u_{k_n}(t)$ and $u_{k_{\pi-2a/q}}(t)$ are equivalent: $u_{k_n}(t) = u_{k_{\pi-2a/q}}(t)$

Heat Capacity for 1D Chain of Atoms

For a one-dimensional chain of atoms, the heat capacity can be derived using the phonon model. The heat capacity C at temperature T is given by: $C = \sum_k \left(\frac{\partial \langle E_k \rangle}{\partial T} \right)$ where $\langle E_k \rangle$ is the average energy of the phonon mode with wave vector k.