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Quantum Mechanics Problems and Solutions

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1 Schrödinger Equation for Tunneling Effect (E ¡ U_0)

Question: What does the Schrödinger equation and the continuity conditions looks like for the tunneling effect in the case E smaller than U_0? Derive equations for a rectangular barrier.

Solution:

Consider a particle with energy E encountering a rectangular potential barrier:

- Region I (x ¡ 0): V(x) = 0
- Region II ($0 \leq$ x $\leq$ L): V(x) = U_0 (where E ¡ U_0)
- Region III (x ¿ L): V(x) = 0

why stationary equation can be used?

1.1 Time-Independent Schrödinger Equation

The one-dimensional Schrödinger equation is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{1}$$

Let's solve this for each region:

Region I (x ¡ 0):

$$\frac{d^2\psi_I(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi_I(x) = 0 \tag{2}$$

With $k = \sqrt{\frac{2mE}{\hbar^2}}$, the general solution is:

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx} \tag{3}$$

Where Ae^{ikx} represents the incident wave and Be^{-ikx} the reflected wave.

Region II ($0 \leq$ x $\leq$ L):

$$\frac{d^2\psi_{II}(x)}{dx^2} - \frac{2m(U_0 - E)}{\hbar^2}\psi_{II}(x) = 0 \tag{4}$$

With $\alpha = \sqrt{\frac{2m(U_0-E)}{\hbar^2}}$, the general solution is:

$$\psi_{II}(x) = Ce^{\alpha x} + De^{-\alpha x} \tag{5}$$

These exponential solutions (rather than oscillatory) characterize the evanescent wave inside the barrier.

Region III (x ¿ L):

$$\frac{d^2\psi_{III}(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi_{III}(x) = 0 \tag{6}$$

With the same k as in Region I, the solution is:

$$\psi_{III}(x) = Fe^{ikx} \tag{7}$$

where is solution for -ikx ?

We only include the forward-traveling wave since there's no reflection from the right.

1.2 Continuity Conditions

For a physically valid solution, both the wave function and its first derivative must be continuous at the boundaries.

At x = 0:

$$\psi_I(0) = \psi_{II}(0) \tag{8}$$

$$A + B = C + D \tag{9}$$

$$\psi'_I(0) = \psi'_{II}(0) \tag{10}$$

$$ik(A - B) = \alpha(C - D) \tag{11}$$

At x = L:

$$\psi_{II}(L) = \psi_{III}(L) \tag{12}$$

$$Ce^{\alpha L} + De^{-\alpha L} = Fe^{ikL} \tag{13}$$

$$\psi'_{II}(L) = \psi'_{III}(L) \tag{14}$$

$$\alpha(Ce^{\alpha L} - De^{-\alpha L}) = ikFe^{ikL} \tag{15}$$

1.3 Transmission Coefficient Derivation

To find the transmission probability, we need to solve these four equations for the coefficients and calculate:

$$T = \frac{|F|^2}{|A|^2} \tag{16}$$

From equations (11) and (12), we can express C and D in terms of F:

$$Ce^{\alpha L} + De^{-\alpha L} = Fe^{ikL} \tag{17}$$

$$\alpha(Ce^{\alpha L} - De^{-\alpha L}) = ikFe^{ikL} \tag{18}$$

Multiplying the first equation by α and adding to the second:

$$2\alpha Ce^{\alpha L} = Fe^{ikL}(\alpha + ik) \tag{19}$$

Therefore:

$$C = \frac{Fe^{ikL}(\alpha + ik)}{2\alpha e^{\alpha L}} \tag{20}$$

Similarly, we can find D:

$$D = \frac{Fe^{ikL}(\alpha - ik)}{2\alpha e^{-\alpha L}} \tag{21}$$

Substituting these into equations (9) and (10), and after algebraic manipulation, we get:

$$T = \frac{4k^2\alpha^2}{4k^2\alpha^2 + (k^2 + \alpha^2)^2 \sinh^2(\alpha L)} \tag{22}$$

For thick or high barriers ($\alpha L \gg 1$), this simplifies to:

$$T \approx \frac{16k^2\alpha^2}{(k^2 + \alpha^2)^2} e^{-2\alpha L} \tag{23}$$

This exponential dependence on barrier width L is the hallmark of quantum tunneling and explains why the tunneling probability becomes extremely small for macroscopic objects or thick barriers.

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2 Infinite Potential Well

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

Solution:

Let's examine why the probability current density must be zero inside the walls of an infinite potential well.

2.1 Infinite Potential Well Setup

For an infinite potential well, we have:

- Region 1 (x ¡ 0): V(x) = ∞
- Region 2 (0 $\leq$ x $\leq$ L): V(x) = 0
- Region 3 (x ¿ L): V(x) = ∞

2.2 Wave Function in the Regions

First, let's consider what happens to the wave function in regions 1 and 3 where V = ∞.

The time-independent Schrödinger equation is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{24}$$

In regions 1 and 3 where V = ∞:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \infty \cdot \psi(x) = E\psi(x) \tag{25}$$

This equation can only be satisfied if:

$$\psi(x) = 0 \tag{26}$$

Since any non-zero value multiplied by infinity would be infinite and could not equal the finite energy E.

2.3 Probability Current Density

The probability current density j(x) is defined as:

$$j(x) = \frac{\hbar}{2mi}[\psi^*(x)\frac{d\psi(x)}{dx} - \psi(x)\frac{d\psi^*(x)}{dx}] \tag{27}$$

Or in a simpler form:

$$j(x) = \frac{\hbar}{m}\mathrm{Im}[\psi^*(x)\frac{d\psi(x)}{dx}] \tag{28}$$

Now, in regions 1 and 3, we've established that $\psi(x) = 0$. When we substitute this into the probability current density equation:

$$j(x) = \frac{\hbar}{2mi}[0 \cdot \frac{d\psi(x)}{dx} - 0 \cdot \frac{d\psi^*(x)}{dx}] = 0 \tag{29}$$

Therefore, the probability current density in the regions where V = ∞ is zero.

2.4 Physical Interpretation

This result makes physical sense for several reasons:

1. **No Probability**: Since $\psi(x) = 0$ in the infinite potential regions, the probability density $|\psi(x)|^2 = 0$, meaning there is zero probability of finding the particle in these regions.

2. **No Flow**: The probability current density represents the flow of probability. Since no probability exists in these regions, there can be no flow of probability.
3. **No Tunneling**: Unlike finite barriers where tunneling can occur, infinite barriers completely prevent the particle from entering the forbidden regions.
4. **Conservation of Probability**: Since particles cannot exist within or beyond the infinite barriers, the total probability must be contained within the well, requiring zero current at the boundaries.

In essence, the infinite potential creates an impenetrable boundary for the quantum particle, forcing both the wave function and the probability current to be zero in these regions.

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3 Finite Potential Well

Question: Why zero energy solution (E=0) of equation $\tan\left(a\sqrt{\frac{2mE}{\hbar^2}}\right) = \frac{2\sqrt{E(U_0-E)}}{2E-U_0}$ should be ignored?

Solution:

Let's analyze why the zero energy solution (E=0) of the transcendental equation should be ignored for a finite potential well.

For the E = 0 case:

1. **Left side**: When E = 0, we have $\tan\left(a\sqrt{\frac{2m(0)}{\hbar^2}}\right) = \tan(0) = 0$
2. **Right side**: When E = 0, the numerator becomes $2\sqrt{0 \cdot (U_0 - 0)} = 2\sqrt{0} = 0$

   And the denominator becomes $2(0) - U_0 = -U_0$

   So the right side evaluates to $\frac{0}{-U_0} = 0$

While mathematically both sides equal zero (suggesting E = 0 could be a solution), there are important physical reasons why this solution should be ignored:

1. **Wavefunction behavior**: For E = 0, the wavefunction inside the well would have to be a straight line (constant or linear function), which cannot satisfy both continuity conditions at the boundaries.
2. **Normalization issue**: A particle with exactly zero energy would have an infinite de Broglie wavelength, making proper normalization of the wavefunction impossible within a finite well.
3. **Physical reality**: A particle with E = 0 would have no kinetic energy inside the well and would not exhibit quantum confinement properties.

4. **Mathematical singularity approach**: As E approaches 0, the equation approaches a special case that requires careful limit analysis rather than direct substitution.

5. **Analytical derivation assumption**: The transcendental equation was derived assuming E ¿ 0, as the bound state energies of interest are positive values less than U_0.

The E = 0 case represents a boundary case that falls outside the valid range of the transcendental equation's physical interpretation for bound states. This is why we ignore the E = 0 solution when solving for the energy levels of the finite potential well.

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4 Classical Harmonic Oscillator

Question: Show that for classical harmonic oscillator average value of kinetic and potential energies are equal: $\langle E_k \rangle = \langle E_{pot} \rangle$. PS! The classical expression for calculate average value of classical physical quantity is $\langle A \rangle = \frac{1}{T} \int_0^T A(t)dt$ where T is the averaging time.

Solution:

I'll demonstrate that for a classical harmonic oscillator, the average kinetic energy equals the average potential energy.

4.1 Classical Harmonic Oscillator Properties

For a classical harmonic oscillator:

- Position varies as: $x(t) = A\cos(\omega t + \phi)$ where A is amplitude, ω is angular frequency
- Velocity is: $v(t) = -A\omega \sin(\omega t + \phi)$
- Force is: $F = -kx$
- $\omega = \sqrt{\frac{k}{m}}$ where k is the spring constant and m is mass

4.2 Energies of the Harmonic Oscillator

Kinetic Energy:

$$\begin{aligned} E_k(t) &= \frac{1}{2}mv^2(t) && (30) \\ &= \frac{1}{2}m(-A\omega \sin(\omega t + \phi))^2 && (31) \\ &= \frac{1}{2}mA^2\omega^2 \sin^2(\omega t + \phi) && (32) \end{aligned}$$

Potential Energy:

$$E_p(t) = \frac{1}{2}kx^2(t) \tag{33}$$

$$= \frac{1}{2}kA^2\cos^2(\omega t + \phi) \tag{34}$$

Since $k = m\omega^2$, we can rewrite the potential energy as:

$$E_p(t) = \frac{1}{2}m\omega^2A^2\cos^2(\omega t + \phi) \tag{35}$$

4.3 Time Averages

The classical time average of a physical quantity $A(t)$ is:

$$\langle A \rangle = \frac{1}{T}\int_0^T A(t)dt \tag{36}$$

where T is the period of oscillation. For the harmonic oscillator, $T = \frac{2\pi}{\omega}$.
Average Kinetic Energy

$$\langle E_k \rangle = \frac{1}{T}\int_0^T \frac{1}{2}mA^2\omega^2\sin^2(\omega t + \phi)dt \tag{37}$$

Let's use $\omega t + \phi = u$, so $dt = \frac{du}{\omega}$:

$$\langle E_k \rangle = \frac{1}{T}\int_{\phi}^{\omega T + \phi} \frac{1}{2}mA^2\omega^2\sin^2(u)\frac{du}{\omega} \tag{38}$$

$$= \frac{1}{T}\cdot\frac{1}{2}mA^2\omega\int_{\phi}^{2\pi+\phi}\sin^2(u)du \tag{39}$$

Since the period is $T = \frac{2\pi}{\omega}$:

$$\langle E_k \rangle = \frac{\omega}{2\pi}\cdot\frac{1}{2}mA^2\omega\int_{\phi}^{2\pi+\phi}\sin^2(u)du \tag{40}$$

Using the identity $\sin^2(u) = \frac{1-\cos(2u)}{2}$:

$$\langle E_k \rangle = \frac{\omega}{2\pi}\cdot\frac{1}{2}mA^2\omega\int_{\phi}^{2\pi+\phi}\frac{1-\cos(2u)}{2}du \tag{41}$$

$$= \frac{\omega}{2\pi}\cdot\frac{1}{4}mA^2\omega\left[u - \frac{\sin(2u)}{2}\right]_{\phi}^{2\pi+\phi} \tag{42}$$

Since $\sin(2(\phi + 2\pi)) = \sin(2\phi)$:

$$\langle E_k \rangle = \frac{\omega}{2\pi}\cdot\frac{1}{4}mA^2\omega\cdot 2\pi \tag{43}$$

$$= \frac{1}{4}mA^2\omega^2 \tag{44}$$

Average Potential Energy

$$\langle E_p \rangle = \frac{1}{T}\int_0^T \frac{1}{2}m\omega^2 A^2 \cos^2(\omega t + \phi)dt \tag{45}$$

Following similar steps as above and using $\cos^2(u) = \frac{1+\cos(2u)}{2}$:

$$\begin{aligned}
\langle E_p \rangle &= \frac{\omega}{2\pi}\cdot\frac{1}{2}m\omega^2 A^2 \int_\phi^{2\pi+\phi} \frac{1+\cos(2u)}{2}du \tag{46}\\
&= \frac{\omega}{2\pi}\cdot\frac{1}{4}m\omega^2 A^2 \left[u + \frac{\sin(2u)}{2}\right]_\phi^{2\pi+\phi} \tag{47}\\
&= \frac{\omega}{2\pi}\cdot\frac{1}{4}m\omega^2 A^2 \cdot 2\pi \tag{48}\\
&= \frac{1}{4}m\omega^2 A^2 \tag{49}
\end{aligned}$$

4.4 Comparison of Averages

We've found:

$$\begin{aligned}
\langle E_k \rangle &= \frac{1}{4}mA^2\omega^2 \tag{50}\\
\langle E_p \rangle &= \frac{1}{4}m\omega^2 A^2 \tag{51}
\end{aligned}$$

Therefore:

$$\langle E_k \rangle = \langle E_p \rangle \tag{52}$$

This proves that for a classical harmonic oscillator, the average kinetic energy equals the average potential energy over a complete cycle. This is a manifestation of the virial theorem for this specific potential and demonstrates the equal sharing of energy between kinetic and potential forms in simple harmonic motion.

20 5 Heat Capacity for 1D Chain of Atoms

Question: Potential energy of interacting nearby atoms in a 1d crystal is looks like: $V = \frac{1}{2}g\sum_n(u_n - u_{n-1})^2$. Get the expression for force acting on atom with number k+1. Here u_n - displacement of atom with number n from its equilibrium position.

Solution:

I'll derive the expression for the force acting on atom k+1 in a one-dimensional chain where atoms interact with their nearest neighbors through a harmonic potential.

5.1 Starting with the Potential Energy

The potential energy of the 1D crystal is given by:

$$V = \frac{1}{2} g \sum_n (u_n - u_{n-1})^2 \tag{53}$$

Where:

- u_n is the displacement of atom n from its equilibrium position
- g is the spring constant
- The sum runs over all atoms in the chain

5.2 Force Calculation

The force on an atom is the negative gradient of the potential energy with respect to the atom's displacement:

$$F_{k+1} = -\frac{\partial V}{\partial u_{k+1}} \tag{54}$$

Let's expand the potential energy sum and identify all terms that contain u_{k+1}:

$$V = \frac{1}{2} g \sum_n (u_n - u_{n-1})^2 \tag{55}$$

The terms in this sum that involve u_{k+1} are:

1. The term where n = k+1: $(u_{k+1} - u_k)^2$
2. The term where n = k+2: $(u_{k+2} - u_{k+1})^2$

Let's calculate the derivative with respect to u_{k+1} for each of these terms:
For the first term (n = k+1):

$$\frac{\partial}{\partial u_{k+1}} (u_{k+1} - u_k)^2 = 2(u_{k+1} - u_k) \tag{56}$$

For the second term (n = k+2):

$$\frac{\partial}{\partial u_{k+1}} (u_{k+2} - u_{k+1})^2 = -2(u_{k+2} - u_{k+1}) \tag{57}$$

Now we can calculate the force:

$$\begin{align} F_{k+1} &= -\frac{\partial V}{\partial u_{k+1}} \tag{58} \\ &= -\frac{1}{2} g \left[2(u_{k+1} - u_k) - 2(u_{k+2} - u_{k+1})\right] \tag{59} \end{align}$$

Simplifying:

$$F_{k+1} = -g(u_{k+1} - u_k) + g(u_{k+2} - u_{k+1}) \tag{60}$$
$$= g(u_{k+2} - 2u_{k+1} + u_k) \tag{61}$$

This is the force acting on atom k+1. It depends on the displacement of atom k+1 as well as its nearest neighbors k and k+2.

This result makes physical sense: if atom k+1 is exactly halfway between atoms k and k+2, the force is zero. If it's closer to one of its neighbors, it experiences a restoring force proportional to the displacement difference, in accordance with Hooke's law.