

# UPSC PHYSICS PYQ SOLUTION

## Quantum Mechanics - Part 5

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**41 A beam of particles of energy 9 eV is incident on a potential step 8 eV high from the left. What percentage of particles will reflect back?**

**Introduction:**

In quantum mechanics, the reflection and transmission of particles at a potential step is a fundamental problem. When a particle encounters a potential step, part of the wave function is reflected, and part is transmitted. The reflection coefficient ( $R$ ) gives the probability of the particle being reflected.

**Solution:**

The energy of the incident particles is  $E = 9 \text{ eV}$ , and the height of the potential step is  $V_0 = 8 \text{ eV}$ . The reflection coefficient ( $R$ ) is given by:

$$R = \left( \frac{k_1 - k_2}{k_1 + k_2} \right)^2$$

where  $k_1$  and  $k_2$  are the wave numbers of the particle in the regions before and after the potential step, respectively.

The wave number  $k$  is related to the energy  $E$  and the potential  $V$  by:

$$k = \sqrt{\frac{2m(E - V)}{\hbar^2}}$$

For the region before the potential step ( $E = 9 \text{ eV}$  and  $V = 0 \text{ eV}$ ):

$$k_1 = \sqrt{\frac{2m(9 \text{ eV})}{\hbar^2}}$$

For the region after the potential step ( $E = 9 \text{ eV}$  and  $V = 8 \text{ eV}$ ):

$$k_2 = \sqrt{\frac{2m(9 \text{ eV} - 8 \text{ eV})}{\hbar^2}} = \sqrt{\frac{2m(1 \text{ eV})}{\hbar^2}}$$

The ratio of the wave numbers is:

$$\frac{k_1}{k_2} = \frac{\sqrt{9 \text{ eV}}}{\sqrt{1 \text{ eV}}} = 3$$

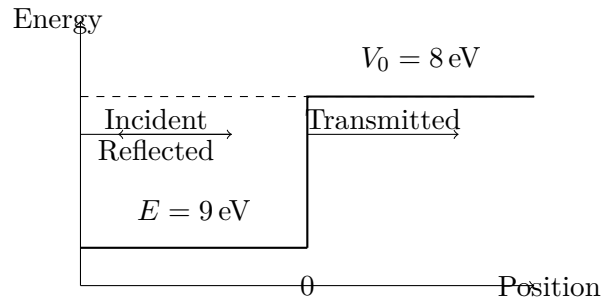
Substituting into the reflection coefficient formula:

$$R = \left( \frac{3 - 1}{3 + 1} \right)^2 = \left( \frac{2}{4} \right)^2 = \left( \frac{1}{2} \right)^2 = 0.25$$

Therefore, the reflection percentage is:

$$R \times 100\% = 0.25 \times 100\% = 25\%$$

The following diagram illustrates the potential step and the wave function behavior:



### Conclusion:

The reflection coefficient indicates that 25% of the particles will reflect back when a beam of particles with energy 9 eV encounters a potential step of 8 eV. This result highlights the wave nature of particles, where partial reflection and transmission occur due to quantum mechanical effects.

### Applications:

1. **Tunneling in Semiconductors:** Quantum tunneling is crucial in the operation of semiconductor devices such as diodes and transistors.
2. **Scanning Tunneling Microscopy (STM):** STM relies on the quantum tunneling of electrons to image surfaces at the atomic level.
3. **Nuclear Fusion:** Quantum tunneling allows particles to overcome the Coulomb barrier, facilitating nuclear reactions in stars and experimental fusion reactors.

## 42 Estimate the size of hydrogen atom and the ground state energy from the uncertainty principle.

**Introduction:** The problem requires an estimation of the characteristic size (Bohr radius) and ground state energy of a hydrogen atom using the Heisenberg uncertainty principle. The hydrogen atom consists of an electron bound to a proton via Coulomb attraction. We aim to estimate:

- The approximate radius  $r$  of the hydrogen atom,
- The ground state energy  $E$  of the electron.

We assume a non-relativistic quantum mechanical model and apply the uncertainty relation  $\Delta x \Delta p \sim \hbar$ .

**Solution:**

Let the electron be confined within a region of size  $r$ , so the uncertainty in position is  $\Delta x \sim r$ . Then the uncertainty in momentum is:

$\Delta p \sim \frac{\hbar}{r}$  order of magnitude is satisfied even when we don't take 1/2 as a factor

The kinetic energy of the electron can be approximated using:

$$T \sim \frac{(\Delta p)^2}{2m} = \frac{\hbar^2}{2mr^2},$$

where  $m$  is the mass of the electron.

The potential energy due to Coulomb attraction between the proton and the electron is:

$$V \sim -\frac{e^2}{4\pi\epsilon_0 r},$$

where  $e$  is the elementary charge and  $\epsilon_0$  is the vacuum permittivity.

The total energy of the electron is approximately:

$$E(r) = T + V \sim \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\epsilon_0 r}.$$

To find the equilibrium (ground state), we minimize  $E(r)$  with respect to  $r$ :

$$\frac{dE}{dr} = -\frac{\hbar^2}{mr^3} + \frac{e^2}{4\pi\epsilon_0 r^2} = 0.$$

The second derivative greater than 0, confirms a minimum.

Solving for  $r$ :

$$\frac{\hbar^2}{mr^3} = \frac{e^2}{4\pi\epsilon_0 r^2} \Rightarrow r = \frac{4\pi\epsilon_0 \hbar^2}{me^2}.$$

This is the Bohr radius:

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{me^2} \approx 5.29 \times 10^{-11} \text{ m}.$$

Substitute  $r = a_0$  into the expression for energy:

$$E = \frac{\hbar^2}{2ma_0^2} - \frac{e^2}{4\pi\epsilon_0 a_0}.$$

This gives the ground state energy:

$$E_0 = -13.6 \text{ eV}.$$

**Conclusion:** By applying the uncertainty principle, we estimate the size of the hydrogen atom to be approximately  $a_0 = 5.29 \times 10^{-11} \text{ m}$ , known as the Bohr radius. The ground state energy is approximately  $E_0 = -13.6 \text{ eV}$ , consistent with experimental results and Bohr's model.

A/P

**43 Write down the Hamiltonian operator for a linear harmonic oscillator. Show that the energy eigenvalue of the same can be given by  $E_n = (n + \frac{1}{2}) \hbar \omega_0$  at energy state  $n$  with  $\omega_0$  being the natural frequency of vibration of the linear oscillator. Prove that  $n = 0$  energy state has a wave function of typical Gaussian form.**

**Introduction:** The problem involves analyzing the quantum harmonic oscillator. We are asked to:

- Write the Hamiltonian operator for a linear harmonic oscillator.
- Derive the energy eigenvalues, demonstrating the quantized form  $E_n = (n + \frac{1}{2}) \hbar \omega_0$ .
- Show that the ground state wavefunction ( $n = 0$ ) has a Gaussian form.

Assumptions include a one-dimensional oscillator and standard canonical quantization with position operator  $\hat{x}$  and momentum operator  $\hat{p}$  satisfying  $[\hat{x}, \hat{p}] = i\hbar$ .

**Solution:**

The Hamiltonian for a one-dimensional quantum harmonic oscillator is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2.$$

This represents the total energy of the system the sum of kinetic and potential energies in quantum mechanical form.

To simplify the problem and reveal its underlying algebraic structure, we introduce ladder (creation and annihilation) operators:

$$\begin{aligned}\hat{a} &= \sqrt{\frac{m\omega_0}{2\hbar}} \left( \hat{x} + \frac{i}{m\omega_0} \hat{p} \right), \\ \hat{a}^\dagger &= \sqrt{\frac{m\omega_0}{2\hbar}} \left( \hat{x} - \frac{i}{m\omega_0} \hat{p} \right).\end{aligned}$$

These satisfy the commutation relation:

$$[\hat{a}, \hat{a}^\dagger] = 1.$$

Ladder operators provide an elegant way to analyze the harmonic oscillator because they allow us to raise or lower the energy levels of the system in discrete steps, corresponding to the quantized nature of energy in quantum mechanics.

In terms of these operators, the Hamiltonian becomes:

$$\hat{H} = \hbar\omega_0 \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right).$$

The number operator is defined as  $\hat{n} = \hat{a}^\dagger \hat{a}$ , and its eigenstates  $|n\rangle$  satisfy:

$$\hat{n} |n\rangle = n |n\rangle, \quad n = 0, 1, 2, \dots$$

Hence, the energy eigenvalues are:

$$E_n = \hbar\omega_0 \left( n + \frac{1}{2} \right).$$

This result shows that the energy levels are quantized and equally spaced, with a minimum energy of  $\frac{1}{2}\hbar\omega_0$ , known as the zero-point energy. This non-zero minimum energy reflects the Heisenberg uncertainty principle: even in the ground state, the particle cannot have both definite position and momentum.

Now consider the ground state  $|0\rangle$ , which satisfies:

$$\hat{a}|0\rangle = 0.$$

Using the coordinate representation, we have:

$$\begin{aligned}\hat{x} &= x, \\ \hat{p} &= -i\hbar \frac{d}{dx}.\end{aligned}$$

Thus the annihilation operator becomes:

$$\hat{a} = \sqrt{\frac{m\omega_0}{2\hbar}} \left( x + \frac{\hbar}{m\omega_0} \frac{d}{dx} \right).$$

Apply  $\hat{a}$  to the ground state wavefunction  $\psi_0(x)$ :

$$\hat{a}\psi_0(x) = 0 \quad \Rightarrow \quad \left( x + \frac{\hbar}{m\omega_0} \frac{d}{dx} \right) \psi_0(x) = 0.$$

Solving this differential equation:

$$\frac{d\psi_0}{dx} = -\frac{m\omega_0}{\hbar} x \psi_0(x).$$

This is a separable differential equation. Integrating both sides:

$$\begin{aligned}\int \frac{1}{\psi_0} d\psi_0 &= -\frac{m\omega_0}{\hbar} \int x dx, \\ \ln \psi_0 &= -\frac{m\omega_0}{2\hbar} x^2 + C, \\ \psi_0(x) &= A e^{-\frac{m\omega_0}{2\hbar} x^2},\end{aligned}$$

where  $A = e^C$  is the normalization constant.

To normalize, we impose:

$$\int_{-\infty}^{\infty} |\psi_0(x)|^2 dx = 1 \Rightarrow A = \left( \frac{m\omega_0}{\pi\hbar} \right)^{1/4}.$$

**Conclusion:** The Hamiltonian operator for a linear harmonic oscillator is  $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2$ . Its energy eigenvalues are quantized as  $E_n = \left( n + \frac{1}{2} \right) \hbar\omega_0$ , reflecting the discrete and equally spaced energy levels characteristic of quantum oscillators. The ground state ( $n = 0$ ) wavefunction is of Gaussian form:

$$\psi_0(x) = \left( \frac{m\omega_0}{\pi\hbar} \right)^{1/4} e^{-\frac{m\omega_0}{2\hbar} x^2}.$$

This confirms both the quantized energy spectrum and the Gaussian nature of the ground state in quantum harmonic oscillators. Moreover, excited states can be generated by applying the creation operator repeatedly on the ground state.

## 44 Prove that Bohr hydrogen atom approaches classical conditions, when $n$ becomes very large and small quantum jumps are involved.

### Introduction:

The correspondence principle, formulated by Niels Bohr, states that the behavior of systems described by quantum mechanics replicates classical physics in the limit of large quantum numbers. For the Bohr model of the hydrogen atom, this principle can be demonstrated by showing that the energy levels become closely spaced and the frequency of radiation approaches the classical orbital frequency as  $n$  becomes very large.

### Solution:

#### 1. Energy Levels in Bohr Model:

The energy levels of a hydrogen atom in the Bohr model are given by:

$$E_n = -\frac{13.6 \text{ eV}}{n^2}$$

where  $n$  is the principal quantum number.

#### 2. Frequency of Radiation:

When an electron transitions from a higher energy level  $n_i$  to a lower energy level  $n_f$ , the frequency of the emitted photon is:

$$f = \frac{E_i - E_f}{h}$$

Substituting the energy levels:

$$f = \frac{-\frac{13.6 \text{ eV}}{n_i^2} + \frac{13.6 \text{ eV}}{n_f^2}}{h}$$

Let  $n_i = n$  and  $n_f = n - \Delta n$  where  $\Delta n$  is small compared to  $n$ . Then,

$$f = \frac{13.6 \text{ eV}}{h} \left( \frac{1}{(n - \Delta n)^2} - \frac{1}{n^2} \right)$$

For large  $n$  and small  $\Delta n$ , we can use the binomial approximation:

$$(n - \Delta n)^2 \approx n^2 - 2n\Delta n$$

So,

$$\frac{1}{(n - \Delta n)^2} \approx \frac{1}{n^2} \left( 1 + \frac{2\Delta n}{n} \right)$$

Therefore,

$$f \approx \frac{13.6 \text{ eV}}{h} \left( \frac{1}{n^2} - \frac{1}{n^2} \left( 1 + \frac{2\Delta n}{n} \right) \right) = \frac{13.6 \text{ eV}}{h} \frac{2\Delta n}{n^3}$$



### 3. Classical Orbital Frequency:

The classical orbital frequency  $f_{\text{classical}}$  of an electron in the  $n$ th orbit is given by:

$$f_{\text{classical}} = \frac{\omega}{2\pi} = \frac{v}{2\pi r}$$

Using Bohr's model,  $v = \frac{e^2}{2\epsilon_0 h} \frac{1}{n}$  and  $r = \frac{4\pi\epsilon_0 h^2 n^2}{e^2 m}$ , we get:

$$f_{\text{classical}} = \frac{\left(\frac{e^2}{2\epsilon_0 h} \frac{1}{n}\right)}{2\pi \left(\frac{4\pi\epsilon_0 h^2 n^2}{e^2 m}\right)} = \frac{e^4 m}{16\pi^3 \epsilon_0^2 h^3} \frac{1}{n^3}$$

### 4. Comparison and Conclusion:

For large  $n$ ,

$$f \approx \frac{13.6 \text{ eV}}{h} \frac{2\Delta n}{n^3} = f_{\text{classical}} \Delta n$$

Thus, the frequency of the radiation approaches the classical orbital frequency when the quantum number  $n$  is very large, confirming Bohr's correspondence principle.

#### Conclusion:

As the quantum number  $n$  becomes very large, the energy levels of the Bohr hydrogen atom become closely spaced, and the frequency of emitted radiation for small quantum jumps approaches the classical orbital frequency. This demonstrates that the Bohr model converges to classical physics in the limit of large quantum numbers, highlighting the correspondence principle. Practical applications include understanding atomic spectra and transitions in high-energy physics and astrophysics.

**45 Find the probability current density for the wave function  $\Psi(x, t) = [Ae^{ipx/\hbar} + Be^{-ipx/\hbar}] e^{-ip^2t/2m\hbar}$ . Interpret the result physically.**

**Introduction:**

In quantum mechanics, the probability current density  $\mathbf{j}(x, t)$  represents the flow of probability associated with the wave function  $\Psi(x, t)$ . It is defined as:

$$\mathbf{j}(x, t) = \frac{\hbar}{2mi} \left( \Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right)$$

where  $\Psi^*$  is the complex conjugate of  $\Psi$ .

**Solution:**

Given the wave function:

$$\Psi(x, t) = [Ae^{ipx/\hbar} + Be^{-ipx/\hbar}] e^{-ip^2t/2m\hbar}$$

First, find the partial derivatives of  $\Psi$  and  $\Psi^*$  with respect to  $x$ .

**1. Partial Derivative of  $\Psi$  with Respect to  $x$ :**

$$\frac{\partial \Psi}{\partial x} = \frac{\partial}{\partial x} [ (Ae^{ipx/\hbar} + Be^{-ipx/\hbar}) e^{-ip^2t/2m\hbar} ]$$

Since  $e^{-ip^2t/2m\hbar}$  is a constant with respect to  $x$ :

$$\begin{aligned} \frac{\partial \Psi}{\partial x} &= e^{-ip^2t/2m\hbar} \left[ \frac{\partial}{\partial x} (Ae^{ipx/\hbar} + Be^{-ipx/\hbar}) \right] \\ &= e^{-ip^2t/2m\hbar} \left[ \frac{ip}{\hbar} Ae^{ipx/\hbar} - \frac{ip}{\hbar} Be^{-ipx/\hbar} \right] \\ &= \frac{ip}{\hbar} e^{-ip^2t/2m\hbar} [Ae^{ipx/\hbar} - Be^{-ipx/\hbar}] \end{aligned}$$

**2. Partial Derivative of  $\Psi^*$  with Respect to  $x$ :**

The complex conjugate of  $\Psi(x, t)$  is:

$$\Psi^*(x, t) = [A^*e^{-ipx/\hbar} + B^*e^{ipx/\hbar}] e^{ip^2t/2m\hbar}$$

$$\begin{aligned} \frac{\partial \Psi^*}{\partial x} &= e^{ip^2t/2m\hbar} \left[ \frac{\partial}{\partial x} (A^*e^{-ipx/\hbar} + B^*e^{ipx/\hbar}) \right] \\ &= e^{ip^2t/2m\hbar} \left[ -\frac{ip}{\hbar} A^*e^{-ipx/\hbar} + \frac{ip}{\hbar} B^*e^{ipx/\hbar} \right] \\ &= \frac{ip}{\hbar} e^{ip^2t/2m\hbar} [-A^*e^{-ipx/\hbar} + B^*e^{ipx/\hbar}] \end{aligned}$$

### 3. Probability Current Density:

Using the definition of  $\mathbf{j}(x, t)$ :

$$\mathbf{j}(x, t) = \frac{\hbar}{2mi} \left( \Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right)$$

Substitute  $\Psi$ ,  $\Psi^*$ , and their derivatives:

$$\begin{aligned} \Psi^* \frac{\partial \Psi}{\partial x} &= \left[ A^* e^{-ipx/\hbar} + B^* e^{ipx/\hbar} \right] e^{ip^2 t/2m\hbar} \cdot \frac{ip}{\hbar} e^{-ip^2 t/2m\hbar} \left[ A e^{ipx/\hbar} - B e^{-ipx/\hbar} \right] \\ &= \frac{ip}{\hbar} \left[ A^* e^{-ipx/\hbar} A e^{ipx/\hbar} - A^* e^{-ipx/\hbar} B e^{-ipx/\hbar} + B^* e^{ipx/\hbar} A e^{ipx/\hbar} - B^* e^{ipx/\hbar} B e^{-ipx/\hbar} \right] \\ &= \frac{ip}{\hbar} \left[ A^* A - A^* B e^{-2ipx/\hbar} + B^* A e^{2ipx/\hbar} - B^* B \right] \end{aligned}$$

Similarly,

$$\begin{aligned} \Psi \frac{\partial \Psi^*}{\partial x} &= \left[ A e^{ipx/\hbar} + B e^{-ipx/\hbar} \right] e^{-ip^2 t/2m\hbar} \cdot \frac{ip}{\hbar} e^{ip^2 t/2m\hbar} \left[ -A^* e^{-ipx/\hbar} + B^* e^{ipx/\hbar} \right] \\ &= \frac{ip}{\hbar} \left[ A e^{ipx/\hbar} (-A^* e^{-ipx/\hbar}) + A e^{ipx/\hbar} B^* e^{ipx/\hbar} + B e^{-ipx/\hbar} (-A^* e^{-ipx/\hbar}) + B e^{-ipx/\hbar} B^* e^{ipx/\hbar} \right] \\ &= \frac{ip}{\hbar} \left[ -AA^* + AB^* e^{2ipx/\hbar} - BA^* e^{-2ipx/\hbar} + BB^* \right] \end{aligned}$$

Therefore, the probability current density is:

$$\begin{aligned} \mathbf{j}(x, t) &= \frac{\hbar}{2mi} \left[ \frac{ip}{\hbar} \left( A^* A - A^* B e^{-2ipx/\hbar} + B^* A e^{2ipx/\hbar} - B^* B \right) - \frac{ip}{\hbar} \left( -AA^* + AB^* e^{2ipx/\hbar} - BA^* e^{-2ipx/\hbar} + BB^* \right) \right] \\ &= \frac{\hbar}{2mi} \cdot \frac{2ip}{\hbar} (A^* A - B^* B) \\ \mathbf{j}(x, t) &= \frac{p}{m} (A^* A - B^* B) \end{aligned}$$

### Conclusion:

The probability current density for the given wave function is:

$$\mathbf{j}(x, t) = \frac{p}{m} (A^* A - B^* B)$$

**Interpretation:**

This result indicates that the probability current density depends on the coefficients  $A$  and  $B$ . If  $|A|^2 = |B|^2$ , the probability current density  $\mathbf{j}(x, t)$  is zero, implying no net flow of probability. If  $|A|^2 \neq |B|^2$ , there is a net flow of probability in the direction of the momentum  $p$ .

This reflects the physical interpretation that the probability current density represents the flow of probability for a particle described by the wave function  $\Psi(x, t)$ . The terms  $|A|^2$  and  $|B|^2$  represent the probabilities of the particle moving in positive and negative directions, respectively. The difference between these probabilities determines the net flow of probability in the system.

A/P

**46** A particle is described by the wave function  $\Psi(x) = \left(\frac{\pi}{2}\right)^{-1/4} e^{-ax^2/2}$ . Calculate  $\Delta x$  and  $\Delta p$  for the particle, and verify the uncertainty relation  $\Delta x \Delta p = \frac{\hbar}{2}$ .

**Introduction:** The given wave function is a Gaussian:

$$\Psi(x) = \left(\frac{\pi}{2}\right)^{-1/4} e^{-ax^2/2},$$

where  $a > 0$  is a real constant. We are asked to find the uncertainties  $\Delta x$  and  $\Delta p$  and verify the Heisenberg uncertainty relation:

$$\Delta x \Delta p \geq \frac{\hbar}{2}.$$

To compute uncertainties, we need:

1.  $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ ,
2.  $\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$ ,

where  $\langle x \rangle$  and  $\langle p \rangle$  are expectation values of position and momentum, respectively.

**Solution:**

**1. Expectation values:**

Since  $\Psi(x)$  is an even function and complete integrand is odd function:

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\Psi(x)|^2 dx = 0.$$

For momentum, we use  $\hat{p} = -i\hbar \frac{d}{dx}$ :

$$\langle p \rangle = \int_{-\infty}^{\infty} \Psi^*(x) \left( -i\hbar \frac{d}{dx} \right) \Psi(x) dx.$$

Since  $\frac{d\Psi}{dx} = -ax\Psi(x)$ :

$$\langle p \rangle = \int_{-\infty}^{\infty} \Psi^*(x) (-i\hbar) (-ax) \Psi(x) dx = i\hbar a \int_{-\infty}^{\infty} x |\Psi(x)|^2 dx = 0,$$

because the integrand is odd.

**2. Compute  $\langle x^2 \rangle$ :**

$$|\Psi(x)|^2 = \left(\frac{\pi}{2}\right)^{-1/2} e^{-ax^2}.$$

Then,

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\Psi(x)|^2 dx = \left(\frac{\pi}{2}\right)^{-1/2} \int_{-\infty}^{\infty} x^2 e^{-ax^2} dx.$$

Using the standard integral:

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{\sqrt{\pi}}{2a^{3/2}},$$

we get:

$$\langle x^2 \rangle = \left(\frac{\pi}{2}\right)^{-1/2} \cdot \frac{\sqrt{\pi}}{2a^{3/2}} = \frac{1}{2a}.$$

Thus,

$$\Delta x = \sqrt{\langle x^2 \rangle} = \sqrt{\frac{1}{2a}} = \frac{1}{\sqrt{2a}}.$$

### 3. Compute $\langle p^2 \rangle$ :

We calculate  $\langle p^2 \rangle = \langle -\hbar^2 \frac{d^2}{dx^2} \rangle$ :

First, compute derivatives:

$$\frac{d\Psi}{dx} = -ax\Psi(x), \quad \frac{d^2\Psi}{dx^2} = -a\Psi(x) - ax(-ax)\Psi(x) = (-a + a^2x^2)\Psi(x).$$

So:

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} \Psi^*(x) \left( -\hbar^2 \frac{d^2}{dx^2} \right) \Psi(x) dx = -\hbar^2 \int_{-\infty}^{\infty} |\Psi(x)|^2 (-a + a^2x^2) dx.$$

$$\langle p^2 \rangle = \hbar^2 \int_{-\infty}^{\infty} |\Psi(x)|^2 (a - a^2x^2) dx = \hbar^2 \left( a \int_{-\infty}^{\infty} |\Psi(x)|^2 dx - a^2 \int_{-\infty}^{\infty} x^2 |\Psi(x)|^2 dx \right).$$

Using  $\int |\Psi(x)|^2 dx = 1$  and  $\langle x^2 \rangle = \frac{1}{2a}$ :

$$\langle p^2 \rangle = \hbar^2 \left( a - a^2 \cdot \frac{1}{2a} \right) = \hbar^2 \left( a - \frac{a}{2} \right) = \frac{a\hbar^2}{2}.$$

Therefore:

$$\Delta p = \sqrt{\frac{a\hbar^2}{2}} = \frac{\hbar\sqrt{a}}{\sqrt{2}}.$$

### 4. Uncertainty product:

$$\Delta x \Delta p = \frac{1}{\sqrt{2a}} \cdot \frac{\hbar\sqrt{a}}{\sqrt{2}} = \frac{\hbar\sqrt{a}}{\sqrt{2a} \cdot \sqrt{2}} = \frac{\hbar\sqrt{a}}{2\sqrt{a}} = \frac{\hbar}{2}.$$

**Conclusion:** The uncertainties in position and momentum are:

$$\Delta x = \frac{1}{\sqrt{2a}}, \quad \Delta p = \frac{\hbar\sqrt{a}}{\sqrt{2}},$$

and their product satisfies the Heisenberg uncertainty principle exactly:

$$\Delta x \Delta p = \frac{\hbar}{2}.$$

This confirms the wave function is a minimum uncertainty Gaussian state.

**47** A beam of 12eV electron is incident on a potential barrier of height 25eV and width 0.05 nm. Calculate the transmission coefficient.

**Solution:**

Given:

- Electron energy,  $E = 12 \text{ eV}$
- Barrier height,  $V_0 = 25 \text{ eV}$
- Barrier width,  $a = 0.05 \text{ nm} = 5 \times 10^{-11} \text{ m}$

For a rectangular barrier with  $E < V_0$ , the transmission coefficient is:

$$T = \left[ 1 + \frac{V_0^2 \sinh^2(\kappa a)}{4E(V_0 - E)} \right]^{-1}$$

where

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

Constants:

$$m = 9.11 \times 10^{-31} \text{ kg}, \quad \hbar = 1.055 \times 10^{-34} \text{ Js}, \quad 1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$$

Compute:

$$\kappa = \frac{\sqrt{2 \cdot 9.11 \times 10^{-31} \cdot 13 \cdot 1.602 \times 10^{-19}}}{1.055 \times 10^{-34}} = \frac{\sqrt{3.785 \times 10^{-48}}}{1.055 \times 10^{-34}} \approx \frac{6.15 \times 10^{-24}}{1.055 \times 10^{-34}} \approx 5.83 \times 10^{10} \text{ m}^{-1}$$

Now:

$$\kappa a = 5.83 \times 10^{10} \cdot 5 \times 10^{-11} = 2.915$$

$$\sinh(\kappa a) \approx \sinh(2.915) \approx 9.18$$

Now plug into the full expression:

$$T = \left[ 1 + \frac{(25)^2 \cdot (9.18)^2}{4 \cdot 12 \cdot 13} \right]^{-1} = \left[ 1 + \frac{625 \cdot 84.29}{624} \right]^{-1} = \left[ 1 + \frac{52681.25}{624} \right]^{-1} \approx [1 + 84.42]^{-1}$$

$$T \approx \frac{1}{85.42} \approx 0.0117$$

**Answer:** The transmission coefficient is approximately  $\boxed{0.012}$ , meaning there is about a 1.2% probability of the electron tunneling through the barrier.

48 Solve the Schrödinger equation for a step potential and calculate the transmission and reflection coefficients for the case when the kinetic energy of the particle  $E_0$  is greater than the potential energy  $V$  (i.e.,  $E_0 > V$ ).

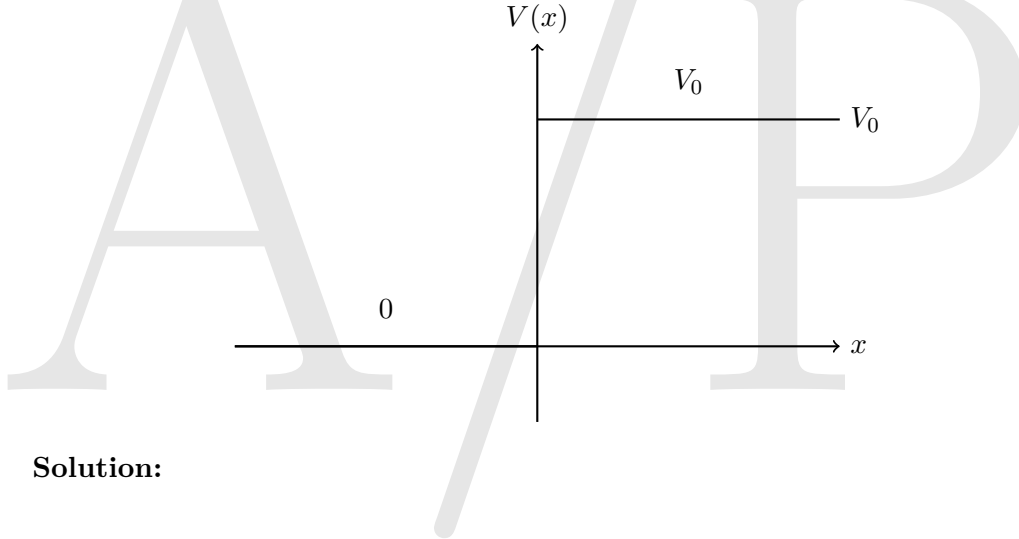
**Introduction:**

The step potential is a fundamental problem in quantum mechanics that illustrates the behavior of a particle encountering a sudden change in potential energy. This problem is essential for understanding phenomena such as quantum tunneling and reflection.

Consider a particle encountering a step potential:

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x \geq 0 \end{cases}$$

Below is a diagram illustrating the step potential:



**Solution:**

Consider a particle encountering a step potential:

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x \geq 0 \end{cases}$$

The Schrödinger equation in regions where  $V(x)$  is constant is:

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

For  $x < 0$  (Region I), where  $V(x) = 0$ :

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E_0\psi(x)$$

The general solution is:

$$\psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x}$$



where:

$$k_1 = \sqrt{\frac{2mE_0}{\hbar^2}}$$

For  $x \geq 0$  (Region II), where  $V(x) = V_0$ :

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V_0\psi(x) = E_0\psi(x)$$

This simplifies to:

$$\frac{d^2\psi(x)}{dx^2} = k_2^2\psi(x)$$

where:

$$k_2 = \sqrt{\frac{2m(E_0 - V_0)}{\hbar^2}}$$

The general solution is:

$$\psi_{II}(x) = Ce^{ik_2x}$$

Since we consider the particle coming from the left and moving to the right, there will be no wave traveling to the left in Region II ( $D = 0$ ):

$$\psi_{II}(x) = Ce^{ik_2x}$$

### Boundary Conditions:

At  $x = 0$ , the wavefunctions and their first derivatives must be continuous:

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

$$\left. \frac{d\psi_I}{dx} \right|_{x=0} = \left. \frac{d\psi_{II}}{dx} \right|_{x=0}$$

Applying these conditions:

1. Continuity of wavefunction:

$$A + B = C$$

2. Continuity of derivative:

$$ik_1A - ik_1B = ik_2C$$

Solving these equations for  $A$ ,  $B$ , and  $C$ :

From the first equation:

$$C = A + B$$

Substituting into the second equation:

$$ik_1A - ik_1B = ik_2(A + B)$$

Rearranging:

$$k_1A - k_1B = k_2A + k_2B$$

$$(k_1 - k_2)A = (k_1 + k_2)B$$

$$\frac{A}{B} = \frac{k_1 + k_2}{k_1 - k_2}$$

Therefore, the reflection coefficient  $R$  is:

$$R = \left| \frac{B}{A} \right|^2 = \left| \frac{k_1 - k_2}{k_1 + k_2} \right|^2$$

To correctly compute the transmission coefficient  $T$ , we must account for the difference in group velocities across regions. This gives:

$$T = \frac{k_2}{k_1} \left| \frac{C}{A} \right|^2 = \frac{4k_1 k_2}{(k_1 + k_2)^2}$$

**Conclusion:**

For a particle encountering a step potential with  $E_0 > V_0$ , the reflection and transmission coefficients are:

$$R = \left| \frac{k_1 - k_2}{k_1 + k_2} \right|^2, \quad T = \frac{4k_1 k_2}{(k_1 + k_2)^2}$$

These coefficients describe the probability of the particle being reflected or transmitted at the potential step and obey the conservation law  $R + T = 1$ .

**49 Write the wave functions for a particle on both sides of a step potential, for  $E > V_0$ :**

$$V(x) = \begin{cases} V_0, & x > 0 \\ 0, & x < 0 \end{cases}$$

**Interpret the results physically.**

**Introduction:** This problem involves a quantum particle encountering a 1D step potential. The potential energy function is piecewise constant, and the total energy of the particle satisfies  $E > V_0$ . Our goal is to determine the wavefunctions in both regions and interpret the behavior of the particle, including any reflection or transmission effects due to the step.

**Solution:**

The time-independent Schrödinger equation is given by:

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

We solve this separately in regions I ( $x < 0$ ) and II ( $x > 0$ ).

**Region I:**  $x < 0$  (where  $V(x) = 0$ )

The Schrödinger equation becomes:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi,$$

which simplifies to:

$$\frac{d^2\psi}{dx^2} + k_1^2\psi = 0, \quad \text{where } k_1 = \frac{\sqrt{2mE}}{\hbar}.$$

General solution:

$$\psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x}.$$

Here,  $Ae^{ik_1x}$  represents the incident wave, and  $Be^{-ik_1x}$  is the reflected wave.

**Region II:**  $x > 0$  (where  $V(x) = V_0$ )

The Schrödinger equation becomes:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V_0\psi = E\psi \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} + k_2^2\psi = 0,$$

where

$$k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}.$$

General solution:

$$\psi_{II}(x) = Ce^{ik_2x}.$$

We exclude the term  $De^{-ik_2x}$  because it would represent a wave incoming from  $x \rightarrow \infty$ , which contradicts the physical setup of a wave incident from the left.

**Boundary Conditions:**

Continuity of the wavefunction and its derivative at  $x = 0$ :

$$\begin{aligned}\psi_I(0) &= \psi_{II}(0) \Rightarrow A + B = C, \\ \psi'_I(0) &= \psi'_{II}(0) \Rightarrow ik_1(A - B) = ik_2C.\end{aligned}$$

Solving this system:

$$\begin{aligned}A + B &= C \\ k_1(A - B) &= k_2(A + B)\end{aligned}$$

Solving for  $B/A$  and  $C/A$ :

$$\begin{aligned}\frac{B}{A} &= \frac{k_1 - k_2}{k_1 + k_2}, \\ \frac{C}{A} &= \frac{2k_1}{k_1 + k_2}.\end{aligned}$$

**Interpretation:**

Even though the energy  $E > V_0$ , the particle has a finite probability of being reflected. The reflection coefficient  $R$  and transmission coefficient  $T$  are given by:

$$\begin{aligned}R &= \left| \frac{B}{A} \right|^2 = \left( \frac{k_1 - k_2}{k_1 + k_2} \right)^2, \\ T &= \frac{k_2}{k_1} \left| \frac{C}{A} \right|^2 = \frac{4k_1k_2}{(k_1 + k_2)^2}.\end{aligned}$$

Note that  $R + T = 1$ , as required by probability conservation.

Physically, even when the particle has enough energy to surpass the potential step, there is a non-zero probability of reflection due to the abrupt change in potential, a purely quantum mechanical phenomenon with no classical analog.

**Conclusion:** The wavefunctions in each region are:

$$\begin{aligned}\psi_I(x) &= Ae^{ik_1x} + Be^{-ik_1x}, \quad x < 0, \\ \psi_{II}(x) &= Ce^{ik_2x}, \quad x > 0.\end{aligned}$$

Despite having energy  $E > V_0$ , the particle experiences partial reflection and transmission due to the discontinuity in potential. This highlights the wave nature of particles in quantum mechanics and the non-classical behavior at potential boundaries.

## 50 Normalize the 1s state of the hydrogen atom in the ground state and calculate the expectation value of position

### Introduction:

The hydrogen atom's ground state (1s) wave function in spherical coordinates is given by:

$$\psi_{100}(r, \theta, \phi) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

where  $a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}$  is the Bohr radius. This function includes both the radial and angular dependence. For the 1s state, the angular dependence is constant:  $Y_{00} = \frac{1}{\sqrt{4\pi}}$ , and hence we focus primarily on the radial part for normalization and expectation value computations.

Our goal is to: 1. Normalize the wave function, and 2. Compute the expectation value of the radial distance  $\langle r \rangle$ .

### 1. Normalization of the wave function:

The normalization condition in three dimensions is:

$$\int |\psi_{100}(r, \theta, \phi)|^2 d^3r = 1$$

In spherical coordinates, this becomes:

$$\int_0^{2\pi} \int_0^\pi \int_0^\infty |\psi_{100}(r)|^2 r^2 \sin \theta dr d\theta d\phi = 1$$

Substituting  $\psi_{100}(r) = Ae^{-r/a_0}$ , we write:

$$\int_0^{2\pi} d\phi \int_0^\pi \sin \theta d\theta \int_0^\infty |A|^2 e^{-2r/a_0} r^2 dr = 1$$

Evaluating the angular integrals:

$$\int_0^{2\pi} d\phi = 2\pi, \quad \int_0^\pi \sin \theta d\theta = 2$$

So the normalization condition becomes:

$$4\pi |A|^2 \int_0^\infty e^{-2r/a_0} r^2 dr = 1$$

Using the standard integral:

$$\int_0^\infty r^2 e^{-2r/a_0} dr = \left(\frac{a_0}{2}\right)^3 \cdot \int_0^\infty x^2 e^{-x} dx = \frac{a_0^3}{8} \cdot 2 = \frac{a_0^3}{4}$$

Hence:

$$4\pi |A|^2 \cdot \frac{a_0^3}{4} = 1 \quad \Rightarrow \quad |A|^2 \pi a_0^3 = 1 \quad \Rightarrow \quad |A| = \frac{1}{\sqrt{\pi a_0^3}}$$

So the normalized wave function is:

$$\psi_{100}(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

## 2. Expectation value of position $\langle r \rangle$ :

The expectation value of the position is given by:

$$\langle r \rangle = \int_0^{2\pi} \int_0^\pi \int_0^\infty \psi_{100}^*(r) r \psi_{100}(r) r^2 \sin \theta dr d\theta d\phi$$

Substitute the normalized wave function:

$$\langle r \rangle = \frac{1}{\pi a_0^3} \int_0^{2\pi} d\phi \int_0^\pi \sin \theta d\theta \int_0^\infty r^3 e^{-2r/a_0} dr$$

Evaluate the angular integrals:

$$\int_0^{2\pi} d\phi = 2\pi, \quad \int_0^\pi \sin \theta d\theta = 2$$

So:

$$\langle r \rangle = \frac{2}{a_0^3} \int_0^\infty r^3 e^{-2r/a_0} dr$$

Using the standard integral:

$$\int_0^\infty r^3 e^{-2r/a_0} dr = \frac{6}{(2/a_0)^4} = \frac{3a_0^4}{4}$$

Then:

$$\langle r \rangle = \frac{2}{a_0^3} \cdot \frac{3a_0^4}{4} = \frac{3a_0}{2}$$

### Conclusion:

- The normalized wave function for the hydrogen atom in the 1s state is:

$$\psi_{100}(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

- The expectation value of the radial distance in this state is:

$$\langle r \rangle = \frac{3a_0}{2}$$

This result shows that the average distance of the electron from the nucleus in the ground state is 1.5 times the Bohr radius. This reflects the quantum mechanical nature of the atom, where the electron does not orbit at a fixed radius but has a spread-out probability distribution.