

1 K simus 9:

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$$\psi = c_1\psi_1 + c_2\psi_2 \quad (1)$$

$$\langle E \rangle = \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle} \quad (2)$$

Using the linearity of the Hamiltonian operator:

$$\hat{H}\psi = \hat{H}(c_1\psi_1 + c_2\psi_2) = c_1\hat{H}\psi_1 + c_2\hat{H}\psi_2 \quad (3)$$

Since ψ_1 and ψ_2 are eigenfunctions of $\hat{H}$ with eigenvalues E_1 and E_2 , we substitute:

$$\hat{H}\psi_1 = E_1\psi_1, \quad \hat{H}\psi_2 = E_2\psi_2 \quad (4)$$

$$\hat{H}\psi = c_1E_1\psi_1 + c_2E_2\psi_2 \quad (5)$$

Calculate $\langle \psi | \hat{H} | \psi \rangle$

$$\langle \psi | \hat{H} | \psi \rangle = \langle (c_1\psi_1 + c_2\psi_2) | (c_1E_1\psi_1 + c_2E_2\psi_2) \rangle \quad (6)$$

Expanding:

$$= c_1^*c_1E_1\langle \psi_1 | \psi_1 \rangle + c_1^*c_2E_2\langle \psi_1 | \psi_2 \rangle + c_2^*c_1E_1\langle \psi_2 | \psi_1 \rangle + c_2^*c_2E_2\langle \psi_2 | \psi_2 \rangle \quad (7)$$

Since ψ_1 and ψ_2 are orthonormal:

$$\langle \psi_1 | \psi_1 \rangle = 1, \quad \langle \psi_2 | \psi_2 \rangle = 1, \quad \langle \psi_1 | \psi_2 \rangle = 0 \quad (8)$$

$$\langle \psi | \hat{H} | \psi \rangle = c_1^*c_1E_1 + c_2^*c_2E_2 \quad (9)$$

Calculate $\langle \psi | \psi \rangle$

$$\langle \psi | \psi \rangle = \langle c_1\psi_1 + c_2\psi_2 | c_1\psi_1 + c_2\psi_2 \rangle \quad (10)$$

$$= c_1^*c_1\langle \psi_1 | \psi_1 \rangle + c_1^*c_2\langle \psi_1 | \psi_2 \rangle + c_2^*c_1\langle \psi_2 | \psi_1 \rangle + c_2^*c_2\langle \psi_2 | \psi_2 \rangle \quad (11)$$

Since ψ_1 and ψ_2 are orthonormal:

$$\langle \psi | \psi \rangle = c_1^*c_1 + c_2^*c_2 \quad (12)$$

Calculate the Expectation Value of Energy

$$\langle E \rangle = \frac{c_1^*c_1E_1 + c_2^*c_2E_2}{c_1^*c_1 + c_2^*c_2} \quad (13)$$

Condition on coefficients c_1 and c_2 For ψ to be a valid quantum state, it must be normalized:

$$\langle \psi | \psi \rangle = 1 \quad (14)$$

Thus, the coefficients must satisfy:

$$|c_1|^2 + |c_2|^2 = 1 \quad (15)$$

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The kinetic energy operator is given by:

$$\hat{T} = \frac{-\hbar^2}{2m} \nabla^2 \quad (16)$$

where ∇^2 is the Laplacian operator.

An operator $\hat{A}$ is Hermitian if it satisfies the condition:

$$\langle \phi | \hat{A} \psi \rangle = \langle \hat{A} \phi | \psi \rangle \quad (17)$$

for all well-behaved functions ϕ and ψ .

To check whether $\hat{T}$ is Hermitian, we evaluate the inner product:

$$I = \int \phi^*(\mathbf{r}) \hat{T} \psi(\mathbf{r}) d^3r. \quad (18)$$

Substituting $\hat{T}$:

$$I = \int \phi^*(\mathbf{r}) \left(\frac{-\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}) \right) d^3r. \quad (19)$$

Using integration by parts and assuming that ϕ and ψ vanish at infinity, the boundary terms disappear, leaving:

$$I = \int \left(\frac{-\hbar^2}{2m} \nabla^2 \phi^*(\mathbf{r}) \right) \psi(\mathbf{r}) d^3r. \quad (20)$$

Rewriting:

$$I = \int \left(\hat{T} \phi(\mathbf{r}) \right)^* \psi(\mathbf{r}) d^3r. \quad (21)$$

This shows that:

$$\langle \phi | \hat{T} \psi \rangle = \langle \hat{T} \phi | \psi \rangle, \quad (22)$$

which confirms that $\hat{T}$ is Hermitian.

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The momentum operator in the x -direction is given by:

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}. \quad (23)$$

The eigenvalue equation for the momentum operator is:

$$\hat{p}_x \psi_n = p_n \psi_n, \quad (24)$$

where p_n is the eigenvalue corresponding to the eigenfunction ψ_n .

The expectation value of momentum for a state ψ is given by:

$$\langle p \rangle_n = \int \psi_n^* \hat{p}_x \psi_n dv. \quad (25)$$

Substituting $\hat{p}_x \psi_n = p_n \psi_n$:

$$\langle p \rangle_n = \int \psi_n^* p_n \psi_n dv. \quad (26)$$

Since p_n is a constant, it can be factored out:

$$\langle p \rangle_n = p_n \int \psi_n^* \psi_n dv. \quad (27)$$

For a normalized wavefunction, $\int |\psi_n|^2 dv = 1$, so we obtain:

$$\langle p \rangle_n = p_n. \quad (28)$$

Thus, if ψ_n is a pure eigenstate of $\hat{p}_x$, then the expectation value $\langle p \rangle_n$ is equal to p_n .

However, if the wavefunction is a superposition of multiple eigenstates:

$$\psi = \sum_n c_n \psi_n, \quad (29)$$

then the expectation value of momentum is given by:

$$\langle p \rangle = \sum_n |c_n|^2 p_n, \quad (30)$$

which is a weighted sum of eigenvalues, not necessarily equal to any single eigenvalue.

The expectation value $\langle p \rangle_n = p_n$ holds only if the system is in a pure eigenstate of the momentum operator. If the state is a superposition of eigenstates, the expectation value is generally different from any individual eigenvalue.

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The Heisenberg uncertainty principle states that the product of the uncertainties in position (Δx) and momentum (Δp) is bounded by:

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2} \quad (31)$$

Derivation

We derive this using the Schwarz inequality and the properties of quantum operators.

Step 1:

The position $\hat{x}$ and momentum $\hat{p}$ operators satisfy the canonical commutation relation:

$$[\hat{x}, \hat{p}] = i\hbar \quad (32)$$

where $\hat{p} = -i\hbar \frac{d}{dx}$ in the position representation.

Step 2:

For an observable $\hat{A}$, its expectation value in a state $|\psi\rangle$ is given by:

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle \quad (33)$$

The uncertainty in $\hat{A}$ is:

$$\Delta A = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2} \quad (34)$$

For position and momentum:

$$\Delta x = \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2}, \quad \Delta p = \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2} \quad (35)$$

Deviation operators:

$$\hat{A} = \hat{x} - \langle \hat{x} \rangle, \quad \hat{B} = \hat{p} - \langle \hat{p} \rangle \quad (36)$$

Step 3:

The Schwarz inequality states:

$$\langle \psi | \hat{A}^\dagger \hat{A} | \psi \rangle \langle \psi | \hat{B}^\dagger \hat{B} | \psi \rangle \geq \left| \langle \psi | \hat{A} \hat{B} | \psi \rangle \right|^2 \quad (37)$$

Expanding in terms of variances:

$$(\Delta x)^2 (\Delta p)^2 \geq \left| \frac{1}{2} \langle [\hat{x}, \hat{p}] \rangle \right|^2 \quad (38)$$

Using the commutator relation $[\hat{x}, \hat{p}] = i\hbar$, we get:

$$\left| \frac{1}{2} i\hbar \right|^2 = \frac{\hbar^2}{4} \quad (39)$$

We obtain the final result:

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2} \quad (40)$$

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For a step potential where $E > U_0$, the flux of incident particles (probability current density) is given by:

$$j_i = \frac{\hbar k_1 A^2}{m} \quad (41)$$

where

$$k_1 = \frac{\sqrt{2mE}}{\hbar} \quad (42)$$

Step 1: Define the Wavefunction

In the region before the barrier (Region I), the wavefunction can be written as:

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \quad (43)$$

Step 2: Probability Current Density Definition

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

$$j = \frac{\hbar}{2mi} \left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right) \quad (44)$$

For the incident wave $\psi_i(x) = Ae^{ik_1x}$, we compute its derivative:

$$\frac{d\psi_i}{dx} = ik_1 Ae^{ik_1x} \quad (45)$$

$$\frac{d\psi_i^*}{dx} = -ik_1 A^* e^{-ik_1x} \quad (46)$$

Step 3: Compute Incident Flux j_i

Substituting into the probability current density equation:

$$j_i = \frac{\hbar}{2mi} (A^* e^{-ik_1x} \cdot ik_1 Ae^{ik_1x} - Ae^{ik_1x} \cdot (-ik_1 A^* e^{-ik_1x})) \quad (47)$$

$$= \frac{\hbar}{2mi} (ik_1 A^* A - (-ik_1 AA^*)) \quad (48)$$

$$= \frac{\hbar}{2mi} (ik_1 |A|^2 + ik_1 |A|^2) \quad (49)$$

$$= \frac{\hbar}{m} k_1 |A|^2 \quad (50)$$

We obtain:

$$j_i = \frac{\hbar k_1}{m} A^2 \quad (51)$$