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# 1 General Eigenvalue Problem in Quantum Mechanics 20

In quantum mechanics, an observable is represented by an operator $\hat{A}$, and its eigenvalue equation is given by:

$$\hat{A}\psi = \lambda\psi$$

where $\psi$ is the eigenfunction and $\lambda$ is the corresponding eigenvalue.

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

$$\hat{p}_x = -i\hbar\frac{d}{dx}$$

Solving the eigenvalue equation:

$$\hat{p}_x\psi(x) = p\psi(x)$$

leads to the differential equation:

$$-i\hbar\frac{d\psi}{dx} = p\psi$$

which has solutions of the form:

$$\psi(x) = Ae^{ikx}$$

where the eigenvalues are:

$$p = \hbar k$$

These eigenvalues represent the possible momentum values of the particle.

The kinetic energy operator is given by:

$$\hat{T} = \frac{\hat{p}_x^2}{2m} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

The corresponding eigenvalue equation:

$$\hat{T}\psi(x) = E\psi(x)$$

results in:

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

Substituting $\psi(x) = Ae^{ikx}$ into the equation, we get:

$$\frac{\hbar^2 k^2}{2m}\psi = E\psi$$

Thus, the eigenvalues are:

$$E = \frac{\hbar^2 k^2}{2m}$$

which represent the kinetic energy of the system.

The wavefunctions used in both eigenvalue problems are the same (plane waves $e^{ikx}$), because the kinetic energy operator is derived from the momentum operator. Since kinetic energy depends on momentum via the relation $T = \frac{p^2}{2m}$, any eigenfunction of $\hat{p}_x$ must also be an eigenfunction of $\hat{T}$.

- The eigenvalues of $\hat{p}_x$ correspond to the possible momentum values of the quantum system.
- The eigenvalues of $\hat{T}$ correspond to the possible kinetic energy values.

The eigenvalues of both operators are real. This is because:

- Physical quantities such as momentum and kinetic energy must be real for meaningful measurements.
- The operators $\hat{p}_x$ and $\hat{T}$ are Hermitian, ensuring that their eigenvalues are always real.
- If an operator representing a physical observable had complex eigenvalues, the results of measurements would not correspond to real physical values.

Thus, the eigenvalues of both $\hat{p}_x$ and $\hat{T}$ are necessarily real.

## 2 Proof that the Potential Energy Operator is Hermitian 5

For a quantum harmonic oscillator, the potential energy operator is given by:

$$\hat{V} = \frac{1}{2}m\omega^2\hat{x}^2$$

where $m$ is the mass of the particle, $\omega$ is the angular frequency, and $\hat{x}$ is the position operator.

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

$$\langle\psi|\hat{A}\phi\rangle = \langle\hat{A}\psi|\phi\rangle$$

for all wavefunctions $\psi$ and $\phi$ in the Hilbert space.

Since the position operator $\hat{x}$ is known to be Hermitian, it satisfies:

$$\langle\psi|\hat{x}\phi\rangle = \langle\hat{x}\psi|\phi\rangle$$

Now, consider the potential energy operator:

$$\hat{V} = \frac{1}{2}m\omega^2\hat{x}^2$$

Applying it to a wavefunction $\phi$:

$$\langle\psi|\hat{V}\phi\rangle = \left\langle\psi\middle|\frac{1}{2}m\omega^2\hat{x}^2\phi\right\rangle$$

Since $\frac{1}{2}m\omega^2$ is a real constant, it can be factored out:

$$\langle\psi|\hat{V}\phi\rangle = \frac{1}{2}m\omega^2\langle\psi|\hat{x}^2\phi\rangle$$

Using the fact that $\hat{x}$ is Hermitian: you have to proof it

$$\langle\psi|\hat{x}^2\phi\rangle = \langle\hat{x}^2\psi|\phi\rangle$$

Thus, we obtain:

$$\langle\psi|\hat{V}\phi\rangle = \frac{1}{2}m\omega^2\langle\hat{x}^2\psi|\phi\rangle$$

Since this expression is of the form $\langle\hat{V}\psi|\phi\rangle$, we conclude that:

$$\langle\psi|\hat{V}\phi\rangle = \langle\hat{V}\psi|\phi\rangle$$

which proves that $\hat{V}$ is Hermitian.

Since the potential energy operator $\hat{V}$ satisfies the Hermitian condition for all wavefunctions $\psi$ and $\phi$, it follows that $\hat{V}$ is a Hermitian operator. This ensures that the potential energy has real eigenvalues that correspond to physically meaningful energy measurements.

## 3 Can you show (explain) that for a highly localized wave function (which allows one to precisely determine the position of a particle), the momentum of that particle cannot be accurately measured (calculated)? NB! The movement of particles is free and one-dimensional.

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In quantum mechanics, the Heisenberg uncertainty principle states that the uncertainties in position $\Delta x$ and momentum $\Delta p_x$ satisfy the relation:

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}$$

where $\hbar$ is the reduced Planck's constant.

This implies that as the uncertainty in position $\Delta x$ decreases, the uncertainty in momentum $\Delta p_x$ must increase.

A highly localized wave function means that the particle's position is known with high precision, i.e., $\Delta x$ is very small. Mathematically, this can be represented by a wave packet that is sharply peaked in real space.

For example, consider a wave function that approximates a Dirac delta function:

$$\psi(x) \approx \delta(x - x_0)$$

This means the particle is almost exactly at position $x_0$, so $\Delta x \to 0$.

The momentum-space wave function is given by the Fourier transform of the position-space wave function:

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar} dx$$

For a sharply peaked $\psi(x)$, this integral spreads over a wide range of momenta, meaning $\tilde{\psi}(p)$ is broadly distributed.

Since $\psi(x)$ is highly localized, its Fourier transform $\tilde{\psi}(p)$ must be widely spread. This results in a large uncertainty in momentum:

$$\Delta p_x \to \infty$$

Thus, when position is precisely determined ($\Delta x \to 0$), the momentum uncertainty increases dramatically.

This result is a direct consequence of the wave-particle duality. A localized wave packet requires a superposition of many momentum components, making it impossible to determine a precise momentum value. Physically, this means that a free particle whose position is well-defined does not have a well-defined momentum, as its wave function contains a broad spectrum of momentum values.

We have shown that for a highly localized wave function, the momentum of the particle becomes highly uncertain. This is a fundamental consequence of Heisenberg's uncertainty principle, illustrating that precise knowledge of a particle's position inherently prevents precise knowledge of its momentum.

# 4 32. For stepped barrier: Show that for potential barrier for (E>U0) the flux of particles ....

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In quantum mechanics, the probability current density (or flux) describes the flow of probability associated with a quantum state. It is defined as:

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

For a stepped potential barrier, we analyze the probability flux of incident and reflected particles when the energy of the particle is greater than the barrier height ($E > U_0$).

Consider a one-dimensional step potential barrier given by:

$$V(x) = \begin{cases} 0, & x < 0 \\ U_0, & x \geq 0 \end{cases}$$

For an incident plane wave traveling towards the barrier from the left ($x < 0$), the wavefunction is:

$$\psi_1(x) = Ae^{ik_1 x} + Be^{-ik_1 x}$$

where:

$$k_1 = \frac{\sqrt{2mE}}{\hbar}$$

Here: - $Ae^{ik_1 x}$ represents the incident wave with amplitude $A$. - $Be^{-ik_1 x}$ represents the reflected wave with amplitude $B$.

Using the definition of probability current density:

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

For the incident wave $\psi_i = Ae^{ik_1 x}$, we calculate:

$$\frac{d\psi_i}{dx} = ik_1 Ae^{ik_1 x}$$

Thus, the probability current density of the incident wave is:

$$j_i = \frac{\hbar}{2mi}\left(A^* e^{-ik_1 x}(ik_1 Ae^{ik_1 x}) - Ae^{ik_1 x}(-ik_1 A^* e^{-ik_1 x})\right)$$

$$= \frac{\hbar}{2mi}\left(ik_1|A|^2 - (-ik_1|A|^2)\right)$$

$$= \frac{\hbar}{2mi}\left(2ik_1|A|^2\right) = \frac{\hbar k_1}{m}|A|^2$$

Thus, the probability flux for the incident wave is:

$$j_i = \frac{\hbar k_1}{m}|A|^2$$

For the reflected wave $\psi_r = Be^{-ik_1 x}$, we calculate:

$$\frac{d\psi_r}{dx} = -ik_1 Be^{-ik_1 x}$$

The probability current density for the reflected wave is:

$$j_R = \frac{\hbar}{2mi}\left(B^* e^{ik_1 x}(-ik_1 Be^{-ik_1 x}) - Be^{-ik_1 x}(ik_1 B^* e^{ik_1 x})\right)$$

$$= \frac{\hbar}{2mi}\left(-ik_1|B|^2 + ik_1|B|^2\right) = -\frac{\hbar k_1}{m}|B|^2$$

Thus, the probability flux for the reflected wave is:

$$j_R = -\frac{\hbar k_1}{m}|B|^2$$

For a particle encountering a step potential with $E > U_0$: - The probability flux of the incident wave is:

$$j_i = \frac{\hbar k_1}{m}|A|^2$$

- The probability flux of the reflected wave is:

$$j_R = -\frac{\hbar k_1}{m}|B|^2$$

This result shows that the probability flux is conserved, as expected in quantum mechanics.

## 5 26. Heisenberg uncertainty principle. Derive it ? 10

The Heisenberg Uncertainty Principle states that the product of the uncertainties in position and momentum measurements cannot be arbitrarily small. Mathematically, it is expressed as:

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \tag{1}$$

We start with the definitions of the standard deviations of position and momentum:

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2, \tag{2}$$

$$(\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2. \tag{3}$$

Using the Schrödinger representation, the position and momentum operators are:

$$\hat{x} = x, \tag{4}$$

$$\hat{p} = -i\hbar \frac{d}{dx}. \tag{5}$$

For any two operators $A$ and $B$, the commutator is defined as:

$$[A, B] = AB - BA. \tag{6}$$

For position and momentum, we have:

$$[x, p] = i\hbar. \tag{7}$$

Using the Cauchy-Schwarz inequality in Hilbert space:

$$\langle \psi | A^2 | \psi \rangle \langle \psi | B^2 | \psi \rangle \geq \frac{1}{4} |\langle \psi | [A, B] | \psi \rangle|^2. \tag{8}$$

Substituting $A = x - \langle x \rangle$ and $B = p - \langle p \rangle$, we get:

$$(\Delta x)^2 (\Delta p)^2 \geq \frac{1}{4} |\langle [x, p] \rangle|^2. \tag{9}$$

Since $\langle [x, p] \rangle = i\hbar$, we obtain:

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \tag{10}$$

The Heisenberg Uncertainty Principle imposes a fundamental limit on the precision of simultaneous measurements of position and momentum, arising directly from the non-commutativity of quantum operators.