Quantum mechanics II

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1 Derive the continuity equation for wave function and give it a classical physical interpretation.(3)

Starting from the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

taking its complex conjugate:

$$-i\hbar\frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^*$$

Defining probability density $\rho = \psi^*\psi$. Then:

$$\frac{\partial\rho}{\partial t} = \psi^*\frac{\partial\psi}{\partial t} + \psi\frac{\partial\psi^*}{\partial t}$$

Substituting from the equations gives:

$$\frac{\partial\rho}{\partial t} = \frac{\hbar}{2mi}(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*)$$

Defining the probability current:

$$\vec{j} = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*)$$

Then we obtain the continuity equation:

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{j} = 0$$

This expresses conservation of probability, similar to conservation of mass or charge in classical physics.

2 Why in quantum mechanics should we use Hermitian operators to solve the eigenvalue problem? Definition of Hermite operators. Show that eigenfunctions of Hermitian opera tors form the set of orthonormal functions.(12)

In quantum mechanics, observables such as energy, position, momentum etc. are represented by operators. To ensure that measurement eigenvalues are **real**, these operators must be **Hermitian**. An operator $\hat{A}$ is said to be **Hermitian** if

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

Proof of Orthonormality

We consider the case where the eigenvalues are discrete and distinct, and each eigenvalue a_n corresponds to a single eigenfunction φ_n. Since Hermitian operators have real eigenvalues, we consider the inner product:

$$(a_n - a_m)\langle \varphi_m | \varphi_n \rangle = 0$$

Now, for $n \neq m$, it follows that $a_n - a_m \neq 0$, and thus:

$$\langle \varphi_m | \varphi_n \rangle = 0$$

This implies that eigenfunctions corresponding to different eigenvalues are **orthogonal**. For the case $n = m$, we have:

$$\langle \varphi_n | \varphi_n \rangle \neq 0$$

So each eigenfunction can be normalized to satisfy:

$$\langle \varphi_n | \varphi_n \rangle = 1$$

In conclusion, the eigenfunctions satisfy the orthonormality condition:

$$\langle \varphi_m | \varphi_n \rangle = \delta_{mn} \quad \text{or} \quad \int \varphi_m^*(x)\, \varphi_n(x)\, dV = \delta_{mn}$$

In conclusion Hermitian operators guarantee:

- **Real eigenvalues**
- **Orthonormal eigenfunctions**

3 The task for free one-dimensional motion of particle is stationary? Why? Write the corresponding Schrodinger equation for this task. Find the solution of it (wavefunction and en ergy of free particle). What gives the periodic boundary conditions (quantum number aka the physical state number)? Give the mathematical representation for it. Normalize the wavefunction. Calculate the probability density function. Is it depend on coordinate x, give the physical interpretation of the answer and relation one to Heisenberg uncertainty principle? (17)

Starting with the time-independent Schrödinger equation for a single particle:

$$\hat{H}\varphi_n = E_n \varphi_n$$

For a free particle, the Hamiltonian is:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

Thus, the equation becomes:

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi_n}{dx^2} = E_n \varphi_n$$

We rewrite it as:

$$\frac{d^2\varphi_n}{dx^2} + k^2\varphi_n = 0, \quad \text{where } k = \frac{\sqrt{2mE_n}}{\hbar}$$

The general solution is:

$$\varphi_n(x) = c_1 e^{ikx} + c_2 e^{-ikx}$$

From the definition of k, the energy is:

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

Assuming periodic boundary conditions $\varphi(x+L) = \varphi(x)$, we require:

$$e^{ikL} = 1 \Rightarrow k_n = \frac{2\pi n}{L}, \quad n \in Z$$

Substituting k_n into the energy formula:

$$E_n = \frac{2\pi^2 \hbar^2 n^2}{mL^2}$$

Solving for n in terms of E:

$$n = \frac{L}{2\pi}\sqrt{\frac{mE}{\hbar^2}}$$

The normalized wavefunction is:

$$\varphi_n(x) = \frac{1}{\sqrt{L}} e^{ik_n x}$$

The probability density is:

$$|\varphi_n(x)|^2 = \frac{1}{L}$$

This implies a uniform probability distribution within the box.

4 Operators are commute: (29)

(a.) $\hat{p}_x$ and $\hat{p}_y$?

(b.) $\hat{p}_x$ and $\hat{x}^2$ (x^2)?

a.)

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x}, \quad \hat{p}_y = -i\hbar\frac{\partial}{\partial y}$$

$$[\hat{p}_x, \hat{p}_y] = \hat{p}_x\hat{p}_y - \hat{p}_y\hat{p}_x = (-i\hbar)^2\frac{\partial^2}{\partial x \partial y} - (-i\hbar)^2\frac{\partial^2}{\partial y \partial x} = 0$$

Therefore operators $\hat{p}_x$ and $\hat{p}_y$ are commute.

b.)

$$[\hat{p}_x, \hat{x}^2] = \hat{p}_x\hat{x}^2 - \hat{x}^2\hat{p}_x$$

Let $\psi(x)$ be an arbitrary function:

$$\hat{p}_x\hat{x}^2\psi(x) = -i\hbar\frac{\partial}{\partial x}\left(x^2\psi(x)\right) = -i\hbar\left(2x\psi(x) + x^2\frac{\partial\psi(x)}{\partial x}\right)$$

$$\hat{x}^2\hat{p}_x\psi(x) = x^2\left(-i\hbar\frac{\partial\psi(x)}{\partial x}\right) = -i\hbar x^2\frac{\partial\psi(x)}{\partial x}$$

$$\Rightarrow [\hat{p}_x, \hat{x}^2]\psi(x) = -i\hbar(2x\psi(x)) = -2i\hbar x\psi(x) \Rightarrow [\hat{p}_x, \hat{x}^2] = -2i\hbar x \neq 0$$

Hence operators $\hat{p}_x$ and $\hat{x}^2$ are not commute.

5 What do the dependencies of transition and reflection coefficients on particle energy look like in the classical case? Why? (36)

The two coefficients, R and L, represent the probabilities of a particle being reflected or transmitted when encountering a potential barrier. In classical physics, if the particle's energy is less than the barrier height, it is completely reflected (hence $R = 1$ and $L = 0$); if the energy exceeds the barrier, the particle passes through entirely (hence $R = 0$ and $L = 1$). This is because classical physics does not allow quantum tunneling. In contrast, quantum mechanics permits a nonzero probability of transmission even when the particle's energy is less than the barrier height, meaning R and L can take values between 0 and 1.