Quantum Mechanics in Medicine
Lecture 5

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For Third-year Students

Probability Conservation and the Hermiticity of the Hamiltonian

In quantum mechanics, probability conservation implies that the Hamiltonian operator $\hat{H}$, which governs the dynamics of a quantum system, must be ** **Hermitian****. A Hermitian operator has the important property that its eigenvalues are real, which corresponds to observable quantities being real in physical systems.

Hermitian Operator Condition:

$$\hat{H} = \hat{H}^\dagger$$

This property ensures that the total probability in a closed quantum system remains constant over time, which is crucial for the conservation of probability.

The Schrödinger equation, written as:

$$i\hbar \frac{\partial}{\partial t}\Psi = \hat{H}\Psi$$

represents the time evolution of the wave function Ψ of a particle. For the system's energy to be conserved, the Hamiltonian must be Hermitian.

Probability Current Density

The **probability current density** $\mathbf{j}$ is a vector quantity that describes the flow of probability in space over time. It is defined as:

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

This equation provides information about how the probability density $\rho(r,t)$ changes in space and time.

Equation of Continuity:

$$\nabla \cdot \mathbf{j} = -\frac{\partial \rho}{\partial t}$$

This equation shows that the rate of change of the probability density in space is equal to the divergence of the probability current.

If $\nabla \cdot \mathbf{j} = 0$, this implies that the probability density is constant in time, describing **stationary states**.

Expectation Values of Dynamical Variables

In quantum mechanics, dynamical variables such as position and momentum are represented by operators acting on the wave function Ψ. However, exact values of these variables cannot be known simultaneously due to the **uncertainty principle**. Instead, we calculate the **expectation value**, which is the average value of the observable over many measurements.

Position Expectation Value:

$$\langle r \rangle = \int \Psi^* r \Psi \, dr$$

Momentum Expectation Value:

$$\langle p \rangle = \int \Psi^* \hat{p} \Psi \, dr$$

The expectation value of a physical quantity is always real, which aligns with the fact that observable quantities are real.

Since the wave function Ψ has a probabilistic interpretation, the expectation value represents the **average** outcome of measuring a given observable in quantum mechanics.

Expectation Values (cont.)

The expectation value is calculated by integrating the product of the complex conjugate of the wave function Ψ^*, the operator $\hat{A}$, and the wave function Ψ over the entire space.

General Expectation Value Formula:

$$\langle A \rangle = \int \Psi^* \hat{A} \Psi \, dr$$

For quantities like momentum or energy, the operators involved depend on the physical system being analyzed. The expectation values for quantities that depend on both position and momentum can also be calculated using the operator representations.

The expectation value is an important concept because it allows us to make probabilistic predictions about the outcomes of measurements in quantum mechanics.

Multiple-Choice Questions (MCQs) 1-2

1. **What does the Schrödinger equation describe in quantum mechanics?**
   a) Energy levels of a system
   b) Probability distribution of a particle
   c) Conservation of energy
   d) Thermodynamic properties of matter
2. **Which of the following is a key property of a Hermitian operator?**
   a) Its eigenvalues are always complex.
   b) It is always diagonalizable.
   c) It has real eigenvalues.
   d) It does not commute with other operators.

Multiple-Choice Questions (MCQs) 3-4

3. What does the equation of continuity represent in quantum mechanics?

a) The time rate of change of a probability density
b) The relationship between position and momentum
c) The conservation of probability
d) The uncertainty principle

4. What is the definition of stationary states in quantum mechanics?

a) States where the probability density changes with time
b) States where the probability density remains constant over time
c) States with uncertain energy
d) States with zero probability

Multiple-Choice Questions (MCQs) 5-6

5. What does the expectation value of a physical quantity represent in quantum mechanics?

a) The exact value of the quantity

b) The average of a large number of measurements

c) The minimum possible value of the quantity

d) The value of the quantity at a specific time

6. What is the general form of the expectation value of position $\langle r \rangle$?

a) $\langle r \rangle = \int \Psi^* r \Psi \, dr$

b) $\langle r \rangle = \int \Psi r \, dr$

c) $\langle r \rangle = \int \Psi^2 r \, dr$

d) $\langle r \rangle = \int \Psi^* \Psi \, dr$

Multiple-Choice Questions (MCQs) 7-8

7. Which of the following does the Schrödinger equation relate to in terms of probability conservation?

a) The continuity equation

b) The energy operator

c) The momentum operator

d) The Hamiltonian operator

8. Which statement is true regarding the expectation value of any physical quantity in quantum mechanics?

a) It is always complex.

b) It is always real.

c) It is the same as the particle's exact value.

d) It is time-dependent only.

Multiple-Choice Questions (MCQs) 9-10

9. **What is a key feature of a Hermitian operator in terms of expectation values?**
   a) It leads to complex expectation values.
   b) It results in real expectation values.
   c) It violates the principle of conservation of energy.
   d) It does not affect the wave function.
10. **Which of the following is the probability current density equation derived from?**
   a) The wave function's time-dependent Schrödinger equation
   b) The equation of continuity
   c) The momentum operator
   d) The expectation value of position

11. What condition must be satisfied for a system's wave function to be considered normalized?

a) The wave function must be zero at infinity.

b) The integral of the squared wave function over all space must equal one.

c) The wave function must be complex.

d) The wave function must have both real and imaginary components.

12. Which equation represents the expectation value of a dynamical variable (A)?

a) $\langle A \rangle = \int \Psi^* A \Psi \, dr$

b) $\langle A \rangle = \int A \Psi \, dr$

c) $\langle A \rangle = \int \Psi^2 A \, dr$

d) $\langle A \rangle = \int A \Psi^* \, dr$

Multiple-Choice Questions (MCQs) 13-14

13. What is the condition for an operator ($\hat{A}$) to represent a physical quantity in quantum mechanics?

a) It must be time-independent.

b) It must be Hermitian.

c) It must have complex eigenvalues.

d) It must commute with all other operators.

14. In the context of quantum mechanics, which of the following represents a probabilistic interpretation?

a) Energy of the particle at a given time

b) Exact position of the particle

c) The wave function's square modulus

d) The momentum of the particle

Multiple-Choice Questions (MCQs) 15-16

15. What is implied when $\nabla \cdot \mathbf{j} = 0$?

a) The system is in a non-stationary state.

b) The probability density is constant over time.

c) The particle's energy is conserved.

d) The wave function is not normalized.

16. What happens to the probability density in a stationary state in quantum mechanics?

a) It oscillates with time.

b) It remains constant in time.

c) It exponentially decays over time.

d) It changes based on the position of the particle.

Multiple-Choice Questions (MCQs) 17-18

17. Which mathematical operation is used to calculate the expectation value of momentum in quantum mechanics?

a) Integration of the wave function over space

b) Multiplying the wave function by the momentum operator

c) Taking the derivative of the wave function with respect to time

d) Solving the Hamiltonian for the particle's energy

18. How is the expectation value of a dynamical variable generally calculated?

a) By using the particle's energy equation.

b) By integrating the product of the wave function and the operator.

c) By solving the Schrödinger equation for the particle's state.

d) By differentiating the wave function with respect to position.

Multiple-Choice Questions (MCQs) 19-20

19. **What is the primary feature of a Hermitian operator regarding its eigenvalues?**
    a) They are always complex.
    b) They are always real.
    c) They depend on the wave function.
    d) They can vary with time.
20. **What does the normalized wave function ($\Psi(r, t)$) describe in quantum mechanics?**
    a) The exact position of the particle at any time
    b) The probability distribution of the particle's position
    c) The energy of the system
    d) The momentum of the system