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Summary: From Classical Mechanics to the Schrödinger Equation

1. Classical Hamiltonian

$$\textbf{Hamiltonian: } H(q, p) = \frac{p^2}{2m} + V(q)$$

$$\text{Where: } T = \frac{p^2}{2m} \quad (\text{kinetic energy}), \quad V(q) \quad (\text{potential energy})$$

2. Hamilton's Equations of Motion

The equations that describe the temporal evolution of a system are:

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q}$$

$$\text{The first gives the velocity: } \frac{dq}{dt} = \frac{p}{m}$$

$$\text{The second gives the force: } \frac{dp}{dt} = F = -\frac{dV}{dq}$$

3. From the Hamiltonian to the Schrödinger Equation

In quantum mechanics, we cannot know position and momentum exactly. Thus, we introduce the **wave function** ($\Psi(x, t)$).

We "quantize" the Hamiltonian by substituting:

$$\hat{q} = x, \quad \hat{p} = -i\hbar \frac{d}{dx}$$

Therefore, the quantum Hamiltonian is:

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

The time-dependent Schrödinger equation is:

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

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x) \Psi$$

4. Probabilistic Interpretation

$$|\Psi(x, t)|^2 = \text{probability density}$$

Probability of finding the particle between a and b:

$$\int_a^b |\Psi(x, t)|^2 dx$$

Normalization:

$$\int_{-\infty}^{+\infty} |\Psi(x, t)|^2 dx = 1$$

If

$$\Psi(x)$$

is not normalized:

$$|N| = \frac{1}{\sqrt{\int |\Psi(x)|^2 dx}}$$

5. Final Summary

Classical	Quantum
q (position)	x (multiplication operator)
p (momentum)	$-i\hbar \frac{d}{dx}$ (derivative)
$H = T + V$	$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$
$\frac{dq}{dt}, \frac{dp}{dt}$	$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi$

2. The Measurement Problem and Stationary States

The measurement problem in quantum mechanics arises when we try to understand how the act of measurement affects the state of a quantum system. Before measurement, a system is described by a wave function that represents a superposition of all possible states. Upon measurement, the wave function collapses to a specific state, leading to the question of how and why this collapse occurs.

Stationary states are particular solutions to the Schrödinger equation that do not change in time, except for a phase factor. These states are characterized by having a definite energy and are crucial for understanding the behavior of quantum systems. In stationary states, the probability density remains constant over time, allowing for a stable description of the system's properties.

Measurement Problem and Time-Independent Schrödinger Equation

Measurement and Wavefunction Collapse

Electrons were measured as particles by Thomson and Millikan. A widely accepted explanation today is that **a measurement collapses the wavefunction**:

$$\text{If I measure the position, } \Psi(x, t) \rightarrow \delta(x - x_0)$$

This means: *"Now I know for sure that the particle is at (x_0)"*

The Dirac delta is zero everywhere, except at ($x = x_0$), where it is infinite, but in such a way that:

$$\int_{-\infty}^{\infty} \delta(x - x_0) dx = 1$$

The symbol ($\delta(x - x_0)$) is called the **Dirac delta function**. It is not a regular function, but a "generalized function" or "distribution" used in theoretical physics and mathematics.

Conceptually:

$$\delta(x - x_0) = 0 \quad \text{for all } x \neq x_0$$

$$\int_{-\infty}^{\infty} \delta(x - x_0) f(x) dx = f(x_0) \quad \text{for any continuous function } f$$

That is, it "picks out" the value of a function at (x_0). This reflects the idea that the wavefunction collapses to a precise location after measurement.

Double-Slit Experiment

Even when electrons are sent one at a time through the slits, interference patterns emerge:

The electron interferes with itself.

This demonstrates the **wave nature** of particles.

Heisenberg Uncertainty Principle

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

The more precisely one measures position, the less precisely momentum can be known, and vice versa. This arises from the properties of Fourier transforms: a function and its transform cannot both be arbitrarily narrow.

Expectation Values

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

Operators for position and momentum:

$$\hat{x} = x, \quad \hat{p} = -i\hbar \frac{d}{dx}$$

Thus:

$$\langle x \rangle = \int \Psi^* x \Psi dx, \quad \langle p \rangle = \int \Psi^* (-i\hbar \frac{d}{dx}) \Psi dx$$

For a general operator (\hat{Q})

$$\langle Q \rangle = \int \Psi^* \hat{Q} \Psi dx, \quad \langle Q^2 \rangle = \int \Psi^* \hat{Q}^2 \Psi dx$$

Variance:

$$\sigma_Q^2 = \langle Q^2 \rangle - \langle Q \rangle^2$$

Variance of an Operator

Given a general operator (\hat{Q}), its expectation values are defined as:

$$\langle Q \rangle = \int \Psi^*(x) \hat{Q} \Psi(x) dx, \quad \langle Q^2 \rangle = \int \Psi^*(x) \hat{Q}^2 \Psi(x) dx$$

The **variance** (σ_Q^2) quantifies the uncertainty of measuring the observable (Q) in the quantum state (Ψ), and is defined as:

$$\sigma_Q^2 = \langle (\hat{Q} - \langle Q \rangle)^2 \rangle$$

Expanding the square:

$$\sigma_Q^2 = \langle \hat{Q}^2 - 2\langle Q \rangle \hat{Q} + \langle Q \rangle^2 \rangle$$

Since $\langle \hat{Q} \rangle = \langle Q \rangle$ is a scalar, we can take it outside the integral:

$$\sigma_Q^2 = \langle \hat{Q}^2 \rangle - 2\langle Q \rangle^2 + \langle Q \rangle^2 = \langle Q^2 \rangle - \langle Q \rangle^2$$

Thus, the variance of (Q) is:

$$\sigma_Q^2 = \langle Q^2 \rangle - \langle Q \rangle^2$$

This expression reflects how much the measurement outcomes of the observable (Q) deviate from the mean value ($\langle Q \rangle$).

Solving Schrödinger's Equation via Separation of Variables

Time-dependent equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi$$

Assume a solution of the form:

$$\Psi(x, t) = \psi(x)\phi(t)$$

Substitute into the equation:

$$i\hbar \psi(x) \frac{d\phi}{dt} = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} \phi(t) + V(x)\psi(x)\phi(t)$$

Divide both sides:

$$\frac{1}{\phi(t)} \frac{d\phi}{dt} = -\frac{i}{\hbar} E, \quad \Rightarrow \phi(t) = e^{-iEt/\hbar}$$

Time-independent Schrödinger equation:

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

Stationary States

Solving the time-independent equation yields stationary states ($\psi_n(x)$) and corresponding energies (E_n):

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

Stationary states are orthogonal and form a complete set:

$$\int \psi_m^*(x) \psi_n(x) dx = \delta_{mn}$$

Any quantum state can be written as:

$$\Psi(x, t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t / \hbar}$$

At ($t = 0$):

$$\Psi(x, 0) = \sum_{n=1}^{\infty} c_n \psi_n(x), \quad \text{with } c_n = \int \psi_n^*(x) \Psi(x, 0) dx$$

Normalization condition:

$$\sum_{n=1}^{\infty} |c_n|^2 = 1$$