Quantum Mechanics

Introduction to Quantum Mechanics

Quantum mechanics is a fundamental theory in physics that describes the behavior of matter and energy at the atomic and subatomic scale. Unlike classical physics, which deals with predictable, deterministic systems, quantum mechanics deals with probabilistic systems where particles exhibit both wave and particle characteristics. This revolutionary theory emerged in the early 20th century and has become the foundation for understanding the microscopic world.

The development of quantum mechanics began with Max Planck's solution to the black-body radiation problem in 1900, followed by Einstein's explanation of the photoelectric effect in 1905, and culminated in the comprehensive formulations by Heisenberg, Schrödinger, and others in the 1920s. Today, quantum mechanics is not only essential for understanding atomic and molecular physics but also forms the basis for modern technologies such as lasers, semiconductors, and quantum computers.

Wave-Particle Duality

Historical Development

The concept of wave-particle duality emerged from observations that could not be explained by classical physics. Light, traditionally understood as a wave phenomenon, was found to exhibit particle-like behavior in certain experiments, while particles like electrons showed wave-like properties under specific conditions.

Key Experiments:

1. **Photoelectric Effect (Einstein, 1905):** Demonstrated the particle nature of light
2. **Compton Scattering (1923):** Further confirmed photon behavior
3. **Davisson-Germer Experiment (1927):** Demonstrated electron diffraction, proving the wave nature of matter

De Broglie Hypothesis

In 1924, Louis de Broglie proposed that all matter possesses wave-like properties. He suggested that any particle with momentum p has an associated wavelength λ, known as the de Broglie wavelength:

$$\lambda = \frac{h}{p} = \frac{h}{mv}$$

where:

- h = Planck's constant (6.626×10^{-34} J·s)
- p = momentum of the particle
- m = mass of the particle

- v = velocity of the particle

Relativistic Form

For relativistic particles, the de Broglie wavelength becomes:

$$\lambda = \frac{hc}{\sqrt{E_k(E_k + 2mc^2)}}$$

where E_k is the kinetic energy and mc^2 is the rest energy.

Examples and Applications

Example 1: Electron Wavelength
Calculate the de Broglie wavelength of an electron moving at 10^6 m/s.

Given: $m = 9.1 \times 10^{-31}$ kg, $v = 10^6$ m/s, $h = 6.626 \times 10^{-34}$ J·s

$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34}}{9.1 \times 10^{-31} \times 10^6} = 7.28 \times 10^{-10}\ \mathrm{m} = 0.728\ \mathrm{nm}$$

This wavelength is comparable to atomic dimensions, explaining why electron diffraction is observable.

Example 2: Macroscopic Object
For a 1 kg ball moving at 10 m/s:

$$\lambda = \frac{6.626 \times 10^{-34}}{1 \times 10} = 6.626 \times 10^{-35}\ \mathrm{m}$$

This wavelength is extremely small, which is why wave properties are not observed for macroscopic objects.

Significance

The wave-particle duality concept revolutionized our understanding of matter and energy:

1. **Complementarity Principle:** Wave and particle descriptions are complementary; both are needed for a complete description of quantum objects.
2. **Measurement Problem:** The act of measurement determines which aspect (wave or particle) is observed.
3. **Technological Applications:** Understanding wave-particle duality led to the development of electron microscopes, which use the wave nature of electrons to achieve much higher resolution than light microscopes.

Schrödinger Wave Equation

Introduction

The Schrödinger equation, formulated by Erwin Schrödinger in 1926, is the fundamental equation of quantum mechanics. It describes how the quantum state of a physical system changes with time and space. The equation is based on the wave nature of matter and provides a mathematical framework for calculating the probability of finding a particle in a particular state.

Schrödinger developed his equation by combining:

1. Classical plane wave equation
2. De Broglie's hypothesis of matter waves
3. Conservation of energy principle

Mathematical Formulation

Time-Dependent Schrödinger Equation:

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

In expanded form:

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

Time-Independent Schrödinger Equation:

$$\hat{H}\Psi = E\Psi$$

In one dimension:

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

where:

- Ψ (psi) = wave function
- ħ = reduced Planck's constant (h/2π)
- Ĥ = Hamiltonian operator
- E = energy eigenvalue
- V(x) = potential energy function
- m = mass of the particle

Derivation of the Schrödinger Equation

Step 1: Classical Wave Equation

Starting with the general wave equation:

$$\frac{\partial^2 y}{\partial t^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial x^2}$$

Step 2: Matter Wave Representation

For a matter wave:

$$\Psi = Ae^{i(kx-\omega t)}$$

where k = 2π/λ and ω = 2πν

Step 3: De Broglie Relations

- $$\lambda = \frac{h}{p} \Rightarrow k = \frac{p}{\hbar}$$
- $$E = h\nu \Rightarrow \omega = \frac{E}{\hbar}$$

Step 4: Partial Derivatives

$$\frac{\partial \Psi}{\partial t} = -i\omega\Psi = -i\frac{E}{\hbar}\Psi$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2\Psi = -\frac{p^2}{\hbar^2}\Psi$$

Step 5: Conservation of Energy

Total energy: E = KE + PE =

$$\frac{p^2}{2m} + V(x)$$

Step 6: Substitution

Substituting the energy relation and rearranging gives the time-dependent Schrödinger equation.

Physical Interpretation of Wave Function

The wave function Ψ itself is not directly observable, but $|\Psi|^2$ has a clear physical meaning:

Born Interpretation: $|\Psi(x,t)|^2$ represents the probability density of finding the particle at position x at time t.

Normalization Condition:

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

This ensures that the total probability of finding the particle somewhere is unity.

Properties of Wave Functions

For a wave function to be physically acceptable, it must satisfy certain conditions:

1. **Single-valued:** Ψ must have a unique value at each point in space and time
2. **Continuous:** Ψ and its first derivative must be continuous
3. **Finite:** Ψ must be finite everywhere
4. **Normalizable:** The integral of $|\Psi|^2$ over all space must be finite

Qualitative Understanding

The Schrödinger equation can be rewritten in the form:

$$\frac{d^2\Psi}{dx^2} = -\frac{2m}{\hbar^2}(E - V(x))\Psi$$

This reveals important physical insights:

In Classically Allowed Regions (E > V):

- The kinetic energy (E - V) is positive
- The wave function oscillates
- The wavelength is inversely related to √(kinetic energy)

In Classically Forbidden Regions (E < V):

- The kinetic energy (E - V) is negative
- The wave function shows exponential behavior
- This leads to quantum tunneling

Applications

1. **Hydrogen Atom:** Solving the Schrödinger equation for hydrogen gives the correct energy levels and wave functions
2. **Harmonic Oscillator:** Describes vibrational states of molecules
3. **Particle in a Box:** Fundamental quantum system for understanding quantization
4. **Quantum Tunneling:** Predicts barrier penetration probability

Quantum Mechanical Tunneling

Introduction

Quantum mechanical tunneling is a phenomenon where a particle can pass through a potential energy barrier even when its kinetic energy is less than the barrier height. This is impossible in classical mechanics but is a natural consequence of the wave nature of matter in quantum mechanics.

Tunneling occurs because the wave function of a particle does not abruptly go to zero at a potential barrier. Instead, it decays exponentially within the barrier and can have a non-zero amplitude on the other side, giving the particle a finite probability of being found there.

Mathematical Description

Consider a particle with energy E approaching a rectangular potential barrier of height V_0 and width a, where $E < V_0$.

Region I (x < 0): Incident and Reflected Waves

$$\Psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

where

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

Region II (0 < x < a): Inside the Barrier

$$\Psi_{II}(x) = Ce^{\kappa x} + De^{-\kappa x}$$

where

$$\kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Region III (x > a): Transmitted Wave

$$\Psi_{III}(x) = Fe^{ik_1x}$$

Transmission Coefficient

The probability of transmission through the barrier is given by the transmission coefficient:

$$T = \frac{|F|^2}{|A|^2}$$

For a high, wide barrier (κa >> 1), the transmission coefficient can be approximated as:

$$T \approx \frac{16E(V_0 - E)}{V_0^2} e^{-2\kappa a}$$

The exponential factor e^(-2κa) shows that transmission decreases exponentially with:

- Increasing barrier width (a)
- Increasing barrier height (V_0 - E)
- Increasing particle mass (m)

WKB Approximation

For more general barrier shapes, the Wentzel-Kramers-Brillouin (WKB) approximation gives:

$$T \approx e^{-2\gamma}$$

where

$$\gamma = \int_{x_1}^{x_2} \sqrt{\frac{2m(V(x) - E)}{\hbar^2}} dx$$

and x_1, x_2 are the classical turning points.

Examples and Applications

Nuclear Physics

Alpha Decay: Alpha particles tunnel through the Coulomb barrier of atomic nuclei. The Gamow theory of alpha decay, based on tunneling, successfully explains:

- Half-lives of radioactive nuclei
- Relationship between decay energy and half-life
- Why some nuclei are stable while others decay

Nuclear Fusion: In stellar cores, protons tunnel through their mutual Coulomb repulsion barrier to undergo fusion, enabling stellar energy production despite temperatures being insufficient for classical barrier crossing.

Electronic Devices

Tunnel Diodes: These devices exploit quantum tunneling for:

- High-frequency oscillations
- Fast switching applications
- Negative resistance characteristics

Scanning Tunneling Microscope (STM): Uses tunneling current between a sharp tip and sample surface to:

- Image surfaces at atomic resolution
- Measure local electronic properties
- Manipulate individual atoms

Flash Memory: Uses tunneling through oxide barriers to:

- Store charge on floating gates
- Enable non-volatile data storage
- Allow electrical erasure and reprogramming

Chemical Reactions

Hydrogen Transfer: Quantum tunneling affects reaction rates, especially for light particles like hydrogen, explaining:

- Temperature-independent reaction rates at low temperatures
- Isotope effects in reaction kinetics
- Enzyme catalysis mechanisms

Factors Affecting Tunneling

1. **Barrier Width:** Narrower barriers have higher transmission probability
2. **Barrier Height:** Lower barriers are more easily tunneled
3. **Particle Mass:** Lighter particles tunnel more easily
4. **Energy:** Higher energy particles have better tunneling probability

Example Problem

Problem: An electron with kinetic energy 5 eV approaches a rectangular barrier of height 10 eV and width 0.2 nm. Calculate the transmission coefficient.

Solution:
Given: E = 5 eV, V_0 = 10 eV, a = 0.2 nm = 2×10^{-10} m

$$\kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} = \sqrt{\frac{2 \times 9.1 \times 10^{-31} \times 5 \times 1.6 \times 10^{-19}}{(1.054 \times 10^{-34})^2}}$$

$$\kappa = 1.15 \times 10^{10} \text{ m}^{-1}$$

$$\kappa a = 1.15 \times 10^{10} \times 2 \times 10^{-10} = 2.3$$

Since κa >> 1, using the approximation:

$$T \approx \frac{16E(V_0 - E)}{V_0^2} e^{-2\kappa a} = \frac{16 \times 5 \times 5}{100} e^{-4.6} = 4 \times 10^{-2} \times e^{-4.6} = 4 \times 10^{-4}$$

Therefore, T ≈ 0.04%, showing that even with significant tunneling parameters, the transmission probability is quite low.

Wave Functions and Their Physical Significance

Nature of Wave Functions

The wave function Ψ(x,t) is the central concept in quantum mechanics. It contains all the information that can be known about a quantum system. However, the wave function itself is not directly measurable; only certain quantities derived from it have physical significance.

Mathematical Properties

Complex Nature: Wave functions are generally complex functions:

$$\Psi(x,t) = R(x,t) + iI(x,t)$$

where R and I are real functions.

Probability Density: The probability of finding a particle between x and x + dx is:

$$P(x)dx = |\Psi(x,t)|^2 dx = \Psi^*(x,t)\Psi(x,t)dx$$

where Ψ* is the complex conjugate of Ψ.

Normalization

For a physically meaningful wave function, the total probability must equal unity:

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

This normalization condition ensures that the particle exists somewhere in space with 100% probability.

Expectation Values

The expectation value of any observable quantity A is calculated using:

$$\langle A \rangle = \int_{-\infty}^{+\infty} \Psi^* \hat{A} \Psi dx$$

where Â is the corresponding quantum mechanical operator.

Common Operators:

- Position: $\hat{x} = x$
- Momentum: $\hat{p} = -i\hbar\frac{\partial}{\partial x}$
- Kinetic Energy: $\hat{T} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
- Total Energy: $\hat{H} = \hat{T} + V(x)$

Uncertainty Principle

Heisenberg's uncertainty principle is a fundamental consequence of the wave nature of matter:

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

This principle states that the position and momentum of a particle cannot both be determined with perfect accuracy simultaneously.

Physical Interpretation: The more precisely we know a particle's position, the less precisely we can know its momentum, and vice versa. This is not due to measurement limitations but is a fundamental property of quantum systems.

Examples of Wave Functions

Free Particle:

$$\Psi(x,t) = Ae^{i(kx-\omega t)}$$

This represents a particle with definite momentum but completely uncertain position.

Particle in a Box:

$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

where n = 1, 2, 3, ... and L is the box length. This shows quantized energy levels.

Gaussian Wave Packet:

$$\Psi(x,0) = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} e^{-\frac{x^2}{2\sigma^2}} e^{ik_0 x}$$

This represents a particle with some localization in both position and momentum.

Applications of Quantum Mechanics

Atomic Structure

Quantum mechanics successfully explains:

1. **Electron Energy Levels:** Discrete energy states in atoms
2. **Atomic Spectra:** Emission and absorption lines
3. **Chemical Bonding:** Formation of molecules through orbital overlap
4. **Periodic Table:** Electronic structure determines chemical properties

Solid State Physics

1. **Band Theory:** Explains electrical conductivity in metals, semiconductors, and insulators
2. **Superconductivity:** Quantum mechanical pairing of electrons
3. **Magnetic Properties:** Quantum spin effects
4. **Crystal Structure:** Quantum mechanical bonding in solids

Modern Technology

Lasers: Based on stimulated emission and population inversion

Transistors: Quantum mechanical behavior of electrons in semiconductor junctions

Magnetic Resonance Imaging (MRI): Uses quantum spin properties of nuclei

Quantum Computing: Exploits superposition and entanglement for computation

Nuclear Physics

1. **Nuclear Decay:** Alpha, beta, and gamma decay processes
2. **Nuclear Reactions:** Fusion and fission processes
3. **Nuclear Models:** Shell model and collective motion
4. **Particle Physics:** Behavior of fundamental particles

Conceptual Problems and Examples

Problem 1: De Broglie Wavelength

Calculate the de Broglie wavelength of:
(a) An electron accelerated through 100 V
(b) A proton with kinetic energy 1 MeV

Solution (a):
For an electron accelerated through potential V:
KE = eV = 100 eV = 100 × 1.6 × 10^{-19} J

$$p = \sqrt{2mKE} = \sqrt{2 \times 9.1 \times 10^{-31} \times 100 \times 1.6 \times 10^{-19}} = 5.4 \times 10^{-24}\ \text{kg}{\cdot}\text{m/s}$$

$$\lambda = \frac{h}{p} = \frac{6.626 \times 10^{-34}}{5.4 \times 10^{-24}} = 1.23 \times 10^{-10}\ \text{m} = 0.123\ \text{nm}$$

Solution (b):
For a proton with KE = 1 MeV:

$$p = \sqrt{2m_p KE} = \sqrt{2 \times 1.67 \times 10^{-27} \times 1 \times 10^{6} \times 1.6 \times 10^{-19}} = 4.6 \times 10^{-20}\ \text{kg}{\cdot}\text{m/s}$$

$$\lambda = \frac{6.626 \times 10^{-34}}{4.6 \times 10^{-20}} = 1.44 \times 10^{-14}\ \text{m} = 0.0144\ \text{fm}$$

Problem 2: Uncertainty Principle

A particle is confined to a region of width 10^{-10} m. What is the minimum uncertainty in its momentum?

Solution:
Given: $\Delta x = 10^{-10}$ m

From the uncertainty principle:

$$\Delta p \geq \frac{\hbar}{2\Delta x} = \frac{1.054 \times 10^{-34}}{2 \times 10^{-10}} = 5.27 \times 10^{-25} \text{ kg·m/s}$$

This minimum momentum uncertainty corresponds to a kinetic energy uncertainty of:

$$\Delta E = \frac{(\Delta p)^2}{2m} = \frac{(5.27 \times 10^{-25})^2}{2 \times 9.1 \times 10^{-31}} = 1.53 \times 10^{-19} \text{ J} = 0.95 \text{ eV}$$

This shows why atomic energy levels have finite widths and why electrons in atoms have significant kinetic energies.

Conclusion

Quantum mechanics represents one of the most profound revolutions in our understanding of the physical world. From the wave-particle duality that challenges our classical intuitions to the Schrödinger equation that governs quantum systems, this theory has revealed the probabilistic nature of matter and energy at the microscopic scale.

The phenomenon of quantum tunneling demonstrates how particles can overcome classically impossible barriers, leading to applications ranging from nuclear decay to modern electronic devices. Wave functions, while not directly observable, encode all possible information about quantum systems and provide the mathematical framework for calculating observable quantities.

The success of quantum mechanics extends far beyond theoretical physics, forming the foundation for numerous technologies that define our modern world, including lasers, semiconductors, and emerging quantum technologies. Understanding these concepts is essential for grasping how the microscopic world operates and how it manifests in the macroscopic phenomena we observe daily.

As we continue to push the boundaries of quantum technology with developments in quantum computing, quantum cryptography, and quantum materials, the fundamental principles covered in this unit remain as relevant and important as ever. Quantum mechanics continues to be one of the most successful and thoroughly tested theories in physics, providing both deep insights into the nature of reality and practical tools for technological advancement.