Lesson 6.1: Schrödinger Equation

Mathematical Intuition · Module 6 — Capstone

Node 6.1

Overview

Complete decoding of the Schrödinger equation—the fundamental equation of quantum mechanics.

The Equation

Time-Dependent Schrödinger Equation

$\mathtt{i}\hbar\ \partial\psi/\partial\mathtt{t} = \hat{\mathtt{H}}\psi$

Time-Independent Schrödinger Equation

$\hat{\mathtt{H}}\psi = \mathtt{E}\psi$

Symbol-by-Symbol Breakdown

Time-Dependent Form: $\mathtt{i}\hbar\ \partial\psi/\partial\mathtt{t} = \hat{\mathtt{H}}\psi$

Left Side: $\mathtt{i}\hbar\ \partial\psi/\partial\mathtt{t}$ $\mathbf{i}$ (imaginary unit) - **Value**: $\sqrt{}(-1)$ - **Purpose**: Makes time evolution unitary (preserves normalization) - **Effect**: Without i, probability wouldn't be conserved - **Physical meaning**: Quantum mechanics is fundamentally complex-valued

$\hbar$ (reduced Planck's constant) - **Value**: $1.054571817\ldots \times 10^{-34}$ J · s - **Units**: Action (energy × time) - **Purpose**: Sets quantum scale - **Physical meaning**: Fundamental constant relating energy and frequency

$\partial\psi/\partial\mathbf{t}$ (partial time derivative) - **Operation**: Rate of change of wavefunction with time - ψ: Wavefunction (complex-valued function) - **Interpretation**: "How fast is the quantum state changing?" - **Units**: $[\psi]$/time

Combined: $\mathbf{i}\hbar\ \partial\psi/\partial\mathbf{t}$ - **Meaning**: "Quantum rate of change" - **Units**: Energy × $[\psi]$ - **Role**: Describes time evolution

Right Side: $\hat{\mathtt{H}}\psi$ $\hat{\mathbf{H}}$ (Hamiltonian operator) - **Definition**: Energy operator - **Typical form**: $\hat{\mathrm{H}} = -\hbar^2/(2\mathrm{m})\nabla^2 + \mathrm{V(x)}$ - **Components**: Kinetic energy + potential energy - **Physical meaning**: Total energy of system

ψ (wavefunction) - **Domain**: ψ(x,t) or $|\psi(\mathrm{t})\rangle$ - **Values**: Complex numbers - **Normalization**: $\int|\psi|^2\mathrm{dx} = 1$ - **Physical meaning**: Encodes all information about quantum state

$\hat{\mathbf{H}}\psi$ (Hamiltonian acting on wavefunction) - **Operation**: Operator multiplication - **Result**: Another wavefunction - **Meaning**: "Energy operator acting on state" - **Units**: Energy × $[\psi]$

The Equation as a Whole

$\mathbf{i}\hbar\ \partial\psi/\partial\mathbf{t} = \hat{\mathbf{H}}\psi$

Plain language: "The rate at which a quantum state changes in time is determined by the energy operator acting on that state."

Deeper meaning: - Time evolution is generated by energy (Hamiltonian) - Unitary evolution (i ensures probability conservation) - Deterministic: given $\psi(0)$, can predict $\psi(t)$ - Linear: superpositions evolve as superpositions

Expanded Form

Position Representation

$i\hbar \, \partial\psi(x,t)/\partial t = [-\hbar^2/(2m) \, \partial^2/\partial x^2 + V(x)]\psi(x,t)$

Breaking down the Hamiltonian:

$-\hbar^2/(2m)$ $\partial^2/\partial \mathbf{x}^2$ (kinetic energy operator) - $\partial^2/\partial \mathbf{x}^2$: Second spatial derivative (curvature) - **$-\hbar^2/(2m)$**: Converts curvature to kinetic energy - **Physical meaning**: Kinetic energy from momentum p = $-i\hbar\partial/\partial x$

V(x) (potential energy) - **Function of position**: Different for each system - **Examples**: V(x) = ½kx^2 (harmonic oscillator), V(x) = $-e^2/r$ (hydrogen atom) - **Physical meaning**: External forces, interactions

Time-Independent Form

Eigenvalue Equation: $\hat{H}\psi = E\psi$

Meaning: "The Hamiltonian acting on ψ just scales it by E"

Interpretation: - ψ is an energy eigenstate (stationary state) - E is the energy eigenvalue - These states don't change shape over time (only phase)

Time evolution of eigenstate:

$\psi(x,t) = \psi(x)e^{(-iEt/\hbar)}$

- Only phase changes: e^(-iEt/$\hbar$)
- Probability $|\psi|^2$ is time-independent

Physical Interpretation

What the Equation Tells Us

1. **Determinism**: Given initial state $\psi(0)$, evolution is determined
2. **Linearity**: If ψ_1 and ψ_2 are solutions, so is $\alpha\psi_1 + \beta\psi_2$
3. **Unitarity**: Probability is conserved: $d/dt\int|\psi|^2dx = 0$
4. **Energy generates time**: $\hat{H}$ is the generator of time evolution

What It Doesn't Tell Us

1. **Measurement outcomes**: Born rule ($|\langle\varphi|\psi\rangle|^2$) is separate postulate
2. **Collapse**: Measurement process not described
3. **Why complex numbers**: Fundamental mystery
4. **Relativistic effects**: Need Dirac equation or QFT

Examples

Free Particle (V = 0)

$i\hbar \, \partial\psi/\partial t = -\hbar^2/(2m) \, \partial^2\psi/\partial x^2$

Solution: Plane waves $\psi(x,t)$ = Ae^(i(kx-ωt)) - k: wave vector (momentum p = $\hbar$k) - ω: angular frequency (energy E = $\hbar\omega$) - Dispersion relation: $\omega = \hbar k^2/(2m)$

Harmonic Oscillator ($V = \frac{1}{2}m\omega^2x^2$)

$i\hbar\ \partial\psi/\partial t = [-\hbar^2/(2m)\ \partial^2/\partial x^2 + \frac{1}{2}m\omega^2x^2]\psi$

Energy eigenvalues: $E_n = \hbar\omega(n + \frac{1}{2})$ - Quantized in units of $\hbar\omega$ - Zero-point energy: $E_0 = \hbar\omega/2$ - Equally spaced levels

Hydrogen Atom ($V = -e^2/r$)

$i\hbar\ \partial\psi/\partial t = [-\hbar^2/(2m)\nabla^2 - e^2/r]\psi$

Energy eigenvalues: $E_n = -13.6\ \text{eV}/n^2$ - Bound states: $n = 1, 2, 3, \ldots$ - Ground state: $n = 1$ (lowest energy) - Explains atomic spectra

Deeper Connections

Relation to Classical Mechanics

Ehrenfest theorem: Quantum expectation values obey classical equations

$d\langle x\rangle/dt = \langle p\rangle/m$
$d\langle p\rangle/dt = -\langle dV/dx\rangle$

Correspondence principle: Quantum $\rightarrow$ classical as $\hbar \rightarrow 0$ or large quantum numbers

Relation to Path Integrals

Feynman formulation: Sum over all paths

$\psi(x_f,t_f) = \int \psi(x_i,t_i)e^{iS[path]/\hbar}D[path]$

- S: Classical action
- Equivalent to Schrödinger equation

Relation to Heisenberg Picture

Schrödinger picture: States evolve, operators fixed **Heisenberg picture**: Operators evolve, states fixed

$d\hat{A}/dt = (i/\hbar)[\hat{H},\hat{A}] + \partial\hat{A}/\partial t$

- Equivalent formulations
- Different perspectives on time evolution

Practice Problems

1. **Dimensional analysis**: Verify that both sides of $i\hbar\partial\psi/\partial t = \hat{H}\psi$ have the same units.
2. **Probability conservation**: Show that $d/dt\int|\psi|^2dx = 0$ using the Schrödinger equation.
3. **Stationary states**: If $\psi(x,t) = \varphi(x)e^{-iEt/\hbar})$, show that $\varphi(x)$ satisfies $\hat{H}\varphi = E\varphi$.
4. **Expectation values**: Show that $d\langle x\rangle/dt = \langle p\rangle/m$ using the Schrödinger equation.
5. **Uncertainty principle**: Derive $\Delta x\Delta p \geq \hbar/2$ from $[x,p] = i\hbar$.

Key Takeaways

- Schrödinger equation governs quantum time evolution
- $i\hbar$ ensures unitary evolution (probability conservation)
- Hamiltonian $\hat{H}$ = kinetic + potential energy
- Time-independent form gives energy eigenstates
- Linear equation $\rightarrow$ superposition principle

- Deterministic evolution, probabilistic measurement

Historical Note

Erwin Schrödinger (1926): Formulated wave mechanics - Inspired by de Broglie's matter waves - Equivalent to Heisenberg's matrix mechanics - Nobel Prize 1933 (shared with Dirac) - "Schrödinger's cat" thought experiment (1935)

Next Steps

Next, we'll decode QAOA—the Quantum Approximate Optimization Algorithm that uses quantum circuits to solve combinatorial problems.

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Concepts: hilbert-space, unitary-evolution, eigenvalue-decomposition, superposition, dynamical-systems

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