Chapter 1
Foundations of Wave Mechanics

A compact chapter-style exposition

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Abstract

This chapter introduces the fundamental postulates and mathematical framework of non-relativistic quantum mechanics: wave functions, operators, measurement postulates, the Schrödinger equation, stationary states, simple one-dimensional examples, and the Ehrenfest theorem. The presentation stresses derivations, physical interpretation, and common worked examples.

Contents

1 Introduction and historical motivation

Classical mechanics describes particles via definite position and momentum trajectories. Quantum phenomena (black-body radiation, photoelectric effect, atomic spectra) cannot be reconciled with classical particle dynamics. Wave-particle duality prompts a new framework: the *wave function* ψ encodes probability amplitudes; observable quantities become operators acting on state vectors.

2 Mathematical preliminaries

2.1 State space and wave functions

For a single non-relativistic particle in $\mathbb{R}^3$ the pure state is represented by a square-integrable complex function

$$\psi(\mathbf{x},t): \ \mathbb{R}^3 \times \mathbb{R} \to \mathbb{C}, \qquad \int_{\mathbb{R}^3} |\psi(\mathbf{x},t)|^2 \, d^3x < \infty.$$

Normalization: $\int |\psi|^2 = 1$ (if the particle is certainly present somewhere).

Bra–ket notation: $|\psi\rangle$ denotes the state vector; $\langle\phi|\psi\rangle = \int \phi^*(\mathbf{x})\psi(\mathbf{x})\, d^3x$.

2.2 Operators and expectation values

An observable A corresponds to a linear Hermitian operator $\hat{A}$ on the Hilbert space $L^2(\mathbb{R}^3)$. Expectation value:

$$\langle A\rangle_\psi = \langle\psi|\hat{A}|\psi\rangle.$$

In position representation, position and momentum operators are

$$\hat{\mathbf{x}} = \mathbf{x}, \qquad \hat{\mathbf{p}} = -\mathrm{i}\hbar\nabla,$$

satisfying canonical commutation relations

$$[\hat{x}_i, \hat{p}_j] = \mathrm{i}\hbar\delta_{ij}.$$

2.3 Probability density and current

Probability density $\rho(\mathbf{x},t) = |\psi(\mathbf{x},t)|^2$. For a particle governed by the Schrödinger equation (below) the probability current is

$$\mathbf{j}(\mathbf{x},t) = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*),$$

obeying the continuity equation $\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{j} = 0$.

3 Time-dependent Schrödinger equation

3.1 Heuristics and derivation

Start from de Broglie relations: $E = \hbar\omega$, $\mathbf{p} = \hbar\mathbf{k}$. For a free wave $\psi(\mathbf{x},t) = \exp(\mathrm{i}(\mathbf{k}\cdot\mathbf{x} - \omega t))$, the classical energy $E = \frac{p^2}{2m}$ suggests the operator correspondence

$$E \mapsto \mathrm{i}\hbar\frac{\partial}{\partial t}, \qquad \mathbf{p} \mapsto -\mathrm{i}\hbar\nabla.$$

Apply these to $E = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x},t)$ to obtain the time-dependent Schrödinger equation (TDSE)

$$\mathrm{i}\hbar\frac{\partial\psi(\mathbf{x},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x},t)\right)\psi(\mathbf{x},t) = \hat{H}\psi(\mathbf{x},t). \tag{1}$$

3.2 Properties of TDSE

- Linear: superposition principle applies.
- Unitary time evolution: norm preserved; evolution operator $U(t, t_0)$ is unitary.
- Conservation of probability via continuity equation.

4 Separation of variables and the time-independent Schrödinger equation

For time-independent potential $V(\mathbf{x})$ seek separable solutions $\psi(\mathbf{x}, t) = \phi(\mathbf{x})T(t)$. Plugging into (1) and dividing by ϕT yields separation constant E:

$$\mathrm{i}\hbar\frac{\dot{T}}{T} = \frac{-\hbar^2}{2m}\frac{\nabla^2\phi}{\phi} + V(\mathbf{x}) = E.$$

Temporal part: $T(t) = \exp(-\mathrm{i}Et/\hbar)$. Spatial part (time-independent Schrödinger equation, TISE):

$$\hat{H}\phi(\mathbf{x}) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})\right)\phi(\mathbf{x}) = E\phi(\mathbf{x}). \tag{2}$$

Solutions ϕ_n with eigenvalues E_n yield stationary states $\psi_n(\mathbf{x}, t) = \phi_n(\mathbf{x})e^{-iE_nt/\hbar}$.

5 Postulates (concise)

1. A system is described by a normalized state vector $|\psi\rangle$ in a Hilbert space.
2. Observables correspond to Hermitian operators $\hat{A}$.
3. Measurement of A yields an eigenvalue a of $\hat{A}$ with probability $|\langle a|\psi\rangle|^2$; immediately after measurement the state collapses to the eigenstate $|a\rangle$ (projection postulate).
4. Time evolution is given by the Schrödinger equation with Hamiltonian $\hat{H}$.

6 Expectation values, uncertainty and Ehrenfest theorem

6.1 Expectation values and variance

Expectation value:

$$\left\langle \hat{A} \right\rangle = \langle\psi| \hat{A} |\psi\rangle .$$

Variance (uncertainty):

$$(\Delta A)^2 = \left\langle \hat{A}^2 \right\rangle - \left\langle \hat{A} \right\rangle^2 .$$

6.2 Ehrenfest theorem

For operator $\hat{A}$ with no explicit time dependence,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \hat{A} \right\rangle = \frac{1}{\mathrm{i}\hbar}\left\langle [\hat{A}, \hat{H}] \right\rangle .$$

Apply to position and momentum to obtain

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle \hat{\mathbf{x}} \rangle = -\langle \nabla V(\hat{\mathbf{x}}) \rangle ,$$

showing that expectation values obey Newton-like laws (classical limit).

7 One-dimensional examples

7.1 Infinite square well (particle in a box)

Potential:

$$V(x) = \begin{cases} 0, & 0 < x < L, \\ \infty, & \text{otherwise.} \end{cases}$$

TISE inside the well:

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} = E\phi.$$

Solutions satisfying $\phi(0) = \phi(L) = 0$:

$$\phi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), \qquad E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2}, \quad n = 1, 2, \dots$$

Key features: discrete spectrum, orthonormal eigenfunctions.

7.2 Harmonic oscillator (sketch)

Potential: $V(x) = \frac{1}{2}m\omega^2 x^2$. Introducing ladder operators or solving Hermite equation yields discrete energies

$$E_n = \hbar\omega\left(n + \tfrac{1}{2}\right), \qquad n = 0, 1, 2, \dots$$

and Hermite-function eigenstates $\phi_n(x)$ (Gaussian times Hermite polynomial).

8 Measurement, collapse, and physical interpretation

Measurement yields eigenvalues probabilistically. Repeated measurements of an observable immediately after a projective measurement give the same eigenvalue (state collapsed to eigenstate). Discusses Copenhagen-style interpretation and remarks on alternatives (many-worlds, decoherence) — introduction only.

9 Worked example: Gaussian wave packet free evolution (outline)

Initial Gaussian wave packet in 1D

$$\psi(x, 0) = \frac{1}{(2\pi\sigma_0^2)^{1/4}}\exp\left(-\frac{(x - x_0)^2}{4\sigma_0^2} + \frac{\mathrm{i}p_0 x}{\hbar}\right).$$

Under free Hamiltonian $H = p^2/2m$ the packet disperses; width grows in time as

$$\sigma(t) = \sigma_0\sqrt{1 + \left(\frac{\hbar t}{2m\sigma_0^2}\right)^2}.$$

This illustrates wavepacket spreading and semiclassical motion of the center.

10 Boundary conditions and self-adjointness

Physical operators representing observables must be self-adjoint. For differential operators domain and boundary conditions matter. Example: the momentum operator $-i\hbar d/dx$ on the interval requires suitable boundary conditions to be self-adjoint.

11 Exercises

Exercise 11.1. Normalize the ground-state harmonic oscillator wave function

$$\phi_0(x) = A \exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

and compute $\langle x \rangle, \langle x^2 \rangle, \Delta x$.

Exercise 11.2. Compute the time evolution of a particle initially in a superposition of the first two infinite-well eigenstates:

$$\psi(x, 0) = c_1\phi_1(x) + c_2\phi_2(x).$$

Find $\psi(x, t)$ and the probability density $|\psi(x, t)|^2$.

Exercise 11.3. Show explicitly that the continuity equation holds for the Schrödinger equation with a real potential.

12 Summary and outlook

This chapter introduced the wave-function formalism and the Schrödinger equation, plus the operator view of observables and measurement. Later chapters will treat angular momentum, scattering, perturbation theory, identical particles, and the formal spectral theory of operators.

References

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