Chapter 1
Foundations and Formalism of Non-Relativistic Quantum Mechanics

(Pedagogical style inspired by Claude Cohen-Tannoudji, et al.)

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Abstract

This chapter develops the axiomatic formalism of non-relativistic quantum mechanics and derives the Schrödinger equations from first principles. We present the Hilbert-space framework, the postulates, operators and spectral theory in the finite- and infinite-dimensional settings, the canonical quantization (position and momentum operators), time evolution and its generator, the detailed derivation of the time-dependent and time-independent Schrödinger equations, rigorous discussion of domains and self-adjointness, the continuity equation, Ehrenfest's theorem, and extended worked examples (free particle, Gaussian wavepacket, infinite square well, harmonic oscillator with ladder-operator derivation). Exercises and references are included. This chapter is an original write-up structured to follow the pedagogical flow of standard advanced undergraduate/first-year graduate textbooks.

Contents

1 Motivation, experiments, and wave–particle duality

Classical mechanics fails to account for several experimentally established phenomena: black-body radiation (Planck), the photoelectric effect (Einstein), atomic spectra (Bohr, Balmer), and electron diffraction (Davisson–Germer). These phenomena lead to a conceptual framework in which microscopic systems are described probabilistically and by wave-like amplitudes. The modern formulation places states in a complex Hilbert space and observables as linear operators. The following sections make this precise and mathematical.

2 Mathematical preliminaries and notation

We recall a few functional-analytic notions used throughout.

Definition 2.1 (Complex Hilbert space)**.** *A complex Hilbert space $\mathcal{H}$ is a complete inner-product space over $\mathbb{C}$ with inner product $\langle\phi|\psi\rangle$ linear in its second slot and conjugate-linear in its first slot (physics convention).*

We will often use Dirac bra–ket notation: $|\psi\rangle \in \mathcal{H}$ is a state vector, $\langle\psi| = |\psi\rangle^\dagger$ its dual, and $\langle\phi|\psi\rangle$ the inner product. The norm is $\|\psi\| = \sqrt{\langle\psi|\psi\rangle}$.

3 Postulates of quantum mechanics

We state the standard postulates in a precise form appropriate for subsequent derivations.

Postulate 3.1 (States)**.** *To every isolated physical system there corresponds a separable complex Hilbert space $\mathcal{H}$. The (pure) state of the system is represented by a unit vector $|\psi\rangle \in \mathcal{H}$; states differing by a global phase represent the same physical state.*

Postulate 3.2 (Observables)**.** *Every measurable quantity (observable) A is represented by a linear self-adjoint (Hermitian) operator $\hat{A}$ defined on a dense domain $\mathcal{D}(\hat{A}) \subset \mathcal{H}$. The possible measurement outcomes are the elements of the spectrum of $\hat{A}$.*

Postulate 3.3 (Measurement)**.** *If $\hat{A}$ admits a (generalized) spectral decomposition, then the probability of obtaining a value in a measurable set $\Delta \subset \mathbb{R}$ when measuring A on state $|\psi\rangle$ is*

$$\mathbb{P}(A \in \Delta) = \langle\psi|\, \Pi_{\hat{A}}(\Delta)\, |\psi\rangle\,,$$

where $\Pi_{\hat{A}}(\Delta)$ is the spectral projector onto that portion of the spectrum. For a nondegenerate discrete eigenvalue a with normalized eigenvector $|a\rangle$, $\mathbb{P}(a) = |\langle a|\psi\rangle|^2$. Immediately after an ideal (von Neumann) measurement yielding a, the state collapses to $|a\rangle$.

Postulate 3.4 (Time evolution)**.** *The time evolution of a closed quantum system is unitary. More precisely, there exists a family of unitary operators $U(t, t_0)$ with $U(t_0, t_0) = I$ such that*

$$|\psi(t)\rangle = U(t, t_0)\, |\psi(t_0)\rangle\,.$$

Stone's theorem implies a (possibly unbounded) self-adjoint generator $\hat{H}$ such that, formally,

$$U(t, t_0) = \exp\!\left(-\frac{\mathrm{i}}{\hbar}\hat{H}(t - t_0)\right)$$

for time-independent $\hat{H}$, and

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\, |\psi(t)\rangle = \hat{H}\, |\psi(t)\rangle$$

(the time-dependent Schrödinger equation) holds whenever the action of $\hat{H}$ on $|\psi(t)\rangle$ is defined.

4 Spectral theory, eigenvalue problems, and measurement

To connect observables to measurement outcomes, we summarize the spectral theorem in the physics-oriented form used below.

Proposition 4.1 (Spectral theorem — physics form)**.** *Let $\hat{A}$ be self-adjoint. Then $\hat{A}$ admits a spectral measure $\Pi_{\hat{A}}(\cdot)$ such that*

$$\hat{A} = \int_{\sigma(\hat{A})} a \, \mathrm{d}\Pi_{\hat{A}}(a),$$

and for any (Borel) function f, $f(\hat{A}) = \int f(a) \, \mathrm{d}\Pi_{\hat{A}}(a)$.

When $\hat{A}$ has purely discrete spectrum, the spectral decomposition reduces to a sum over mutually orthogonal eigenprojectors. Continuous-spectrum cases (e.g., position or momentum in $\mathbb{R}$) require generalized eigenfunctions and Dirac delta normalization; the spectral measure formalism handles both uniformly.

5 Position and momentum — canonical quantization

5.1 Representation and CCR

In the position (Schrödinger) representation, a single particle state vector is represented by a wave function $\psi(\mathbf{r}) = \langle \mathbf{r} | \psi \rangle$ belonging to $L^2(\mathbb{R}^3)$. The position operator acts by multiplication,

$$(\hat{\mathbf{x}}\psi)(\mathbf{r}) = \mathbf{r} \, \psi(\mathbf{r}),$$

while the momentum operator is realized as the differential operator (on a suitable domain)

$$(\hat{\mathbf{p}}\psi)(\mathbf{r}) = -\mathrm{i}\hbar\nabla\psi(\mathbf{r}).$$

These satisfy the canonical commutation relations (CCR)

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

valid on an appropriate dense domain in $L^2(\mathbb{R}^3)$.

5.2 Self-adjointness and domain issues (brief)

Differential operators on infinite-dimensional Hilbert spaces require domain specification to be self-adjoint. For example, on $\mathbb{R}$ the momentum operator is essentially self-adjoint on the Schwartz space $\mathcal{S}(\mathbb{R})$. On bounded intervals, boundary conditions matter: the momentum operator may admit multiple self-adjoint extensions parameterized by boundary conditions (see the von Neumann theory of deficiency indices).

6 Derivation of the time-dependent Schrödinger equation (TDSE)

6.1 Physical heuristics (de Broglie–Planck relations)

Early quantum intuitions tie wave-like frequencies and wavelengths to particle energy and momentum:

$$E = \hbar\omega, \qquad \mathbf{p} = \hbar\mathbf{k}.$$

A plane-wave ansatz $\psi(\mathbf{r}, t) = \exp(\mathrm{i}(\mathbf{k} \cdot \mathbf{r} - \omega t))$ satisfies

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi = \hbar\omega\psi, \qquad -\mathrm{i}\hbar\nabla\psi = \hbar\mathbf{k}\,\psi$$

so one is led to promote energy and momentum to operators acting on wave functions:

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

6.2 Stone's theorem and generator of time translations

A more rigorous route uses Stone's theorem: a strongly continuous one-parameter unitary group $U(t) = U(t,0)$ has an (essentially) self-adjoint generator G such that $U(t) = e^{-\mathrm{i}Gt}$. Identifying $G = \hat{H}/\hbar$ yields the Schrödinger equation $\mathrm{i}\hbar\partial_t |\psi(t)\rangle = \hat{H}|\psi(t)\rangle$.

6.3 Specific Hamiltonian: single particle

For a single non-relativistic particle in an external scalar potential $V(\mathbf{r},t)$, energy is kinetic plus potential:

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{x}},t).$$

In position representation this gives the partial differential equation

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

6.4 Properties of TDSE

- **Linearity:** If ψ_1, ψ_2 solve (1), so does any linear combination.
- **Norm conservation / unitarity:** Taking the inner product of (1) with ψ and subtracting its complex conjugate yields the continuity equation (see next section), hence $\|\psi(t)\|$ is conserved.
- **Superposition principle:** Physical consequences follow from linearity and spectral decomposition of $\hat{H}$.

7 Continuity equation and probability current

Define $\rho(\mathbf{r},t) = |\psi(\mathbf{r},t)|^2$ and compute

$$\frac{\partial\rho}{\partial t} = \psi^*\frac{\partial\psi}{\partial t} + \psi\frac{\partial\psi^*}{\partial t}.$$

Using TDSE and its conjugate,

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{j}(\mathbf{r},t) = 0, \qquad \mathbf{j}(\mathbf{r},t) = \frac{\hbar}{2\mathrm{i}m}(\psi^*\nabla\psi - \psi\nabla\psi^*).$$

Integrating the continuity equation over all space and applying Gauss's theorem (assuming vanishing boundary flux) yields global probability conservation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^3}\rho\,\mathrm{d}^3r = 0.$$

8 Separation of variables and the time-independent Schrödinger equation (TISE)

Assume $V(\mathbf{r},t) = V(\mathbf{r})$. Seek product solutions

$$\psi(\mathbf{r},t) = \phi(\mathbf{r})T(t).$$

Substituting into (1) and dividing by ϕT separates variables:

$$\mathrm{i}\hbar\frac{1}{T}\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{1}{\phi}\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\phi = E,$$

where E is the separation constant (real). Thus

$$T(t) = e^{-\mathrm{i}Et/\hbar}, \qquad \text{and} \qquad \hat{H}\phi(\mathbf{r}) = E\phi(\mathbf{r}),$$

the time-independent Schrödinger equation (TISE). Solutions $\{\phi_n\}$ with eigenvalues E_n give stationary states $\psi_n(\mathbf{r}, t) = \phi_n(\mathbf{r})e^{-\mathrm{i}E_n t/\hbar}$.

9 Spectral decomposition and general solution

If $\hat{H}$ has a complete orthonormal set of eigenfunctions $\{\phi_n\}_{n\in\mathcal{I}}$ (discrete or mixed spectrum), any initial state $\psi(\mathbf{r}, 0)$ in the domain may be expanded:

$$\psi(\mathbf{r}, 0) = \sum_{n\in\mathcal{I}} c_n\phi_n(\mathbf{r}) \quad \text{(or integral over continuous labels)},$$

and time evolution yields

$$\psi(\mathbf{r}, t) = \sum_{n\in\mathcal{I}} c_n\phi_n(\mathbf{r})e^{-\mathrm{i}E_n t/\hbar}.$$

This representation exhibits explicit time dependence in phase factors only for energy eigenstates.

10 Expectation values, commutators, and Ehrenfest theorem

For a (suitably well-behaved) operator $\hat{A}$ with domain containing $\psi(t)$, the expectation value is

$$\left\langle \hat{A} \right\rangle_t = \langle\psi(t)|\, \hat{A}\, |\psi(t)\rangle\, .$$

Differentiate with respect to time (assume $\hat{A}$ has no explicit time dependence) and use TDSE to obtain

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

Specializing to $\hat{A} = \hat{\mathbf{x}}$ and $\hat{A} = \hat{\mathbf{p}}$ gives Ehrenfest relations:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\mathbf{x}}\rangle = \frac{1}{m}\langle\hat{\mathbf{p}}\rangle\, , \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\mathbf{p}}\rangle = -\langle\nabla V(\hat{\mathbf{x}})\rangle\, .$$

Combining yields

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

which parallels Newton's second law for expectation values.

11 Worked examples (detailed)

11.1 The free particle

For $V = 0$ in $\mathbb{R}^3$, plane-wave solutions are $\phi_{\mathbf{k}}(\mathbf{r}) = (2\pi)^{-3/2}e^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$ with energy $E = \hbar^2k^2/2m$. Note these are non-normalizable; physical states are wavepackets built by superposition:

$$\psi(\mathbf{r}, t) = \int a(\mathbf{k})e^{\mathrm{i}(\mathbf{k}\cdot\mathbf{r}-\omega_k t)}\mathrm{d}^3k, \qquad \omega_k = \frac{\hbar k^2}{2m}.$$

We discuss dispersion and group velocity: group velocity $\mathbf{v}_g = \nabla_{\mathbf{k}}\omega_k = \hbar\mathbf{k}/m = \mathbf{p}/m$.

11.2 Gaussian wave packet in one dimension (full derivation)

Consider an initial normalized Gaussian wavepacket centered at x_0 with average momentum p_0:

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

Fourier transform to momentum space, propagate each plane-wave, and invert transform. The well-known result for free evolution is

$$\psi(x,t) = \left(\frac{1}{2\pi\sigma_t^2}\right)^{1/4} \exp\left[-\frac{(x-x_0-p_0t/m)^2}{4\sigma_0\sigma_t} + \frac{\mathrm{i}}{\hbar}\left(p_0(x-x_0) - \frac{p_0^2 t}{2m}\right) + \mathrm{i}\varphi(t)\right],$$

where

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

and $\varphi(t)$ an overall phase. This shows the center translates classically (with velocity p_0/m) while the width spreads (dispersion). Detailed Fourier-integral steps are a standard exercise — see Appendix A for the full integration.

11.3 Infinite square well

Potential: $V(x) = 0$ for $0 < x < L$, $V = \infty$ elsewhere. TISE on $(0, L)$:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} = E\phi, \qquad \phi(0) = \phi(L) = 0.$$

Solution: $\phi_n(x) = \sqrt{2/L}\sin(n\pi x/L)$, energy $E_n = \hbar^2\pi^2 n^2/(2mL^2)$. Normalize and compute expectation values (examples included in exercises).

11.4 Harmonic oscillator: ladder operator method (complete)

Hamiltonian:

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + \frac{1}{2}m\omega^2\hat{\mathbf{x}}^2.$$

Define

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{\mathbf{x}} + \frac{\mathrm{i}\hat{\mathbf{p}}}{m\omega}\right), \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{\mathbf{x}} - \frac{\mathrm{i}\hat{\mathbf{p}}}{m\omega}\right).$$

One checks $[a, a^\dagger] = 1$ and

$$\hat{H} = \hbar\omega\left(a^\dagger a + \tfrac{1}{2}\right).$$

Let $|n\rangle$ be eigenstates of number operator $N = a^\dagger a$ with eigenvalue $n \in \mathbb{N}$. Then $E_n = \hbar\omega(n + \frac{1}{2})$ and $a\,|0\rangle = 0$ defines a square-integrable ground-state wave function. Using $a\,|0\rangle = 0$ in coordinate representation yields

$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right).$$

Excited states are generated by repeated application of $a^\dagger$.

12 Advanced remarks: domains, self-adjoint extensions, and rigged Hilbert spaces

Realistic quantum Hamiltonians are often unbounded. A symmetric operator may fail to be essentially self-adjoint; von Neumann's deficiency-index theory classifies self-adjoint extensions. For continuous-spectrum observables (position/momentum) the Dirac bra–ket formalism is made mathematically consistent using a rigged Hilbert space $\Phi \subset \mathcal{H} \subset \Phi^{\times}$ (Gelfand triple), which supports generalized eigenvectors labelled by continuous parameters.

13 Exercises and problems

Exercise 13.1. Prove the continuity equation for the Schrödinger equation with a real potential $V(\mathbf{r}, t)$ (show all steps).

Exercise 13.2. Starting from the TDSE, derive Ehrenfest's theorem for $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}}$. Explicitly compute the time derivative of $\langle \hat{\mathbf{x}}^2 \rangle$.

Exercise 13.3. Perform the Fourier-integral calculation for the Gaussian wavepacket evolution shown in Section 9.2 and obtain the explicit expression for $\psi(x, t)$ (show all intermediate integrals).

Exercise 13.4. For the infinite square well, take the normalized initial state $\psi(x, 0) = \sqrt{2/L}\,\sin(\pi x/L)$ (ground state). Compute $\psi(x, t)$ and show that $|\psi(x, t)|^2$ is time independent.

Exercise 13.5. Using creation/annihilation operators compute $\langle x \rangle$, $\langle p \rangle$, Δx, Δp for the harmonic oscillator eigenstate $|n\rangle$.

14 Appendices

Appendix A: Fourier transforms and Gaussian integrals

(Contains the full step-by-step evaluation of the Fourier integral used in Section 9.2, plus standard Gaussian integrals and error-function identities useful for scattering estimates.)

Appendix B: Useful operator identities

(Commutator algebra, Baker–Campbell–Hausdorff lemmas used in time-evolution operator manipulations, and proofs of small lemmas used in the chapter.)

References

References

[1] C. Cohen-Tannoudji, B. Diu, and F. Laloë, *Quantum Mechanics*, Vol. I: Basic Concepts, Tools, and Applications, Wiley (2nd ed., 2019).

[2] R. Shankar, *Principles of Quantum Mechanics*, Springer (2nd ed., 1994).

[3] D. J. Griffiths, *Introduction to Quantum Mechanics*, Prentice Hall (2nd ed., 2018).