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An introduction

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Quantum gates Programming • Quantum Entanglement • Quantum Protocols
Quantum Algorithms • Hybrid Quantum-classical algorithms • Hardware

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Quantum Computing: An introduction

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To all the women who made science
in laboratories where no chair awaited them,
who persevered against closed doors,
unsigned papers and unspoken names,
and built, step by step,
the luminous path we walk today.

To Marie Curie and Lise Meitner;
to Emmy Noether, who revealed that symmetry
is the deepest grammar of the universe;
to Grete Hermann, who dared to question
a proof that no one else questioned;
to Maria Goeppert Mayer and Chien-Shiung Wu;
to Ada Lovelace and Grace Hopper,
who first imagined that a machine could think.

And to those who are writing the present:
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and Ana María Rey, who carried the light
of these same mountains to the coldest atoms.

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To Professor Mario Trujillo Vargas, whose teaching has transformed the lives of his students. He taught us that physics is not a collection of formulas to be memorized but a way of looking at the world, and that a teacher's true measure is not what he knows, but what he awakens in others. His vision continues to shape those of us who had the fortune of learning from him.

To the young minds of Engineering Physics, who with their genuine questions and tireless curiosity have shaped every page of this text. Their doubts became clarities, their difficulties became opportunities to explain things better. This book is, in reality, an extended dialogue with all those restless souls seeking to understand.

Finally, to the students of the quantum computing course, who read these pages with a critical eye and helped correct the errors that inevitably inhabit a work of this length, and to all those who have helped and will help to improve it: you are a fundamental part of this collective process of building knowledge. In every correction, in every suggestion, lives the spirit of collaboration that makes the advancement of science possible.

Contents

Chapter 1

Quantum Mechanics

The mathematical foundations developed in Chapter 2—Hilbert spaces, linear operators, eigenvalue equations, and unitary transformations—provide the algebraic framework for quantum computing. The quantum algorithms surveyed in Chapter 1—from Shor's factoring algorithm to quantum simulation of molecular systems—exploit quantum phenomena that have no classical analog. Yet between the abstract mathematics of Chapter 2 and the practical algorithms of quantum computing lies quantum mechanics itself: the physical theory that explains why qubits behave as they do, why quantum gates must be unitary, and why measurement irreversibly collapses superpositions. Understanding quantum mechanics is not merely background knowledge but essential preparation for designing quantum circuits, analyzing quantum algorithms, and interpreting experimental results from quantum hardware.

This chapter develops quantum mechanics from first principles, progressing from classical physics through canonical quantization to the postulates that govern quantum systems. We begin with the historical evolution, tracing how Heisenberg's matrix formulation emerged as the first complete quantum theory, followed by Schrödinger's wave mechanics and other equivalent formulations. The Lagrangian and Hamiltonian formalisms of classical mechanics provide the conceptual bridge to quantum theory: these energy-based descriptions translate naturally into quantum operators through canonical quantization, the systematic procedure that converts classical dynamical variables into quantum observables. The derivation of Schrödinger's equation reveals the wave-particle duality underlying quantum behavior, connecting de Broglie's matter waves with the differential equations governing quantum state evolution. Schrödinger's equation, in both time-dependent and time-independent forms, becomes the central tool for calculating quantum states, energy levels, and transition probabilities.

The matrix formulation of quantum mechanics, developed by Heisenberg, Born, and Jordan in 1925, proves particularly relevant for quantum computing. Where Schrödinger's wave functions describe continuous probability distributions, matrix quantum mechanics represents states as finite-dimensional vectors and observables as matrices—precisely the representation used in quantum circuits. A single-qubit state is a vector in $\mathbb{C}^2$, a quantum gate is a 2×2 unitary matrix, and measurement corresponds to projecting onto eigenvectors of observable matrices. The quantum harmonic oscillator, solved elegantly using creation and annihilation operators, illustrates how discrete quantum states emerge from continuous classical motion. These ladder operators appear throughout quantum computing: in quantum error correction codes, in quantum optics descriptions of photonic qubits, and in theoretical analyses of quantum field theories.

The postulates of quantum mechanics, presented at chapter's end, consolidate these mathematical structures into physical principles. The state postulate establishes that quantum systems inhabit Hilbert spaces, justifying the vector space framework developed in Chapter 2. The observable postulate links Hermitian operators to measurable quantities, explaining why quantum gates must preserve probability (hence must be unitary). The measurement postulate, incorporating Born's rule, determines how probability amplitudes $|\alpha|^2$ convert to measurement outcomes—the fundamental probabilistic character distinguishing quantum from classical computing. The evolution postulate, embodied in Schrödinger's equation, ensures quantum dynamics are deterministic and reversible between measurements, enabling the controlled interference that powers quantum algorithms. The composition postulate introduces tensor products for multi-qubit systems, giving rise to entanglement—the resource that enables exponential quantum speedups.

Readers approaching quantum mechanics for the first time will find connections to familiar classical physics: energy conservation, momentum operators, and Hamiltonian dynamics all persist in modified form. Those already familiar with quantum mechanics from physics courses will encounter the material reorganized with quantum computing applications in mind: emphasis falls on discrete systems, finite-dimensional Hilbert spaces, and matrix representations rather than continuous wavefunctions and infinite-dimensional spaces. Throughout this chapter, we highlight how each quantum mechanical concept translates directly into quantum computing practice: the Hamiltonian becomes the generator of quantum gate sequences, eigenstates become the computational basis for algorithms, and unitary evolution becomes the mechanism for quantum logic operations. By chapter's end, the abstract postulates transform into practical tools for understanding and implementing quantum computation.

1.1 Historical Evolution

Classical mechanics has undergone a long development process, generating multiple theoretical formulations to describe physical systems. Among the most notable are: the **Newtonian** formulation, arising from Isaac Newton's works in his *Philosophiae Naturalis Principia Mathematica* (1687); the **Lagrangian**, whose foundations were established by Joseph-Louis Lagrange in the 18th century; the **Hamiltonian**, proposed by William Rowan Hamilton at the beginning of the 19th century; the **formulation based on the principle of least action** (or Hamilton's principle), whose origins date back to Pierre de Fermat, Gottfried Leibniz, Pierre Louis Maupertuis and Leonhard Euler, and which was later systematized by Lagrange and Hamilton; as well as the formulations of **Euler, Lagrange and Jacobi**, which offer complementary perspectives for solving classical dynamics problems [8]. Each of these formulations provides a distinct conceptual framework for analyzing and predicting the behavior of bodies in motion.

In an analogous development, **quantum mechanics**—which emerged in the early years of the 20th century—also has a varied set of formulations (currently at least nine are recognized). Among them stand out:

1. Heisenberg's **matrix formulation** (1925)
2. Schrödinger's **wave function formulation** (1926)
3. Feynman's **path integral formulation**
4. Wigner's **phase space formulation**
5. The **density matrix-based formulation** (related to von Neumann's contributions)
6. **Second quantization** (introductory to quantum field theory)
7. The **variational formulation**, which extends the action principle in quantum contexts
8. The **de Broglie-Bohm formulation** (pilot wave)
9. The **Hamilton-Jacobi formulation** in quantum mechanics

For a more extensive discussion of these nine formulations, as well as their implications and equivalences, the references of Styer et al. in *Nine Formulations of Quantum Mechanics* [15] may be consulted.

A Historical Glimpse at the Matrix Formulation

The first quantum formulation to see the light was the **matrix** one, developed by Werner Heisenberg and published in June 1925 in the article *Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen*. Subsequently, Max Born and Pascual Jordan made essential contributions to formalize the interpretation and mathematical structure of this theory. Barely six months later, in January 1926, Erwin Schrödinger presented his formulation based on the wave function, inaugurating the so-called "wave mechanics."

In Heisenberg's formulation, each physical observable—for example, position, momentum and energy—is represented mathematically by **matrices**, which in the modern language of quantum mechanics are called **operators**. More strictly speaking, these are linear operators (generally Hermitian) that act on a state space, commonly identified with a Hilbert space.

Representation of States and Observables

For a quantum system with N basis states, an observable is associated with a Hermitian square matrix of dimension $N \times N$. A quantum state, described by a vector $|\psi\rangle$, is represented as a column matrix of dimension $N \times 1$. Any magnitude we wish to measure, denoted by A, is described with the operator $\hat{A}$. The *expectation value* of A in state $|\psi\rangle$ is calculated through the inner product:

$$\left\langle \psi \mid f(\hat{A}) \mid \psi \right\rangle,$$

where $f(\hat{A})$ is a function of operator $\hat{A}$, which could simply be $\hat{A}$ or some algebraic combination of operators.

The importance of this matrix vision lies in the fact that the concept of *eigenvectors* and *eigenvalues* becomes central to the physical interpretation of the theory. The operator corresponding to the energy observable is called the **Hamiltonian**, represented by $\hat{H}$. The temporal evolution of any operator $\hat{A}$ is given by the so-called *Heisenberg equation*:

$$\frac{d\hat{A}}{dt} = -\frac{i}{\hbar}[\hat{A}(t), \hat{H}] + \frac{\partial \hat{A}}{\partial t}. \tag{1.1}$$

This result contains the operator dynamics: the first term on the right side explains unitary evolution (generated by $\hat{H}$), while the second term represents the possible explicit time dependence in $\hat{A}$.

Throughout this chapter—and the book in general—we will delve into the principles governing quantum dynamics and how each of these formulations fits into the general framework of the theory. However, from a historical point of view, we have introduced here the basic elements of Heisenberg's matrix formulation, which marked the formal beginning of quantum mechanics and opened the way for the other interpretations and formulations that followed.

1.2 Energy and the Lagrangian Function of a System

Energy, as a fundamental physical quantity, plays a central role in both classical and quantum mechanics. In classical physics, energy conservation emerges from the time-invariance of physical laws—a profound connection established by Emmy Noether in 1918. Noether's theorem demonstrates that every differentiable symmetry of a physical system corresponds to a conserved quantity. Time translation symmetry (the invariance of physical laws under time shifts) implies energy conservation. Rotational symmetry in three-dimensional space, characterized mathematically by the $SO(3)$ group, implies conservation of angular momentum. Spatial translation symmetry implies momentum conservation. This deep relationship between symmetries and conservation laws permeates all of physics, from classical mechanics through quantum field theory [11].

Noether's theorem provides the conceptual foundation for understanding why certain quantities remain constant during the evolution of physical systems. In quantum mechanics, these conserved quantities correspond to Hermitian operators that commute with the Hamiltonian. The Hamiltonian itself—representing the system's total energy—generates time evolution through Schrödinger's equation. For isolated quantum systems, energy eigenstates evolve only in phase, preserving their energy values indefinitely. This connection between classical conservation laws and quantum operators is formalized through canonical quantization, the procedure we develop later in this chapter that systematically converts classical dynamical variables into quantum observables.

The mathematical description of classical mechanics through energy functions—specifically the Lagrangian and Hamiltonian formulations—provides the natural pathway to quantum mechanics. Rather than describing motion through Newton's forces and accelerations, these energy-based formulations express dynamics through scalar functions of position, momentum, and time. This reformulation, while equivalent to Newtonian mechanics for classical systems, generalizes more naturally to the quantum domain. The Lagrangian approach, developed by Joseph-Louis Lagrange in the 18th century, uses the principle of least action to derive equations of motion. The Hamiltonian formulation, introduced by William Rowan Hamilton in the 19th century, expresses dynamics through conjugate variables that translate directly into the position and momentum operators of quantum mechanics. We now develop these classical formulations as preparation for their quantum extensions.

Historical Note: The Development of Energy Concepts

The concept of **energy** as a unifying principle in physics emerged gradually over the 19th century, driven by technological advances and theoretical insights that revealed deep connections between mechanics, heat, and electromagnetic phenomena.

Early Terminology and Concepts

British scientist **Thomas Young** first used the term *energy* in a lecture at the Royal Society in 1802, developing the concept further in his 1807 lectures on natural philosophy [16]. The specific forms of energy received distinct names over subsequent decades: **Gustave-Gaspard Coriolis** formally introduced **kinetic energy** in 1829 [6], while **William Rankine** coined the term **potential energy** in 1853 [13]. Throughout this period, physicists debated whether energy should be considered a substance flowing between systems or an abstract quantity characterizing system states—a debate resolved only with the development of modern thermodynamics and quantum mechanics.

Thermodynamics and the Conservation Principle

The Industrial Revolution and the invention of the steam engine catalyzed practical investigations into energy transformation and mechanical efficiency. **Sadi Carnot**'s theoretical analysis of heat engines (1824) established fundamental limits on thermodynamic efficiency [4]. **James Prescott Joule** demonstrated experimentally that mechanical work and heat are equivalent forms of energy (1850), establishing the quantitative conversion factor now known as the mechanical equivalent of heat [9]. These discoveries led to the first law of thermodynamics—energy conservation in thermodynamic processes.

Rudolf Clausius extended these insights by introducing entropy in 1865, the second law of thermodynamics, and the concept of irreversible processes [5]. The study of radiant energy and electromagnetic radiation culminated in the black body radiation problem. Classical physics predicted the ultraviolet catastrophe—infinite energy emission at short wavelengths—contradicting experimental observations. **Max Planck**'s revolutionary solution in 1900, introducing energy quantization $E = h\nu$, marked the birth of quantum mechanics [12].

Noether's Theorem and Symmetry Principles

The deepest understanding of energy conservation emerged from **Emmy Noether**'s 1918 theorem connecting symmetries to conservation laws [11]. Noether demonstrated that energy conservation holds if and only if physical laws are time-independent. More generally, her theorem establishes that every continuous symmetry of a physical system's action corresponds to a conserved quantity:

- **Time translation symmetry** (laws unchanged at different times) $\rightarrow$ Energy conservation
- **Spatial translation symmetry** (laws unchanged at different positions) $\rightarrow$ Momentum conservation
- **Rotational symmetry** (laws unchanged under rotations) $\rightarrow$ Angular momentum conservation
- **Gauge symmetry** (phase invariance) $\rightarrow$ Charge conservation

Noether's theorem applies across all of physics: classical mechanics, electromagnetism, general relativity, and quantum field theory. In quantum mechanics, symmetries correspond to unitary transformations that commute with the Hamiltonian, and conserved quantities correspond to Hermitian operators whose expectation values remain constant during unitary evolution.

Modern Perspective

The historical development of energy concepts reveals a progression from practical engineering concerns (steam engine efficiency) through thermodynamic principles to the profound symmetry-based understanding provided by Noether's theorem. In quantum computing, energy and its associated operator—the Hamiltonian—remain central: quantum gates implement unitary transformations generated by Hamiltonians, quantum annealing exploits energy landscapes to solve optimization problems, and adiabatic quantum computation evolves systems through Hamiltonian interpolation. The conservation laws rooted in symmetries constrain which quantum operations are physically implementable and which computational resources can be created or preserved through quantum protocols.

1.3 Lagrangian Formulation of Classical Physics

Joseph-Louis Lagrange (1736-1813), born in Italy and naturalized in France, was a mathematician and astronomer whose contributions spanned multiple areas, including mathematical analysis, number theory, classical mechanics and celestial mechanics. In 1766, thanks to recommendations from Euler and d'Alembert, Lagrange replaced the latter at the Prussian Academy of Sciences, where, over the next 20 years, he wrote his treatise on *Analytical Mechanics*. This treatise is considered one of the most important texts in physics since Isaac Newton's *Principia*.

Before Lagrange, classical mechanics was described primarily through Newton's laws, which were based on forces and accelerations. Although this approach was effective for many problems, it proved complicated and inelegant when dealing with complex systems or with non-inertial reference frames.

Lagrange, in an attempt to simplify and generalize mechanics, introduced a new way of formulating the laws of motion. Instead of focusing on forces, Lagrange proposed a scalar function called the Lagrangian, which depended on the system's generalized coordinates and their velocities. From this function, the system's equations of motion could be obtained using the Euler-Lagrange equations.

Between 1772 and 1778, Lagrange worked on reformulating Newtonian mechanics, seeking to simplify the equations and improve calculation procedures. This achievement gave rise to what we know today as *Lagrangian mechanics*, a formulation that is not only different but also more sophisticated than Newtonian mechanics. Its key features are:

1. Lagrangian mechanics dispenses with the individual forces acting on the system, which allows avoiding the use of vectors and the direct sum of forces

2. Equations referring only to constraint forces, such as tensions or reactions, are eliminated, involving only forces that actually contribute to the system's motion

3. A scalar function called the **Lagrangian** is introduced, from which the system's differential equations of motion are derived

In general terms, the generalized Newton equations can be expressed by the following differential equation:

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j} = Q_j, \tag{1.2}$$

where T represents the system's kinetic energy, q_j are the generalized coordinates, and $\dot{q}_j$ their generalized velocities. The function Q_j is the generalized force, which includes both conservative and non-conservative components:

$$Q_j = -\frac{\partial V}{\partial q_j} + Q_j^{NC}, \tag{1.3}$$

where V is the potential energy and Q_j^{NC} represents non-conservative forces.

Lagrange defined the **Lagrangian L** as the difference between kinetic energy **T** and potential energy **V**:

$$\mathbf{L}(q_j, \dot{q}_j; t) = \mathbf{T}(q_j, \dot{q}_j; t) - \mathbf{V}(q_j; t). \tag{1.4}$$

The equations of motion, known as **Lagrange equations**, are then derived as follows:

$$\frac{d}{dt}\left(\frac{\partial \mathbf{L}}{\partial \dot{q}_j}\right) - \frac{\partial \mathbf{L}}{\partial q_j} = Q_j^{NC}, \tag{1.5}$$

where Q_j^{NC} represents non-conservative forces. If only conservative forces exist, the term Q_j^{NC} vanishes, thus simplifying the Lagrange equations.

This formulation not only provides a powerful tool for solving problems in classical mechanics, but also lays the foundations for the Hamiltonian formulation, which will be key in developing Schrödinger's equation and, therefore, in understanding quantum mechanics.

We will proceed to summarize and connect the Lagrangian formulation with the Hamiltonian formulation, from which we will introduce Schrödinger's equation.

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Historical Note: The Development of Analytical Mechanics

The evolution from Newtonian mechanics to the analytical formulations of Lagrange and Hamilton represents one of the most profound conceptual advances in theoretical physics. This transformation not only simplified mechanical calculations but revealed deep mathematical structures that would later prove essential for quantum mechanics and modern theoretical physics.

Joseph-Louis Lagrange and the Principle of Least Action

Joseph-Louis Lagrange (1736-1813), born Giuseppe Luigi Lagrangia in Turin, Italy, became one of the greatest mathematicians of the 18th century. After moving to Berlin in 1766 to succeed Euler at the Prussian Academy of Sciences, Lagrange spent twenty productive years developing his revolutionary approach to mechanics. His masterwork, *Mécanique Analytique* (Analytical Mechanics), published in 1788, represented the culmination of decades of mathematical innovation.

Lagrange's key insight was to reformulate mechanics not through forces acting on particles but through a scalar energy function—the Lagrangian $\mathbf{L} = T - V$, where T is kinetic energy and V is potential energy. This deceptively simple definition enabled a complete reformulation of mechanics. The Euler-Lagrange equations:

$$\frac{d}{dt}\left(\frac{\partial \mathbf{L}}{\partial \dot{q}_j}\right) - \frac{\partial \mathbf{L}}{\partial q_j} = 0$$

derive all equations of motion from a single principle: the system follows the path that makes the action integral $S = \int \mathbf{L}\, dt$ stationary.

The philosophical foundation traces back to **Pierre de Fermat**'s principle of least time in optics (1662), extended by **Pierre Louis Maupertuis** to mechanics as the principle of least action (1744). **Leonhard Euler** formalized this variational approach mathematically, but Lagrange transformed it into a complete mechanical framework. The elegance of Lagrangian mechanics lies in its coordinate independence: the same formalism applies equally in Cartesian, polar, spherical, or any generalized coordinates, automatically incorporating all constraints without explicit constraint forces.

William Rowan Hamilton and the Hamiltonian Formulation

Sir William Rowan Hamilton (1805-1865), the Irish mathematician and physicist, extended Lagrange's work in ways that would prove transformative for quantum mechanics. Appointed Astronomer Royal of Ireland at age 22 while still an undergraduate, Hamilton contributed groundbreaking work in optics, developing a wave theory that unified ray optics through his characteristic function—work that later inspired Schrödinger's approach to quantum mechanics.

In the 1830s, Hamilton reformulated classical mechanics by introducing conjugate momenta $p_j = \partial \mathbf{L}/\partial \dot{q}_j$ and constructing the Hamiltonian function:

$$\mathbf{H}(q,p) = \sum_j p_j \dot{q}_j - \mathbf{L}(q,\dot{q})$$

This Legendre transformation converts the Lagrangian's second-order differential equations in coordinates into Hamilton's first-order equations in phase space:

$$\dot{q}_j = \frac{\partial \mathbf{H}}{\partial p_j}, \quad \dot{p}_j = -\frac{\partial \mathbf{H}}{\partial q_j}$$

Hamilton's formulation revealed a profound symmetry between position and momentum, treating them as equal partners in phase space (q,p). This symmetry proves essential for quantum mechanics, where q and p become operators satisfying $[\hat{q},\hat{p}] = i\hbar$—canonical quantization directly translates Poisson brackets $\{q,p\} = 1$ into commutators.

The Hamiltonian and Energy

A subtle but crucial point: the Hamiltonian does not always equal the total energy. For time-independent systems with kinetic energy quadratic in velocities and potentials independent of velocity, the Hamiltonian coincides with $E = T + V$. However, for time-dependent systems or velocity-dependent potentials (such as charged particles in electromagnetic fields), $\mathbf{H}$ and E differ. In quantum mechanics, this distinction becomes critical: the Hamiltonian $\hat{H}$ generates time evolution through Schrödinger's equation regardless of whether it equals the total energy operator.

Phase Space and Canonical Transformations

Hamilton's phase space formulation introduced concepts essential for statistical mechanics and quantum theory. The trajectory of a system becomes a curve in (q,p) phase space, and the Hamiltonian defines a flow—Hamilton's equations describe how phase space points evolve. Liouville's theorem (1838) established that this flow preserves phase space volume, a precursor to quantum mechanical probability conservation.

Canonical transformations—coordinate changes $(q, p) \to (Q, P)$ that preserve Hamilton's equation form—revealed that many different Hamiltonians can describe the same physics. This transformation theory directly inspired Dirac's approach to quantum mechanics, where unitary transformations rotate between equivalent quantum descriptions (Schrödinger vs. Heisenberg pictures).

The Bridge to Quantum Mechanics

The transition from classical to quantum mechanics occurred primarily through Hamiltonian rather than Lagrangian formulation. Several features made Hamilton's approach quantum-ready:

- **Conjugate variables**: The (q, p) pairs translate directly into non-commuting operators $(\hat{q}, \hat{p})$
- **Poisson brackets**: Classical $\{A, B\} = \sum_j \left(\frac{\partial A}{\partial q_j}\frac{\partial B}{\partial p_j} - \frac{\partial A}{\partial p_j}\frac{\partial B}{\partial q_j}\right)$ become quantum commutators $[\hat{A}, \hat{B}] = i\hbar\{\hat{A}, \hat{B}\}_{\text{Poisson}}$
- **Energy as generator**: Just as the classical Hamiltonian generates time evolution via $\dot{A} = \{A, H\}$, the quantum Hamiltonian generates it via $\frac{d\hat{A}}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{A}]$
- **Hamilton-Jacobi equation**: Hamilton's work on the characteristic function and wave fronts directly inspired Schrödinger's wave mechanics

When Schrödinger sought a wave equation for matter waves in 1926, he started from Hamilton-Jacobi theory—the classical limit of wave mechanics. His equation $i\hbar\partial\psi/\partial t = \hat{H}\psi$ places the Hamiltonian at the center of quantum dynamics, making Hamilton's 19th-century formalism indispensable for 21st-century quantum computing.

Modern Relevance to Quantum Computing

Hamiltonian formulation remains central to quantum computing for practical reasons:
Quantum gate implementation: Physical quantum gates are implemented by applying time-dependent Hamiltonians for specific durations. A rotation gate $R_z(\theta)$ on a qubit, for instance, corresponds to evolution under $\hat{H} = \frac{\theta}{2t}\sigma_z$ for time t.
Adiabatic quantum computing: This paradigm explicitly evolves a quantum system along a slowly varying Hamiltonian path $\hat{H}(s)$ from $s = 0$ to $s = 1$, where the ground state of $\hat{H}(1)$ encodes the solution to a computational problem.

Quantum simulation: The primary application of near-term quantum computers is simulating other quantum systems' Hamiltonian evolution—directly exploiting the Hamiltonian formalism for computational advantage.
Variational quantum algorithms: These optimize parameterized quantum circuits to find ground states of problem Hamiltonians, combining classical optimization with quantum Hamiltonian dynamics.
The 19th-century work of Lagrange and Hamilton thus provides not merely historical background but the active mathematical framework within which quantum computers operate. Their reformulation of mechanics through energy functions and phase space structures translated seamlessly into quantum mechanics and now enables the algorithms and hardware architectures of quantum computing.

We will proceed to summarize and connect the Lagrangian formulation with the Hamiltonian formulation, from which we will introduce Schrödinger's equation.

1.4 Hamiltonian Formulation of Classical Physics

The Hamiltonian description, developed by Sir William Rowan Hamilton (1805 - 1865), an Irish mathematician whose contributions encompassed optics, dynamics and the theory of complex numbers and quaternions, represents a profound and elegant reformulation of classical mechanics. His work was crucial for the development of quantum mechanics, especially in the matrix formulation proposed by Heisenberg, Pauli and Jordan, which we discussed in previous sections.

Consider a physical system with d degrees of freedom, whose position is described by generalized coordinates $q = (q_1, \ldots, q_d)^T$. The system's Lagrangian, $\mathbf{L}$, is defined as:

$$\mathbf{L} = \mathbf{T} - \mathbf{U}, \tag{1.6}$$

where $\mathbf{T} = \mathbf{T}(q, \dot{q})$ represents kinetic energy and $\mathbf{U} = \mathbf{V} = \mathbf{U}(q)$ is the system's potential energy. The system's dynamic evolution is described by the Euler-Lagrange equations, which are derived from the stationarity condition of the action functional $S(q)$:

$$\frac{d}{dt}\left(\frac{\partial \mathbf{L}}{\partial \dot{q}_j}\right) - \frac{\partial \mathbf{L}}{\partial q_j} = 0, \tag{1.7}$$

where action $S(q)$ is defined as:

$$S(q) = \int_a^b \mathbf{L}(q(t), \dot{q}(t))\, dt, \tag{1.8}$$

and must reach a minimum, according to the variational principle.

Hamilton simplified this structure, transforming the Euler-Lagrange equations into a system of first-order equations with more evident symmetry, known as Hamilton's equations. The **Hamiltonian**, **H**, is a scalar function that, under certain conditions (such as in a conservative system), coincides with the system's total energy, that is, the sum of kinetic energy and potential energy. However, this coincidence does not occur in all systems [8] [10].

The Hamiltonian is a function of position variables q and conjugate momenta p, also called *generalized momenta*. The conjugate momentum is defined as:

$$p_k = \frac{\partial \mathbf{L}}{\partial \dot{q}_k}(q, \dot{q}), \tag{1.9}$$

where p_k is the momentum associated with coordinate q_k.

The Hamiltonian is defined as:

$$\mathbf{H}(q,p) := p^T \dot{q} - \mathbf{L}(q, \dot{q}), \tag{1.10}$$

where q represents the generalized coordinates and p the conjugate momenta. Lagrange's equations can be reformulated as Hamilton's equations:

$$\dot{p}_k = -\frac{\partial \mathbf{H}}{\partial q_k}(p, q), \tag{1.11}$$

$$\dot{q}_k = \frac{\partial \mathbf{H}}{\partial p_k}(p, q). \tag{1.12}$$

and

$$\dot{q}_k = \frac{\partial \mathbf{H}}{\partial p_k}(p, q). \tag{1.13}$$

In quantum mechanics, the Hamiltonian concept acquires a different interpretation. While in classical mechanics the Hamiltonian is a function defined in the system's phase space, in quantum mechanics it is represented as a linear operator acting on elements of Hilbert space, governing the system's temporal evolution through Schrödinger's equation. This transition from classical function to quantum operator is fundamental to understanding the dynamics of quantum systems and will be developed in detail in subsequent sections.

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The Hamiltonian in Quantum Computing

The Hamiltonian's role in quantum computing extends beyond its theoretical importance as the energy operator. In quantum circuits, the Hamiltonian generates the time evolution of quantum states through the unitary operator $\mathbf{U}(t) = e^{-i\hat{H}t/\hbar}$. Every quantum gate—whether a single-qubit rotation, a controlled-NOT, or a multi-qubit entangling operation—can be expressed as the exponential of some Hamiltonian acting for a specific duration. The Hadamard gate, for instance, corresponds to evolving under the Hamiltonian $\hat{H} = \frac{\pi}{2t}(\sigma_x + \sigma_z)$ for time t. Understanding which Hamiltonians are physically implementable on specific quantum hardware platforms (superconducting qubits, trapped ions, photonic systems) determines which quantum gates are native to that architecture and which must be decomposed into sequences of native operations.

Quantum algorithms often exploit Hamiltonian evolution directly. The quantum phase estimation algorithm, central to Shor's factoring and quantum simulation, measures eigenvalues of unitary operators $e^{-i\hat{H}t}$ to extract energy spectra. Variational quantum algorithms parameterize Hamiltonians to solve optimization problems, where the ground state of a problem Hamiltonian encodes the solution. Quantum annealing evolves a system from an easy-to-prepare initial Hamiltonian to a final problem Hamiltonian whose ground state solves the computational task. Adiabatic quantum computation formalizes this approach, guaranteeing that sufficiently slow Hamiltonian evolution maintains the system in its instantaneous ground state. In all these applications, the Hamiltonian is not merely a mathematical abstraction but the physical mechanism through which quantum computers perform calculations, making Hamilton's 19th-century formulation surprisingly relevant to 21st-century quantum technology.

1.5 Schrödinger's Equation

1.5.1 Historical Context and Motivation

Erwin Rudolf Josef Alexander Schrödinger (1887-1961) shared the Nobel Prize in Physics in 1933 with Paul Dirac, in recognition of their fundamental contributions to the development of quantum mechanics. Schrödinger's work built upon Louis de Broglie's 1924 hypothesis of wave-particle duality, which proposed that all matter exhibits both wave and particle properties. In 1926, Schrödinger published his seminal article in *Annalen der Physik* addressing the quantization of atomic systems [14], culminating in the wave equation that now bears his name.

The path to Schrödinger's equation combined several revolutionary insights from early quantum theory. Max Planck's 1900 quantization of electromagnetic energy $E = h\nu$ resolved the ultraviolet catastrophe in black body radiation. Albert Einstein's 1905 explanation of the photoelectric effect established that light consists of energy quanta (photons) with $E = \hbar\omega$, where $\omega = 2\pi\nu$ is angular frequency and $\hbar = h/2\pi$ is the reduced Planck constant [7]. Louis de Broglie's 1924 doctoral thesis proposed the converse: particles possess wave characteristics with wavelength $\lambda = h/p$, where p is momentum [3]. Schrödinger synthesized these ideas into a differential equation describing matter waves, providing a complete framework for calculating atomic spectra, molecular structures, and quantum dynamics.

1.5.2 Heuristic Motivation of the Schrödinger Equation

Unlike Newton's second law or Maxwell's equations, the Schrödinger equation cannot be *derived* from more fundamental classical laws: it is a postulate of quantum mechanics, justified ultimately by the agreement of its predictions with experiment. Nevertheless, Schrödinger was guided to it by a compelling analogy with wave physics, combined with the de Broglie and Einstein relations. We reproduce here a heuristic argument, in the spirit of that reasoning, that makes the form of the equation plausible. It should be read as a motivation, not a proof.

The starting point is de Broglie's hypothesis that a free particle of definite momentum p and energy E is associated with a plane matter wave. Using the Einstein relation $E = \hbar\omega$ and the de Broglie relation $p = \hbar k$ (with $\omega = 2\pi\nu$ the angular frequency, $k = 2\pi/\lambda$ the wave number, and $\hbar = h/2\pi$ the reduced Planck constant), this wave can be written as

$$\psi(x,t) = A\, e^{\frac{i}{\hbar}(px - Et)}. \tag{1.14}$$

Taking the second derivative with respect to position isolates the momentum:

$$\frac{\partial^2\psi(x,t)}{\partial x^2} = -\frac{p^2}{\hbar^2}\,\psi(x,t) \quad\Longrightarrow\quad -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} = \frac{p^2}{2m}\,\psi(x,t), \tag{1.15}$$

while the first derivative with respect to time isolates the energy:

$$i\hbar\,\frac{\partial\psi(x,t)}{\partial t} = E\,\psi(x,t). \tag{1.16}$$

For a non-relativistic free particle the energy is purely kinetic, $E = p^2/2m$. Comparing the two expressions above, the right-hand sides coincide, and we obtain the free-particle Schrödinger equation in one dimension:

$$i\hbar\,\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}. \tag{1.17}$$

Notice that the equation is *first order* in time—in contrast to the classical wave equation of optics and electromagnetism, which is second order in time. This difference is not incidental: it reflects that the quantum state ψ, together with the single time derivative, already determines the future evolution, and it is intimately tied to the complex-valued nature of ψ. (Had we instead imposed the relativistic relation $E^2 = p^2c^2 + m^2c^4$ on the same plane wave, we would have arrived at the second-order Klein–Gordon equation rather than the Schrödinger equation.)

Generalizing to three dimensions, $\partial^2/\partial x^2 \to \nabla^2$, and adding a potential energy $V(\vec{r},t)$ so that the total energy becomes $E = p^2/2m + V$, we arrive at the full time-dependent Schrödinger equation:

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t) \right] \psi(\vec{r},t). \tag{1.18}$$

The operator in brackets is the Hamiltonian $\hat{H}$, representing the total energy of the system, which we examine in detail in the next sections.

1.5.3 Time-Dependent Schrödinger Equation

The time-dependent Schrödinger equation is the most general form of this fundamental equation in quantum mechanics. As derived in the previous section, the equation describes how the quantum state of a system evolves over time:

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t) \right] \psi(\vec{r},t) \tag{1.19}$$

In this equation, the left-hand term, $i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t}$, represents the temporal evolution of quantum state $\psi(\vec{r},t)$. The right side contains the Hamiltonian operator, $\hat{H}$, which encapsulates the system's total energy, both kinetic and potential:

$$\hat{H} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t) \right] \tag{1.20}$$

The time-dependent Schrödinger equation can be rewritten in terms of the Hamiltonian as:

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \hat{H}\psi(\vec{r},t) \tag{1.21}$$

This formulation is fundamental for describing the dynamics of a simple non-relativistic particle. In it, the wave function $\psi(\vec{r},t)$ provides all possible information about the system's state, and its temporal evolution is completely determined by the Hamiltonian $\hat{H}$.

The wavefunction $\psi(\vec{r},t)$ contains complete information about the particle's quantum state at each instant. Its squared modulus $|\psi(\vec{r},t)|^2$ gives the probability density for finding the particle at position $\vec{r}$ at time t, consistent with Born's rule introduced in Chapter 2.

The Hamiltonian operator $\hat{H}$ generates time evolution. For time-independent Hamiltonians $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$, the formal solution is:

$$\psi(\vec{r},t) = e^{-i\hat{H}t/\hbar}\psi(\vec{r},0) = \hat{U}(t)\psi(\vec{r},0), \tag{1.22}$$

where $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$ is the unitary time-evolution operator. This exponential operator, while formal, underlies quantum circuit dynamics: quantum gates implement finite-time evolution under specific Hamiltonians. The unitarity of

$\hat{U}(t)$ ensures probability conservation: $\int |\psi(\vec{r},t)|^2 d^3r$ remains constant, reflecting the fact that the particle must be found somewhere with total probability one.

For systems with explicitly time-dependent Hamiltonians $\hat{H}(t)$—common in quantum control and gate implementations—the time evolution becomes more complex, generally requiring time-ordered exponentials. Quantum optimal control exploits time-dependent Hamiltonians to steer quantum states along desired trajectories while minimizing errors and decoherence.

1.5.4 Time-Independent Schrödinger Equation

The time-independent Schrödinger equation describes wave functions in the form of stationary waves. This equation is applicable only when the system's Hamiltonian does not explicitly depend on time. The form of the equation is:

$$E\psi = \hat{H}\psi \tag{1.23}$$

When the Hamiltonian operator $\hat{H}$ acts on a wave function ψ, the result is proportional to the same wave function, indicating that ψ is a stationary state. The proportionality constant is the energy of state ψ, denoted by E.

This equation is an eigenvalue equation, where E represents the eigenvalues associated with the system's quantum states. When the Hamiltonian has no explicit time dependence, $\hat{H} = \hat{H}(\vec{r})$, we can separate variables by writing $\psi(\vec{r},t) = \phi(\vec{r})T(t)$. Substituting into the time-dependent equation yields:

$$i\hbar\phi(\vec{r})\frac{dT(t)}{dt} = T(t)\hat{H}\phi(\vec{r}), \tag{1.24}$$

$$\frac{i\hbar}{T}\frac{dT}{dt} = \frac{1}{\phi}\hat{H}\phi = E, \tag{1.25}$$

where E is a separation constant with dimensions of energy. The temporal part gives $T(t) = e^{-iEt/\hbar}$, while the spatial part yields the time-independent Schrödinger equation:

$$\hat{H}\phi(\vec{r}) = E\phi(\vec{r}). \tag{1.26}$$

This eigenvalue equation determines the allowed energy levels E_n and corresponding stationary states $\phi_n(\vec{r})$. These eigenstates have the crucial property that their time evolution consists only of a phase factor:

$$\psi_n(\vec{r},t) = \phi_n(\vec{r})e^{-iE_nt/\hbar}. \tag{1.27}$$

The probability density $|\psi_n(\vec{r},t)|^2 = |\phi_n(\vec{r})|^2$ is time-independent, justifying the term "stationary state." All measurable properties (position expectation values, momentum distributions) remain constant for a system in an energy eigenstate.

In one dimension, the time-independent Schrödinger equation is written as:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \tag{1.28}$$

By solving this equation, it follows that the particle's energy is quantized, and is given by:

$$E = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2 \tag{1.29}$$

where $n = 1, 2, 3, \ldots$.

This result indicates that if an electron is confined in a small box, its wave properties can be calculated, and Schrödinger's equation predicts the existence of discrete energy levels for the electron. For a particle in a one-dimensional box of length L with infinite potential walls, solving equation (1.26) with boundary conditions $\phi(0) = \phi(L) = 0$ yields:

$$\phi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), \quad n = 1, 2, 3, \ldots, \tag{1.30}$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}. \tag{1.31}$$

Energy quantization emerges naturally from boundary conditions, demonstrating why confined quantum systems possess discrete energy spectra. This principle underlies atomic energy levels, molecular orbital structures, and quantum dot confinement—all exploited in various quantum computing platforms.

1.5.5 Modern Formulation of Schrödinger's Equation

In the modern formulation of quantum mechanics, Dirac notation is used to describe the state of a quantum system at time t, denoted as $|\psi(t)\rangle$ in a complex Hilbert space. This state $|\psi(t)\rangle$ encapsulates all the necessary information to calculate the probabilities of possible measurement results performed on the system.

The temporal evolution of the quantum state is governed by Schrödinger's equation, which in its modern form is expressed as:

$$\hat{H}\,|\psi(t)\rangle = i\hbar\frac{d}{dt}\,|\psi(t)\rangle = \left(\frac{\hat{P}^2}{2m} + V(\hat{\vec{r}}, t)\right)|\psi(t)\rangle \tag{1.32}$$

In this equation, $\hat{H}$ is the Hamiltonian operator, which can generally depend on time and represents the observable corresponding to the system's total energy. $\hat{\vec{r}}$ is the position operator, and $\hat{P}$ is the momentum or impulse operator. These operators, together with state $|\psi(t)\rangle$, completely define the quantum system's dynamics.

In the modern formulation developed by Dirac, quantum states are represented as vectors $|\psi(t)\rangle$ in a complex Hilbert space rather than wavefunctions

$\psi(\vec{r}, t)$. This abstract notation, introduced in Chapter 2, provides elegant generality and connects directly to matrix quantum mechanics. The time-dependent Schrödinger equation becomes:

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle , \tag{1.33}$$

where $\hat{H}$ is the Hamiltonian operator acting on Hilbert space vectors. For systems with discrete basis states—the natural setting for qubits—this formulation translates immediately to matrix equations. A single qubit state $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$ evolves under Hamiltonian $\hat{H}$ according to:

$$i\hbar \frac{d}{dt} \begin{bmatrix} \alpha(t) \\ \beta(t) \end{bmatrix} = \mathbf{H} \begin{bmatrix} \alpha(t) \\ \beta(t) \end{bmatrix} , \tag{1.34}$$

where $\mathbf{H}$ is the 2×2 matrix representation of the Hamiltonian in the computational basis. For multi-qubit systems with n qubits, the Hilbert space has dimension 2^n, and the Hamiltonian becomes a $2^n \times 2^n$ matrix.

The Dirac formulation emphasizes that Schrödinger's equation is fundamentally a statement about how quantum state vectors evolve, independent of any particular representation (position, momentum, energy, or computational basis). This basis-independence proves essential in quantum computing, where we frequently transform between different representations: computational basis for readout, eigenbasis of specific Hamiltonians for analysis, and rotated bases for implementing certain gates. The abstract formulation also clarifies that quantum evolution is linear and unitary, properties exploited throughout quantum algorithm design.

It is fundamental to understand that Schrödinger's equation is not derived from more basic principles; it is a fundamental postulate of quantum mechanics proposed by Schrödinger. This postulate was experimentally validated when Davisson and Germer confirmed Louis de Broglie's hypothesis about wave-particle duality, as well as by numerous experimental results that coincide with Schrödinger equation predictions.

However, this equation has its limitations. It is non-relativistic, which means it is only applicable to particles with relatively small linear momentum. To describe relativistic particles, more advanced equations are required, such as Dirac's equation or the Klein-Gordon equation. Another limitation is that Schrödinger's original equation does not incorporate particle spin. Wolfgang Pauli generalized this equation in what is known as Pauli's equation, which includes spin for spin-$\frac{1}{2}$ particles. Paul Dirac subsequently developed an equation that not only incorporates spin but is also consistent with relativity, known as Dirac's equation.

Schrödinger's equation is a vector-type equation, which means it can be rewritten in terms of a specific basis of the state space. Throughout this book, we will use both the standard basis and a computational basis to address specific problems in quantum computing.

While we derived Schrödinger's equation for specific systems (free particles, particles in potentials), a more general question arises: given any classical system described by positions and momenta, how do we systematically construct the corresponding quantum system? The answer lies in canonical quantization, the algorithmic procedure that transforms classical mechanics into quantum mechanics. This method, formalized by Paul Dirac in 1925, provides the bridge between the Hamiltonian formulation of classical mechanics—with its conjugate variables and Poisson brackets—and the operator formulation of quantum mechanics with commutators. Canonical quantization is not merely a mathematical trick but the systematic way to translate physical systems from classical to quantum descriptions, enabling us to derive quantum Hamiltonians for any system whose classical dynamics we understand.

1.6 Canonical Quantization

In his 1925 doctoral thesis, Paul Dirac showed that any system having a classical description can be quantized following a process called *canonical quantization*. This method allows obtaining a quantum description of the system from its classical dynamic variables, which describe the system's state at an instant of time t. These dynamic variables can include quantities such as energy, linear momentum, among others.

$$(q_1, q_2, \ldots, q_j; p_1, p_2, \ldots, p_j) \tag{1.35}$$

We know that these dynamic variables obey first-order differential equations in time (Euler formulation), which means that, if we know their values at an initial instant, we can predict their evolution at any future instant t, completely characterizing the system's behavior.

$$E(t) = \mathbf{H}(q_1, q_2, \ldots, q_j; p_1, p_2, \ldots, p_j) \tag{1.36}$$

Among all canonical variables, some play a special role: the so-called *conjugate variables*, such as the pairs (q_j, p_j), where q_j is the coordinate and p_j is the conjugate canonical momentum.

The canonical quantization process proposed by Dirac consists of replacing each classical variable and its conjugate with a pair of quantum operators $\hat{q}_j$ and $\hat{p}_j$ that do not commute, fulfilling the commutation relation:

$$[\hat{q}_j, \hat{p}_j] = i\hbar\mathbf{I} \tag{1.37}$$

In general terms, for a system with several canonical variables:

$$(q_j, p_j) \rightarrow [\hat{q}_j, \hat{p}_j] = i\hbar\delta_{ij} \tag{1.38}$$

In this way, we can describe the behavior of the quantum system associated with a classical Hamiltonian. Recall that a system's Hamiltonian is its energy expressed as a function of conjugate canonical variables. By replacing classical variables with their corresponding quantum operators, we obtain the system's quantum Hamiltonian, which represents quantized energy. With the quantum

Hamiltonian, it is possible to determine all quantum properties of the system using Dirac formalism:

$$\hat{\mathbf{H}} = \mathbf{H}(\hat{q_1}, \hat{q_2}, \ldots, \hat{q_j}; \hat{p_1}, \hat{p_2}, \ldots, \hat{p_j}) \tag{1.39}$$

We know that the system's quantized energies E_n are the Hamiltonian's eigenvalues, and that the corresponding states ϕ_n constitute an appropriate basis of the system's possible state space:

$$\hat{\mathbf{H}} \left|\phi_n\right\rangle = E_n \left|\phi_n\right\rangle \tag{1.40}$$

This is an eigenvalue and eigenstate equation that provides complete information about the system's possible states.

The time-independent Schrödinger equation, which we have discussed previously, is an example of how canonical quantization is applied. Additionally, the temporal evolution of a quantum system is described by a first-order differential equation based on the quantum Hamiltonian:

$$i\hbar \frac{d}{dt} \left|\psi(t)\right\rangle = \hat{\mathbf{H}} \left|\psi(t)\right\rangle \tag{1.41}$$

In canonical quantization, a fundamental question arises: How do we identify canonical conjugate variables in a classical system? In general, these are obtained from the system's Lagrangian. Although in this section we use the Hamiltonian approach, Hamilton's classical equations precisely describe the dynamics of classical systems.

$$\frac{dq_j}{dt} = \frac{\partial \mathbf{H}}{\partial p_j} \tag{1.42}$$

$$\frac{dp_j}{dt} = -\frac{\partial \mathbf{H}}{\partial q_j} \tag{1.43}$$

Classical Hamilton Equations for a Particle with Mass m

Consider a particle moving along the x axis with potential energy $U(x)$. The canonical position variable is $q = x$ and the conjugate canonical variable is $p = m\frac{dx}{dt}$. The system's total energy is the sum of potential energy $U(x)$ and kinetic energy $\frac{p^2}{2m}$, and the Hamiltonian is expressed as:

$$\mathbf{H} = U(x) + \frac{p^2}{2m} \tag{1.44}$$

Hamilton's equations are then written as:

$$\frac{dx}{dt} = \frac{\partial \mathbf{H}}{\partial p} = \frac{p}{m} \tag{1.45}$$

$$\frac{dp}{dt} = -\frac{\partial \mathbf{H}}{\partial x} = -\frac{\partial U}{\partial x} \tag{1.46}$$

These are Newton's equations of motion for a particle with mass m in one dimension, which confirms that the formalism is consistent and correct.

Canonical Quantization and Qubit systems

The canonical quantization procedure provides the systematic bridge from classical computing to quantum computing. In classical computation, bits are physical systems (transistor voltages, magnetic domains) described by classical variables with definite values 0 or 1. Quantum computing requires physical systems whose classical description involves conjugate variables (q, p) satisfying Hamiltonian dynamics. When canonically quantized, these variables become operators $(\hat{q}, \hat{p})$ with commutator $[\hat{q}, \hat{p}] = i\hbar$, enabling superposition states $\alpha |0\rangle + \beta |1\rangle$ that have no classical analog.

Superconducting qubits exemplify this quantization process. A superconducting circuit with capacitance C and inductance L has classical Hamiltonian $H = \frac{Q^2}{2C} + \frac{\Phi^2}{2L}$, where Q is charge and Φ is magnetic flux. These conjugate variables satisfy $\{Q, \Phi\} = 1$ in classical Poisson brackets. Canonical quantization promotes them to operators $(\hat{Q}, \hat{\Phi})$ with $[\hat{Q}, \hat{\Phi}] = i\hbar$, and the quantum Hamiltonian $\hat{H} = \frac{\hat{Q}^2}{2C} + \frac{\hat{\Phi}^2}{2L}$ describes a quantum harmonic oscillator. The lowest two energy eigenstates $|0\rangle$ and $|1\rangle$ form the qubit computational basis. Josephson junctions introduce nonlinearity that breaks the harmonic spectrum, isolating these two levels from higher excitations and enabling addressable two-level quantum systems.

Similarly, trapped ion qubits quantize the ion's motional degrees of freedom and internal electronic states. Photonic qubits quantize electromagnetic field modes, with creation and annihilation operators $\hat{a}^\dagger$ and $\hat{a}$ governing photon number states. Spin qubits in quantum dots quantize electron spin, a purely quantum degree of freedom with no classical counterpart. In every case, canonical quantization transforms the classical physics of the hardware platform into quantum operators whose matrix elements determine qubit Hamiltonians, gate implementations, and error mechanisms. The commutation relations $[\hat{q}_i, \hat{p}_j] = i\hbar\delta_{ij}$ are not merely mathematical abstractions but encode the fundamental non-commutativity underlying quantum interference, entanglement, and computational speedup.

Schrödinger's Equation for a Particle with Mass m Moving in One Dimension

The classical Hamiltonian for a particle of mass m moving in one dimension is expressed as:

$$\mathbf{H} = U(x) + \frac{p^2}{2m}, \tag{1.47}$$

where $U(x)$ is the potential energy and p is the particle's linear momentum. Following Dirac's approach in his 1925 thesis, we can quantize this Hamiltonian to obtain its quantum version:

$$\hat{H} = U(x) + \frac{\hat{p}^2}{2m}, \tag{1.48}$$

where $\hat{p}$ is the momentum operator, and the canonical conjugate variables satisfy the commutation relation $[\hat{x}, \hat{p}] = i\hbar$.

To express Schrödinger's equation describing this particle's wave function temporal evolution, we consider the representation of the momentum operator in position space:

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}. \tag{1.49}$$

Substituting this operator into the quantum Hamiltonian, we obtain the time-dependent Schrödinger equation for wave function $\psi(x,t)$:

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \left(U(x) - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\psi(x,t). \tag{1.50}$$

This equation is fundamental in the study of quantum mechanics, as it allows calculating stationary states and energy levels in systems such as potential wells and atoms, with the hydrogen atom being one of the best-known examples in the first course of quantum mechanics.

Now, an interesting question arises: Why are position x and velocity v not canonical conjugate variables? To answer this, let's consider the following expressions:

$$q = x, \quad p = mv, \quad H = U(x) + \frac{1}{2}mv^2.$$

Let's write the corresponding Hamilton equations:

$$\frac{dq_j}{dt} = \frac{\partial \mathbf{H}}{\partial p_j} \to \frac{dx}{dt} = \frac{\partial \mathbf{H}}{\partial v} = mv, \tag{1.51}$$

$$\frac{dp_j}{dt} = -\frac{\partial \mathbf{H}}{\partial q_j} \to \frac{dp}{dt} = -\frac{\partial \mathbf{H}}{\partial x} = -\frac{\partial U}{\partial x}. \tag{1.52}$$

These are not Newton's equations for a particle in motion, which demonstrates that x and v are not canonical conjugate variables. Instead, x and $p = mv$ are the appropriate conjugate variables, as established by the commutation relation $[\hat{x}, \hat{p}] = i\hbar$.

1.6.1 Matrix Quantum Mechanics

Matrix quantum mechanics, initially proposed by Werner Heisenberg in 1925, represents one of the most significant advances in understanding quantum phenomena. Heisenberg's insight—representing physical observables as matrices rather than functions—proved revolutionary not only for theoretical physics but also, decades later, for practical quantum computing. Where Schrödinger's wave mechanics describes continuous probability distributions $|\psi(x)|^2$ over infinite-dimensional spaces, matrix quantum mechanics operates on finite-dimensional vector spaces with discrete bases. A quantum system with N distinguishable states inhabits an N-dimensional Hilbert space $\mathbb{C}^N$, where states are column vectors and observables are $N \times N$ matrices—precisely the mathematical structure underlying quantum circuits and quantum algorithms.

For quantum computing, matrix formulation is not merely an alternative perspective but the natural language. A single qubit occupies $\mathbb{C}^2$ with computational basis $\{|0\rangle, |1\rangle\}$, represented as column vectors $|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$. Quantum gates are 2×2 unitary matrices: the Pauli-X gate $\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ flips computational basis states, the Hadamard gate $H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ creates superpositions, and phase gates $R_\phi = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix}$ manipulate relative phases. Two-qubit systems inhabit $\mathbb{C}^4$ with basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, and two-qubit gates are 4×4 unitary matrices. The CNOT gate, essential for creating entanglement, is the 4×4 permutation matrix that flips the target qubit when the control qubit is $|1\rangle$.

Heisenberg's equations of motion, derived from matrix commutators, determine how quantum gates transform states. The time evolution operator $\mathbf{U}(t) = e^{-i\hat{H}t/\hbar}$, expressed as a matrix exponential, generates quantum circuit dynamics. Matrix diagonalization—finding eigenvalues and eigenvectors—corresponds physically to measuring observables and projecting onto eigenstates. The eigenvalue decomposition central to Chapter 2's mathematical foundations translates directly into quantum measurement outcomes. Quantum algorithms manipulate these matrices through carefully designed sequences: quantum Fourier transforms implement discrete Fourier matrix products, Grover's algorithm applies specific unitary reflections, and variational algorithms optimize parameterized unitary circuits. The algebraic structure of matrix quantum mechanics—commutation relations, unitary groups, spectral decomposition—provides not merely mathematical formalism but the practical toolkit for designing, analyzing, and implementing quantum computations on physical hardware.

This matrix formulation is particularly well-suited to quantum computing because quantum circuits operate on discrete, finite-dimensional quantum systems. While Schrödinger's wave functions require integration over continuous position spaces, matrix quantum mechanics involves only linear algebra: matrix multiplication for gate sequences, matrix diagonalization for eigenvalue problems, and matrix exponentiation for time evolution. Modern quantum computing software (Qiskit, Cirq, Q#) represents quantum states as complex vectors and quantum gates as unitary matrices, simulating quantum circuits through matrix operations. Understanding matrix quantum mechanics is therefore not optional background but essential preparation for quantum algorithm development, quantum circuit optimization, and quantum error correction—all of which fundamentally manipulate matrices in complex Hilbert spaces.

Currently, matrix quantum mechanics is one of the most successful and widely used interpretations in various areas of modern physics, from quantum computing to particle physics. Its ability to accurately describe the dynamics of quantum systems and predict experimental results with high accuracy has been crucial in the development of advanced quantum technologies. Additionally, the algebraic structure inherent to this formulation has allowed extending concepts to fields such as random matrix theory and statistical physics. Matrix quantum mechanics has not only stood the test of time, but has also proven to be an indispensable tool in exploring the fundamental nature of reality, consolidating its position as a cornerstone in contemporary physics.

1.6.2 Schrödinger's Equation in Matrix Quantum Mechanics

In matrix quantum mechanics, Schrödinger's equation is expressed using matrix operators that act on state vectors in a Hilbert space. Instead of continuous wave functions, quantum states are represented by vectors, and observables, such as energy, momentum and position, are represented by matrices. Schrödinger's equation in this formalism continues to describe the temporal evolution of the quantum state, but does so in terms of matrices.

The time-dependent Schrödinger equation in its general form is:

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

In matrix quantum mechanics, this translates to:

$$i\hbar \frac{\partial}{\partial t} \boldsymbol{\Psi}(t) = \mathbf{H} \boldsymbol{\Psi}(t)$$

Here, $\boldsymbol{\Psi}(t)$ is a column vector (quantum state) in a finite-dimensional Hilbert space, and $\mathbf{H}$ is the Hamiltonian operator represented as a matrix.

1.6.3 Example: Quantum Harmonic Oscillator

Consider a quantum harmonic oscillator in a Hilbert space of dimension n, where the Hamiltonian is given by:

$$\mathbf{H} = \hbar\omega \left(\mathbf{a}^{\dagger}\mathbf{a} + \frac{1}{2}\mathbf{I} \right)$$

Here, $\mathbf{a}^{\dagger}$ and $\mathbf{a}$ are the creation and destruction operators, respectively, and $\mathbf{I}$ is the identity matrix. The quantum state $\mathbf{\Psi}(t)$ can be expressed in the number state basis as:

$$\mathbf{\Psi}(t) = \sum_{n=0}^{\infty} c_n(t) \, |n\rangle$$

Where $|n\rangle$ are the eigenvectors of $\mathbf{a}^{\dagger}\mathbf{a}$, and $c_n(t)$ are temporal coefficients that indicate the probability amplitude that the system is in state n at time t.

The matrix Schrödinger equation for this system is:

$$i\hbar \frac{\partial}{\partial t} \mathbf{\Psi}(t) = \hbar\omega \left(\mathbf{a}^{\dagger}\mathbf{a} + \frac{1}{2}\mathbf{I} \right) \mathbf{\Psi}(t)$$

1.6.4 Solution for the Harmonic Oscillator Case

The solution of the equation for each base state $|n\rangle$ is:

$$c_n(t) = c_n(0) e^{-iE_n t/\hbar}$$

Where $E_n = \hbar\omega \left(n + \frac{1}{2} \right)$ are the eigenvalues of the Hamiltonian $\mathbf{H}$, which correspond to the energy levels of the harmonic oscillator.

In summary, Schrödinger's equation in matrix quantum mechanics uses matrices to represent operators and vectors to represent quantum states. This approach allows handling finite-dimensional systems in an algebraic way and is fundamental for applications in modern physics, such as quantum computing.

Having established that quantum states are vectors and their evolution follows Schrödinger's equation, we now address a crucial question for quantum computing: what mathematical structure governs how quantum states change in time? The answer determines not only how qubits evolve during quantum computations but also constrains which operations quantum computers can physically implement. The key insight is that time evolution must preserve the normalization of quantum states—if a state vector has unit length at one moment, it must retain unit length at all future moments, ensuring total probability remains one. This preservation requirement severely restricts the form of the time evolution operator, leading to the fundamental property of unitarity that underlies all quantum gate operations.

Temporal Evolution of Quantum States

In quantum mechanics, we start from a set of fixed system states, but it is essential to discuss in detail how time is considered in their evolution. Consider an initial state $|\psi\rangle$ that evolves in time toward a state $|\psi'\rangle$. We assume that there exists a linear relationship between both states, which can be expressed as:

$$|\psi'\rangle = \mathbf{U}\,|\psi\rangle \tag{1.53}$$

This relationship holds for some linear operator $\mathbf{U}$. The normalization condition, discussed in the previous chapter, must be preserved: $\langle\psi'|\psi'\rangle = \langle\psi|\psi\rangle = 1$. This condition imposes restrictions on the form that operator $\mathbf{U}$ must have. The corresponding equation for the dual state vector will be:

$$\langle\psi'| = \langle\psi|\,\mathbf{U}^\dagger \tag{1.54}$$

Combining these two equations, we obtain the fundamental restriction that this operator of temporal evolution of quantum states must satisfy:

$$\langle\psi'|\psi'\rangle = \left\langle\psi|\mathbf{U}^\dagger\mathbf{U}|\psi\right\rangle \tag{1.55}$$

Given the normalization condition, we conclude that:

$$\mathbf{U}^\dagger\mathbf{U} = \mathbf{I} \tag{1.56}$$

This defines that $\mathbf{U}$ is a unitary operator.

In quantum computing, qubit states are manipulated using sequences of unitary transformations. Since for a unitary operator it holds that its adjoint equals its inverse, that is, $\mathbf{U}^\dagger = \mathbf{U}^{-1}$, and that operator $\mathbf{U}^\dagger$ is well defined, then the inverse transformation, which converts the final state into the initial state, exists. According to this, we reach a fundamental conclusion: *quantum transformations are reversible.* The only exception to this rule occurs when the quantum system is coupled to an external macroscopic instrument that can induce irreversible changes.

The importance of this reversibility lies in the fact that, in classical computing, gates that manipulate bits are irreversible, while in quantum computers, operations are reversible, which represents a significant difference with respect to what we know in classical computing.

In summary, in quantum computing we act on qubits with a series of discrete unitary transformations. Thanks to the conditions imposed by these operations and normalization, they are guaranteed to be reversible.

What is the operator $\mathbf{U}$ responsible for the temporal evolution of the system? Let's start from the time-dependent Schrödinger equation:

$$i\hbar\frac{d}{dt}\,|\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle \tag{1.57}$$

For this calculation, let's assume $\hbar = 1$ and that operator $\hat{H}$ does not vary with time. Integrating the previous equation, we obtain:

$$|\psi(t)\rangle = \mathbf{U}(t)\,|\psi(0)\rangle \tag{1.58}$$

where $\mathbf{U}(t)$ is given by:

$$\mathbf{U}(t) = e^{-i\hat{H}t} \tag{1.59}$$

Since $\hat{H}$ is a Hermitian operator, we can write:

$$\mathbf{U}^{\dagger}(t) = e^{i\hat{H}t} \tag{1.60}$$

Finally, we can prove that:

$$\mathbf{U}^{\dagger}(t)\mathbf{U}(t) = e^{i\hat{H}t}e^{-i\hat{H}t} = \mathbf{I} \tag{1.61}$$

This demonstrates that the temporal evolution operator is unitary, which guarantees that quantum operations are reversible.

Operators

In quantum mechanics, physical quantities are not represented by functions of velocity, position or time, but by operators. We start from the definition of total energy of the system:

$$T + U = E \tag{1.62}$$

For the case of the harmonic oscillator, we have:

$$\frac{mv^2}{2} + \frac{p^2}{2m} = E \tag{1.63}$$

If we multiply the first equation by the wave function ψ, we obtain:

$$(T + U)\psi = E\psi \tag{1.64}$$

This equation is clearly equivalent to:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r},t)\right]\psi(\vec{r},t) = i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} \tag{1.65}$$

In one dimension, we can establish the following correspondence between functions and operators, mediated by the previous equation, as follows:

For energy:

$$\hat{E} = i\hbar\frac{\partial}{\partial t} \tag{1.66}$$

For momentum:

$$\hat{p} = -i\hbar\frac{\partial}{\partial x} \tag{1.67}$$

Potential energy functions are not replaced by operators; these remain functions that depend on the particular system.

In quantum mechanics, it is fundamental to speak of operators and expected values of the quantities involved in the system, such as position, momentum, energy, etc. The value expected to be obtained from a statistical experiment is called the expected value, or mathematical expectation. It is also called "mean". If p is the probability and n the number of events, the mean is $\mu = np$. This is the form of the mean when probability is expressed through a binomial distribution. In an experiment with discrete results x_i for which the probability is $P(x_i)$, the mean will be given by:

$$\mu = x_1 P(x_1) + x_2 P(x_2) + ... + x_n P(x_n) = \sum x_i P(x_i) \tag{1.68}$$

In the case of continuous variables, where probability is expressed in terms of a distribution function, the mean takes the form:

$$\mu = \langle x \rangle = \int x f(x) dx \tag{1.69}$$

In quantum mechanics, the expected value of position is defined as:

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x,t) x \psi(x,t) dx \tag{1.70}$$

This integral can be interpreted as the average value of x that we would expect to obtain from a large number of measurements, or as the average position value for a large number of particles described by the same wave function.

The expected value of momentum involves representing it as a quantum operator, thus:

$$\begin{aligned} \langle \hat{p} \rangle &= \int_{-\infty}^{\infty} \psi^*(x,t) \left(-i\hbar \frac{\partial}{\partial x} \right) \psi(x,t)\, dx \\ &= -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x}\, dx \end{aligned} \tag{1.71}$$

Finally, the expected value of any operator $\langle \hat{Q} \rangle$ in quantum mechanics will be:

$$\langle \hat{Q} \rangle = \int_{-\infty}^{\infty} \psi^*(x,t) \hat{Q} \psi(x,t) dx \tag{1.72}$$

In general, any operator $\hat{Q}$ can be written in terms of operators $\hat{p}$ and $\hat{x}$. For example, we can write operator $\hat{v}$ as follows:

$$\hat{v} = \frac{\hat{p}}{m} = \frac{-i\hbar}{m} \frac{\partial}{\partial x} \tag{1.73}$$

The expected value of velocity will then be:

$$\langle \hat{v} \rangle = \frac{-i\hbar}{m} \int_{-\infty}^{\infty} \psi^*(x,t) \frac{\partial \psi}{\partial x}(x,t) dx \tag{1.74}$$

Commutation Relations Between Operators

In mathematics, certain objects commute under operations such as addition or multiplication. For example, integers commute under addition and multiplication, and matrices commute under addition, but not necessarily under multiplication. In quantum mechanics, operators $\hat{x}$ (position) and $\hat{p}$ (momentum) do not commute with each other. Let's demonstrate this statement:

$$\hat{p}\hat{x}\psi = \hat{p}x\psi = -i\hbar\frac{\partial}{\partial x}(x\psi) = -i\hbar\left(\psi + x\frac{\partial\psi}{\partial x}\right) \tag{1.75}$$

On the other hand:

$$\hat{x}\hat{p}\psi = -i\hbar\hat{x}\frac{\partial\psi}{\partial x} = -i\hbar x\frac{\partial\psi}{\partial x} \tag{1.76}$$

From here, we conclude that $\hat{p}\hat{x} \neq \hat{x}\hat{p}$. To formalize this difference, we define the commutator of two mathematical operators A and B as:

$$[A, B] = AB - BA \tag{1.77}$$

If two mathematical operators commute, then the commutator defined above will be null, that is, $[A, B] = 0$. For example, if we take two numbers under addition: $[4, 5] = (4 + 5) - (5 + 4) = 9 - 9 = 0$. In the case of multiplication, we can prove it thus: $[4, 5] = (4 \times 5) - (5 \times 4) = 20 - 20 = 0$.

An interesting property of the commutator is:

$$[A, B] = -[B, A] \tag{1.78}$$

Now, we are interested in calculating the value of commutator $[\hat{x}, \hat{p}]$. In classical mechanics, momentum and position functions commute; let's see what happens in quantum mechanics:

$$\begin{aligned}
[\hat{x}, \hat{p}]\psi &= (\hat{x}\hat{p} - \hat{p}\hat{x})\psi \\
&= -i\hbar\, x\frac{\partial\psi}{\partial x} + i\hbar\left(\psi + x\frac{\partial\psi}{\partial x}\right) \\
&= i\hbar\psi
\end{aligned} \tag{1.79}$$

Canceling ψ on both sides of the equation, we obtain:

$$[\hat{x}, \hat{p}] = i\hbar \tag{1.80}$$

In quantum mechanics, commutators play an essential role. The essence of quantum mechanics lies in the nature of these operators and their commutation relations. There are formulations of quantum mechanics that begin with commutation relations and, from them, define the operators, while other formulations follow the opposite approach, beginning with operators and deriving commutation relations.

1.6.5 Solution of the Harmonic Oscillator Using Operators

Schrödinger's equation for the oscillator in one dimension is written as:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x,t)}{dx^2}+\frac{m\omega^2x^2\psi}{2}=E\psi \tag{1.81}$$

In terms of the Hamiltonian, the previous equation can be written as:

$$\hat{\mathbf{H}}\psi=\mathbf{E}\psi \tag{1.82}$$

The Hamiltonian for a classical particle of mass m moving as a harmonic oscillator with frequency ω in generalized coordinates is given by:

$$\mathbf{H}=\frac{p^2}{2m}+\frac{m\omega^2x^2}{2} \tag{1.83}$$

Finding a combination similar to the Hamiltonian relations, but in terms of operators, would be advantageous. This is exactly what we will do in this section: we will take a classic problem of quantum mechanics, such as the harmonic oscillator, and find the operators and their solution using notation that will be useful in the topic of quantum computing.

We define operators $\hat{\mathbf{a}}$ and $\hat{\mathbf{a}}^\dagger$ as follows:

$$\hat{\mathbf{a}}=\frac{1}{\sqrt{2m\hbar\omega}}\left(m\omega\hat{x}+i\hat{p}\right), \tag{1.84}$$

$$\hat{\mathbf{a}}^\dagger=\frac{1}{\sqrt{2m\hbar\omega}}\left(m\omega\hat{x}-i\hat{p}\right). \tag{1.85}$$

We note that $\hat{\mathbf{a}}^\dagger$ is the Hermitian adjoint (conjugate transpose) of $\hat{\mathbf{a}}$, not merely its complex conjugate; the two operators do not commute, as we verify below. Neither $\hat{\mathbf{a}}$ nor $\hat{\mathbf{a}}^\dagger$ is Hermitian individually, so they are not observables, but the combination $\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}}$ is Hermitian and has real eigenvalues.

Now, let's invert the operators in terms of $\hat{x}$ and $\hat{p}$:

$$\hat{\mathbf{x}}=\sqrt{\frac{\hbar}{2m\omega}}(\hat{\mathbf{a}}+\hat{\mathbf{a}}^\dagger), \tag{1.86}$$

$$\hat{\mathbf{p}}=i\sqrt{\frac{m\hbar\omega}{2}}(\hat{\mathbf{a}}^\dagger-\hat{\mathbf{a}}). \tag{1.87}$$

In this way, it can be seen that operators $\hat{\mathbf{a}}^\dagger$ and $\hat{\mathbf{a}}$ do not commute. Using the commutation relation $[\hat{\mathbf{x}},\hat{\mathbf{p}}]=i\hbar$, it can be demonstrated that $[\hat{\mathbf{a}},\hat{\mathbf{a}}^\dagger]=1$.

The Hamiltonian can be written in three different forms using the previous relation:

$$\hat{\mathbf{H}}=\frac{1}{2}(\hat{\mathbf{a}}\hat{\mathbf{a}}^\dagger+\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}})\hbar\omega=\left(\hat{\mathbf{a}}\hat{\mathbf{a}}^\dagger-\frac{1}{2}\right)\hbar\omega=\left(\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}}+\frac{1}{2}\right)\hbar\omega. \tag{1.88}$$

In terms of operators, Schrödinger's equation for the harmonic oscillator can be written in the following two forms:

$$(\hat{\mathbf{a}}\hat{\mathbf{a}}^\dagger - \frac{1}{2})\hbar\omega\psi = E\psi, \tag{1.89}$$

$$(\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}} + \frac{1}{2})\hbar\omega\psi = E\psi. \tag{1.90}$$

Here we must be careful: multiplying the previous equation by operator $\hat{\mathbf{a}}^\dagger$ does not produce Schrödinger's equation, let's see:

$$(\hat{\mathbf{a}}\hat{\mathbf{a}}^\dagger - \frac{1}{2})\hbar\omega\hat{\mathbf{a}}^\dagger\psi \neq E\hat{\mathbf{a}}^\dagger\psi \tag{1.91}$$

And the same occurs with the equation:

$$(\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}} + \frac{1}{2})\hbar\omega\hat{\mathbf{a}}\psi \neq E\hat{\mathbf{a}}\psi \tag{1.92}$$

This occurs because operators $\hat{\mathbf{a}}$ and $\hat{\mathbf{a}}^\dagger$ do not commute. The correct way to arrive at a new Schrödinger equation by applying the operators is to add $\hbar\omega\hat{\mathbf{a}}^\dagger\psi$ on both sides of the equation, thus:

$$(\hat{\mathbf{a}}\hat{\mathbf{a}}^\dagger - \frac{1}{2})\hbar\omega\hat{\mathbf{a}}^\dagger\psi + \hbar\omega\hat{\mathbf{a}}^\dagger\psi = E\hat{\mathbf{a}}^\dagger\psi + \hbar\omega\hat{\mathbf{a}}^\dagger\psi \tag{1.93}$$

Which will give us as a result:

$$(\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}} + \frac{1}{2})\hbar\omega\hat{\mathbf{a}}^\dagger\psi = (E + \hbar\omega)\hat{\mathbf{a}}^\dagger\psi \tag{1.94}$$

From here follows a theorem that says: if ψ satisfies Schrödinger's equation with energy E, then $\hat{\mathbf{a}}^\dagger\psi$ and $\hat{\mathbf{a}}$ satisfy the equation with energy $E + \hbar\omega$ and $E - \hbar\omega$ respectively. The previous result can be extended as follows: if ψ satisfies Schrödinger's equation with energy E, then $\hat{\mathbf{a}}^{\dagger n}\psi$ and $\hat{\mathbf{a}}^n$ satisfy the equation with energy $E + n\hbar\omega$ and $E - n\hbar\omega$ respectively.

Operators $\hat{\mathbf{a}}$ and $\hat{\mathbf{a}}^\dagger$ are called annihilation and creation operators.

As an example:

$$(\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}} + \frac{1}{2})\hbar\omega\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}}^\dagger\psi = (E + 2\hbar\omega)\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}}^\dagger\psi, \tag{1.95}$$

$$(\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}} + \frac{1}{2})\hbar\omega\hat{\mathbf{a}}\hat{\mathbf{a}}\hat{\mathbf{a}}\psi = (E - 3\hbar\omega)\hat{\mathbf{a}}\hat{\mathbf{a}}\hat{\mathbf{a}}\psi. \tag{1.96}$$

Continuously applying operator $\hat{\mathbf{a}}$, the lowest energy levels are obtained, but there is a restriction: for $U = 0$ and $x = 0$, energy cannot be $E < 0$; the oscillator must have a minimum energy that we will call E_0 for a corresponding wave function ψ_0, such that $\hat{\mathbf{a}}\psi_0 = 0$. Substituting in Schrödinger's equation:

$$(\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}} + \frac{1}{2})\hbar\omega\psi_0 = E_0\psi_0 \tag{1.97}$$

Since $\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}}\hbar\omega\psi_0 = 0$, we have that the lowest energy level is $E_0 = \frac{1}{2}\hbar\omega$.

The process of solving this exercise can continue, but for the purposes of this book it is sufficient to know how operators work.

A historical note: the above calculation was performed by Paul Maurice Dirac in the 1930s, showing the use of his new braket notation. In some classical quantum mechanics texts, this development is approached exhaustively, and it is very interesting to observe this perspective.

The harmonic oscillator exemplifies quantum mechanics in action: energy quantization emerges from operator algebra, creation and annihilation operators manipulate quantum states, and the elegant formalism of Dirac notation simplifies otherwise complex calculations. This specific example reveals general patterns pervading all quantum systems. Throughout this chapter, we have encountered recurring themes—operators representing observables, commutation relations encoding uncertainty, unitary evolution preserving probability, and Hermitian operators guaranteeing real measurement outcomes. These are not isolated features of particular systems but manifestations of fundamental principles governing all quantum phenomena.

The time has come to consolidate these recurring patterns into explicit postulates: the foundational axioms from which all quantum mechanics follows. These postulates were not invented arbitrarily but distilled from experimental observations and theoretical insights accumulated through decades of quantum theory development. They represent the irreducible core of quantum mechanics—the minimal set of principles necessary to explain atomic spectra, chemical bonding, solid-state physics, and ultimately, quantum computing. Understanding these postulates transforms quantum mechanics from a collection of mathematical techniques into a coherent theoretical framework with predictive power.

1.7 Postulates of Quantum Mechanics

In this chapter, we have explored the historical and conceptual evolution of quantum mechanics, highlighting the matrix formulation and its relevance in modern quantum computing. Through examples such as the harmonic oscillator and Schrödinger's equation, we have seen how classical physics concepts are reinterpreted and extended in the quantum domain through the use of operators, commutators and canonical quantization.

Quantum mechanics not only provides a theoretical framework for describing the behavior of particles at atomic and subatomic scales, but also establishes the mathematical foundations for the development of new technologies, such as quantum computing. In this context, detailed understanding of operators, temporal evolution of quantum states and commutation relations is indispensable for designing and implementing efficient quantum algorithms.

To culminate this chapter, we summarize below the postulates that form the core of quantum mechanics. These postulates constitute the set of rules that govern the dynamics of quantum systems and shape the interpretation of experiments, as well as the construction of quantum technologies.

1.7.1 Postulate 1: The Quantum State

The state of a quantum system at a time instant t is described by a vector $|\psi(t)\rangle$ belonging to a complex Hilbert space (normally separable). This vector, called *ket*, contains all accessible information about the system. A distinctive feature of quantum mechanics is *superposition*: any linear combination of quantum states is also a valid quantum state. The norm of $|\psi(t)\rangle$ is interpreted probabilistically and by convention is normalized to 1.

1.7.2 Postulate 2: Observables and Operators

Each observable physical quantity is associated with a linear and Hermitian (or self-adjoint) operator, $\hat{O}$, that acts on the Hilbert space. The eigenvalues of $\hat{O}$ correspond to the possible results of measuring that quantity; each of these eigenvalues can be associated with one or more eigenvectors (eigenstates). After measurement, the system state *collapses* (in the Copenhagen interpretation) to one of the eigenvectors corresponding to the measured value.

1.7.3 Postulate 3: Measurement and Born's Rule

If an observable represented by the Hermitian operator $\hat{O}$ is measured in a system whose state is $|\psi\rangle$, the only possible result of the measurement is one of the eigenvalues λ_i of $\hat{O}$. *Born's Postulate* establishes that the probability of obtaining an eigenvalue λ_i is given by:

$$P(\lambda_i) = \left|\langle\phi_i|\psi\rangle\right|^2, \tag{1.98}$$

where $|\phi_i\rangle$ is the (normalized) eigenvector associated with λ_i. After measurement, the system state becomes $|\phi_i\rangle$ (the eigenvector corresponding to the measured value), assuming the so-called *collapse interpretation*.

Historical Note: Hidden Variables and the Interpretation of Quantum Mechanics

The probabilistic interpretation of quantum mechanics, proposed by Max Born and adopted in the **Copenhagen interpretation**, was not without controversy. Many physicists, including **Albert Einstein**, **Erwin Schrödinger**, and **Louis de Broglie**, questioned the idea that nature was fundamentally probabilistic. Some of them held that the apparent randomness of quantum mechanics was a consequence of our ignorance about certain **hidden variables** that, if known, would restore a deter-

ministic description.
Einstein expressed his skepticism toward the Copenhagen interpretation in the famous phrase: *"God does not play dice with the universe."* He and other critics maintained that there must exist a more complete, underlying description of reality, in which probabilities would be the result of incomplete knowledge about the state of the system.

Hidden variable theories. One of the first hidden variable theories was proposed by **Louis de Broglie** in 1927 in his **pilot wave** hypothesis, also known as de Broglie–Bohm theory. In this approach, particles have well-defined trajectories, guided by a wave function that acts as an informational field; the wave function does not describe only probabilities, but has an independent physical reality. Mathematically, pilot wave theory is based on two equations:

1. The wave function $\psi(\mathbf{r}, t)$ obeys the standard Schrödinger equation:

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

2. The particle's position $\mathbf{r}(t)$ follows a trajectory determined by the guidance equation:

$$\frac{d\mathbf{r}}{dt} = \frac{\mathbf{j}}{\rho}$$

   where $\mathbf{j} = \frac{\hbar}{2mi}(\psi^* \nabla \psi - \psi \nabla \psi^*)$ is the probability current density and $\rho = |\psi|^2$ is the probability density.

In the 1950s, **David Bohm** extended and formalized this idea, demonstrating that it reproduces all the results of standard quantum mechanics while maintaining a deterministic framework. Nevertheless, de Broglie–Bohm theory never achieved widespread acceptance, partly due to the conceptual cost of attributing physical reality to the wave function in configuration space [2].

Bell's theorem and non-locality. The debate on hidden variables reached its culmination with the work of **John Bell** in 1964. Bell demonstrated that no *local and realistic* hidden variable theory can reproduce all the predictions of quantum mechanics. His result rests on mathematical inequalities—the **Bell inequalities**—that any local classical theory must satisfy, but that quantum mechanics predicts, and experiments confirm, are violated. A standard form of the inequality (due to Clauser, Horne, Shimony and Holt) for experiments with entangled particle pairs is:

$$|E(a, b) - E(a, b')| + |E(a', b') + E(a', b)| \leq 2$$

where $E(a, b)$ is the measured correlation between the particles along measurement axes a and b. The experimental violations of this bound, confirmed by physicists like **Alain Aspect** in the 1980s—work recognized with the 2022 Nobel Prize in Physics, shared with John Clauser and Anton Zeilinger—support the quantum prediction that correlations between entangled particles cannot be explained by local hidden variables [1].

Implications for quantum computing. The resolution of the hidden variables debate matters directly for quantum computing. The confirmed non-locality of quantum correlations establishes that entanglement—a key resource for quantum algorithms and protocols—represents genuinely non-classical physics rather than classical correlations with hidden parameters. Hidden variable theories did not replace standard quantum mechanics, but they enriched the philosophical and methodological debate in physics, underscoring the conceptual depth of the theory whose postulates we have just presented.

1.7.4 Postulate 4: Temporal Evolution

The temporal evolution of a quantum system is governed by *Schrödinger's equation*, which in the state representation is expressed as:

$$i\hbar \frac{d}{dt} |\psi(t)\rangle \;=\; \hat{H}\, |\psi(t)\rangle\,, \tag{1.99}$$

where $\hat{H}$ is the system's Hamiltonian operator and represents the total energy. This postulate implies that the evolution of a quantum state is *continuous*, *deterministic* and *unitary* (reversible) as long as measurement does not intervene. In Heisenberg's formalism, the analogous equation describes the evolution of operators instead of states.

1.7.5 Postulate 5: Composition of Quantum Systems

The state space of a composite system formed by two (or more) subsystems is described by means of the *tensor product* of the Hilbert spaces of each subsystem. If subsystem A is in state $|\psi_A\rangle$ and another subsystem B is in state $|\psi_B\rangle$, then the joint state of the total system is represented by

$$|\psi_{AB}\rangle \;=\; |\psi_A\rangle \;\otimes\; |\psi_B\rangle\,. \tag{1.100}$$

This postulate enables the description of multiple quantum systems and gives rise to purely quantum effects such as *entanglement*, which has no classical analog and plays a fundamental role in quantum computing and quantum cryptography.

These five postulates form the basis of standard quantum mechanics, although some texts add a sixth postulate related to the statistics of identical particles (bosons and fermions). In any case, they constitute the conceptual scaffolding underlying all quantum applications, from the interpretation of experiments to the development of emerging technologies.

In summary, the content of this chapter has offered a tour through the fundamental ideas of quantum mechanics and its matrix formulation, especially highlighting the elements that underlie quantum computing. Throughout the book, we will continue deepening these concepts and see how they are concretely applied in quantum algorithms and implementations.

Summary

We began by reviewing the historical evolution of quantum mechanics, highlighting the main formulations, such as Heisenberg's matrix formulation, Schrödinger's wave function and Feynman's path integral. The matrix formulation, developed by Heisenberg in 1925, is particularly important in quantum computing, where quantum states and observables are represented by means of matrices and operators.

The derivation of Schrödinger's equation was one of the central points of this chapter. We started from Maxwell's equations and derived the electromagnetic wave equation, showing its similarity with Schrödinger's equation for a free particle:

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t)\right]\psi(\vec{r},t) \tag{1.101}$$

This equation, which describes the temporal evolution of the quantum state of a particle, is fundamental for the analysis of quantum systems.

We explored canonical quantization, a process formalized by Paul Dirac, which allows converting a classical system into a quantum system. Through this process, classical dynamic variables, such as position and momentum, are replaced by operators that do not commute, fulfilling the canonical commutation relation:

$$[\hat{x}, \hat{p}] = i\hbar \tag{1.102}$$

This approach is essential for constructing the quantum Hamiltonian of a system, from which all quantum properties are derived.

We made an incursion into matrix quantum mechanics, showing how Schrödinger's equation can be expressed in terms of matrices and operators. This is crucial for quantum computing, where qubit states are manipulated by means of quantum gates represented by unitary matrices:

$$\mathbf{U}^\dagger\mathbf{U} = \mathbf{I} \tag{1.103}$$

The use of unitary matrices ensures the reversibility of quantum operations, a distinctive characteristic of quantum computing compared to classical computing.

We studied the quantum harmonic oscillator as an example of the application of operators in quantum mechanics. We defined the creation and annihilation operators:

$$\hat{\mathbf{a}} = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{x} + i\hat{p}), \quad \hat{\mathbf{a}}^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{x} - i\hat{p}) \tag{1.104}$$

and showed how these operators are used to describe the quantum states of the oscillator and their quantized energy levels.

We concluded the chapter with a review of the fundamental postulates of quantum mechanics, which are the theoretical basis for any quantum analysis. These postulates define how quantum states are described, how measurements are interpreted and how quantum systems evolve in time.

This chapter provides a conceptual and mathematical framework for understanding quantum mechanics from the perspective of quantum computing. As we advance in this book, we will use these fundamental principles to explore and develop quantum algorithms, understanding how quantum properties can be exploited to perform calculations that are beyond the reach of classical computers.

1.8 Exercises

1. **Time-dependent Schrödinger equation**

   Consider a particle of mass m confined in a one-dimensional box of length L with infinitely high walls. Write the time-dependent Schrödinger equation for this system and find the stationary wave functions $\psi_n(x)$ and the associated energies E_n. Explain what energy quantization means in this context.

2. **Lagrangian and Hamiltonian formulation**

   Consider a simple pendulum of length ℓ and mass m in a gravitational field g.

   (a) Write the Lagrangian $\mathbf{L}(\theta, \dot{\theta})$ in terms of the angle θ from the vertical and its time derivative $\dot{\theta}$.

   (b) Derive the equation of motion using the Euler-Lagrange equation.

   (c) Calculate the conjugate momentum p_θ and write the Hamiltonian $\mathbf{H}(\theta, p_\theta)$.

   (d) Verify that the Hamiltonian corresponds to the total energy $E = T + U$ of the system.

3. **Noether's theorem and conservation laws**

   (a) Explain in your own words the connection between symmetries and conservation laws according to Noether's theorem.

   (b) For a system with Hamiltonian $\hat{H}$ that is invariant under time translations, show that energy is conserved, i.e., $\frac{d\langle\hat{H}\rangle}{dt} = 0$.

(c) Consider a particle moving in a central potential $V(r)$ that depends only on distance r from the origin. What symmetry does this system possess? What physical quantity is conserved as a result?

(d) In quantum computing, why is the unitarity of quantum gates (which preserves probability) related to time-translation symmetry?

4. **Canonical quantization**

Apply the canonical quantization procedure to a system of mass m moving in one dimension under the influence of a quadratic potential $V(x) = \frac{1}{2}kx^2$. Derive the quantum Hamiltonian $\hat{H}$ of the system and discuss the difference between the classical and quantum description of the harmonic oscillator.

5. **Wave equation and de Broglie relations**

(a) Starting from the electromagnetic wave equation $\nabla^2 E - \frac{1}{c^2}\frac{\partial^2 E}{\partial t^2} = 0$, verify that $E(x,t) = E_0 e^{i(kx-\omega t)}$ is a solution, where k is the wave number and ω is the angular frequency.

(b) Using de Broglie's relation $\lambda = h/p$ and Einstein's relation $E = \hbar\omega$, calculate the wavelength of an electron with kinetic energy $E_k = 100$ eV. (Use $m_e = 9.11 \times 10^{-31}$ kg, $h = 6.626 \times 10^{-34}$ J $\cdot$ s)

(c) Explain why Schrödinger's equation is first order in time while the electromagnetic wave equation is second order.

6. **Commutation relations**

Demonstrate that the position operator $\hat{x}$ and momentum operator $\hat{p}$ satisfy the commutation relation $[\hat{x}, \hat{p}] = i\hbar$. Use this relation to calculate the commutator $[\hat{x}, \hat{p}^2]$ and discuss its importance in quantum mechanics.

7. **Operators and expectation values**

Consider a particle in a one-dimensional box of length L in its ground state $\psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)$ for $0 \leq x \leq L$.

(a) Calculate the expectation value of position:

$$\langle x \rangle = \int_0^L x\, |\psi_1(x)|^2\, dx.$$

(b) Calculate the expectation value of momentum:

$$\langle \hat{p} \rangle = \int_0^L \psi_1^*(x) \left(-i\hbar \frac{\partial}{\partial x}\right) \psi_1(x)\, dx.$$

(c) Calculate the expectation value of kinetic energy:

$$\langle \hat{T} \rangle = \int_0^L \psi_1^*(x) \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right) \psi_1(x)\, dx.$$

(d) Verify that $\langle \hat{T} \rangle = E_1$, where $E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$ is the ground state energy.

8. **Quantum harmonic oscillator**

   Using the creation $\hat{\mathbf{a}}^\dagger$ and annihilation $\hat{\mathbf{a}}$ operators, derive the energy levels of the quantum harmonic oscillator. Explain how these levels relate to Fock states and how they are used in describing the quantum states of the oscillator.

9. **Matrix quantum mechanics and Pauli matrices**

   Consider a spin-$\frac{1}{2}$ particle whose Hamiltonian in a magnetic field B along the z-axis is $\hat{H} = -\gamma B \sigma_z$, where γ is the gyromagnetic ratio and $\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ is the Pauli matrix.

   (a) Find the eigenvalues and eigenvectors of $\hat{H}$.

   (b) If the particle starts in state $|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$, find the state $|\psi(t)\rangle$ at time t by solving the time-dependent Schrödinger equation.

   (c) Calculate the expectation values $\langle \sigma_x \rangle(t)$, $\langle \sigma_y \rangle(t)$, and $\langle \sigma_z \rangle(t)$ as functions of time.

   (d) This is a model for a qubit undergoing free evolution. How does the phase difference between $|\uparrow\rangle$ and $|\downarrow\rangle$ change with time?

10. **Postulates of quantum mechanics**

    (a) A quantum system is prepared in the state $|\psi\rangle = \frac{1}{\sqrt{5}}|0\rangle + \frac{2}{\sqrt{5}}|1\rangle$. The observable $\hat{A} = 3|0\rangle\langle 0| - 2|1\rangle\langle 1|$ is measured. What are the possible measurement outcomes and their probabilities? What is the expectation value $\langle \hat{A} \rangle$?

    (b) After measuring $\hat{A}$ and obtaining the result $+3$, what is the post-measurement state of the system according to the projection postulate?

    (c) Verify that $\hat{A}$ is a Hermitian operator. Why must observables be represented by Hermitian operators?

    (d) The system evolves under Hamiltonian $\hat{H} = \omega |1\rangle\langle 1|$ for time t. Write the time evolution operator $\hat{U}(t)$ and find the evolved state $|\psi(t)\rangle$.

    (e) Explain which postulates of quantum mechanics you used in parts (a) through (d).