



A Century of the Schrödinger Equation Foundations, Structure and Applications

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ABSTRACT

Purpose of the study: This study aims to provide a comprehensive pedagogical review of the Schrödinger equation by integrating its physical derivations, mathematical structure, and applications to support advanced undergraduate and beginning graduate students in understanding quantum mechanics coherently.

Methodology: Literature review, pedagogical synthesis, canonical model analysis, Hilbert-space formalism, self-adjoint operator framework, spectral theory approach, quantum mechanics textbooks and journal sources, mathematical physics methods, conceptual analysis, and visualization of wave packets and quantum phenomena were used as tools and methods in this study.

Main Findings: The study shows that multiple derivations of the Schrödinger equation converge to a unified structure based on linear, unitary evolution with a self-adjoint Hamiltonian. Key quantum phenomena such as superposition, tunnelling, and quantization emerge consistently from canonical models, while mathematical conditions ensure physical consistency and probability conservation.

Novelty/Originality of this study: This study uniquely integrates physical derivations, rigorous mathematical structure, and pedagogical organization into a single coherent framework. It bridges conceptual gaps between theory and application, offering a unified reference that enhances understanding of quantum mechanics and supports both self-study and instructional practices.

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1. INTRODUCTION

The Schrödinger equation is perhaps the most recognizable equation of quantum mechanics. In its time-dependent, single-particle form,

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \hat{H} \Psi(\mathbf{r}, t), \quad \dots(1)$$

where \hat{H} is the Hamiltonian operator, it plays for quantum systems the role that Newton's second law plays in classical mechanics; given an initial state and the forces (encoded in \hat{H}), it determines the future evolution. Yet Eq. (1) is more than a classical-like evolution equation. It embodies several profound physical principles that distinguish quantum theory from its classical counterpart. The linearity of the equation ensures that superpositions evolve as superpositions, providing the mathematical foundation for quantum interference phenomena. The unitarity of the time evolution, guaranteed by the self-adjointness of the Hamiltonian operator, ensures that

probabilities are conserved in time [1]. The essential complex structure, manifested through the imaginary unit i , encodes the phase relationships that are crucial for interference effects [2]. Finally, the spectral structure of the Hamiltonian operator gives rise to stationary states and discrete energy levels through its eigenfunctions and eigenvalues, a cornerstone of quantum theory [3].

Together with the Born rule, which provides the probabilistic interpretation of quantum mechanics [4], [5], these features yield the complete probabilistic predictive structure of quantum theory. More precisely, the Born rule states that the probability density for finding a particle at position \mathbf{r} is given by $|\Psi(\mathbf{r}, t)|^2$, i.e., the absolute square of the wavefunction. The Schrödinger equation thus serves not merely as a dynamical law but as the conceptual framework through which we understand the quantum world.

A large literature on the Schrödinger equation exists in the form of textbooks, lecture notes, and specialized review articles [17]–[20], but these sources are typically optimized for a single purpose. Many texts emphasize historical narrative or physical intuition but treat the mathematical underpinnings (domains, self-adjointness, boundary conditions, and spectral structure) only briefly [17], [18]; conversely, functional-analytic treatments can be rigorous yet pedagogically steep and less connected to standard solvable models and their physical interpretation [21]–[23]. In addition, derivations of the time-dependent Schrödinger equation are often presented in isolation (e.g., only via de Broglie relations or only via canonical quantization) [18], [19], which may leave students unaware that multiple independent lines of reasoning converge to the same dynamical structure. Finally, the expanding role of quantum theory in modern curricula (quantum technologies, decoherence, open systems, and path integrals) has created a need for a coherent reference that links the foundational equation to both its mathematical architecture and to representative applications using a unified notation and a consistent level of detail [24]–[26].

Quantum mechanics is increasingly taught alongside computational visualization and concept-driven learning. Nevertheless, students often encounter conceptual discontinuities between: (i) formal Hilbert-space formulations [22], [27], (ii) boundary-condition subtleties that determine physical spectra [21]–[23], and (iii) model calculations illustrating tunnelling, wave-packet spreading, and symmetry-induced degeneracies [17, 19]. A long-form review that bridges these layers can reduce such fragmentation and provide a structured pathway from fundamental principles to problem solving. The goals of this comprehensive review article are fivefold. First, to derive and motivate the Schrödinger equation from several complementary physical and mathematical perspectives, demonstrating how different lines of reasoning converge on the same fundamental equation. Second, to present its mathematical structure in a detailed yet accessible manner, emphasizing the role of Hilbert spaces, self-adjoint operators, and spectral theory [6], [7]. Third, to analyze key exactly solvable models as archetypes of quantum behavior, illustrating how characteristic quantum phenomena emerge from the equation's solutions [8]. Fourth, to discuss generalizations to many-body, open, and relativistic systems, showing how the basic framework extends to more complex physical contexts [9], [10]. Fifth, to connect the equation to foundational issues and experimental tests, examining its status as a fundamental or effective law of nature [11], [12].

These objectives are guided by the following research questions: What are the distinct yet convergent derivations of the Schrödinger equation, and what assumptions underlie each approach [18], [19], [28]? Which mathematical structures are essential for physical consistency—such as self-adjointness, domains, and spectral decomposition—and how do they manifest in standard boundary-value problems [21–23]? How can a limited set of canonical models be organized to reveal characteristic quantum phenomena (interference, tunnelling, quantization, symmetries) while supporting step-by-step problem solving [17], [19], [20]? Furthermore, how do modern extensions—such as many-body formalisms, approximation schemes, decoherence in open systems, and path-integral methods—connect back to the same structural core [24]–[26]?

Throughout this exposition, the mathematical framework is developed carefully while maintaining a strong emphasis on physical understanding. It is assumed that the reader possesses foundational knowledge of linear algebra and classical mechanics at the intermediate undergraduate level, while more advanced concepts are introduced as needed. Additionally, the discussion is structured to integrate various topics into a coherent narrative rather than presenting them as isolated results. Historically, the Schrödinger equation emerged out of several parallel developments: old quantum theory, wave-particle duality, Hamilton–Jacobi mechanics, and early operator methods [13]. Mathematically, it sits at the intersection of functional analysis, spectral theory, and representation theory of symmetry groups [1], [14]. Physically, it underpins atomic structure, chemical bonding, condensed-matter bands, scattering theory, and much of modern quantum technology [15], [16].

The novelty of this article is the deliberate integration of three dimensions that are often separated in the literature: (a) physical derivations that motivate the equation from complementary viewpoints [18], [19], [28], (b) the mathematical structure required for a well-defined quantum dynamics (Hilbert space, self-adjoint Hamiltonians, probability conservation, and boundary conditions) [21]–[23], [27], and (c) a pedagogical organization centered on canonical solvable models with explicit visualizations [17, 20]. Relative to reviews that focus primarily on historical development or on isolated applications, the present work offers a single self-contained narrative that connects formal structure, exactly solvable archetypes, and modern extensions in a way designed to support both self-study and classroom use [24]–[26]. In particular, the article emphasizes where

conceptual difficulties typically arise (e.g., domains and boundary conditions in operator definitions) and resolves them within the same notation used for standard model problems [21], [23], thereby providing a unified reference for learners and instructors.

This article is a pedagogical review/tutorial rather than an empirical study, employing a structured synthesis of the literature and canonical models to support advanced undergraduate and beginning graduate learning. The selection of materials is based on relevance to core curricula, conceptual leverage in bridging gaps between intuition and formalism, and representativeness across atomic, molecular, condensed-matter, and quantum-technology contexts. The analysis compares complementary derivation routes, clarifies underlying assumptions, identifies minimal mathematical conditions for physical consistency, and connects structural elements to solvable examples and visualizable phenomena such as wave-packet spreading, tunnelling, and symmetry-induced degeneracy, all presented with unified notation and consistent detail to support self-study and classroom use. The article is also modular in design: a core pathway covers motivations, derivations, fundamental spectral concepts, and canonical single-particle examples, while subsequent sections progressively address symmetries, many-body systems, approximation methods, open quantum systems, decoherence, and path-integral formulations, allowing readers to engage selectively based on their level and interests.

2. RESEARCH METHOD

This study adopts a pedagogical review approach rather than an empirical research design. The method is based on a structured synthesis of relevant literature and canonical quantum mechanics models to construct a coherent conceptual framework for understanding the Schrödinger equation. The data sources consist of standard quantum mechanics textbooks and peer-reviewed journal articles, selected based on three main criteria: (1) relevance to core quantum mechanics curricula, (2) conceptual significance in bridging gaps between intuition and formalism, and (3) representativeness across major application domains, including atomic, molecular, condensed-matter, and quantum technology contexts.

The analytical procedure involves (1) comparing multiple derivation approaches of the Schrödinger equation to identify their underlying assumptions, (2) extracting the minimal mathematical conditions required for physical consistency, and (3) mapping theoretical structures to canonical solvable models and observable quantum phenomena such as wave-packet dynamics, tunnelling, and symmetry-related degeneracies. To ensure coherence and pedagogical clarity, the study applies a unified notation system and maintains a consistent level of conceptual and mathematical detail throughout the analysis.

3. RESULTS AND DISCUSSION

3.1. Derivation of Schrödinger Equation

There is no unique, “historically correct” derivation of the Schrödinger equation. Instead, several complementary arguments converge on the same mathematical structure, each emphasizing different physical or mathematical principles. This convergence suggests that the Schrödinger equation is a natural and almost inevitable consequence of fundamental physical requirements. In this section we present four standard derivations and briefly comment on a fifth, more modern, information-theoretic route. Each derivation highlights a different aspect: wave-particle duality, the correspondence principle, canonical structure, and group representation theory.

Throughout this section we provide citations to original works and modern expositions. Schrödinger’s original derivations appear in Refs. [29], [30]; the complementary matrix mechanics formulation was developed by Heisenberg [31] and later unified with wave mechanics by Dirac [28]. We emphasize that the Schrödinger equation historically emerged from Schrödinger’s 1926 wave-mechanics program, with a complementary operator formulation developed in Heisenberg’s matrix mechanics and unified in Dirac’s transformation theory; standard historical and pedagogical sources include Refs. [28]–[31].

3.1.1 De Broglie Waves and Energy–Momentum Relations

The historical path to the Schrödinger equation begins with Louis de Broglie’s revolutionary hypothesis in 1924 that matter possesses wave-like properties. For a free relativistic particle of mass m , the classical energy–momentum relation is

$$E^2 = p^2 c^2 + m^2 c^4 \quad \dots(2)$$

In the nonrelativistic limit $\left(\frac{p^2}{2m} \ll mc^2\right)$, one writes

$$E = mc^2 + \frac{p^2}{2m} + O(p^4) \quad \dots(3)$$

and subtracts the rest energy mc^2 , treating

$$E_{nr} = \frac{p^2}{2m} \quad \dots(4)$$

as the relevant mechanical energy.

de Broglie hypothesized that a particle with energy E and momentum p can be associated with a wave of frequency ω and wave number k via

$$E = \hbar\omega, p = \hbar k \quad \dots(5) \quad \text{so that the plane wave } \Psi(\mathbf{r}, t) = Ae^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \quad \dots(6)$$

encodes the particle's properties.

Combining $E_{nr} = \frac{p^2}{2m}$ with the de Broglie relations gives the dispersion relation

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} \quad \dots(7)$$

Now note that

$$i\hbar \frac{\partial}{\partial t} \Psi = \hbar\omega \Psi \quad \dots(8) \quad -\frac{\hbar^2}{2m} \nabla^2 \Psi = \frac{\hbar^2 k^2}{2m} \Psi \quad \dots(9)$$

Thus, for a free particle, the plane wave is a solution of

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\mathbf{r}, t) \quad \dots(10)$$

which is precisely the Schrödinger equation for a free particle (no potential term).

This heuristic argument motivates the key structure: a first-order time derivative proportional to the Hamiltonian operator, which for a free particle is just the kinetic-energy operator. The appearance of i is necessary to match the phase evolution of the plane wave.

To include a potential $V(\mathbf{r}, t)$, one postulates that the total energy operator (Hamiltonian) is the sum of kinetic and potential energy operators:

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t), \quad \dots(11)$$

yielding the general time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) \right] \Psi(\mathbf{r}, t). \quad \dots(12)$$

While this derivation has the virtue of simplicity, it relies heavily on the de Broglie relations as a postulate and does not explain why the wavefunction should obey a differential equation of this particular form.

From a modern standpoint, this route also emphasizes the role of dispersion relations: for different physical systems (relativistic particles, quasiparticles in solids, photons in media), the dispersion relation $\omega(k)$ changes, and with it the form of the effective wave equation. The Schrödinger equation is therefore the natural nonrelativistic wave equation associated with the quadratic dispersion $E = p^2/2m$.

Schrödinger's own derivation, while distinct, also started from the Hamilton–Jacobi equation; see Refs. [29], [30].

3.1.2. Hamilton–Jacobi Theory and the Semiclassical Limit

A more systematic derivation uses the Hamilton–Jacobi formulation of classical mechanics, which Schrödinger was deeply familiar with. For a particle in a potential $V(\mathbf{r})$, the Hamilton–Jacobi equation for the action function $S(\mathbf{r}, t)$ is

$$\frac{\partial S}{\partial t} + \frac{1}{2m} (\nabla S)^2 + V(\mathbf{r}) = 0. \quad \dots(13)$$

Classical trajectories are obtained from

$$\mathbf{p} = \nabla S, \mathbf{v} = \frac{\mathbf{p}}{m}. \quad \dots(14)$$

Schrödinger considered a wave function of the form

$$\Psi(\mathbf{r}, t) = R(\mathbf{r}, t) \exp \left[\frac{i}{\hbar} S(\mathbf{r}, t) \right], \quad \dots(15)$$

and asked: which equation for Ψ reduces to Eq. (13) in the limit $\hbar \rightarrow 0$? This approach represents a sophisticated form of correspondence principle, demanding that the new quantum theory contain classical mechanics as a limiting case.

Let us insert Eq. (15) into the general TDSE,

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi, \quad \dots(16)$$

and separate real and imaginary parts carefully.

First compute the time derivative:

$$\frac{\partial \Psi}{\partial t} = \left[\frac{\partial R}{\partial t} + \frac{i}{\hbar} R \frac{\partial S}{\partial t} \right] \exp \left[\frac{iS}{\hbar} \right], \quad \dots(17)$$

and the spatial derivatives:

$$\begin{aligned} \nabla \Psi &= \left[\nabla R + \frac{i}{\hbar} R \nabla S \right] \exp \left(\frac{iS}{\hbar} \right), \quad \dots(18) \\ \nabla^2 \Psi &= \left[\nabla^2 R + \frac{2i}{\hbar} \nabla R \cdot \nabla S + \frac{i}{\hbar} R \nabla^2 S - \frac{1}{\hbar^2} R (\nabla S)^2 \right] \exp \left(\frac{iS}{\hbar} \right). \quad \dots(19) \end{aligned}$$

Now substitute into Eq. (16) and divide both sides by $\exp \left(\frac{iS}{\hbar} \right)$:

$$i\hbar \left[\frac{\partial R}{\partial t} + \frac{i}{\hbar} R \frac{\partial S}{\partial t} \right] = -\frac{\hbar^2}{2m} \left[\nabla^2 R + \frac{2i}{\hbar} \nabla R \cdot \nabla S + \frac{i}{\hbar} R \nabla^2 S - \frac{1}{\hbar^2} R (\nabla S)^2 \right] + VR. \quad \dots(20)$$

Collecting real and imaginary parts separately gives us two equations.

a. Imaginary Part. The imaginary terms yield

$$\hbar \frac{\partial R}{\partial t} = -\frac{\hbar^2}{2m} [2\nabla R \cdot \nabla S + R \nabla^2 S]. \quad \dots(21)$$

or after simplification:

$$\frac{\partial R}{\partial t} = -\frac{1}{m} \nabla R \cdot \nabla S - \frac{1}{2m} R \nabla^2 S. \quad \dots(22)$$

It is convenient to work with $\rho = R^2$ (which can be interpreted as the probability density). Then

$$\frac{\partial \rho}{\partial t} = 2R \frac{\partial R}{\partial t}, \quad \dots(23) \quad \text{So} \quad \frac{\partial \rho}{\partial t} = -\frac{2}{m} R \nabla R \cdot \nabla S - \frac{1}{m} \rho \nabla^2 S. \quad \dots(24)$$

Using $\nabla(R^2) = 2R \nabla R$ and rearranging:

$$\frac{\partial \rho}{\partial t} = -\frac{1}{m} [(\nabla \rho) \cdot \nabla S + \rho \nabla^2 S] = -\frac{1}{m} \nabla \cdot (\rho \nabla S). \quad \dots(25)$$

This is a continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0, \quad \mathbf{J} = \frac{\rho}{m} \nabla S. \quad \dots(26)$$

for the density $\rho = |\Psi|^2$ and current \mathbf{J} . This equation ensures probability conservation and emerges naturally from the imaginary part of the Schrödinger equation.

b. Real Part. The real terms yield

$$-R \frac{\partial S}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 R + \frac{1}{2m} R (\nabla S)^2 + VR. \quad \dots(27)$$

or, dividing by R ,

$$\frac{\partial S}{\partial t} + \frac{1}{2m} (\nabla S)^2 + V - \frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} = 0. \quad \dots(28)$$

Comparing with the classical Hamilton–Jacobi equation (13), we see an additional quantum term:

$$Q(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \frac{\nabla^2 R}{R}. \quad \dots(29)$$

which vanishes in the limit $\hbar \rightarrow 0$, provided R varies slowly compared to the de Broglie wavelength.

Thus Eq. (15) reproduces classical Hamilton–Jacobi theory plus a quantum correction term. Conversely, demanding that the wave equation reduce to Eq. (13) in the appropriate limit singles out the Schrödinger equation up to small modifications. This derivation shows clearly how quantum mechanics generalizes rather than contradicts classical mechanics.

The Hamilton–Jacobi route also clarifies how phase and probability density are intertwined: the phase S determines the velocity field, while ρ obeys a continuity equation, linking quantum dynamics to classical hydrodynamical picture, the wavefunction describes a compressible fluid whose velocity field is $\mathbf{v} = \nabla S/m$, with an extra quantum pressure encoded in Q .

It is important to note that this derivation, while in-spired by Schrödinger's work, incorporates later developments such as the Madelung fluid interpretation [32] and the quantum potential highlighted in Bohmian mechanics [33]. The approach presented here is thus a modern syn-thesis rather than a literal reproduction of Schrödinger's original argument.

3.1.3. Canonical Quantization and Operator Postulates

A more abstract but powerful derivation starts from the canonical structure of classical mechanics. In Hamiltonian form, a classical system with coordinates q_i and momenta p_i evolves according to

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \dot{p}_i = -\frac{\partial H}{\partial q_i}. \quad \dots(30)$$

Observables $A(q, p)$ evolve via the Poisson bracket:

$$\dot{A} = \{A, H\} = \sum_i \left(\frac{\partial A}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial H}{\partial q_i} \right). \quad \dots(31)$$

Canonical quantization, developed principally by Dirac, promotes q, p to operators \hat{q}, \hat{p} on a Hilbert space and replaces Poisson brackets by commutators:

$$\{A, B\} \rightarrow \frac{1}{i\hbar} [\hat{A}, \hat{B}]. \quad \dots(32)$$

One postulates the canonical commutation relations

$$[\hat{q}_i, \hat{p}_j] = i\hbar \delta_{ij}, [\hat{q}_i, \hat{q}_j] = 0, [\hat{p}_i, \hat{p}_j] = 0, \quad \dots(33)$$

and assumes that the quantum Hamiltonian is constructed from \hat{q}, \hat{p} by a suitable ordering prescription. In the Schrödinger picture, states $|\psi(t)\rangle$ evolve according to

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle, \quad \dots(34)$$

which is the abstract form of the Schrödinger equation. Representing \hat{q} and \hat{p} in the position basis via

$$\hat{q} \rightarrow x, \hat{p} \rightarrow -i\hbar \frac{d}{dx}, \quad \dots(35)$$

and acting on $\psi(x, t) = \langle x | \psi(t) \rangle$, one obtains the familiar differential equation:

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi(x, t). \quad \dots(36)$$

From this point of view, Eq. (34) is a direct analogue of Hamilton's equations in the operator formalism, with $i\hbar$ generating time translations. This approach emphasizes the deep structural connections between classical and quantum dynamics. In practice, canonical quantization is more than a formal recipe: it guides the construction of quantum models. For example, starting from a classical many-body Hamiltonian of electrons and nuclei and quantizing leads, after suitable approximations, to the electronic Schrödinger equation used in quantum chemistry. The operator formalism described here is equivalent to Heisenberg's matrix mechanics [31], in which observables are represented by infinite matrices and states by vectors; the equivalence was established by Schrödinger and Dirac [28, 34].

3.1.4. Stone's Theorem and Unitary Time Evolution

Finally, one may characterize the Schrödinger equation purely in terms of the mathematical structure of time evolution in quantum theory. Suppose we assume:

1. States are rays in a complex Hilbert space \mathcal{H} .
2. Time evolution from t_0 to t is represented by a unitary operator $U(t, t_0)$.
3. The family $\{U(t, t_0)\}$ has the group property:

$$U(t_2, t_1) U(t_1, t_0) = U(t_2, t_0), U(t, t) = I, \quad \dots(37)$$

and is strongly continuous in t .

Stone's theorem then states that there exists a unique (possibly unbounded) self-adjoint operator \hat{H} such that

$$U(t, t_0) = \exp \left(-\frac{i}{\hbar} \hat{H}(t - t_0) \right) \quad \dots(38)$$

for some constant \hbar with units of action. Differentiating,

$$i\hbar \frac{d}{dt} U(t, t_0) = \hat{H} U(t, t_0), \quad \dots(39)$$

and acting on an initial state $|\psi(t_0)\rangle$ yields Eq. (34).

Thus, under quite general assumptions about the continuous, unitary nature of time evolution, the Schrödinger equation is essentially the statement that the generator of the unitary group is self-adjoint. This is a purely mathematical characterization, independent of any specific representation (position, momentum, etc.), and shows that the Schrödinger equation emerges naturally from very basic physical requirements.

From a conceptual viewpoint, this derivation reverses the usual logic: instead of postulating the explicit differential equation and deducing unitarity, one postulates unitarity and continuity and deduces that there must exist a self-adjoint generator the Hamiltonian governing the evolution through a first-order differential equation in time.

3.1.5. Information-Theoretic and Reconstruction Approaches

A more recent line of work attempts to derive the structure of quantum theory, including linear unitary evolution, from information-theoretic axioms: constraints on probabilities, continuity, composition of systems, and the impossibility of superluminal signaling. Although a full treatment is beyond the scope of this article, it is useful to mention the general logic. One typically starts from:

- A convex state space of generalized probabilistic theories.
- A rule for combining systems (tensor product or a general composition rule).
- Operational constraints such as no-signaling and reversibility.

Under suitable assumptions (for instance, local tomography, continuity of reversible transformations, and the existence of entangled states), one can show that the only consistent theories are classical probability theory and quantum theory over a complex Hilbert space. Within the quantum branch, reversible dynamics are then represented by one-parameter groups of unitary transformations, and Stone's theorem again brings us back to Schrödinger-like evolution.

These reconstruction programs highlight that the Schrödinger equation is not merely a historical accident, but the natural way to implement continuous, reversible dynamics in a theory whose kinematics is that of complex Hilbert space. The details differ between different reconstruction programs, but they converge on the same

structural conclusions: linear, unitary evolution generated by a self-adjoint Hamiltonian. For detailed expositions of information-theoretic reconstructions, see Refs. [35–37]. These approaches demonstrate that the Schrödinger equation can be derived from operational principles without reference to classical mechanics.

The four routes above (de Broglie dispersion, Hamilton–Jacobi/WKB correspondence, canonical quantization, and Stone’s theorem) converge on the same dynamical structure: linear, first-order time evolution generated by a self-adjoint Hamiltonian. Their assumptions differ physical postulates about matter waves, correspondence requirements, canonical commutators, or unitary continuity but the convergence highlights which elements are structurally indispensable and which are model-dependent.

3.2. Mathematical Framework

We now describe in more detail the mathematical setting of the Schrödinger equation. Hilbert spaces, self-adjoint operators, and spectral theory. A proper understanding of these mathematical structures is essential for working with the equation rigorously and for appreciating its physical content.

3.2.1. Hilbert Space and Inner Products

A (complex) Hilbert space \mathcal{H} is a complex vector space equipped with an inner product

$$\langle \phi | \psi \rangle \in \mathbb{C}, \quad \dots(40)$$

that satisfies three fundamental properties:

1. **Linearity in the second argument:**

$$\langle \phi | (a\psi_1 + b\psi_2) \rangle = a \langle \phi | \psi_1 \rangle + b \langle \phi | \psi_2 \rangle. \quad \dots(41)$$

2. **Conjugate symmetry:**

$$\langle \phi | \psi \rangle = \langle \psi | \phi \rangle^*. \quad \dots(42)$$

3. **Positive-definiteness:**

$$\langle \psi | \psi \rangle \geq 0, \text{ with equality iff } \psi = 0. \quad \dots(43)$$

The norm is defined as

$$\| \psi \| = \sqrt{\langle \psi | \psi \rangle},$$

and the space is complete with respect to this norm (every Cauchy sequence converges). In nonrelativistic quantum mechanics for a single spinless particle in \mathbb{R}^3 , the Hilbert space is

$$\mathcal{H} = L^2(\mathbb{R}^3) = \left\{ \psi: \mathbb{R}^3 \rightarrow \mathbb{C} \mid \int_{\mathbb{R}^3} |\psi(\mathbf{r})|^2 d^3r < \infty \right\}, \quad \dots(44)$$

with inner product $\langle \phi | \psi \rangle = \int_{\mathbb{R}^3} \phi^*(\mathbf{r}) \psi(\mathbf{r}) d^3r. \quad \dots(45)$

Physical states are represented by vectors of unit norm:

Global phases are physically irrelevant:

$|\psi\rangle$ and $e^{i\theta} |\psi\rangle$ represent the same physical state. Strictly speaking, the state space is thus the projective Hilbert space of rays.

The requirement of square-integrability is crucial for the probability interpretation: $|\psi(\mathbf{r})|^2$ is interpreted as the probability density for finding the particle at position \mathbf{r} , and the total probability must be normalized to unity.

It is worth emphasizing that $L^2(\mathbb{R}^3)$ is a space of equivalence classes of functions: wavefunctions that differ only on a set of measure zero are identified. This technicality is important when dealing with distributions, potentials with singularities, and boundary conditions.

For systems with internal degrees of freedom (spin, isospin, etc.), the Hilbert space is a tensor product

$$\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^n, \quad \dots(46)$$

where \mathbb{C}^n carries the spin representation (e.g., $n = 2$ for spin- $\frac{1}{2}$). The wavefunction is then a spinor $\psi(\mathbf{r}, t)$ with n complex components.

3.2.2. Observables and Self-Adjoint Operators

In quantum theory, observables are represented by self-adjoint operators on \mathcal{H} . The distinction between Hermitian and self-adjoint operators is subtle but crucial. An operator \hat{A} with dense domain $D(\hat{A}) \subset \mathcal{H}$ is:

- **Hermitian (symmetric)** if

$$\langle \phi | \hat{A}\psi \rangle = \langle \hat{A}\phi | \psi \rangle, \forall \phi, \psi \in D(\hat{A}). \quad \dots(47)$$

- **Self-adjoint** if it is Hermitian and its domain coincides with that of its adjoint:

$$D(\hat{A}) = D(\hat{A}^\dagger), \hat{A}\psi = \hat{A}^\dagger\psi, \forall \psi \in D(\hat{A}). \quad \dots(48)$$

Self-adjointness guarantees real eigenvalues and spectral decomposition that allows the construction of functions of \hat{A} (e.g., $\exp(\hat{A})$).

The Hamiltonian \hat{H} must be self-adjoint to ensure that

$$U(t) = \exp\left(-\frac{i}{\hbar}\hat{H}t\right) \quad \dots(49)$$

is unitary. This unitarity ensures probability conservation:

$$\frac{d}{dt} \langle \psi(t) | \psi(t) \rangle = 0. \quad \dots(50)$$

In the position representation, the momentum operator is

$$\hat{p} = -i\hbar\nabla, \quad \dots(51)$$

acting on wave functions satisfying appropriate boundary conditions so that \hat{p} is self-adjoint. For a particle on a line, this typically requires specifying boundary conditions that make the operator truly self-adjoint.

A simple example illustrating the role of a boundary condition is the Hamiltonian of a particle in a box:

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}, x \in (0, L). \quad \dots(52)$$

The same differential expression can give rise to different self-adjoint operators depending on the boundary conditions (e.g., $\psi(0) = \psi(L) = 0$). Domain choices are not merely mathematical technicalities: they affect physical situations (hard walls, ring geometry, etc.) and lead to different spectra.

In more singular situations (e.g., δ -function potentials), the operator may require self-adjoint extensions. While this level of detail is beyond the scope of this review, it is important to remember that specifying the differential operator is not enough: the domain is part of the definition of the quantum Hamiltonian.

3.2.3. Spectral Theorem and Stationary States

For a self-adjoint operator \hat{H} , the spectral theorem provides the mathematical foundation for quantum mechanics. It states that there exists a projection-valued measure $E(\lambda)$ such that

$$\hat{H} = \int \lambda dE(\lambda), \quad \dots(53)$$

and for any reasonable function f ,

$$f(\hat{H}) = \int f(\lambda) dE(\lambda). \quad \dots(54)$$

In particular, the time evolution operator is given by

$$U(t) = e^{-i\hat{H}t/\hbar} = \int e^{-i\lambda t/\hbar} dE(\lambda). \quad \dots(55)$$

When \hat{H} has purely discrete spectrum $\{E_n\}$ with eigenvectors $|n\rangle$ forming an orthonormal basis,

$$\hat{H}|n\rangle = E_n|n\rangle, \quad \dots(56) \quad \text{we have} \quad |\psi(0)\rangle = \sum_n c_n |n\rangle, \quad \dots(57)$$

and time evolution yields

$$|\psi(t)\rangle = \sum_n c_n e^{-iE_n t/\hbar} |n\rangle. \quad \dots(58)$$

The stationary states $|n\rangle$ solve the time-independent Schrödinger equation (TISE),

$$\hat{H}\psi_n = E_n\psi_n. \quad \dots(59)$$

For operators with continuous spectrum (e.g., the free particle Hamiltonian), one has generalized eigenstates $|E\rangle$ that are not normalizable in the usual sense; these require treatment in a rigged Hilbert space, where distributions such as Dirac delta functions are included.

In practice, physicists work formally with wave packets (superpositions of energy eigenstates) that are normalizable. The spectral theorem thus provides a unified treatment of both discrete and continuous spectra, allowing us to describe bound states and scattering states within a single framework.

From a practical viewpoint, the spectral decomposition of \hat{H} is central to solving quantum mechanical problems. Green's functions, resolvents, and spectral densities all play a role in analyzing the structure of the spectrum and its associated physical consequences.

A rigorous Hilbert space (also known as a Gel'fand triple) extends the Hilbert space to include distributions, providing a consistent mathematical foundation for generalized eigenfunctions.

(e.g., plane waves) and Dirac delta functions; see Ref. [38]. Green's functions $G(\mathbf{r}, \mathbf{r}'; E)$ are resolvent kernels that solve

$$(\hat{H} - E)G(\mathbf{r}, \mathbf{r}'; E) = \delta(\mathbf{r} - \mathbf{r}'),$$

and are essential in scattering theory and many-body physics; see Ref. [39].

The central mathematical requirement for physically consistent quantum dynamics is the self-adjointness of the Hamiltonian (including its domain and boundary conditions), which guarantees unitary evolution and probability conservation. The spectral theorem then unifies bound-state quantization and scattering continua within a single framework, clarifying how physics depends not only on differential expressions but on operator domains and boundary-value specifications.

3.3. Single-Particle Schrödinger Equation: Examples

We now analyze several exactly solvable problems, illustrating bound states, scattering, tunneling, and wave-packet dynamics. These examples serve as archetypes that display characteristic quantum phenomena and provide the building blocks for understanding more complex systems.

In this section we also introduce phase-space concepts and symmetry properties that are often left implicit in elementary treatments. For the harmonic oscillator we discuss the Wigner function, and for the hydrogen atom we mention the hidden $SO(4)$ symmetry.

3.3.1. Free Particle in One Dimension

Consider a free particle of mass m in one dimension:

$$\hat{H} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}. \quad \dots(60)$$

The time-independent Schrödinger equation,

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) = E \psi(x), \quad \dots(61)$$

has general solution

$$\psi_k(x) = Ae^{ikx} + Be^{-ikx}, E = \frac{\hbar^2 k^2}{2m}, k \in \mathbb{R}. \quad \dots(62)$$

These are non-normalizable plane waves, representing states with definite momentum but completely delocalized in space. To construct physical states, we form wave packets—superpositions of plane waves:

$$\psi(x, t) = \int_{-\infty}^{\infty} a(k) e^{i(kx - \omega_k t)} dk, \omega_k = \frac{\hbar k^2}{2m}. \quad \dots(63)$$

For a Gaussian wave packet centered at k_0 with width σ_k ,

$$a(k) = \frac{1}{(2\pi\sigma_k^2)^{1/4}} \exp\left[-\frac{(k-k_0)^2}{4\sigma_k^2}\right]. \quad \dots(64)$$

The time evolution can be computed explicitly. The initial state is

$$\psi(x, 0) = \frac{1}{(2\pi\sigma_x^2)^{1/4}} \exp\left(ik_0x - \frac{x^2}{4\sigma_x^2}\right), \quad \dots(65)$$

where $\sigma_x = \frac{1}{2\sigma_k}$ by the Fourier uncertainty relation.

The time-evolved wavefunction is

$$\Psi(x, t) = \frac{1}{[2\pi\sigma_x^2(1 + i\hbar t/(2m\sigma_x^2))]^{1/4}} \exp\left[-\frac{(x - \hbar k_0 t/m)^2}{4\sigma_x^2(1 + i\hbar t/(2m\sigma_x^2))} + i\left(k_0x - \frac{\hbar k_0^2 t}{2m}\right)\right]. \quad \dots(66-67)$$

The probability density $|\Psi(x, t)|^2$ is a Gaussian that spreads over time:

$$|\Psi(x, t)|^2 = \frac{1}{\sqrt{2\pi}\sigma(t)} \exp\left[-\frac{(x - v_0 t)^2}{2\sigma^2(t)}\right], \quad \dots(68)$$

Where $v_0 = \frac{\hbar k_0}{m}$ and $\sigma(t) = \sigma_x \sqrt{1 + \left(\frac{\hbar t}{2m\sigma_x^2}\right)^2}$. This spreading is a purely quantum phenomenon resulting from the dispersion relation $E \propto k^2$.

The probability density $|\Psi(x, t)|^2$ obeys the continuity equation

$$\frac{\partial}{\partial t} |\Psi(x, t)|^2 + \frac{\partial}{\partial x} J(x, t) = 0, \quad \dots(69)$$

with current

$$J(x, t) = \frac{\hbar}{2mi} \left[\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right]. \quad \dots(70)$$

For a plane wave $\Psi(x, t) = A e^{i(kx - \omega t)}$, the current is $J = \frac{|A|^2 \hbar k}{m} = |A|^2 v_0$, consistent with the classical interpretation. For a Gaussian wave packet, the probability density $|\Psi(x, t)|^2$ remains Gaussian but spreads with time, and the peak propagates with the group velocity $v_0 = \hbar k_0/m$. It is instructive to visualize both the “snapshots” at fixed times and the full space–time pattern.

In Fig. 1, we plot $|\Psi(x, t)|^2$ for a free Gaussian packet at several successive times. One clearly sees the simultaneous translation of the packet and its quantum spreading: later curves are broader and lower, reflecting the uncertainty relation. Figure 2 displays the same dynamics as a density plot in the (x, t) plane; the curvature of the ridge illustrates how dispersion gradually dominates over simple ballistic motion.

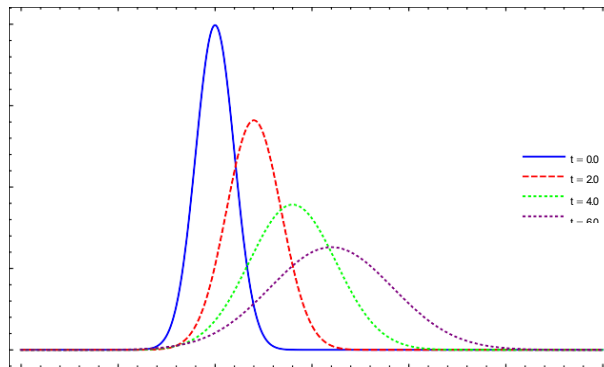


Figure 1. Free-particle Gaussian wave packet $|\Psi(x, t)|^2$ at several times t

The curves show how the initially localized packet moves with the group velocity while spreading over time. The figure is generated from the numerical solution of the Schrödinger equation for an initial Gaussian state.

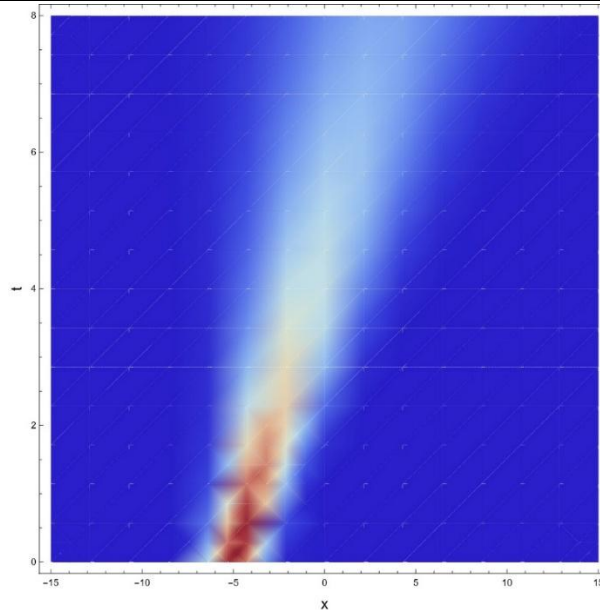


Figure 2 Space–time density plot of the free Gaussian wave packet $|\Psi(x, t)|^2$

The bright ridge corresponds to the peak of the packet moving along the classical trajectory $x = v_0t$, while the widening of the ridge in time indicates quantum spreading.

3.3.2. Potential Step and Barrier: Reflection and Transmission

Consider the potential step

$$V(x) = \begin{cases} 0, & x \leq 0, \\ V_0, & x > 0. \end{cases} \quad \dots(71)$$

For stationary states with energy E , the time-independent Schrödinger equation (TISE) reads

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x). \quad \dots(72)$$

For $x < 0$ (region I),

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx}, k = \frac{\sqrt{2mE}}{\hbar}. \quad \dots(73)$$

For $x > 0$ (region II), assume $E > V_0$,

$$\psi_{II}(x) = Ce^{ik'x}, k' = \frac{\sqrt{2m(E - V_0)}}{\hbar}. \quad \dots(74)$$

To describe an incoming wave from the left, we set $A = 1$ (incident wave), $B = R$ (reflected amplitude), and $C = T$ (transmitted amplitude), so

$$\psi_I(x) = e^{ikx} + Re^{-ikx}, \quad \dots(75) \quad \psi_{II}(x) = Te^{ik'x}. \quad \dots(76)$$

Continuity of ψ and ψ' at $x = 0$ yields

$$1 + R = T, \quad \dots(77) \quad k(1 - R) = k'T. \quad \dots(78)$$

Solving for R and T ,

$$R = \frac{k - k'}{k + k'}, \quad \dots(79) \quad T = \frac{2k}{k + k'}. \quad \dots(80)$$

The probability currents in regions I and II are

$$J_I = \frac{\hbar k}{m} (1 - |R|^2), \quad \dots(81) \quad J_{II} = \frac{\hbar k'}{m} |T|^2. \quad \dots(82)$$

Flux conservation $J_I = J_{II}$ implies

$$1 - |R|^2 = \frac{k'}{k} |T|^2. \quad \dots(83)$$

The reflection and transmission coefficients are

$$\mathcal{R} = |R|^2 = \left(\frac{k - k'}{k + k'} \right)^2, \quad \mathcal{T} = \frac{k'}{k} |T|^2 = \frac{4kk'}{(k + k')^2}, \quad \dots(84)$$

with $\mathcal{R} + \mathcal{T} = 1$.

For a finite barrier,

$$V(x) = \begin{cases} 0, & x < 0, \\ V_0, & 0 \leq x \leq a, \\ 0, & x > a, \end{cases} \quad \dots(85)$$

a similar analysis yields tunneling when $E < V_0$, with an exponentially decaying wave inside the barrier. Transmission coefficient is nonzero even when classically forbidden and is given by

$$T = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(\kappa a)}, \quad \kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}. \quad \dots(86)$$

For $x \geq a$, this simplifies to $T \sim e^{-2\kappa a}$, showing the characteristic exponential decay with barrier width and height.

The step and barrier problems illustrate several key quantum features:

- Partial reflection even when $E > V_0$, in contrast with classical mechanics where a particle with $E > V_0$ would always cross the step.
- Nonzero transmission for $E < V_0$ through a finite barrier (tunneling).
- The role of continuity of the wavefunction and its derivative in matching solutions across potential discontinuities.

In applications, barrier tunneling underlies alpha decay, field emission from metals, electron transport in semiconductor junctions, and Josephson effects in superconductors.

For a finite barrier of width a , one obtains a nonzero transmission coefficient even when $E < V_0$, expressing quantum tunneling. The dependence of $T(E)$ on energy shows oscillatory transmission resonances for $E > V_0$ and classically forbidden exponential suppression (for $E < V_0$).

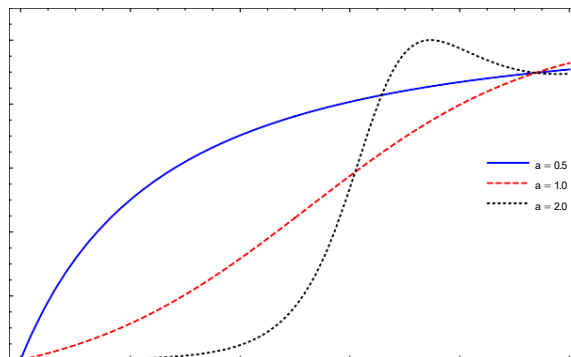


Figure 3. Transmission coefficient $T(E)$ for a finite square barrier of height V_0 and width a , plotted versus the dimensionless energy E/V_0 .

For $E < V_0$, tunneling yields nonzero transmission, while for $E > V_0$, resonant transmission peaks appear due to constructive interference of waves within the barrier region.

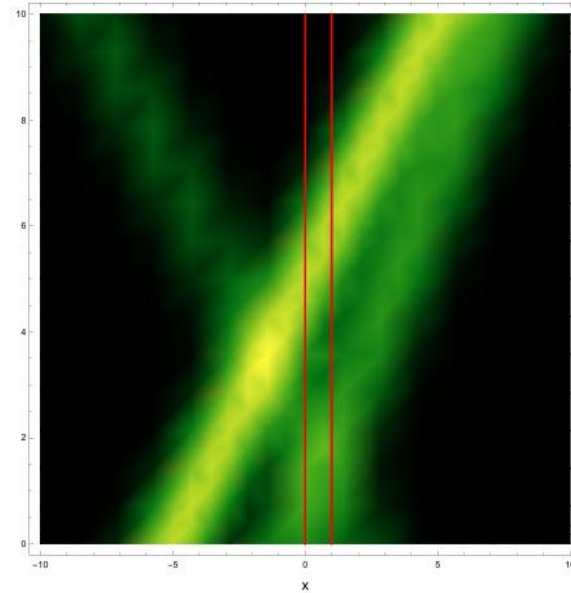


Figure 4. Space-time density plot of a Gaussian wave packet scattering from a finite barrier.

The incoming packet approaches from the left, partially reflects, and partially transmits through the barrier. The density in the barrier region is suppressed but nonzero, illustrating tunneling. The transmitted wave packet emerges on the right with reduced amplitude.

3.3.3. Harmonic Oscillator

The one-dimensional harmonic oscillator has potential

$$V(x) = \frac{1}{2}m\omega^2x^2, \quad \dots(87) \quad \text{and Hamiltonian} \quad \hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2. \quad \dots(88)$$

The time-independent Schrödinger equation (TISE) is

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi. \quad \dots(89)$$

It can be solved by power-series methods or more elegantly by using ladder operators. Define dimensionless variables

$$\xi = \sqrt{\frac{m\omega}{\hbar}} x, \quad \epsilon = \frac{2E}{\hbar\omega}. \quad \dots(90) \quad \text{The TISE becomes} \quad \frac{d^2\psi}{d\xi^2} + (\epsilon - \xi^2)\psi = 0. \quad \dots(91)$$

For large $|\xi|$, the equation is approximately $\frac{d^2\psi}{d\xi^2} \approx \xi^2\psi$, suggesting the asymptotic behavior $\psi \sim e^{-\xi^2/2}$. We therefore write $\psi(\xi) = H(\xi)e^{-\xi^2/2}$, which leads to Hermite's equation for $H(\xi)$:

$$\frac{d^2H}{d\xi^2} - 2\xi \frac{dH}{d\xi} + (\epsilon - 1)H = 0. \quad \dots(92)$$

This equation has polynomial solutions (Hermite polynomials) only when $\epsilon = 2n + 1$, for $n = 0, 1, 2, \dots$, giving the quantized energies

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right). \quad \dots(93)$$

More elegantly, one introduces ladder operators:

$$\hat{a} = \frac{1}{\sqrt{2}} \left(\xi + \frac{d}{d\xi} \right) = \sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{i}{m\omega} \hat{p} \right), \quad \dots(94) \quad \hat{a}^\dagger = \frac{1}{\sqrt{2}} \left(\xi - \frac{d}{d\xi} \right) = \sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{i}{m\omega} \hat{p} \right), \quad \dots(95)$$

which satisfy $[\hat{a}, \hat{a}^\dagger] = 1$. The Hamiltonian becomes

$$\hat{H} = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right), \quad \dots(96)$$

where $\hat{N} = \hat{a}^\dagger \hat{a}$ is the number operator. The eigenstates $|n\rangle$ satisfy

$$\hat{N} |n\rangle = n |n\rangle, n = 0, 1, 2, \dots \quad \dots(97) \quad \text{and are generated by} \quad |n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle, \quad \dots(98)$$

where the ground state $|0\rangle$ obeys $\hat{a} |0\rangle = 0$.

The ladder operators act as

$$\hat{a} |n\rangle = \sqrt{n} |n-1\rangle, \hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle. \quad \dots(99)$$

In the position representation, the wave functions are

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} H_n(\xi) e^{-\xi^2/2}, \quad \dots(100)$$

where H_n are Hermite polynomials.

The harmonic oscillator is ubiquitous: small oscillations in potentials, quantized modes of fields, phonons, photons in cavities, and molecular vibrations.

An especially important class of solutions are coherent states, defined as eigenstates of the annihilation operator:

$$\hat{a} |\alpha\rangle = \alpha |\alpha\rangle. \quad \dots(101) \quad \text{They can be written as} \quad |\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle. \quad \dots(102)$$

Coherent states minimize the Heisenberg uncertainty relation and follow classical oscillator trajectories in phase space. They provide a bridge between classical and quantum descriptions and are central to quantum optics and the description of laser fields.

The Wigner function $W(x, p)$ is defined as $W(x, p) = \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} \psi^*(x+y) \psi(x-y) e^{\frac{2ipy}{\hbar}} dy$. For a coherent state, the Wigner function is a Gaussian centered at the classical phase-space point and is everywhere positive.

3.3.4. Hydrogen Atom

The hydrogen atom problem illustrates the Schrödinger equation in three dimensions with a central potential

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r}. \quad \dots(103)$$

Using spherical coordinates and separating variables $\psi(r, \theta, \phi) = R(r)Y_\ell^m(\theta, \phi)$, the radial equation becomes

$$-\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) - \frac{\ell(\ell+1)}{r^2} R \right] - \frac{e^2}{4\pi\epsilon_0 r} R = ER. \quad \dots(104)$$

Introducing $u(r) = rR(r)$ simplifies the equation to

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + \left[\frac{\hbar^2 \ell(\ell+1)}{2mr^2} - \frac{e^2}{4\pi\epsilon_0 r} \right] u = Eu, \quad \dots(105)$$

which resembles a one-dimensional Schrödinger equation with an effective potential

$$V_{\text{eff}}(r) = -\frac{e^2}{4\pi\epsilon_0 r} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}. \quad \dots(106)$$

Defining dimensionless variables $\rho = \frac{r}{a}$ with $a = \frac{\hbar^2}{me^2}$ and $\epsilon = -\frac{E}{(e^2/2a)} = -\frac{2mEa^2}{\hbar^2}$, one obtains

$$\frac{d^2u}{d\rho^2} + \left[\epsilon + \frac{2}{\rho} - \frac{\ell(\ell+1)}{\rho^2} \right] u = 0. \quad \dots(107)$$

For bound states ($E < 0$), the asymptotic behavior suggests $u(\rho) \sim \rho^{\ell+1}e^{-\rho/n}$, with $n = 1, 2, 3, \dots$. Substituting gives the associated Laguerre equation for $L(\rho)$. The solution is normalizable only when $n - \ell - 1$ is a nonnegative integer, yielding the energy spectrum

$$E_n = -\frac{me^4}{2\hbar^2n^2} = -\frac{13.6 \text{ eV}}{n^2}, n = 1, 2, 3, \dots \quad \dots(108)$$

reproducing the Balmer series. The degeneracy in ℓ reflects rotational symmetry. This hydrogenic spectrum remains one of the most important results in quantum mechanics.

Its spectrum provided crucial early evidence for quantum theory:

- Precision spectroscopy of hydrogen and hydrogenic ions tests quantum electrodynamics and fundamental constants.
- The hydrogen solutions form a basis for understanding multi-electron atoms and for constructing approximate many-electron wavefunctions.

From a mathematical perspective, the hydrogen problem also exhibits a hidden symmetry related to the Runge–Lenz vector, which explains the high degeneracy of the spectrum.

The $SO(4)$ symmetry of the hydrogen atom arises from the conservation of the Runge–Lenz vector $\mathbf{A} \propto \mathbf{p} \times \mathbf{L} - k\hat{\mathbf{r}}$. The generators \mathbf{L} and \mathbf{A} form an $so(4)$ algebra, leading to the degeneracy of states with the same principal quantum number n .

3.4 Symmetries and Conservation Laws

Symmetries play a central role in quantum mechanics. They constrain the form of the Hamiltonian and determine conserved quantities through Noether's theorem, which has a particularly elegant formulation in quantum mechanics.

3.4.1. Time Translation and Energy

Time translation invariance corresponds to a Hamiltonian independent of time. In that case, the evolution operator satisfies

$$U(t_2, t_1) = U(t_2 - t_1). \quad \dots(109)$$

and the generator \hat{H} is conserved:

$$\frac{d}{dt} \langle \hat{H} \rangle = \frac{i}{\hbar} \langle [\hat{H}, \hat{H}] \rangle + \left\langle \frac{\partial \hat{H}}{\partial t} \right\rangle = 0. \quad \dots(110)$$

More generally, for any time-independent operator \hat{A} ,

$$\frac{d}{dt} \langle \hat{A} \rangle = \frac{i}{\hbar} \langle [\hat{H}, \hat{A}] \rangle. \quad \dots(111)$$

A particularly important symmetry is the global phase symmetry:

$$\psi(\mathbf{r}, t) \rightarrow e^{i\theta} \psi(\mathbf{r}, t), \quad \dots(112)$$

where θ is constant. This symmetry underlies the conservation of total probability (or, in field theory contexts, particle number) and can be associated with a $U(1)$ Noether current. In a field-theoretic setting, coupling this symmetry to a gauge field leads to electromagnetism.

3.4.2. Spatial Translations and Momentum

Spatial translation by a vector \mathbf{a} is implemented by a unitary operator

$$\hat{T}(\mathbf{a}) = \exp\left(-\frac{i}{\hbar} \mathbf{a} \cdot \hat{\mathbf{P}}\right), \quad \dots(113)$$

where $\hat{\mathbf{P}}$ is the total momentum operator. If the Hamiltonian is translation invariant, $[\hat{H}, \hat{\mathbf{P}}] = 0$, then momentum is conserved:

$$\frac{d}{dt}\langle \hat{\mathbf{P}} \rangle = \frac{i}{\hbar} \langle [\hat{H}, \hat{\mathbf{P}}] \rangle = 0. \quad \dots(114)$$

In the position representation, infinitesimal translations yield

$$\hat{T}(\mathbf{a})\psi(\mathbf{r}) = \psi(\mathbf{r} - \mathbf{a}) \simeq \psi(\mathbf{r}) - \mathbf{a} \cdot \nabla\psi(\mathbf{r}), \quad \dots(115)$$

which is equivalent to

$$\hat{T}(\mathbf{a})\psi(\mathbf{r}) = \left(1 - \frac{i}{\hbar} \mathbf{a} \cdot \hat{\mathbf{P}}\right)\psi(\mathbf{r}). \quad \dots(116)$$

one recovers $\hat{P} = -i\hbar\nabla$.

In periodic systems such as crystals, exact translational invariance is reduced to discrete lattice translations. The associated symmetry leads to Bloch's theorem and to the band structure of solids, which constitutes a central application of the Schrödinger equation in condensed-matter physics.

3.4.3. Rotations and Angular Momentum

Rotations are generated by the angular momentum operator

$$L = \mathbf{r} \times \mathbf{p} = -i\hbar \mathbf{r} \times \nabla \quad \dots(117)$$

The components satisfy the $\mathfrak{so}(3)$ algebra

$$[L_x, L_y] = i\hbar L_z \quad \dots(118)$$

Rotational invariance, $[H, L_i] = 0$, implies conservation of total angular momentum and degeneracies associated with different m quantum numbers.

For a rotation axis in the direction \hat{n} ,

$$R(\hat{n}, \theta) = \exp\left(-\frac{i}{\hbar} \theta \hat{n} \cdot L\right) \quad \dots(119)$$

The conservation of angular momentum follows from:

$$\frac{d}{dt}(\hat{n} \cdot L) = \frac{i}{\hbar} [H, \hat{n} \cdot L] = 0 \quad \dots(120)$$

when $[H, L_i] = 0$.

In atomic physics, rotational symmetry organizes the spectrum into multiplets labelled by ℓ and m , and selection rules for dipole transitions ($\Delta\ell = \pm 1, \Delta m = 0, \pm 1$) are direct consequences of how the position operator transforms under rotations.

3.4.4. Galilean Invariance and the Schrödinger Equation

Nonrelativistic physics is invariant under the Galilei group of transformations

$$\mathbf{r}' = \mathbf{r} - \mathbf{v}t, t' = t \quad \dots(121)$$

together with translations and rotations.

For a free particle, one can demand that the form of the Schrödinger equation be covariant under such transformations. This requirement fixes the mass-dependent phase transformation of the wavefunction and leads uniquely (up to unitary equivalence) to the kinetic term $-\hbar^2/2m\nabla^2$.

More concretely, under a boost with velocity \mathbf{v} , the wavefunction transforms as

$$\psi'(\mathbf{r}', t') = \exp\left[\frac{im}{\hbar}\left(\mathbf{v} \cdot \mathbf{r} - \frac{1}{2}v^2 t\right)\right]\psi(\mathbf{r} + \mathbf{v}t', t') \quad \dots(122)$$

which leaves the free-particle Schrödinger equation invariant in form.

The transformation law ensures that the probability density transforms correctly: $|\psi'(\mathbf{r}', t')|^2 = |\psi(\mathbf{r} + \mathbf{v}t', t')|^2$ and that phase factors are necessary to compensate the additional terms arising from the time derivative.

In more advanced treatments, the fact that the Galilei group has nontrivial projective representations is what forces the presence of mass as a parameter, and the Schrödinger equation can be seen as the equation for a wavefunction transforming under such a projective representation.

3.5. Many-Particle Systems and Identical Particles

The generalization of the Schrödinger equation to many particles is straightforward in principle but leads to enormously complex and fundamentally new phenomena, particularly for identical particles.

3.5.1. Tensor Products and Configuration Space

For N distinguishable particles, the total Hilbert space is

$$\mathcal{H} = \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_N \quad \dots(123)$$

where $\mathcal{H}_i = L^2(\mathbb{R}^3)$ (ignoring spin for now).

A pure state can be written in the position basis as

$$\psi(\mathbf{r}_1, \dots, \mathbf{r}_N) = \langle \mathbf{r}_1, \dots, \mathbf{r}_N | \psi \rangle(t) \quad \dots(124)$$

The Schrödinger equation then becomes

$$i\hbar \frac{\partial}{\partial t} \psi = \left[- \sum_{i=1}^N \frac{\hbar^2}{2m_i} \nabla_i^2 + V(\mathbf{r}_1, \dots, \mathbf{r}_N) \right] \psi \quad \dots(125)$$

The potential $V(\mathbf{r}_1, \dots, \mathbf{r}_N)$ typically includes external potentials and interparticle interactions. For example, for electrons in an atom with nuclear charge Z :

$$V(\mathbf{r}_1, \dots, \mathbf{r}_N) = - \sum_{i=1}^N \frac{Ze^2}{4\pi\epsilon_0 r_i} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_i - \mathbf{r}_j|} \quad \dots(126)$$

The complexity of solving this equation grows exponentially with N , illustrating the “curse of dimensionality” in many-body quantum mechanics.

In practice, one rarely solves the full $3N$ -dimensional Schrödinger equation directly. Instead, one uses approximations such as mean-field theory (Hartree or Hartree–Fock), configuration interaction expansions, density functional theory, or quantum Monte Carlo methods. These approaches can be even different ways of approximating the many-body wavefunction or its associated reduced density matrices.

3.5.2. Identical Particles and (Anti) Symmetrization

For identical bosons or fermions, the wave function must be symmetric or antisymmetric under particle exchange:

$$\Psi(\dots, r_i, \dots, r_j, \dots) = \begin{cases} +\Psi(\dots, r_j, \dots, r_i, \dots), & \text{bosons,} \\ -\Psi(\dots, r_j, \dots, r_i, \dots), & \text{fermions.} \end{cases} \quad \dots(127)$$

This symmetrization requirement is responsible for Bose–Einstein condensation, Fermi degeneracy pressure, the Pauli exclusion principle, and the structure of the periodic table.

For two identical particles, the symmetrized (bosonic) and antisymmetrized (fermionic) wavefunctions are:

$$\Psi_S(r_1, r_2) = \frac{1}{\sqrt{2}} [\Psi(r_1, r_2) + \Psi(r_2, r_1)], \quad \dots(128) \quad \Psi_A(r_1, r_2) = \frac{1}{\sqrt{2}} [\Psi(r_1, r_2) - \Psi(r_2, r_1)]. \quad \dots(129)$$

For fermions, if $\Psi(r_1, r_2) = \psi_a(r_1)\psi_b(r_2)$ with $a \neq b$, the antisymmetrized wavefunction is the Slater determinant:

$$\Psi_A(r_1, r_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_a(r_1) & \psi_b(r_1) \\ \psi_a(r_2) & \psi_b(r_2) \end{vmatrix}. \quad \dots(130)$$

For N fermions, this generalizes to an $N \times N$ determinant.

Working with fully symmetrized or antisymmetrized wave functions in configuration space quickly becomes cumbersome. This motivates the *second quantization* or Fock-space formalism, in which one introduces creation and annihilation operators acting on occupation-number states.

As a simple application, consider a noninteracting spinless Fermi gas in a box. Filling the one-particle energy levels up to the Fermi energy E_F with one fermion per state yields a many-body ground state described by a single Slater determinant. The resulting pressure and energy as functions of density, entirely due to the Pauli principle, explain the stability of white dwarfs and contribute to the properties of electrons in metals.

For bosons, placing many particles into the same one-particle state is allowed and energetically favorable at low temperatures. This leads to Bose–Einstein condensation, in which a macroscopic fraction of particles occupies the lowest-energy single-particle state, and the many-body wavefunction acquires a coherent macroscopic component described (in mean field) by the Gross–Pitaevskii equation.

The structure imposed by (anti)symmetrization is particularly transparent when expressed in terms of reduced density matrices and correlation functions. The one-body density matrix,

$$\rho^{(1)}(x_1, x_2) = \langle \hat{\psi}^\dagger(x_2) \hat{\psi}(x_1) \rangle, \quad \dots(131)$$

contains information about coherence and off-diagonal order, while the normalized second-order correlation function.

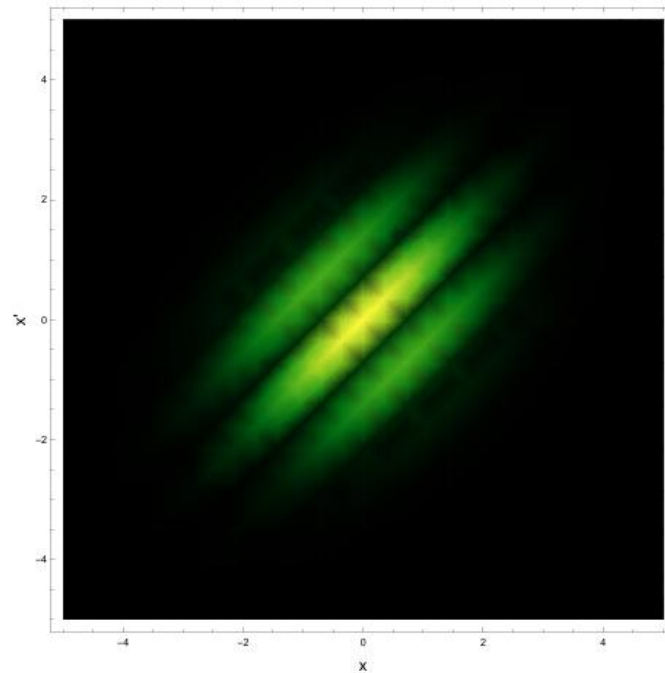


Figure 6. One-body density matrix $\rho^{(1)}(x_1, x_2)$ for a few particles in a harmonic trap (representative example).

The diagonal $x_1 = x_2$ gives the spatial density, while the off-diagonal coherence reflects phase correlations between different positions. diagnoses bunching or antibunching of identical particles.

The reduced density matrix $\rho^{(1)}(x_1, x_2)$ is obtained by tracing out all but one particle from the full N -body density matrix; its eigenvalues (natural occupations) diagnose Bose–Einstein condensation or Fermi-surface structure. The anticommutator of two operators \hat{A} and \hat{B} is defined as $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$, and for fermionic field operators we have $\{\hat{\psi}(r), \hat{\psi}^\dagger(r')\} = \delta(r - r')$. See Refs. [42, 43] for foundational discussions.

Figure 6 shows a representative one-body density matrix $\rho^{(1)}(x_1, x_2)$ for a few particles confined in a harmonic trap. The diagonal $x_1 = x_2$ encodes the local density, while the off-diagonal structure reveals long-range coherence properties across different positions. In Figs. 7 and 8 we compare $g^{(2)}(x_1, x_2)$ for non-interacting bosons and fermions in the same trap; bosons display bunching (enhanced probability along the diagonal), whereas fermions exhibit antibunching and a clear suppression near $x_1 = x_2$ due to the Pauli principle. A one-dimensional cut at fixed $x_2 = x_0$ is plotted in Fig. 9, making the contrast between bosonic and fermionic statistics particularly clear.

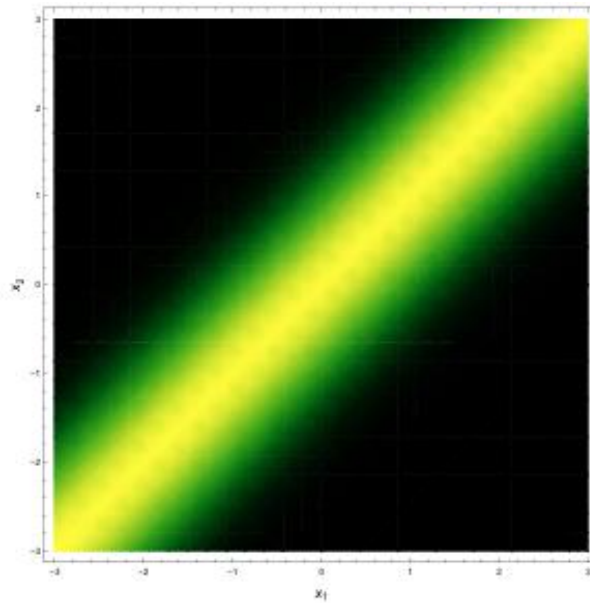


Figure 7. Normalized second-order correlation function $g^{(2)}(x_1, x_2)$ for ideal bosons.

The enhancement along the diagonal ($x_1 = x_2$) illustrates bosonic bunching: the probability to detect two bosons close together is larger than for uncorrelated particles.

3.5.3. Second Quantization and Field Operators

For a set of one-particle states $\{|\phi_n\rangle\}$, define bosonic or fermionic annihilation operators \hat{a}_n and creation operators \hat{a}_n^\dagger satisfying

Bosons:

$$[\hat{a}_m, \hat{a}_n^\dagger] = \delta_{mn}, [\hat{a}_m, \hat{a}_n] = [\hat{a}_m^\dagger, \hat{a}_n^\dagger] = 0, \quad \dots(133)$$

Fermions:

$$\{\hat{a}_m, \hat{a}_n^\dagger\} = \delta_{mn}, \{\hat{a}_m, \hat{a}_n\} = \{\hat{a}_m^\dagger, \hat{a}_n^\dagger\} = 0. \quad \dots(134)$$

The vacuum $|0\rangle$ obeys $\hat{a}_n |0\rangle = 0$ for all n .

The many-body Hilbert space is the Fock space spanned by occupation-number states

$$|n_1, n_2, \dots\rangle = \prod_n \frac{(\hat{a}_n^\dagger)^{n_n}}{\sqrt{n_n!}} |0\rangle. \quad \dots(135)$$

For fermions, n_n can only be 0 or 1 due to the anticommutation relations.

One defines field operators

$$\hat{\psi}(r) = \sum_n \phi_n(r) \hat{a}_n, \quad \dots(136) \quad \hat{\psi}^\dagger(r) = \sum_n \phi_n^*(r) \hat{a}_n^\dagger. \quad \dots(137)$$

For bosons,

$$[\hat{\psi}(r), \hat{\psi}^\dagger(r')] = \delta(r - r'). \quad \dots(138)$$

Explaining research chronological, including research design, research procedure (in the form of algorithms, Pseudocode or other), how to test and data acquisition [1]-[3]. The description of the course of research should be supported references, so the explanation can be accepted scientifically [2], [4].

Tables and Figures are presented center, as shown in Table 1 and Figure 1, and cited in the manuscript before appeared.

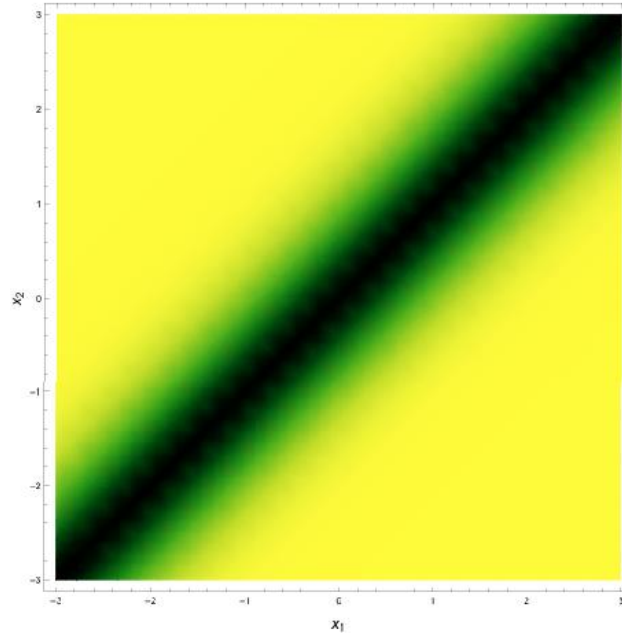


Figure 8. Normalized second-order correlation function $g^{(2)}(x_1, x_2)$ for identical fermions.

The pronounced dip along the diagonal ($x_1 = x_2$) reflects fermionic antibunching and the Pauli exclusion principle, which suppresses joint detection at the same position.

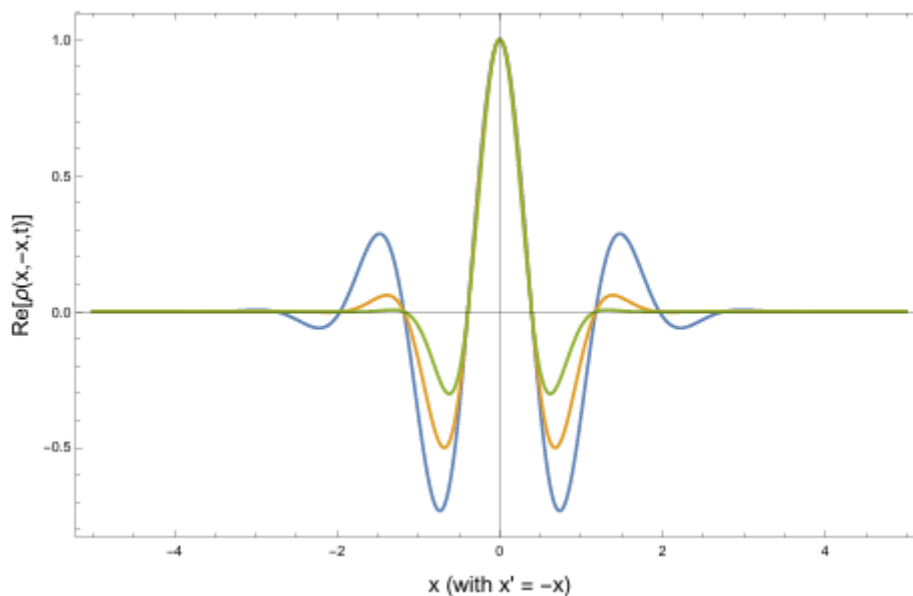


Figure 9. One-dimensional slice of a correlation function $g^{(2)}(x, x_0)$, illustrating the contrast between bosonic bunching and fermionic antibunching along a particular line parallel.

Such slices are directly related to experimentally accessible measurements in cold-atom and quantum-optics setups. And similarly for fermions with anticommutators.

The many-body Hamiltonian for interacting particles can be compactly written as

$$\hat{H} = \int \hat{\psi}^\dagger(r) \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(r) \right) \hat{\psi}(r) dr + \frac{1}{2} \int \hat{\psi}^\dagger(r) \hat{\psi}^\dagger(r') V(r-r') \hat{\psi}(r') \hat{\psi}(r) dr dr'. \quad \dots(139)$$

where U is the interaction potential. The Heisenberg equation.

$$i\hbar \frac{\partial}{\partial t} \hat{\psi}(\mathbf{r}, t) = [\hat{\psi}(\mathbf{r}, t), \hat{H}] \quad \dots(140)$$

It is a field-theoretic generalization of the Schrödinger equation.

This formalism automatically handles the symmetry requirements for identical particles and provides powerful tools for perturbation theory and mean-field approximations.

In condensed-matter and cold-atom physics, the second-quantized Hamiltonian is often projected onto a set of localized orbitals (e.g., Wannier functions), leading to lattice models such as the Bose–Hubbard and Fermi–Hubbard models. These simplified models, though derived from the underlying continuum Schrödinger equation, capture key phenomena such as Mott insulators, superfluid–insulator transitions, and magnetism in correlated electron systems.

3.6. Approximation Methods

Exact solutions of the Schrödinger equation are rare. Much of quantum theory consists of approximation schemes that allow us to extract physical predictions for realistic systems.

3.6.1. Time-Independent Perturbation Theory

Suppose

$$H = H_0 + \lambda V,$$

where H_0 is solvable and λ is a small parameter. Let

$$H_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle. \quad \dots(141)$$

With nondegenerate spectrum. We seek corrections

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots, \quad \dots(142) \quad |n\rangle = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \dots. \quad \dots(143)$$

Substituting into $(H_0 + \lambda V) |n\rangle = E_n |n\rangle$ and equating powers of λ yields the perturbation equations. To first order:

$$(H_0 - E_n^{(0)}) |n^{(1)}\rangle + (V - E_n^{(1)}) |n^{(0)}\rangle = 0. \quad \dots(144)$$

Taking the inner product with $\langle n^{(0)} |$ gives

$$E_n^{(1)} = \langle n^{(0)} | V | n^{(0)} \rangle. \quad \dots(145)$$

The first-order correction to the state is obtained by projecting onto the orthogonal complement:

$$|n^{(1)}\rangle = \sum_{m \neq n} \frac{\langle m^{(0)} | V | n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} |m^{(0)}\rangle. \quad \dots(146)$$

To second order:

$$E_n^{(2)} = \sum_{m \neq n} \frac{| \langle m^{(0)} | V | n^{(0)} \rangle |^2}{E_n^{(0)} - E_m^{(0)}} \quad \dots(147)$$

Higher orders follow similarly. Degenerate perturbation theory requires diagonalizing \hat{V} in the degenerate subspace. This machinery underlies fine-structure corrections in atoms, Stark and Zeeman effects, and many other phenomena. As a simple example, consider a harmonic oscillator subject to a small quartic perturbation

$$\hat{V} = \lambda \hat{x}^4 \quad \dots(148)$$

Using the known eigenstates of \hat{H}_0 and expressing \hat{x} in terms of \hat{a}, \hat{a}^\dagger , one can compute the shifts of the oscillator energy levels order by order in λ . Such anharmonic corrections are important in molecular vibrational spectra and in the physics of nonlinear oscillators and superconducting qubits (transmons).

For the ground state, the first-order energy shift is $E_0^{(1)} = \lambda \langle 0 | x^4 | 0 \rangle$. Using $x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger)$, we obtain

$$E_0^{(1)} = \frac{3}{4} \lambda \left(\frac{\hbar}{m\omega} \right)^2.$$

This explicit calculation illustrates how perturbation theory yields quantitative predictions.

3.6.2. Time-Dependent Perturbation Theory and Fermi's Golden Rule

For a Hamiltonian $\hat{H}(t) = \hat{H}_0 + \hat{V}(t)$ with $\hat{V}(t)$ small, one solves the TDSE in the interaction picture. The time-evolution operator in the interaction picture satisfies

$$i\hbar \frac{\partial}{\partial t} U_I(t, t_0) = \tilde{V}_I(t) U_I(t, t_0), \quad \dots(149) \quad \text{where} \quad \tilde{V}_I(t) = e^{i\hat{H}_0 t/\hbar} \hat{V}(t) e^{-i\hat{H}_0 t/\hbar}.$$

The formal solution is

$$U_I(t, t_0) = \mathcal{T} \exp \left(-\frac{i}{\hbar} \int_{t_0}^t \tilde{V}_I(t') dt' \right), \quad \dots(150)$$

where \mathcal{T} is the time-ordering operator. For small perturbations, we expand to first order:

$$U_I(t, t_0) \approx 1 - \frac{i}{\hbar} \int_{t_0}^t V_I(t') dt'. \quad \dots(151)$$

Writing the state as

$$|\Psi_I(t)\rangle = \sum_n c_n(t) e^{-iE_n t/\hbar} |n\rangle, \quad \dots(152)$$

where $|n\rangle$ are eigenstates of \hat{H}_0 , the coefficients obey

$$i\hbar \dot{c}_n(t) = \sum_m V_{nm}(t) e^{i(E_n - E_m)t/\hbar} c_m(t). \quad \dots(153) \quad \text{with} \quad V_{nm}(t) = \langle n | \hat{V}(t) | m \rangle.$$

To first order, starting with $c_i(0) = 1$, $c_{f \neq i}(0) = 0$, we find

$$c_f^{(1)}(t) = \frac{1}{i\hbar} \int_0^t dt' V_{fi}(t') e^{i(E_f - E_i)t'}. \quad \dots(154)$$

For a constant perturbation turned on at $t = 0$, $V_{fi}(t) = V_{fi}$ for $t > 0$,

$$c_f^{(1)}(t) = \frac{V_{fi}}{i\hbar} \frac{e^{i(E_f - E_i)t} - 1}{i(E_f - E_i)} = \frac{V_{fi}}{E_f - E_i} e^{i(E_f - E_i)t/2} \left[\frac{2\hbar}{E_f - E_i} \sin \left[\frac{(E_f - E_i)t}{2\hbar} \right] \right]. \quad \dots(155)$$

The transition probability is

$$P_{i \rightarrow f}(t) = |c_f^{(1)}(t)|^2 = \frac{|V_{fi}|^2 \sin^2(\omega_{fi}t/2)}{\hbar^2 (\omega_{fi}/2)^2}. \quad \dots(156)$$

where $\omega_{fi} = \frac{E_f - E_i}{\hbar}$.

For a perturbation $\hat{V}(t) = V e^{-i\omega t} + V^\dagger e^{i\omega t}$ switched on for a long time and with a continuum of final states, one obtains the transition rate

$$w_{i \rightarrow f} = \frac{2\pi}{\hbar} |V_{fi}|^2 \rho(E_f), \quad \dots(157)$$

where $\rho(E_f)$ is the density of final states. This is Fermi's golden rule, fundamental for decay rates, absorption and emission of radiation, scattering cross sections, etc.

As an application, consider a atom interacting with a classical monochromatic electric field. The perturbation can be written as $\hat{V}(t) = -\hat{d} \cdot \mathbf{E}_0 \cos \omega t$, where \hat{d} is the dipole operator. Using time-dependent perturbation theory and Fermi's golden rule, one obtains the Einstein B coefficients for absorption and stimulated emission, and, including the quantized field, spontaneous emission as well. This is the foundation of spectroscopy and laser physics.

3.6.3. Variational Principle

The Schrödinger equation can be obtained from a variational principle. Define the functional

$$\mathcal{E}[\psi] = \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle}. \quad \dots(158)$$

The Rayleigh–Ritz principle states that

$$\mathcal{E}[\psi] \geq E_0 \quad \dots(159)$$

for all ψ , with equality when ψ is the ground-state eigenfunction. To prove this, expand ψ in the energy eigenbasis: $\psi = \sum_n c_n \psi_n$. Then

$$\mathcal{E}[\psi] = \frac{\sum_n |c_n|^2 E_n}{\sum_n |c_n|^2} \geq E_0. \quad \dots(160)$$

Taking ψ as a trial function with variational parameters and minimizing \mathcal{E} yields approximate ground-state energies and wave functions. This method is widely used in atomic physics, quantum chemistry, and many-body theory. For example, for the hydrogen atom, one might try a trial wavefunction $\psi(r) = e^{-\alpha r}$ and minimize $\mathcal{E}[\psi]$ with respect to α , obtaining the exact ground state in this case.

The variational method can be extended to excited states by requiring the trial function be orthogonal to lower-energy states. In quantum chemistry, the variational principle underlies the Hartree–Fock method and multiconfigurational self-consistent field approaches. One chooses a parametrized family of Slater determinants or configuration state functions and minimizes the expectation value of the electronic Hamiltonian. Modern density-functional theory (DFT) can also be viewed as a variational approach, but now with the basic variable being the electron density rather than the wavefunction.

3.6.4. Semiclassical Approximations: WKB and Beyond

An important class of approximations exploits the smallness of \hbar compared to classical action scales. In one dimension, the Wentzel–Kramers–Brillouin (WKB) method approximates solutions of

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x) \quad \dots(161)$$

by a phase-amplitude ansatz

$$\psi(x) \approx A(x) \exp \left[\frac{i}{\hbar} S(x) \right] \quad \dots(162)$$

and expands S and A in powers of \hbar . At leading order, one finds

$$\left(\frac{dS}{dx} \right)^2 = 2m(E - V(x)), \quad \dots(163)$$

so that $S(x)$ is the classical action and $p(x) = dS/dx = \sqrt{2m(E - V(x))}$ is the classical momentum. The wavefunction takes the form

$$\psi(x) \approx \frac{C}{\sqrt{p(x)}} \exp \left[\pm \frac{i}{\hbar} \int^x p(x') dx' \right] \quad \dots(164)$$

in classically allowed regions ($E > V$), and

$$\psi(x) \approx \frac{C}{\sqrt{|p(x)|}} \exp \left[\pm \frac{1}{\hbar} \int^x |p(x')| dx' \right]. \quad \dots(165)$$

in classically forbidden regions ($E < V$). Matching the solutions across turning points leads to the Bohr–Sommerfeld quantization condition for bound states between turning points x_1, x_2 :

$$\int_{x_1}^{x_2} p(x) dx = \left(n + \frac{1}{2} \right) \pi \hbar. \quad (166)$$

This semiclassical approximation reproduces the exact spectrum for some systems (harmonic oscillator) and gives good approximations for smooth potentials with large quantum numbers. Semiclassical methods bridge the gap between classical and quantum mechanics and are widely used in molecular spectroscopy, mesoscopic physics (e.g. quantization of electron orbits in magnetic fields), and quantum chaos.

3.7. Open Quantum Systems and Master Equations

So far we have assumed isolated systems evolving unitarily under the Schrödinger equation. Realistic systems interact with environments, leading to decoherence, dissipation, and thermalization.

3.7.1. System–Environment Decomposition

Let the Hilbert space factorize into system and environment:

$$\mathcal{H}_{\text{tot}} = \mathcal{H}_S \otimes \mathcal{H}_E. \quad \dots(167)$$

The total state obeys

$$i\hbar \frac{\partial}{\partial t} | \Psi_{SE}(t) \rangle = \hat{H}_{SE} | \Psi_{SE}(t) \rangle, \quad \dots(168)$$

with

$$\hat{H}_{SE} = \hat{H}_S \otimes \mathbb{I}_E + \mathbb{I}_S \otimes \hat{H}_E + \hat{H}_{\text{int}}. \quad \dots(169)$$

The reduced state of the system is

$$\rho_S(t) = \text{Tr}_E [| \Psi_{SE}(t) \rangle \langle \Psi_{SE}(t) |]. \quad \dots(170)$$

Its dynamics is generally nonunitary and non-Markovian. In the Born–Markov approximation (weak coupling, fast environmental correlation decay), the reduced dynamics becomes Markovian and is described by a master equation.

3.6.2. Lindblad Master Equations

Under the Born–Markov and secular approximations, the reduced state evolves according to a quantum master equation in Lindblad form:

$$\frac{d\rho_S}{dt} = -\frac{i}{\hbar} [\hat{H}_S, \rho_S] + \sum_k \left(L_k \rho_S L_k^\dagger - \frac{1}{2} \{L_k^\dagger L_k, \rho_S\} \right). \quad \dots(171)$$

where \hat{L}_k are Lindblad operators encoding decoherence channels (spontaneous emission, dephasing, thermalization, etc.). This structure ensures complete positivity and trace preservation of $\hat{\rho}_S(t)$. The unitary Schrödinger equation is recovered when all \hat{L}_k vanish. For example, for a two-level system with spontaneous emission,

$$\frac{d}{dt} \hat{\rho}_S = -\frac{i}{\hbar} [\hat{H}_S, \hat{\rho}_S] + \gamma \left(\hat{\sigma}_- \hat{\rho}_S \hat{\sigma}_+ - \frac{1}{2} \{ \hat{\sigma}_+ \hat{\sigma}_-, \hat{\rho}_S \} \right), \quad \dots(172)$$

where $\hat{\sigma}_- = |g\rangle\langle e|$ and $\hat{\sigma}_+ = \hat{\sigma}_-^\dagger$.

Another common example is pure dephasing of a qubit in the $\{|0\rangle, |1\rangle\}$ basis:

$$\frac{d}{dt} \hat{\rho}_S = -\frac{i}{\hbar} [\hat{H}_S, \hat{\rho}_S] + \Gamma_\phi (\hat{\sigma}_z \hat{\rho}_S \hat{\sigma}_z - \hat{\rho}_S), \quad \dots(173)$$

where $\hat{\sigma}_z = |0\rangle\langle 0| - |1\rangle\langle 1|$ and Γ_ϕ is the dephasing rate. This equation leaves populations unchanged but exponentially suppresses off-diagonal coherences, modeling phase noise.

The Lindblad operators \hat{L}_k describe specific decoherence mechanisms. For example, $\hat{L} = \sqrt{\gamma} \hat{\sigma}_-$ models spontaneous emission, while $\hat{L} = \sqrt{\Gamma_\phi} \hat{\sigma}_z$ models pure dephasing. The Lindblad form guarantees that the evolution is completely positive and trace-preserving; see original derivations in Refs. [44, 45].

3.6.3. Decoherence and Emergence of Classicality

Consider a system in a superposition $| \Psi_S \rangle = \sum_i c_i | s_i \rangle$, ... (174)

coupled to an environment initially in $| E_0 \rangle$. Under unitary evolution,

$$| \Psi_{SE}(t) \rangle = \sum_i c_i | s_i \rangle | E_i(t) \rangle, \quad \dots(175)$$

with environment states $| E_i(t) \rangle$ correlated with system states. The reduced density matrix is

$$\hat{\rho}_S(t) = \sum_{i,j} c_i c_j^* \langle E_j(t) | E_i(t) \rangle | s_i \rangle \langle s_j |. \quad \dots(176)$$

If the environment states become approximately orthogonal,

$$\langle E_j(t) | E_i(t) \rangle \approx \delta_{ij}, \quad \dots(177)$$

the off-diagonal elements in the $|s_i\rangle$ basis are suppressed, and $\hat{\rho}_S(t)$ becomes approximately diagonal. This is decoherence. The decoherence timescale is

$$\tau_D \sim \frac{1}{\Gamma}, \quad \dots(178)$$

where Γ is the decoherence rate, which typically grows with the size of the system and the strength of its coupling to the environment.

Decoherence explains why interference between macroscopically distinct states is not observed, even though the total system obeys the Schrödinger equation. It is a crucial ingredient in understanding the quantum-to-classical transition, though it does not by itself select a single measurement outcome. A paradigmatic example is a particle in a superposition of two well-separated positions, interacting with a gas or a bath of photons. Collisions or scattering events imprint “which-path” information in the environment. The reduced density matrix in the position basis,

$$\rho(x, x', t) \quad \dots(179)$$

develops an exponentially decaying factor for $x \neq x'$,

$$\rho(x, x', t) \sim \rho(x, x', 0) \exp[-\Lambda(x - x')^2 t] \quad \dots(180)$$

with a decoherence rate Λ that grows with the square of the separation. For macroscopic separations, the decoherence time can be extremely short, explaining why macroscopic objects appear well localized.

In modern experiments with superconducting circuits, trapped ions, and optomechanical resonators, decoherence and dissipation can be engineered and controlled, allowing detailed tests of open-system dynamics and the interplay between unitary Schrödinger evolution and environmental noise.

3.8. Path Integrals and the Classical Limit

The Schrödinger equation admits an equivalent formulation in terms of path integrals, developed by Richard Feynman. This approach provides deep insights into the relationship between quantum and classical mechanics.

$$\text{The propagator } K(r_b, t_b; r_a, t_a) = \langle r_b | \hat{U}(t_b, t_a) | r_a \rangle \quad \dots(181)$$

$$\text{can be expressed, formally, as } K(r_b, t_b; r_a, t_a) = \int_{r(t_a)=r_a}^{r(t_b)=r_b} \mathcal{D}[r(t)] \exp\left(\frac{i}{\hbar} S[r(t)]\right) \quad \dots(182)$$

$$\text{where the integral is over all paths connecting } (r_a, t_a) \text{ and } (r_b, t_b) \text{ and } S[r(t)] = \int_{t_a}^{t_b} L(r, \dot{r}) dt \quad \dots(183)$$

$$\text{is the classical action. The Lagrangian for a particle in a potential is } L = \frac{1}{2} m \dot{r}^2 - V(r) \quad \dots(184)$$

To make sense of the path integral, we discretize time: $t_a = t_0 < t_1 < \dots < t_N = t_b$ with $\varepsilon = (t_b - t_a)/N$. Then $K(r_b, t_b; r_a, t_a) = \lim_{N \rightarrow \infty} \int d^3 r_1 \dots d^3 r_{N-1} \prod_{j=1}^N K(r_j, t_j; r_{j-1}, t_{j-1}) \quad \dots(185)$

$$\text{where for small } \varepsilon, K(r_j, t_j; r_{j-1}, t_{j-1}) \approx \left(\frac{m}{2\pi i \hbar \varepsilon}\right)^{3/2} \exp\left\{\frac{i\varepsilon}{\hbar} \left[\frac{m}{2} \left(\frac{r_j - r_{j-1}}{\varepsilon}\right)^2 - V\left(\frac{r_j + r_{j-1}}{2}\right)\right]\right\} \quad \dots(186)$$

The continuum path integral is the limit $N \rightarrow \infty$ of this multidimensional integral. In the semiclassical limit $\hbar \rightarrow 0$, the path integral is dominated by stationary points of the action, i.e. classical trajectories obeying the Euler–Lagrange equations. This connects the Schrödinger equation to classical mechanics and underlies the WKB approximation.

For a classical path $r_{cl}(t)$ satisfying $\delta S = 0$, we expand around it: $r(t) = r_{cl}(t) + \delta r(t)$. Then

$$S[r] = S[r_{cl}] + \frac{1}{2} \delta^2 S + \dots \quad \dots(187)$$

The path integral becomes

$$K \approx \exp\left(\frac{i}{\hbar} S[r_{cl}]\right) \int \mathcal{D}[\delta r(t)] \exp\left(\frac{i}{2\hbar} \delta^2 S\right) \quad \dots(188)$$

The Gaussian functional integral can be evaluated, yielding the van Vleck formula:

$$K(r_b, t_b; r_a, t_a) \approx \frac{1}{(2\pi i \hbar)^{3/2}} \sqrt{-\det \left(\frac{\partial^2 S_{cl}}{\partial r_a \partial r_b} \right)} \exp \left(\frac{i}{\hbar} S_{cl} \right) \dots (189)$$

where $S_{cl} = S[r_{cl}]$.

The path integral formulation is particularly powerful for systems with constraints, for quantum field theory, and for explaining topological effects in quantum mechanics. For a free particle, the path integral can be performed exactly, yielding

$$K_{free}(x_b, t_b; x_a, t_a) = \sqrt{\frac{m}{2\pi i \hbar (t_b - t_a)}} \exp \left(\frac{im(x_b - x_a)^2}{2\hbar(t_b - t_a)} \right) \dots (190)$$

which is the same propagator obtained by solving the Schrödinger equation directly. For the harmonic oscillator, the path integral can also be evaluated exactly, and the result matches the known operator-based solution. These examples illustrate the equivalence of the two formulations.

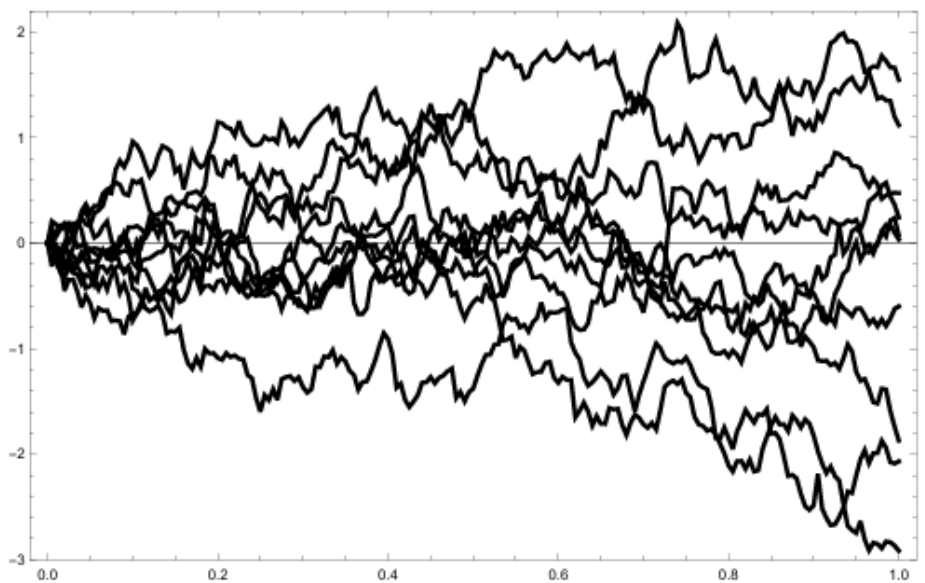


Figure 10. Representative sample paths in the one-dimensional path integral for a free particle between fixed endpoints

The jagged quantum paths dominate the functional integral, while the smooth classical path corresponds to the stationary point of the action. The classical trajectory emerges in the semiclassical limit from interference among these fluctuations. Path integrals also provide a natural route to quantum statistical mechanics: replacing real time t by imaginary time $\tau = -it$ transforms the propagator into a Boltzmann factor, and the partition function can be written as a path integral over closed imaginary-time paths. This connects the Schrödinger equation to the theory of Euclidean field integrals and Monte Carlo methods.

The path integral representation emphasizes that quantum amplitudes arise from a coherent sum over all paths connecting initial and final points, each weighted by $\exp(iS/\hbar)$. Typical paths sampled from the free-particle path integral are highly irregular and nowhere differentiable, in stark contrast to the smooth classical trajectory which extremizes the action. This qualitative difference is illustrated in Fig. 10, where several representative paths contributing to the propagator are shown together with the classical solution.

In Fig. 10, the classical axis represents position x and the vertical axis represents time t , showing sample paths between fixed endpoints. The path integral formulation is particularly powerful for systems with constraints (e.g., a particle on a sphere) because it naturally incorporates constraints by restricting the domain of integration. In quantum field theory, it provides a systematic way to quantize fields and compute correlation functions via generating functionals. Topological effects such as the Aharonov–Bohm effect appear through nontrivial phases $\exp(ie\oint A \cdot dx/\hbar)$ in the path integral; see Ref. [46].

3.9. Nonlinear Modifications and Collapse Models

The standard Schrödinger equation is linear. Several proposals modify it by adding nonlinear or stochastic terms, often motivated by the measurement problem or attempts to unify quantum mechanics with gravity.

3.9.1. Nonlinear Deterministic Modifications

One class of proposals adds nonlinear, state-dependent terms,

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi + \lambda F[\psi]\psi, \quad \dots(191)$$

where $F[\psi]$ is a functional of the state (e.g., depending on $|\psi|^2$). Such models can in principle reproduce the Born rule and introduce new phenomena (self-focusing, solitons, etc.), but are tightly constrained by the requirement of no superluminal signaling. Gisin and others showed that generic nonlinear modifications of the Schrödinger equation, when combined with entanglement, can lead to faster-than-light communication unless very special conditions are satisfied. This severely limits viable nonlinear theories. Presently, there is no compelling experimental evidence for such nonlinear effects.

$$\text{One example is: } i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}} + g |\psi|^2 \right) \psi, \quad \dots(192)$$

where the nonlinear term arises from mean-field interactions. However, this is an effective equation for a condensate, not a fundamental modification. More generally, effective nonlinear Schrödinger-type equations appear in nonlinear optics, where the refractive index depends on the intensity of the light, and in mean-field descriptions of many-body systems. In these contexts, the underlying microscopic dynamics (atoms, fields) still obey linear quantum mechanics, and the nonlinearity is an emergent approximation.

3.9.2. Objective Collapse Models

Objective collapse models modify the Schrödinger equation to produce spontaneous localization of wave functions. For example, in the Ghirardi–Rimini–Weber (GRW) model, each particle undergoes random, instantaneous localization events at a rate λ , with localization width r_c . For a macroscopic object with many particles, the effective collapse rate is $N\lambda$, making macroscopic superpositions extremely short-lived. The Continuous Spontaneous Localization (CSL) model replaces discrete jumps with a continuous stochastic evolution:

$$d|\psi_t\rangle = \left[-\frac{i}{\hbar} \hat{H} dt + \sqrt{\lambda} \int d^3x (\hat{A}(x) - \langle \hat{A}(x) \rangle_t) dW_t(x) - \frac{\lambda}{2} \int d^3x (\hat{A}(x) - \langle \hat{A}(x) \rangle_t)^2 dt \right] |\psi_t\rangle, \quad \dots(193)$$

where $\hat{n}(x)$ is a smeared mass density operator and $dW_t(x)$ are independent Wiener process (white noise). The noise drives the state towards superpositions localized in x , suppressing macroscopic superpositions.

Such models make experimentally testable predictions (heating, spontaneous radiation, loss of interference) and are the subject of ongoing experimental tests. To date, no deviations from standard quantum mechanics have been observed, placing bounds on the parameters λ and r_c .

Current and proposed experiments testing collapse models include:

- Matter-wave interferometry with large molecules and nanoparticles, where CSL predicts loss of interference at large masses and path separations.
- Precision heating measurements in ultracold cantilevers and levitated nanoparticles, where CSL noise would induce energy.
- Spontaneous X-ray emission from bulk matter, arising from CSL-induced excitations.

The interplay between environmental decoherence and intrinsic collapse is subtle: both tend to suppress interference, but with different parameter dependences. Carefully designed experiments aim to separate these effects.

3.10. Relativistic Extensions and Quantum Fields

The Schrödinger equation is nonrelativistic. Incorporating relativity leads to new structures and ultimately to quantum field theory.

3.10.1. Relativistic Wave Equations

Starting from the relativistic dispersion relation $E^2 = p^2 c^2 + m^2 c^4$ and promoting $E \rightarrow i\hbar \partial_t$, $p \rightarrow -i\hbar \nabla$ gives the Klein–Gordon equation:

$$\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 + \frac{m^2 c^2}{\hbar^2} \right) \psi(x, t) = 0, \quad \dots(194)$$

This is second order in time and describes spin-0 particles. It has issues with probability interpretation (the conserved current is not positive-definite), and its solutions include negative-energy states. For spin- $\frac{1}{2}$ particles, Dirac sought a first-order equation that would avoid these problems. The result is the Dirac equation:

$$(i\hbar\gamma^\mu \partial_\mu - mc)\psi = 0, \quad \dots(195)$$

with gamma matrices γ^μ obeying the Clifford algebra

$$\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}. \quad \dots(196)$$

The Dirac equation has a conserved positive-definite probability density and predicts spin and antimatter through its four-component structure. Both Klein–Gordon and Dirac equations lead naturally to quantum field theory, where creation and annihilation operators are allowed and the negative-energy solutions are reinterpreted. Taking the nonrelativistic limit of the Dirac equation recovers the Pauli equation for spin- $\frac{1}{2}$ particles, including relativistic corrections such as spin–orbit coupling and magnetic interactions.

3.10.2. Functional Schrödinger Picture in QFT

Even in relativistic quantum field theory, one may adopt a Schrödinger picture, where states are functionals of field configurations and obey a functional Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} \Psi[\phi(x), t] = \hat{H}[\phi(x), -i\hbar \frac{\delta}{\delta\phi(x)}] \Psi[\phi(x), t], \quad \dots(197)$$

with Hamiltonian

$$\hat{H} = \int d^3x \left[\frac{1}{2} \left(-\hbar^2 \frac{\delta^2}{\delta\phi(x)^2} + (\nabla\phi(x))^2 + V(\phi) \right) \right]. \quad \dots(198)$$

This formulation is useful in canonical quantization (and in certain approaches to quantum gravity). However, the nonrelativistic Schrödinger equation remains the primary tool for low-energy systems (atoms, molecules, condensed matter, ultracold gases) where relativistic effects and quantum field effects are negligible.

3.11. Foundational Status and Outlook

As a long-form pedagogical review, the present scope is necessarily selective. We prioritize structural clarity and canonical models over exhaustive coverage of specialized applications (e.g., advanced scattering theory, numerical spectral methods, or full quantum chemistry workflows). We also emphasize conceptual and operator-theoretic issues (self-adjointness, domain questions) at a level suitable for advanced undergraduate and early graduate students, rather than presenting full proofs in functional analysis.

After nearly a century, how should one view the Schrödinger equation? As a fundamental law, in many interpretations (Everett, Bohm, the Schrödinger equation is taken as universally valid, with all apparent collapse phenomena arising from decoherence and branching or from hidden variables. In this view, the equation describes the complete evolution of the quantum state at all scales. In Everett (many-worlds) type interpretations, the universal wavefunction never collapses; measurements correspond to branching of the state into decohering sectors, each containing different outcomes. The Schrödinger equation is exact, and probabilities are interpreted in terms of branch weights. Decoherence theory, discussed in Sec. VII, provides the dynamical mechanism for branching and for the emergence of quasi-classical worlds.

In Bohmian mechanics, the wavefunction obeys the Schrödinger equation, but particles also have definite positions guided by the wavefunction through the guidance equation $\dot{x} = \nabla S/m$. The Schrödinger equation thus governs the evolution of the pilot wave, which in turn determines the trajectories of particles. The Born rule emerges from typicality arguments given suitable initial conditions. As an effective law, in collapse models and some quantum-gravity scenarios, the Schrödinger equation is regarded as an approximation valid for microscopic systems, replaced at larger scales or higher energies by a more general nonlinear or stochastic dynamics. This view suggests that laboratory tests will increasingly measure quantum superpositions with eventually revealed deviations.

As a structural constraint from information-theoretic principles, recent reconstructions of quantum theory emphasize axioms about information, probability, and symmetry that single out the Schrödinger equation as a unique dynamical law compatible with consistency requirements (no-signaling, continuity, reversibility, dynamics). From this perspective, the Schrödinger equation appears as a consequence of very general principles

about information processing. Experimentally, the Schrödinger equation has passed every test to date, from atomic spectra to interference with large molecules and macroscopic quantum states in superconducting circuits and mechanical resonators. Future experiments with increasingly massive superpositions, precision tests of collapse models, and probes of quantum gravity may yet reveal deviations or may further reinforce the equation's status as a central pillar of physics.

Regardless of its ultimate fate at the deepest level, the Schrödinger equation will continue to structure how we model, compute, and understand quantum systems across physics, chemistry, and emerging quantum technologies. Its combination of mathematical elegance and empirical success has made it one of the most profound and useful equations in all of science. In addition to Bohmian mechanics and many-worlds, the Copenhagen interpretation remains the most widely taught view: it treats the wavefunction as a complete description of an individual system, with measurement causing an irreversible collapse. The statistical interpretation, advocated by Einstein and others, regards the wavefunction as describing an ensemble of similarly prepared systems. All interpretations share the Schrödinger equation as the dynamical core; their differences lie in the ontology and the treatment of measurement. See Ref. [47] for a comprehensive overview.

4. CONCLUSION

This study provides a coherent pedagogical synthesis of the Schrödinger equation by integrating its physical derivations, mathematical structure, and key applications. The results show that different derivation approaches consistently lead to a unified framework characterized by linear, unitary evolution governed by a self-adjoint Hamiltonian. This structure ensures probability conservation and explains fundamental quantum phenomena such as superposition, tunnelling, and quantization. The integration of Hilbert-space formalism with canonical models helps bridge the gap between abstract theory and physical interpretation, supporting clearer conceptual understanding in quantum mechanics learning. Future research is recommended to empirically test the effectiveness of this framework in educational settings, develop interactive digital learning tools, and extend the approach to emerging areas such as quantum computing and quantum information.

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