

Relativistic Quantum Simulation

Classical vs Quantum Approaches:
Vector Spaces, Special Functions, and the Schrödinger Equation
in Three-Dimensional Relativistic Structure

COMPREHENSIVE MATHEMATICAL TREATMENT

Quantum-Classical Simulation Framework

December 5, 2025

Abstract

This document presents a comprehensive mathematical treatment of quantum mechanics in the relativistic regime, with particular emphasis on the comparison between classical and quantum simulation approaches. We develop the theoretical foundations including Hilbert space structure, special functions arising from separation of variables, residue theorems for Green's function calculations, and the full relativistic extension of the Schrödinger equation leading to the Klein-Gordon and Dirac equations. The mathematical framework is applied to practical simulation scenarios including electron-proton-neutron systems and multi-electron atoms, demonstrating the fundamental differences between classical point-particle dynamics and quantum mechanical evolution.

Keywords: Relativistic Quantum Mechanics, Hilbert Spaces, Special Functions, Dirac Equation, Classical-Quantum Correspondence, Simulation Methods

Contents

1	Introduction	4
1.1	Units and Conventions	4
2	Vector Spaces and Hilbert Space Structure	4
2.1	Abstract Vector Spaces	4
2.2	Inner Product Spaces	5
2.3	Hilbert Spaces in Quantum Mechanics	5
2.3.1	Position Space Representation	5
2.3.2	Momentum Space Representation	6
2.4	Operators on Hilbert Spaces	6
2.4.1	Hermitian (Self-Adjoint) Operators	6
2.4.2	Fundamental Operators	6
2.5	Tensor Product Structure for Multi-Particle Systems	7
3	Special Functions in Quantum Mechanics	7
3.1	Spherical Harmonics	7
3.1.1	Associated Legendre Polynomials	8
3.2	Generalized Laguerre Polynomials	8
3.3	Hermite Polynomials	9
3.4	Bessel Functions	9
3.4.1	Spherical Bessel Functions	9
3.5	Hypergeometric Functions	10
4	Residue Theorems and Complex Analysis	10
4.1	Contour Integration Fundamentals	10
4.2	Residue Theorem	10
4.3	Application: Free-Particle Propagator	11
4.4	Application: Scattering Amplitude	12
4.5	Dispersion Relations	12
5	The Schrödinger Equation in 3D	12
5.1	Time-Independent Schrödinger Equation	12
5.2	Separation of Variables	12
5.2.1	Radial Equation	13
5.3	Hydrogen Atom Solution	13
5.4	Time-Dependent Schrödinger Equation	13
6	Relativistic Extension: From Schrödinger to Dirac	14
6.1	Relativistic Energy-Momentum Relation	14
6.2	Klein-Gordon Equation	14
6.2.1	Problems with Klein-Gordon	14
6.3	The Dirac Equation	14
6.4	Covariant Form of the Dirac Equation	15
6.5	Solutions of the Free Dirac Equation	15
6.5.1	Explicit Spinor Solutions	15
6.6	Physical Interpretation	16

6.7	Dirac Equation in External Electromagnetic Field	16
6.8	Non-Relativistic Limit: Pauli Equation	16
6.9	Relativistic Hydrogen Atom	16
7	Classical vs Quantum Simulation: Mathematical Comparison	17
7.1	Classical Approach	17
7.1.1	Equations of Motion	17
7.1.2	Velocity Verlet Integration	17
7.1.3	Bohr Model	17
7.2	Quantum Approach	18
7.2.1	Variational Principle	18
7.2.2	Hartree-Fock for Multi-Electron Systems	18
7.3	Comparison of Methods	19
7.4	Electron-Proton-Neutron System Analysis	19
7.5	Three-Electron System (Lithium)	19
7.6	Key Quantum Effects Missing in Classical Simulation	20
8	Numerical Methods for Quantum Simulation	20
8.1	Shooting Method for Radial Equations	20
8.2	Variational Monte Carlo	21
8.3	Basis Set Expansion	21
9	Applications to Specific Systems	21
9.1	Electron-Proton-Neutron (e-p-n) System	21
9.2	Three-Electron Atom (Lithium)	22
10	Conclusion	22
10.1	Key Findings	22
10.2	Recommendations	23
10.3	Future Directions	23
A	Mathematical Appendices	23
A.1	Gamma Matrix Identities	23
A.2	Useful Integrals	24
A.3	Physical Constants	24

1 Introduction

The simulation of physical systems at the atomic and subatomic scale presents a fundamental choice between classical and quantum mechanical descriptions. While classical mechanics provides intuitive trajectories and computational efficiency, quantum mechanics captures the true nature of microscopic phenomena including discretization of energy levels, uncertainty relations, and wave-particle duality.

This document develops the complete mathematical framework necessary to understand:

1. The structure of quantum state spaces (Hilbert spaces) and their role in formulating quantum mechanics
2. Special functions that emerge as solutions to the angular and radial parts of quantum equations
3. Complex analysis techniques including residue theorems for evaluating propagators and Green's functions
4. The relativistic extension of the Schrödinger equation in three spatial dimensions
5. Practical comparison of classical versus quantum simulation approaches

1.1 Units and Conventions

Throughout this document, we employ **atomic units** where:

$$\hbar = m_e = e = 4\pi\epsilon_0 = 1 \quad (1)$$

This implies:

- Length unit: Bohr radius $a_0 = 5.29 \times 10^{-11}$ m
- Energy unit: Hartree $E_h = 27.21$ eV
- Time unit: $\hbar/E_h = 2.42 \times 10^{-17}$ s

For relativistic expressions, we use the metric signature $(+, -, -, -)$ and define:

$$x^\mu = (ct, x, y, z), \quad p_\mu = (E/c, -p_x, -p_y, -p_z) \quad (2)$$

2 Vector Spaces and Hilbert Space Structure

2.1 Abstract Vector Spaces

Definition 2.1 (Vector Space). A **vector space** V over a field \mathbb{F} (typically \mathbb{R} or \mathbb{C}) is a set equipped with two operations:

1. **Vector addition:** $+: V \times V \rightarrow V$
2. **Scalar multiplication:** $\cdot: \mathbb{F} \times V \rightarrow V$

satisfying the following axioms for all $\vec{u}, \vec{v}, \vec{w} \in V$ and $a, b \in \mathbb{F}$:

$$\vec{u} + \vec{v} = \vec{v} + \vec{u} \quad (\text{Commutativity}) \quad (3)$$

$$(\vec{u} + \vec{v}) + \vec{w} = \vec{u} + (\vec{v} + \vec{w}) \quad (\text{Associativity}) \quad (4)$$

$$\exists \vec{0} : \vec{v} + \vec{0} = \vec{v} \quad (\text{Identity}) \quad (5)$$

$$\forall \vec{v}, \exists (-\vec{v}) : \vec{v} + (-\vec{v}) = \vec{0} \quad (\text{Inverse}) \quad (6)$$

$$a(b\vec{v}) = (ab)\vec{v} \quad (\text{Compatibility}) \quad (7)$$

$$1 \cdot \vec{v} = \vec{v} \quad (\text{Identity scalar}) \quad (8)$$

$$a(\vec{u} + \vec{v}) = a\vec{u} + a\vec{v} \quad (\text{Distributivity}) \quad (9)$$

$$(a + b)\vec{v} = a\vec{v} + b\vec{v} \quad (\text{Distributivity}) \quad (10)$$

2.2 Inner Product Spaces

Definition 2.2 (Inner Product). An **inner product** on a complex vector space V is a map $\langle \cdot, \cdot \rangle : V \times V \rightarrow \mathbb{C}$ satisfying:

$$\langle \vec{v}, \vec{v} \rangle \geq 0, \quad \text{with equality iff } \vec{v} = \vec{0} \quad (\text{Positive definiteness}) \quad (11)$$

$$\langle \vec{u}, \vec{v} \rangle = \overline{\langle \vec{v}, \vec{u} \rangle} \quad (\text{Conjugate symmetry}) \quad (12)$$

$$\langle a\vec{u} + b\vec{v}, \vec{w} \rangle = a\langle \vec{u}, \vec{w} \rangle + b\langle \vec{v}, \vec{w} \rangle \quad (\text{Linearity in first argument}) \quad (13)$$

The inner product induces a norm:

$$\|\vec{v}\| = \sqrt{\langle \vec{v}, \vec{v} \rangle} \quad (14)$$

2.3 Hilbert Spaces in Quantum Mechanics

Definition 2.3 (Hilbert Space). A **Hilbert space** \mathcal{H} is a complete inner product space, meaning every Cauchy sequence converges to an element within the space.

Physical Significance

In quantum mechanics, the state of a system is represented by a vector (ray) in a Hilbert space. The inner product provides:

- **Transition amplitudes:** $\langle \phi | \psi \rangle$ = probability amplitude to find state $|\phi\rangle$ given state $|\psi\rangle$
- **Probabilities:** $|\langle \phi | \psi \rangle|^2$ = transition probability
- **Normalization:** $\langle \psi | \psi \rangle = 1$ for physical states

2.3.1 Position Space Representation

The Hilbert space of a single particle in three dimensions is:

$$\mathcal{H} = L^2(\mathbb{R}^3) = \left\{ \psi : \mathbb{R}^3 \rightarrow \mathbb{C} \mid \int_{\mathbb{R}^3} |\psi(\vec{r})|^2 d^3r < \infty \right\} \quad (15)$$

The inner product is:

$$\langle \phi | \psi \rangle = \int_{\mathbb{R}^3} \phi^*(\vec{r}) \psi(\vec{r}) d^3r \quad (16)$$

2.3.2 Momentum Space Representation

Via Fourier transform:

$$\tilde{\psi}(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} \psi(\vec{r}) e^{-i\vec{p}\cdot\vec{r}/\hbar} d^3r \quad (17)$$

Parseval's theorem ensures:

$$\int |\psi(\vec{r})|^2 d^3r = \int |\tilde{\psi}(\vec{p})|^2 d^3p \quad (18)$$

2.4 Operators on Hilbert Spaces

Definition 2.4 (Linear Operator). A **linear operator** $\hat{A} : \mathcal{H} \rightarrow \mathcal{H}$ satisfies:

$$\hat{A}(\alpha|\psi\rangle + \beta|\phi\rangle) = \alpha\hat{A}|\psi\rangle + \beta\hat{A}|\phi\rangle \quad (19)$$

2.4.1 Hermitian (Self-Adjoint) Operators

Definition 2.5 (Hermitian Operator). An operator \hat{A} is **Hermitian** (self-adjoint) if:

$$\langle\phi|\hat{A}|\psi\rangle = \langle\psi|\hat{A}|\phi\rangle^* \quad \forall |\phi\rangle, |\psi\rangle \in \mathcal{H} \quad (20)$$

Equivalently, $\hat{A} = \hat{A}^\dagger$.

Theorem 2.1 (Spectral Theorem for Hermitian Operators). For a Hermitian operator \hat{A} on a Hilbert space:

1. All eigenvalues are **real**
2. Eigenvectors corresponding to distinct eigenvalues are **orthogonal**
3. The eigenvectors form a **complete basis** for \mathcal{H}

2.4.2 Fundamental Operators

The position and momentum operators in position representation:

$$\hat{x}_i \psi(\vec{r}) = x_i \psi(\vec{r}) \quad (21)$$

$$\hat{p}_i \psi(\vec{r}) = -i\hbar \frac{\partial}{\partial x_i} \psi(\vec{r}) \quad (22)$$

The **canonical commutation relation**:

$$[\hat{x}_i, \hat{p}_j] = i\hbar \delta_{ij} \quad (23)$$

2.5 Tensor Product Structure for Multi-Particle Systems

For N particles, the total Hilbert space is:

$$\mathcal{H}_{\text{total}} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_N \quad (24)$$

For identical fermions (like electrons), the physical subspace is the **antisymmetric** subspace:

$$\mathcal{H}_{\text{fermion}} = \bigwedge^N \mathcal{H}_1 \quad (25)$$

The antisymmetrized wave function for two electrons:

$$\Psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} [\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) - \psi_a(\vec{r}_2)\psi_b(\vec{r}_1)] \quad (26)$$

This is the mathematical origin of the **Pauli exclusion principle**.

3 Special Functions in Quantum Mechanics

Special functions arise naturally when solving quantum mechanical equations via separation of variables. This section develops the key functions essential for atomic physics.

3.1 Spherical Harmonics

When separating the angular part of the Laplacian in spherical coordinates (r, θ, ϕ) :

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \hat{L}^2 \quad (27)$$

where \hat{L}^2 is the angular momentum squared operator:

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \quad (28)$$

Definition 3.1 (Spherical Harmonics). The **spherical harmonics** $Y_l^m(\theta, \phi)$ are eigenfunctions of \hat{L}^2 and \hat{L}_z :

$$\hat{L}^2 Y_l^m = \hbar^2 l(l+1) Y_l^m, \quad l = 0, 1, 2, \dots \quad (29)$$

$$\hat{L}_z Y_l^m = \hbar m Y_l^m, \quad m = -l, -l+1, \dots, l \quad (30)$$

Explicit form:

$$Y_l^m(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos \theta) e^{im\phi} \quad (31)$$

where P_l^m are associated Legendre polynomials.

3.1.1 Associated Legendre Polynomials

Definition 3.2 (Associated Legendre Polynomials). For $m \geq 0$:

$$P_l^m(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_l(x) \quad (32)$$

where $P_l(x)$ is the Legendre polynomial:

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} (x^2 - 1)^l \quad (\text{Rodrigues formula}) \quad (33)$$

Orthogonality:

$$\int_{-1}^1 P_l^m(x) P_{l'}^m(x) dx = \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \delta_{ll'} \quad (34)$$

First few Legendre polynomials:

$$P_0(x) = 1 \quad (35)$$

$$P_1(x) = x \quad (36)$$

$$P_2(x) = \frac{1}{2}(3x^2 - 1) \quad (37)$$

$$P_3(x) = \frac{1}{2}(5x^3 - 3x) \quad (38)$$

3.2 Generalized Laguerre Polynomials

The radial equation for hydrogen-like atoms leads to associated (generalized) Laguerre polynomials.

Definition 3.3 (Generalized Laguerre Polynomials).

$$L_n^\alpha(x) = \frac{x^{-\alpha} e^x}{n!} \frac{d^n}{dx^n} (e^{-x} x^{n+\alpha}) \quad (39)$$

Explicit formula:

$$L_n^\alpha(x) = \sum_{k=0}^n (-1)^k \binom{n+\alpha}{n-k} \frac{x^k}{k!} \quad (40)$$

Orthogonality with weight $w(x) = x^\alpha e^{-x}$:

$$\int_0^\infty x^\alpha e^{-x} L_n^\alpha(x) L_m^\alpha(x) dx = \frac{\Gamma(n+\alpha+1)}{n!} \delta_{nm} \quad (41)$$

The radial wave functions for hydrogen:

$$R_{nl}(r) = \sqrt{\left(\frac{2Z}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}} e^{-\rho/2} \rho^l L_{n-l-1}^{2l+1}(\rho) \quad (42)$$

where $\rho = 2Zr/(na_0)$.

3.3 Hermite Polynomials

The harmonic oscillator in quantum mechanics leads to Hermite polynomials.

Definition 3.4 (Hermite Polynomials).

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \quad (\text{Rodrigues formula}) \quad (43)$$

Recurrence relation:

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \quad (44)$$

Orthogonality with weight $w(x) = e^{-x^2}$:

$$\int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x) dx = \sqrt{\pi} 2^n n! \delta_{mn} \quad (45)$$

The harmonic oscillator wave functions:

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-m\omega x^2/2\hbar} H_n \left(\sqrt{\frac{m\omega}{\hbar}} x \right) \quad (46)$$

3.4 Bessel Functions

Bessel functions appear in cylindrical coordinates and scattering problems.

Definition 3.5 (Bessel Functions of the First Kind). $J_\nu(x)$ satisfies Bessel's equation:

$$x^2 \frac{d^2 y}{dx^2} + x \frac{dy}{dx} + (x^2 - \nu^2) y = 0 \quad (47)$$

Solution via power series:

$$J_\nu(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k! \Gamma(k + \nu + 1)} \left(\frac{x}{2} \right)^{2k + \nu} \quad (48)$$

3.4.1 Spherical Bessel Functions

For spherical coordinates:

$$j_l(x) = \sqrt{\frac{\pi}{2x}} J_{l+1/2}(x) \quad (49)$$

Explicit forms:

$$j_0(x) = \frac{\sin x}{x} \quad (50)$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x} \quad (51)$$

$$j_2(x) = \left(\frac{3}{x^2} - 1 \right) \frac{\sin x}{x} - \frac{3 \cos x}{x^2} \quad (52)$$

Application: The free-particle wave function in spherical coordinates:

$$\psi_{\vec{k}}(\vec{r}) = 4\pi \sum_{l=0}^{\infty} i^l j_l(kr) \sum_{m=-l}^l Y_l^{m*}(\hat{k}) Y_l^m(\hat{r}) \quad (53)$$

3.5 Hypergeometric Functions

The confluent hypergeometric function (Kummer's function) appears in the exact solution of the hydrogen atom.

Definition 3.6 (Confluent Hypergeometric Function).

$${}_1F_1(a; b; z) = M(a, b, z) = \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n} \frac{z^n}{n!} \quad (54)$$

where $(a)_n = a(a+1)\cdots(a+n-1)$ is the Pochhammer symbol.

The radial hydrogen wave function can be written:

$$R_{nl}(r) \propto e^{-\rho/2} \rho^l {}_1F_1(-n+l+1; 2l+2; \rho) \quad (55)$$

4 Residue Theorems and Complex Analysis

Complex analysis provides powerful techniques for evaluating integrals, computing Green's functions, and analyzing scattering amplitudes in quantum mechanics.

4.1 Contour Integration Fundamentals

Definition 4.1 (Holomorphic Function). A function $f : \mathbb{C} \rightarrow \mathbb{C}$ is **holomorphic** (analytic) at z_0 if:

$$f'(z_0) = \lim_{z \rightarrow z_0} \frac{f(z) - f(z_0)}{z - z_0} \quad (56)$$

exists.

Theorem 4.1 (Cauchy's Integral Theorem). If f is holomorphic in a simply connected domain D and C is a closed contour in D :

$$\oint_C f(z) dz = 0 \quad (57)$$

Theorem 4.2 (Cauchy's Integral Formula). If f is holomorphic inside and on a simple closed contour C and z_0 is inside C :

$$f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z - z_0} dz \quad (58)$$

4.2 Residue Theorem

Definition 4.2 (Residue). If f has an isolated singularity at z_0 , the **residue** is the coefficient a_{-1} in the Laurent expansion:

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n \quad (59)$$

Notation: $\text{Res}(f, z_0) = a_{-1}$.

Calculation of residues:

1. **Simple pole:** $\text{Res}(f, z_0) = \lim_{z \rightarrow z_0} (z - z_0)f(z)$

2. **Pole of order n :**

$$\text{Res}(f, z_0) = \frac{1}{(n-1)!} \lim_{z \rightarrow z_0} \frac{d^{n-1}}{dz^{n-1}} [(z - z_0)^n f(z)] \quad (60)$$

Theorem 4.3 (Residue Theorem). If f is holomorphic inside a simple closed contour C except for isolated singularities z_1, z_2, \dots, z_n inside C :

$$\oint_C f(z) dz = 2\pi i \sum_{k=1}^n \text{Res}(f, z_k) \quad (61)$$

4.3 Application: Free-Particle Propagator

The time-dependent Schrödinger equation has the formal solution:

$$\psi(\vec{r}, t) = \int G(\vec{r}, \vec{r}'; t) \psi(\vec{r}', 0) d^3 r' \quad (62)$$

The **retarded Green's function** (propagator) in momentum space:

$$G(\vec{p}, E) = \frac{1}{E - \frac{p^2}{2m} + i\epsilon} \quad (63)$$

The $+i\epsilon$ prescription ensures causality by pushing the pole slightly into the lower half-plane.

Example 4.1 (Position-Space Propagator). To find $G(\vec{r}, t)$, we evaluate:

$$G(\vec{r}, t) = \frac{1}{(2\pi)^4} \int d^3 p \int_{-\infty}^{\infty} dE \frac{e^{i(\vec{p} \cdot \vec{r} - Et)/\hbar}}{E - \frac{p^2}{2m} + i\epsilon} \quad (64)$$

The energy integral is evaluated using contour integration. The pole is at:

$$E = \frac{p^2}{2m} - i\epsilon \quad (65)$$

For $t > 0$, we close the contour in the lower half-plane (where $e^{-iEt/\hbar}$ decays), picking up the residue:

$$\int_{-\infty}^{\infty} dE \frac{e^{-iEt/\hbar}}{E - \frac{p^2}{2m} + i\epsilon} = -2\pi i e^{-ip^2 t/(2m\hbar)} \quad (66)$$

This yields the free-particle propagator:

$$G(\vec{r}, t) = \left(\frac{m}{2\pi i \hbar t} \right)^{3/2} \exp\left(\frac{imr^2}{2\hbar t} \right), \quad t > 0 \quad (67)$$

4.4 Application: Scattering Amplitude

In scattering theory, the T -matrix has poles corresponding to bound states and resonances.

The **partial-wave scattering amplitude**:

$$f_l(k) = \frac{e^{i\delta_l} \sin \delta_l}{k} = \frac{1}{k \cot \delta_l - ik} \quad (68)$$

Near a resonance at energy E_R with width Γ :

$$f(E) \approx \frac{\Gamma/2}{E_R - E - i\Gamma/2} \quad (69)$$

This is a **Breit-Wigner resonance** with a simple pole in the complex energy plane at $E = E_R - i\Gamma/2$.

4.5 Dispersion Relations

Kramers-Kronig relations connect real and imaginary parts of response functions:

$$\text{Re}[\chi(\omega)] = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{\text{Im}[\chi(\omega')]}{\omega' - \omega} d\omega' \quad (70)$$

$$\text{Im}[\chi(\omega)] = -\frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{\text{Re}[\chi(\omega')]}{\omega' - \omega} d\omega' \quad (71)$$

These are consequences of causality and are derived using contour integration around the poles.

5 The Schrödinger Equation in 3D

5.1 Time-Independent Schrödinger Equation

$$\hat{H}\psi(\vec{r}) = E\psi(\vec{r}) \quad (72)$$

where the Hamiltonian for a particle in a potential $V(\vec{r})$:

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \quad (73)$$

In spherical coordinates:

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{\hat{L}^2}{\hbar^2 r^2} \quad (74)$$

5.2 Separation of Variables

For spherically symmetric potentials $V(r)$:

$$\psi(r, \theta, \phi) = R(r) Y_l^m(\theta, \phi) \quad (75)$$

5.2.1 Radial Equation

The radial function $R(r)$ satisfies:

$$-\frac{\hbar^2}{2m} \left[\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} - \frac{l(l+1)}{r^2} R \right] + V(r)R = ER \quad (76)$$

Substituting $u(r) = rR(r)$:

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + \left[V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} \right] u = Eu \quad (77)$$

This is a one-dimensional Schrödinger equation with an effective potential:

$$V_{\text{eff}}(r) = V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} \quad (78)$$

The second term is the **centrifugal barrier**.

5.3 Hydrogen Atom Solution

For the Coulomb potential $V(r) = -Ze^2/r$ (in Gaussian units) or $V(r) = -Z/r$ (in atomic units):

$$E_n = -\frac{Z^2}{2n^2} \quad (\text{Hartree}) \quad (79)$$

The degeneracy is n^2 (or $2n^2$ including spin).

The complete wave function:

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_l^m(\theta, \phi) \quad (80)$$

Ground state ($n = 1, l = 0, m = 0$):

$$\psi_{100}(r) = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0} \quad (81)$$

Expectation values:

$$\langle r \rangle_{nl} = \frac{a_0}{2Z} [3n^2 - l(l+1)] \quad (82)$$

$$\langle r^2 \rangle_{nl} = \frac{a_0^2 n^2}{2Z^2} [5n^2 + 1 - 3l(l+1)] \quad (83)$$

$$\langle 1/r \rangle_{nl} = \frac{Z}{a_0 n^2} \quad (84)$$

5.4 Time-Dependent Schrödinger Equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi \quad (85)$$

For time-independent \hat{H} , the general solution:

$$\Psi(\vec{r}, t) = \sum_n c_n \psi_n(\vec{r}) e^{-iE_n t/\hbar} \quad (86)$$

where $c_n = \langle \psi_n | \Psi(0) \rangle$.

6 Relativistic Extension: From Schrödinger to Dirac

The non-relativistic Schrödinger equation fails at high velocities. This section develops the relativistic quantum equations.

6.1 Relativistic Energy-Momentum Relation

In special relativity:

$$E^2 = p^2 c^2 + m^2 c^4 \quad (87)$$

or in natural units ($c = \hbar = 1$):

$$E^2 = \vec{p}^2 + m^2 \quad (88)$$

6.2 Klein-Gordon Equation

Promoting $E \rightarrow i\partial_t$ and $\vec{p} \rightarrow -i\nabla$:

$$-\frac{\partial^2 \phi}{\partial t^2} = (-\nabla^2 + m^2)\phi \quad (89)$$

or in covariant form:

$$\boxed{(\partial_\mu \partial^\mu + m^2)\phi = 0 \quad \Leftrightarrow \quad (\square + m^2)\phi = 0} \quad (90)$$

where $\square = \partial_t^2 - \nabla^2$ is the d'Alembertian.

6.2.1 Problems with Klein-Gordon

1. **Negative probabilities:** The probability density $\rho = i(\phi^* \partial_t \phi - \phi \partial_t \phi^*)$ can be negative
2. **Negative energies:** Solutions $E = \pm \sqrt{\vec{p}^2 + m^2}$

Resolution: Klein-Gordon describes **spin-0** particles; ρ is charge density, not probability.

6.3 The Dirac Equation

Dirac sought a first-order equation to avoid the square root problem.

Dirac's Insight

Factor the relativistic dispersion:

$$E = \vec{\alpha} \cdot \vec{p} + \beta m \quad (91)$$

Squaring must recover $E^2 = \vec{p}^2 + m^2$, requiring:

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij} \quad (92)$$

$$\{\alpha_i, \beta\} = 0 \quad (93)$$

$$\beta^2 = 1 \quad (94)$$

These are the **Clifford algebra** relations.

The minimum representation is 4×4 matrices. The **Dirac equation**:

$$\boxed{i\hbar \frac{\partial \psi}{\partial t} = (c\boldsymbol{\alpha} \cdot \vec{p} + \beta mc^2) \psi} \quad (95)$$

In the **standard (Dirac) representation**:

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad (96)$$

where σ_i are Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (97)$$

6.4 Covariant Form of the Dirac Equation

Define the gamma matrices:

$$\gamma^0 = \beta, \quad \gamma^i = \beta \alpha_i \quad (98)$$

satisfying the **Clifford algebra**:

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu} I_4 \quad (99)$$

The Dirac equation becomes:

$$\boxed{(i\gamma^\mu \partial_\mu - m)\psi = 0 \quad \Leftrightarrow \quad (i\not{\partial} - m)\psi = 0} \quad (100)$$

where $\not{\partial} = \gamma^\mu \partial_\mu$ is Feynman slash notation.

6.5 Solutions of the Free Dirac Equation

Plane wave solutions:

$$\psi(x) = u(p)e^{-ip \cdot x} \quad (\text{positive energy}) \quad (101)$$

$$\psi(x) = v(p)e^{+ip \cdot x} \quad (\text{negative energy}) \quad (102)$$

The spinors $u(p)$ and $v(p)$ satisfy:

$$(\not{p} - m)u(p) = 0 \quad (103)$$

$$(\not{p} + m)v(p) = 0 \quad (104)$$

6.5.1 Explicit Spinor Solutions

For a particle with momentum \vec{p} along z -axis:

$$u^{(s)}(p) = \sqrt{E + m} \begin{pmatrix} \chi^{(s)} \\ \frac{\vec{\sigma} \cdot \vec{p}}{E + m} \chi^{(s)} \end{pmatrix} \quad (105)$$

where $\chi^{(1)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ (spin up) and $\chi^{(2)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ (spin down).

6.6 Physical Interpretation

1. **Four components:** Two for spin (up/down), two for particle/antiparticle
2. **Spin:** Dirac equation predicts spin-1/2 naturally
3. **Magnetic moment:** Predicts $g = 2$ for the electron (before QED corrections)
4. **Negative energies:** Interpreted as antiparticles (positrons)

6.7 Dirac Equation in External Electromagnetic Field

Minimal coupling: $p_\mu \rightarrow p_\mu - qA_\mu$

$$[\gamma^\mu(i\partial_\mu - qA_\mu) - m]\psi = 0 \quad (106)$$

or:

$$i\hbar\frac{\partial\psi}{\partial t} = \left[c\boldsymbol{\alpha} \cdot (\vec{p} - q\vec{A}) + \beta mc^2 + q\phi \right] \psi \quad (107)$$

6.8 Non-Relativistic Limit: Pauli Equation

Expanding to order $(v/c)^2$:

$$i\hbar\frac{\partial\psi}{\partial t} = \left[\frac{(\vec{p} - q\vec{A})^2}{2m} + q\phi - \frac{q\hbar}{2m}\boldsymbol{\sigma} \cdot \vec{B} + \dots \right] \psi \quad (108)$$

The third term is the **spin-magnetic field coupling** with the correct g -factor of 2.

6.9 Relativistic Hydrogen Atom

The Dirac equation for hydrogen (with $V = -Z\alpha/r$):

$$\left[c\boldsymbol{\alpha} \cdot \vec{p} + \beta mc^2 - \frac{Z\alpha\hbar c}{r} \right] \psi = E\psi \quad (109)$$

The **exact energy levels** (Sommerfeld fine structure formula):

$$E_{n,j} = mc^2 \left[1 + \frac{(Z\alpha)^2}{\left(n - j - \frac{1}{2} + \sqrt{(j + \frac{1}{2})^2 - (Z\alpha)^2} \right)^2} \right]^{-1/2} \quad (110)$$

where $j = l \pm 1/2$ is the total angular momentum.

Expansion to order $(Z\alpha)^4$:

$$E_{n,j} \approx mc^2 - \frac{mc^2(Z\alpha)^2}{2n^2} - \frac{mc^2(Z\alpha)^4}{2n^3} \left(\frac{1}{j + 1/2} - \frac{3}{4n} \right) \quad (111)$$

The second term is the non-relativistic energy; the third is the **fine structure correction**.

7 Classical vs Quantum Simulation: Mathematical Comparison

7.1 Classical Approach

7.1.1 Equations of Motion

Newton's second law for N particles:

$$m_i \frac{d^2 \vec{r}_i}{dt^2} = \vec{F}_i = -\nabla_i V(\vec{r}_1, \dots, \vec{r}_N) \quad (112)$$

For the electron-proton-neutron system:

$$V = -\frac{e^2}{|\vec{r}_e - \vec{r}_p|} + V_{\text{nuclear}}(\vec{r}_p - \vec{r}_n) \quad (113)$$

7.1.2 Velocity Verlet Integration

$$\vec{v}_i(t + \Delta t/2) = \vec{v}_i(t) + \frac{\Delta t}{2m_i} \vec{F}_i(t) \quad (114)$$

$$\vec{r}_i(t + \Delta t) = \vec{r}_i(t) + \Delta t \vec{v}_i(t + \Delta t/2) \quad (115)$$

$$\vec{F}_i(t + \Delta t) = \vec{F}_i(\{\vec{r}_j(t + \Delta t)\}) \quad (116)$$

$$\vec{v}_i(t + \Delta t) = \vec{v}_i(t + \Delta t/2) + \frac{\Delta t}{2m_i} \vec{F}_i(t + \Delta t) \quad (117)$$

Properties:

- Time-reversible
- Symplectic (preserves phase space volume)
- Energy drift: $\mathcal{O}(\Delta t^2)$ per step

7.1.3 Bohr Model

For hydrogen in the ground state:

$$r_n = n^2 a_0 \quad (\text{quantized radius}) \quad (118)$$

$$v_n = \frac{e^2}{n\hbar} = \frac{\alpha c}{n} \quad (\text{orbital velocity}) \quad (119)$$

$$E_n = -\frac{Z^2 e^2}{2a_0 n^2} = -\frac{Z^2}{2n^2} \text{ Hartree} \quad (120)$$

Remarkable result: The Bohr model gives the *exact* energy levels (though for the wrong physical reasons).

7.2 Quantum Approach

7.2.1 Variational Principle

For any trial wavefunction ψ_{trial} :

$$E_{\text{trial}} = \frac{\langle \psi_{\text{trial}} | \hat{H} | \psi_{\text{trial}} \rangle}{\langle \psi_{\text{trial}} | \psi_{\text{trial}} \rangle} \geq E_0 \quad (121)$$

Example: Trial function $\psi = e^{-\alpha r}$ for hydrogen:

$$\langle T \rangle = \frac{\alpha^2}{2} \quad (122)$$

$$\langle V \rangle = -Z\alpha \quad (123)$$

$$E(\alpha) = \frac{\alpha^2}{2} - Z\alpha \quad (124)$$

Minimizing: $\frac{dE}{d\alpha} = \alpha - Z = 0 \Rightarrow \alpha = Z$

Result: $E_{\text{min}} = -\frac{Z^2}{2}$ (exact!)

7.2.2 Hartree-Fock for Multi-Electron Systems

The Hartree-Fock equations:

$$\hat{f}(1)\phi_i(1) = \epsilon_i\phi_i(1) \quad (125)$$

where the Fock operator:

$$\hat{f}(1) = \hat{h}(1) + \sum_j \left[\hat{J}_j(1) - \hat{K}_j(1) \right] \quad (126)$$

Coulomb operator:

$$\hat{J}_j(1)\phi_i(1) = \left[\int \frac{|\phi_j(2)|^2}{r_{12}} d\vec{r}_2 \right] \phi_i(1) \quad (127)$$

Exchange operator:

$$\hat{K}_j(1)\phi_i(1) = \left[\int \frac{\phi_j^*(2)\phi_i(2)}{r_{12}} d\vec{r}_2 \right] \phi_j(1) \quad (128)$$

7.3 Comparison of Methods

Table 1: Classical vs Quantum Simulation Comparison

Aspect	Classical	Quantum
State description	Point particles (\vec{r}, \vec{p})	Wave function $\psi(\vec{r})$
Dimensions	$6N$ phase space	$3N$ -dim Hilbert space
Scaling	$\mathcal{O}(N^2)$ for pairwise forces	Exponential in N
Energy spectrum	Continuous	Discrete (bound states)
Ground state	Can have $E = 0$	Zero-point energy > 0
Uncertainty	None (deterministic)	$\Delta x \Delta p \geq \hbar/2$
Exchange	None	Pauli exclusion
Tunneling	Forbidden	Allowed
Speed	Fast (simple ODE)	Slow (PDE/integral eq.)
Accuracy	Qualitative	Quantitative

7.4 Electron-Proton-Neutron System Analysis

Classical simulation:

- Electron orbits proton in Bohr-like trajectory
- Energy: $E = -0.5$ Hartree (exact by construction)
- Radius: $r = a_0 = 1$ Bohr (average)
- Angular momentum: $L = \hbar$ (quantized by fiat)

Quantum simulation:

- Electron probability cloud around nucleus
- Energy: $E_1 = -\mu Z^2 / (2n^2) \approx -0.4997$ Hartree (with reduced mass)
- $\langle r \rangle = 1.5a_0$, but $\sqrt{\langle r^2 \rangle} \neq \langle r \rangle$
- Uncertainty: $\Delta r \cdot \Delta p_r \geq \hbar/2$

7.5 Three-Electron System (Lithium)

Classical simulation:

- Three electrons with Coulomb repulsion
- Chaotic dynamics (no stable orbits for 3-body problem)
- Average energy depends on initial conditions
- No exchange effects

Quantum simulation:

- Antisymmetric wave function (Slater determinant)
- Exact energy: $E_{\text{Li}} = -7.478$ Hartree
- Hartree-Fock captures 99% of energy
- Electron correlation: remaining 1%

7.6 Key Quantum Effects Missing in Classical Simulation

1. **Discretization:** Classical gives continuous spectrum

$$E_n = -\frac{Z^2}{2n^2}, \quad n = 1, 2, 3, \dots \text{ (quantum)} \quad (129)$$

2. **Zero-point energy:** Classical allows $E = 0$

$$E_0 = \frac{1}{2}\hbar\omega > 0 \text{ (harmonic oscillator)} \quad (130)$$

3. **Tunneling:** Classical forbids passage through barriers

$$T \approx e^{-2\kappa a}, \quad \kappa = \sqrt{2m(V_0 - E)}/\hbar \quad (131)$$

4. **Exchange symmetry:** Classical particles are distinguishable

$$\Psi(\vec{r}_1, \vec{r}_2) = -\Psi(\vec{r}_2, \vec{r}_1) \text{ (fermions)} \quad (132)$$

5. **Heisenberg uncertainty:**

$$\Delta x \Delta p \geq \frac{\hbar}{2} \quad (133)$$

8 Numerical Methods for Quantum Simulation

8.1 Shooting Method for Radial Equations

For the radial Schrödinger equation with $u(r) = rR(r)$:

$$\frac{d^2 u}{dr^2} = \left[\frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2} V(r) - \frac{2mE}{\hbar^2} \right] u \quad (134)$$

Numerov's method (4th-order accurate):

$$u_{n+1} = \frac{2u_n(1 - \frac{5\hbar^2}{12}k_n^2) - u_{n-1}(1 + \frac{\hbar^2}{12}k_{n-1}^2)}{1 + \frac{\hbar^2}{12}k_{n+1}^2} \quad (135)$$

where $k^2(r) = \frac{2m}{\hbar^2}[E - V_{\text{eff}}(r)]$.

8.2 Variational Monte Carlo

Expectation value via Monte Carlo integration:

$$\langle \hat{H} \rangle = \frac{\int |\psi_T(\vec{R})|^2 E_L(\vec{R}) d\vec{R}}{\int |\psi_T(\vec{R})|^2 d\vec{R}} \quad (136)$$

where the local energy:

$$E_L(\vec{R}) = \frac{\hat{H}\psi_T(\vec{R})}{\psi_T(\vec{R})} \quad (137)$$

Metropolis algorithm generates samples from $|\psi_T|^2$.

8.3 Basis Set Expansion

Expand in a complete set:

$$\psi = \sum_{i=1}^N c_i \phi_i \quad (138)$$

The Schrödinger equation becomes a matrix eigenvalue problem:

$$\sum_j H_{ij} c_j = E \sum_j S_{ij} c_j \quad (139)$$

where:

$$H_{ij} = \langle \phi_i | \hat{H} | \phi_j \rangle \quad (140)$$

$$S_{ij} = \langle \phi_i | \phi_j \rangle \quad (141)$$

9 Applications to Specific Systems

9.1 Electron-Proton-Neutron (e-p-n) System

Physical interpretation: Hydrogen atom with deuteron-like nucleus (or isotope effects).

Hamiltonian (in atomic units):

$$\hat{H} = -\frac{1}{2\mu} \nabla^2 - \frac{1}{r} \quad (142)$$

where the reduced mass:

$$\mu = \frac{m_e(m_p + m_n)}{m_e + m_p + m_n} \approx \frac{m_e M}{m_e + M} \quad (143)$$

Reduced mass correction:

$$E_n = -\frac{\mu}{2n^2} = -\frac{1}{2n^2} \left(1 - \frac{m_e}{m_p + m_n} \right) \quad (144)$$

For hydrogen: $E_1 = -0.499728$ Hartree For deuterium: $E_1 = -0.499864$ Hartree

9.2 Three-Electron Atom (Lithium)

Hamiltonian:

$$\hat{H} = \sum_{i=1}^3 \left(-\frac{1}{2} \nabla_i^2 - \frac{Z}{r_i} \right) + \sum_{i<j} \frac{1}{r_{ij}} \quad (145)$$

Configuration: $(1s)^2(2s)^1$

Variational wave function (simple form):

$$\Psi = \mathcal{A} \left[\psi_{1s}^{\zeta_1}(\vec{r}_1) \alpha(1) \psi_{1s}^{\zeta_1}(\vec{r}_2) \beta(2) \psi_{2s}^{\zeta_2}(\vec{r}_3) \alpha(3) \right] \quad (146)$$

where \mathcal{A} is the antisymmetrizer.

Energy breakdown:

- One-electron: $2E_{1s} + E_{2s}$
- $J_{1s,1s}$: Coulomb between 1s electrons
- $J_{1s,2s}$: Coulomb between 1s and 2s
- $K_{1s,2s}$: Exchange between 1s and 2s (same spin)

Analytical integrals:

$$J_{1s,1s} = \frac{5\zeta_1}{8} \quad (147)$$

$$J_{1s,2s} \approx \frac{17(\zeta_1 + \zeta_2)}{162} \quad (148)$$

$$K_{1s,2s} \approx \frac{8\zeta_1^{3/2}\zeta_2^{3/2}}{(\zeta_1 + \zeta_2)^3} \quad (149)$$

10 Conclusion

This document has presented a comprehensive mathematical framework for understanding quantum mechanics in the relativistic regime, with particular emphasis on the comparison between classical and quantum simulation approaches.

10.1 Key Findings

1. **Vector Space Structure:** Quantum mechanics fundamentally requires the Hilbert space formulation, with observables as Hermitian operators and states as vectors (rays).
2. **Special Functions:** The separation of variables in spherical coordinates naturally leads to Legendre, Laguerre, and Hermite polynomials, which form orthonormal bases for angular and radial wave functions.
3. **Residue Theorems:** Complex analysis provides powerful tools for evaluating propagators, computing scattering amplitudes, and establishing dispersion relations through analytic continuation.

4. **Relativistic Extension:** The Schrödinger equation's relativistic generalization leads to the Klein-Gordon equation (spin-0) and Dirac equation (spin-1/2), with the Dirac equation naturally predicting electron spin and the fine structure of hydrogen.
5. **Classical vs Quantum:** While classical simulations are computationally faster, they fundamentally cannot capture:
 - Energy quantization
 - Heisenberg uncertainty
 - Pauli exclusion and exchange effects
 - Quantum tunneling
 - Spin and its coupling to magnetic fields

10.2 Recommendations

- Use **classical simulation** for: qualitative dynamics, large systems where quantum effects average out, initial explorations
- Use **quantum simulation** for: accurate energy calculations, spectroscopy, chemical reactions, any system where electron correlation matters
- Use **relativistic quantum mechanics** for: heavy elements (high Z), high-energy processes, systems where spin-orbit coupling is important

10.3 Future Directions

The framework presented here can be extended to:

- Quantum electrodynamics (QED) for radiative corrections
- Density functional theory (DFT) for many-electron systems
- Relativistic many-body perturbation theory
- Lattice QCD for nuclear structure

A Mathematical Appendices

A.1 Gamma Matrix Identities

$$\text{Tr}(I) = 4 \tag{150}$$

$$\text{Tr}(\gamma^\mu) = 0 \tag{151}$$

$$\text{Tr}(\gamma^\mu \gamma^\nu) = 4g^{\mu\nu} \tag{152}$$

$$\text{Tr}(\gamma^\mu \gamma^\nu \gamma^\rho \gamma^\sigma) = 4(g^{\mu\nu} g^{\rho\sigma} - g^{\mu\rho} g^{\nu\sigma} + g^{\mu\sigma} g^{\nu\rho}) \tag{153}$$

$$\gamma^\mu \gamma_\mu = 4 \tag{154}$$

$$\gamma^\mu \not{a} \gamma_\mu = -2\not{a} \tag{155}$$

$$\gamma^\mu \not{a} \not{b} \gamma_\mu = 4(a \cdot b) \tag{156}$$

A.2 Useful Integrals

Gaussian integrals:

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}} \quad (157)$$

$$\int_{-\infty}^{\infty} x^{2n} e^{-ax^2} dx = \frac{(2n-1)!!}{(2a)^n} \sqrt{\frac{\pi}{a}} \quad (158)$$

Radial integrals:

$$\int_0^{\infty} r^n e^{-\alpha r} dr = \frac{n!}{\alpha^{n+1}} \quad (159)$$

Fourier transform of Coulomb potential:

$$\int \frac{e^{i\vec{q}\cdot\vec{r}}}{r} d^3r = \frac{4\pi}{q^2} \quad (160)$$

A.3 Physical Constants

Table 2: Physical Constants in SI and Atomic Units

Quantity	SI Value	Atomic Units
\hbar	1.055×10^{-34} J·s	1
m_e	9.109×10^{-31} kg	1
e	1.602×10^{-19} C	1
a_0	5.292×10^{-11} m	1
E_h	4.360×10^{-18} J	1
c	2.998×10^8 m/s	137.036
α	1/137.036	1/137.036
m_p/m_e	1836.15	1836.15

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