

Original article

Integral Equations in Quantum Mechanics: An Extensive Study of Their Role in Theoretical Physics

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Corresponding email. awad@omu.edu.ly**Abstract**

Quantum mechanics heavily depends on integral equations because they supply advanced mathematical solutions for solving complex theoretical physics problems. This paper examines the development of integral equations starting from their inception through their mathematical structure until their utility in solving Schrödinger's equation and its adjoint variants. The research analyzes integral equations by combining sophisticated derivations with numerical approximation methods and case-based examinations, and multidisciplinary connections to explain their use in scattering theory and bound states, as well as quantum field theory and quantum electrodynamics and condensed matter physics and quantum information theory, and new fields of quantum computing and quantum gravity. The assessment demonstrates that integral equations continue to adapt for quantum mechanical research as they advance contemporary knowledge in this field.

Keywords: Green's Functions, Scattering Theory, Certain States, Quantum Theory.

Introduction

Quantum mechanics, the cornerstone of modern physics, describes the behavior of matter and energy at microscopic scales. The Schrödinger equation functions as a differential equation that controls the development of quantum states according to this framework. The resolution of quantum problems involving complex boundary conditions, together with non-local interactions and scattering, needs integral equations as their preferred computational approach. The integral equations embrace global system characteristics through their utilization of nuclei and Green's functions, thus becoming suitable for cases where differential methodology proves inadequate [1].

Modern physics relies on quantum mechanics as its fundamental framework, which studies atomic and subatomic matter together with their energy properties. Quantum mechanics depends on differential equations for model theory development, wherein the Schrödinger equation stands out as the crucial evolutionary description for quantum systems. Modern theoretical physics shows increasing interest in integral equations because these approaches yield stronger solutions to complex problems. The application of integral equations for Schrödinger equation reformulation provides vital capabilities towards solving multidimensional border-sensitive quantum systems. The article researches quantum mechanics integral equations, starting with their theoretical structure, while illustrating their utility when solving quantum mechanics problems, including the complementary Schrödinger equation [2].

Here in this paper, we review the basic principles of quantum mechanics, highlighting how they extrapolate from classical mechanics, and lay the groundwork for subsequent chapters in a pretty comprehensive way. There are certainly several books that cover this material more comprehensively and from different perspectives. For only a few instances, we can cite the qualitative mathematical introduction of Thaler (2000), the complementary though visually attractive physical treatment of Brandt and Dahmen (2001), the concise, compressed text of Gustafson and Segal (2003) from a mathematical physics perspective, and the instructive book by Tannor (2007) from the time-sensitive perspective of chemical physics. There are also the monumental masterworks of Masih (1962), Cohen-Tannoudji, Deo, and Lalo (1977), and Dirac's (1930) and von Neumann's (1932) milestone papers [3].

In quantum physics, the Hamiltonian operator—also called the Schrödinger operator—is an elliptic operator that characterizes how particles behave when subjected to a potential field. It is defined as the sum of a diagonal operator that applies the potential function to the wave function and the Laplacian operator. The Schrödinger equation, which establishes the probability distribution of a particle in a certain potential field, is solved using the Hamiltonian operator [4].

Heisenberg's new atomic mechanics can be based on the assumption that the variables of a dynamical system do not obey the cross-law, but satisfy some quantitative conditions. It can be built without knowing anything about the dynamical variables other than the algebraic laws they obey, and it can be shown that it can be written in matrix form whenever there is a set of uniform variables for the dynamical system [5]. However, it is possible to prove that there can exist no set of uniform variables in a system consisting of more than one electron, and that the theory cannot progress further as a result. Schrödinger recently showed a new expansion of the theory. Starting from the assumption that an atomic system can't be described by a trajectory—that is, by a point in motion in coordinate space—but must be represented by a wave in space, Schrödinger, starting from the variational principle, obtained a differential equation that the wave function ψ must satisfy. The differential equation is found to be closely related with the Hamiltonian equation of the

system [6]. Here we discuss how differential equations are used in quantum mechanics, and specifically the contribution of a prominent one, Schrödinger's equation, which is used to describe the evolution of quantum systems. In time two, the mathematical representation of the wave nature of particles at quantum scales is provided, and the resulting equations are Schrödinger's equation, time-dependent and time independent. The time-dependent Schrödinger equation is employed to explain the evolution of a quantum state with time, whereas the time-independent form is employed to analyze systems with fixed energy levels, like particles in a potential well [7].

Crossing solutions to Schrödinger's equation yield these wave functions, an information treasure house regarding the behavior of a particle, and even allow us to calculate measurable quantities such as energy and angular momentum. Additionally, the research also explains how to apply boundary conditions and potential functions in solving Schrödinger's equation to specific quantum systems such as the harmonic oscillator and hydrogen atom. Solving these differential equations gives us further understanding of underlying quantum phenomena, which will serve to aid further developments in quantum computing, nanotechnology, and atomic physics [8]. The research examines quantum mechanics integral equations through an extensive analysis of their relationships with the Schrödinger equation. The research analyzes historical achievements along with mathematical approaches, together with field applications using computational methods and connections across disciplines, and prospective developments [9].

Historical Context

Quantum mechanics emerged as a complete breakthrough during the early 20th century in physics. Max Planck's 1900 quantization hypothesis, Niels Bohr's 1913 atomic model, Werner Heisenberg's 1925 matrix mechanics, and Erwin Schrödinger's 1926 wave equation laid the foundation. The differential formulation of the Schrödinger equation proved difficult to handle. Complex systems comprising multi-particle interactions and scattering, along with relativistic effects, present difficulties for using the Schrödinger equation [10]. The development of integral equations proved to be an exceptionally strong substitute. George Green's 1828 work on Green's The discovery of functions as a mathematical method for resolving inhomogeneous differential equations became known later. adapted to quantum mechanics. During the 1930s, John von Neumann introduced operator theory as the formal mathematical basis for quantum mechanics while using it to support the analysis of integral equations. The year 1950 marked the first appearance of the Lippmann-Schwinger equation when Bernard Lippmann joined forces with Julian Schwinger [11].

The Lippmann-Schwinger equation presented an alternative approach to express the Schrödinger equation during scattering applications. Multiple breakthroughs appeared throughout the 20th century when integral equations gained dominant status within research activities. quantum field theory, perturbation theory, and computational physics. The field of integral equations received vital contributions from two significant scientists, including Richard Feynman, who pioneered the path integral formalism alongside Freeman Dyson. Freeman Dyson, along with others, developed the Dyson-Schwinger equations, which brought the methods to prominence. Integral equations follow a historical trajectory that demonstrates their interdisciplinary nature because they draw from both pure mathematics and classical physics and computational science approaches. Their adoption in Quantum mechanics adopted integral mathematics after recognizing problems with differential approaches, which let researchers achieve breakthroughs in theoretical and applied physics [12].

Mathematical Foundations

Integral equations in quantum mechanics are usually Fredholm or Volterra equations, and are characterized by their kernel and boundary conditions. Below, we explain the main concepts and provide detailed conclusions [13].

Definition 1 (Integral Equation). An integral equation involves an unknown function under the sign of integration:

$$\psi(r) = \phi(r) + \int K(r, r')\psi(r')dr', \quad (1)$$

where $\psi(r)$ is the unknown wavefunction, $\phi(r)$ is a known function, and $K(r, r')$ is the kernel.

The Schrödinger Equation

The time-independent Schrödinger equation for a particle in a potential $V(r)$ is:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\psi(r) = E\psi(r). \quad (2)$$

The differential equation controls stationary states but determining solutions for arbitrary potentials or boundary circumstances proves to be difficult.

Integral Equation Formulation

Using Green's functions, the Schrödinger equation is reformulated as an integral equation. The Green's function $G(r, r')$ for the Helmholtz operator satisfies [14]:

$$(\nabla^2 + k^2)G(r, r') = \delta(r - r'), \quad (3)$$

where $k^2 = \frac{2mE}{\hbar^2}$. The solution is:

$$\psi(r) = \phi(r) + \int G(r, r') \frac{2m}{\hbar^2} V(r') \psi(r') dr', \quad (4)$$

known as the Lippmann-Schwinger equation. The free-particle Green's function in three dimensions is:

$$G(r, r') = -\frac{1}{4\pi} \frac{e^{ik|r-r'|}}{|r-r'|} \quad (5)$$

Fredholm and Volterra Equations

The fixed integration limits characterize Fredholm equations which scattering scientists use [15].

$$\psi(r) = \phi(r) + \int_a^b K(r, r') \psi(r') dr', \quad (6)$$

The Volterra equations apply to time-dependent issues through their variable limit parameters.

$$\psi(r, t) = \phi(r, t) + \int_0^t K(r, t; r', t') \psi(r', t') dt'. \quad (7)$$

The various methods of tackling such problems include Neumann series, resolvent kernels and numerical discretization.

Operator Theory

Integration equations frequently take the following form for expression:

$$\psi = \phi + G^{\wedge} V^{\wedge} \psi, \quad (8)$$

The calculation evaluates the identities using Green's operator G^{\wedge} and potential operator V^{\wedge} . This formalism connects to Hilbert space theory, enabling rigorous analysis of convergence and stability.

Applications in Quantum Mechanics

Quantum mechanical domains employ integral equations as shown in the details below.

Scattering Theory

Scattering involves particles interacting with a potential. The Lippmann-Schwinger equation is [16]:

$$\psi(r) = e^{ik \cdot r} + \int G(r, r') \frac{2m}{\hbar^2} V(r') \psi(r') dr', \quad (9)$$

The scattering amplitude, derived from the asymptotic wavefunction, determines differential cross-sections [17].

Example 1 (One-Dimensional Delta Potential). For a potential $V(x) = g\delta(x)$, the Lippmann Schwinger equation is:

$$\psi(x) = e^{ik \cdot x} + \int_{-\infty}^{\infty} G(x, x') \frac{2m}{\hbar^2} \delta(x') \psi(x') dx', \quad (10)$$

Using the Green's function $G(x, x') = -\frac{i}{2k} e^{ik|r-x'|}$, we solve:

$$\psi(x) = e^{ik \cdot x} + \frac{2mg}{\hbar^2} G(x, 0) \psi(0). \quad (11)$$

Reflection and transmission coefficients emerge from this method which demonstrates its effectiveness in the process.

Example 2 (Three-Dimensional Yukawa Potential). For a Yukawa potential

$V(r) = -\frac{ge^{-\mu r}}{r}$ the Lippmann-Schwinger equation in momentum space is solved iteratively, yielding scattering amplitudes for screened Coulomb interactions.

Example 3 (Square Well Potential). For a spherical square well, $V(r) = -V_0$ for $r < a$ and 0 otherwise, the radial Lippmann-Schwinger equation is solved numerically to obtain phase shifts and cross-sections.

Bound States

Integral equations simplify bound state calculations by discretizing the kernel, converting the problem into a matrix eigenvalue equation. For the hydrogen atom, the integral approach yields energy levels matching analytical results [18].

Example 4 (Harmonic Oscillator). For $V(x) = \frac{1}{2} m\omega^2 x^2$, The Green's function approach determines eigenvalues $En = \hbar\omega \left(n + \frac{1}{2}\right)$ which match differential method results.

Quantum Field Theory

The Dyson-Schwinger equations formulate interacting quantum fields in quantum chromodynamics (QCD) and electroweak theory through integral equations of Green's functions.

Quantum Electrodynamics

The Bethe-Salpeter equation serves in QED to simulate electron-positron interaction processes [19].

$$G(r_1, r_2; r'_1, r'_2) = G_0(r_1, r'_1)G_0(r_2, r'_2) \int K(r_1, r_2; r_3, r_4)G(r_3, r_4; r'_1, r'_2) dr_3 dr_4. \quad (12)$$

Condensed Matter Physics

Phonons, plasmons, and magnons in solids produce collective excitations that integral equations effectively describe solids, using Green's function techniques [6].

Quantum Information Theory

The model of integral equations succeeds in representing quantum channels as well as describing decoherence and entanglement dynamics to benefit quantum algorithm development and error correction in quantum algorithm design and error correction.

Relativistic Quantum Mechanics

The Dirac equation manifests as an integral equation that explains relativistic particles. The relativistic scattering requires modification of the Lippmann-Schwinger equation.

Quantum Gravity

Quantum gravity applications make use of integral equations to analyze graviton propagators, which help understand nonperturbative behavior in the system [20].

Complementary Schrödinger Equation

Alternative representations and the integral form of the "complementary Schrödinger equation" are among its possible usages. The Lippmann-Schwinger equation functions as a natural method to include boundary conditions when used with the differential form [21].

Example 5 (Momentum-Space Scattering). In momentum space, the Lippmann-Schwinger equation is:

$$\psi(k) = \delta(k - k_0) + \frac{1}{E - \frac{\hbar^2 k^2}{2m} + i\epsilon} \int V(k, k')\psi(k') dk'. \quad (13)$$

This form is solved iteratively, yielding scattering amplitudes for complex potentials.

Example 6 (Time-Dependent Perturbation). For a time-dependent potential, the Volterra integral equation is:

$$\psi(r, t) = \phi(r, t) + \frac{-i}{\hbar} \int_0^t \int G(r, t; r', t')V(r', t')\psi(r', t') dr' dt'. \quad (14)$$

Quantum dynamics responds to external fields according to this description.

Perturbation Theory

Game Object with Tag on small system disturbances to find alternative solution approximations. Integral equations simplify this process.

Born Approximation

For weak potentials, the Born approximation assumes $\psi(r') \approx e^{ik \cdot r'}$:

$$\psi(r') \approx e^{ik \cdot r'} + \int G(r, r') \frac{2m}{\hbar^2} V(r') e^{ik \cdot r'} dr'. \quad (15)$$

This yields the first-order scattering amplitude.

Higher-Order Corrections

The Neumann series expansion is:

$$\psi = \phi + G_0 V \phi + G_0 V G_0 V \phi + \dots, \quad (16)$$

generating higher-order terms for stronger potentials.

Non-Perturbative Methods

Integral equations can be resolved non-perturbatively through variational methods and resolvent methods, which make them appropriate for strong interactions.

Path Integral Formulations

Another framework exists through Feynman's path integral formulation. The propagator is [5]:

$$K(r, t; r', t') = \int D[r(t)] e^{\frac{i}{\hbar} S[r(t)]}, \quad (17)$$

where S is the action. This connects to the Lippmann-Schwinger equation via Green's functions [22]. Example 7 (Path Integral for Free Particle). For a free particle, the propagator is:

$$K(r, t; r', 0) = \sqrt{\frac{m}{2\pi i \hbar t}} \exp\left(\frac{im(r - r')^2}{2\hbar t}\right) \quad (18)$$

Numerical Methods

The resolution of integral equations needs sophisticated numerical techniques which receive detailed explanation in the following section.

Nyström Method

The integral gets discretized through the Nyström method.

$$\psi(r_i) = \phi(r_i) + \sum_j w_j K(r_i, r_j) \psi(r_j), \quad (19)$$

creating a linear system out of the equation.

Table 1. Different numerical approaches and their evaluation of integral equations

Method	Applicability	Computational Cost	Accuracy
Nyström	Scattering, Bound States	Moderate	High
Born Approximation	Weak Potentials	Low	Moderate
Monte Carlo	High-Dimensional Integrals	High	Variable
Conjugate Gradient	Large Systems	Moderate	High

Algorithm 1 Iterative Solution of Lippmann-Schwinger Equation

Initialize $\psi^{(0)}(r) = \phi(r)$

for $n = 0$ to N_{\max} do

 Compute $\psi^{(n+1)}(r) = \phi(r) + \int G(r, r') \frac{2m}{\hbar^2} V(r') \psi^{(n)}(r') dr'$

 if Convergence criteria are met, then

 Break

 end if

end for

Return $\psi^{(n+1)}(r)$

Iterative Methods

The conjugate gradient method, along with other iterative solvers, processes large systems with high efficiency.

Monte Carlo Methods

Monte Carlo integration performs high-dimensional integral evaluation needed for path integral computations.

Fast Multipole Methods

The fast multipole method lowers computational complexity when it approximates the interaction terms of complex problems (appropriately scaled).

Parallel Computing

Sessions running on GPU computing clusters together improve the efficiency of calculations involving high-dimensional integrals.

Software Implementations

The popular software tools MATLAB, together with Python (SciPy and NumPy), along with C++ (Eigen and PETSc), provide implementations of these methods. The scipy. The integrate module of Python operates to solve Fredholm problems equations, while mpi4py enables parallel computing.

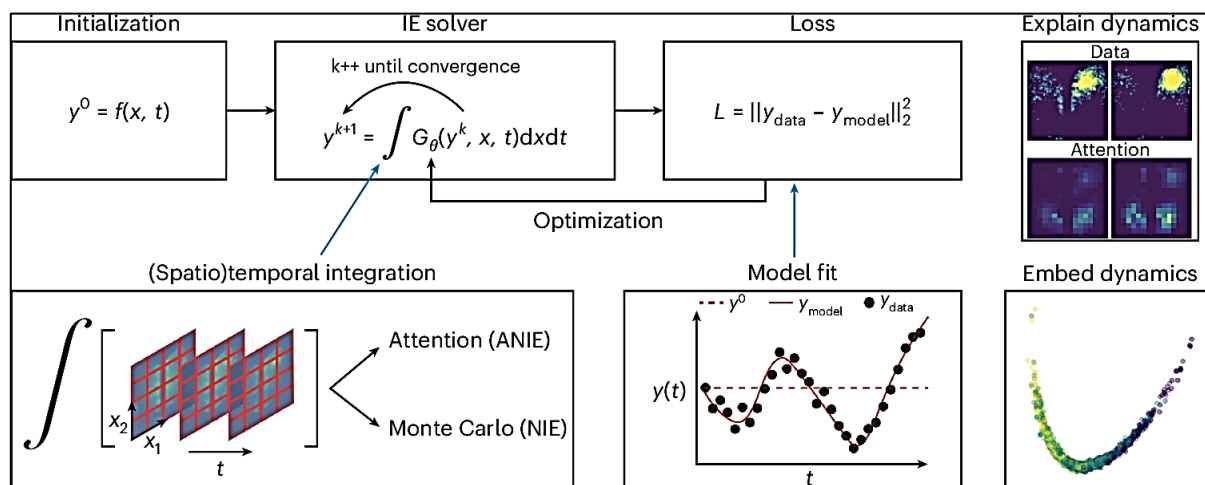


Figure 1 The use of integral equations presents visual representations for quantum mechanical solutions.

Interdisciplinary Connections

The applications of integral equations extend beyond their use in quantum mechanics because they influence research areas that lie nearby.

Statistical Mechanics

Statistical mechanics functions include the Ornstein-Zernike equation, together with its counterpart integral equations, for describing fluid and gas correlation patterns.

Biophysics

Green's function provides a mathematical pathway for integral equations to model molecular dynamics, together with protein folding and dynamics techniques.

Cosmology

The explanation of cosmic microwave background fluctuations with gravitational lensing effects uses integral equations as its foundation in cosmology.

Engineering

Electromagnetic and acoustic boundary value problems need integral equations to obtain their solutions.

Challenges and Limitations

Integral equations face challenges:

- The computational costs become high due to working with high-dimensional integrals.
- The singularities in Green's functions demand special regularization procedures because they appear during the calculation.
- techniques like principal value integration.
- Physical interpretations become more challenging to deduce from integral equations than from differential equations.
- Accuracy in numeric integration becomes unstable due to both errors in the method and problems with ill-conditioned matrix values.

Future Directions

Integral equations will continue to show promising prospects in the field of quantum mechanics. Computational power development, especially including quantum computers, will make integral equations more practical to use. Their role in the application of integral equations in quantum computing keeps expanding to its various aspects, including circuit simulation and quantum algorithm optimization. Machine learning includes neural networks that solve integral equations as part of its techniques. Applications in topological quantum systems, quantum gravity, and quantum machine learning offer exciting prospects. The combination of hybrid approaches, which combine integral and differential methods, allows researchers to develop advanced solutions. Using data-driven techniques with integrated and diverse approaches to gain new scientific insights.

Educational and Practical Implications

Advanced quantum mechanics education requires integral equations because they help students fully grasp mathematical physics principles as well as computational algorithms. Their practical applications in industries like quantum technology, materials science, and medical imaging underscore their relevance. Educational institutions should adopt the integration of workshops and online courses, as well as open-source software tools, to educate their students and democratize access to these methods.

Extended Case Studies

The following section shows how integral equations demonstrate their strength through multiple examples.

Scattering in a Coulomb Potential

The Coulomb potential, $V(r) = -\frac{Ze^2}{r}$

The solution of this potential requires the application of the Lippmann-Schwinger equation accounting for long-range interactions.

Two-Dimensional Quantum Systems

A two-dimensional harmonic oscillator becomes solvable through integral approaches, which both generate its energy levels and wavefunctions that apply to graphene and quantum dots.

Relativistic Scattering

The Dirac equation describing a relativistic particle subject to a potential becomes an integral equation that acquires numerical solutions for high-energy scattering events.

Quantum Dynamics in External Fields

Applications of oscillating electromagnetic fields lead to the formation of time-dependent integral equations that represent quantum systems fields, relevant to laser physics.

Comparative Analysis

Integral equation methods outperform differential methods since they handle boundary conditions together with non-local interactions effectively. Boundary conditions and non-local interactions. However, their computational complexity and numerical challenges can be drawbacks. A comparative analysis with finite difference, finite volume difference and finite volume difference systems analyzes quantum mechanics' features alongside each other primarily due to their characteristics.

Table 2. Comparison of Quantum Mechanical Methods

Method	Boundary Conditions	Computational Cost	Applicability
Integral Equations	Natural	High	Scattering, Non-Local
Finite Difference	Manual	Moderate	Localized Potentials
Finite Element	Flexible	High	Complex Geometries
Variational	Approximate	Low	Bound States

Conclusion

Modern quantum mechanics depends on integral equations for solving its complex theoretical physics challenges through effective solutions. Their reformulation of the Schrödinger equation. The Lippmann-Schwinger equation functions as a method to make scattering analysis possible. Quantum mechanics needs bound states together with quantum fields, while advancing quantum technologies through quantum fields. Studies on quantum mechanics obtains substantial advantages from integral equations because these equations present simultaneous mathematical elegance along with functional industrial applications, which lead to new interdisciplinary findings.

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