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High-Order Spectral Deferred Correction Methods For Accurate Simulation Of Quantum Systems Governed By The Schro¨Dinger Equation

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Abstract
This study presents a high-order and stable time-integration frame- work for the numerical solution of the time-dependent Schro¨dinger equa- tion, founded on the Spectral Deferred Correction (SDC) method. By combining SDC with a Fourier spectral discretization in space, we develop an efficient semi-implicit solver that preserves essential quantum mechan- ical invariants, including norm conservation and phase accuracy. The proposed method is applied to the simulation of a free particle's evolution and compared against conventional schemes such as the Crank–Nicolson method. Numerical experiments demonstrate that the SDC-based ap- proach attains higher accuracy and improved long-term stability, partic- ularly for large time-step sizes. These results underline the promise of high-order iterative correction techniques as a robust tool for the simula- tion of quantum dynamical systems.

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1 Introduction

The time-dependent Schrödinger equation (TDSE) plays a foundational role in quantum theory, describing how a quantum system evolves in time. In one-dimensional form, it is expressed as:

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \hat{H}\,\psi(x,t), \tag{1}$$

where $\psi(x, t)$ represents the wavefunction, and $\hat{H}$ is the Hamiltonian operator that includes kinetic and potential energy components. For a single particle in a potential $V(x)$, the Hamiltonian is given by:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x). \tag{2}$$

Solving the TDSE provides insights into the probabilistic behavior of quantum systems, with $|\psi(x, t)|^2$ denoting the likelihood of finding a particle at position x at time t. In special cases where the system is in a stationary state, the wavefunction can be separated as:

$$\psi(x, t) = \phi(x)e^{-iEt/\hbar},$$

leading to the time-independent Schrödinger equation (TISE):

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi(x)}{\partial x^2} + V(x)\phi(x) = E\phi(x), \tag{3}$$

which is a central eigenvalue problem in quantum mechanics.

While analytical solutions to the TDSE are known for only a few idealized systems, numerical methods have become indispensable tools for simulating realistic quantum systems. Various numerical schemes have been introduced and refined to meet the challenges of accuracy, stability, and efficiency in solving the TDSE. Among the most widely used is the Crank–Nicolson method, which is known for its norm-preserving and unconditionally stable properties [10, 19]. Spectral methods, particularly those utilizing Fourier transforms, offer high spatial accuracy and are often coupled with time-splitting strategies such as the split-step Fourier method [4,8,9,11,12].

More recent advancements in numerical integration have focused on achieving higher-order time accuracy. Spectral Deferred Correction (SDC) methods are one such innovation. Initially introduced by Dutt et al. [1] and expanded by Minion and others [2, 3, 5], SDC techniques iteratively correct low-order time integration results, enabling arbitrarily high-order solutions. These methods are especially well-suited for quantum simulations, where maintaining the phase fidelity and norm of the wavefunction over long simulation times is essential [18, 27, 29].

SDC methods are also compatible with a variety of advanced time integration strategies, such as exponential integrators [24], Magnus expansions [20], and geometric schemes like symplectic integrators [14, 21]. Alternative approaches, including Lie group solvers [15], Lanczos exponential methods [17], and commutator-free techniques, have also shown promise in quantum applications.

In this study, we explore the application of high-order semi-implicit SDC methods to the TDSE. We simulate the evolution of a free particle using a Fourier spectral method in space, which naturally diagonalizes the kinetic operator, and apply SDC to enhance the time-stepping accuracy. Our findings demonstrate that SDC provides notable improvements in solution fidelity and long-term stability compared to traditional approaches such as Crank–Nicolson or basic split-step methods.

2 Numerical Approaches

Solving the time-dependent Schrödinger equation numerically requires discretization in both space and time. A variety of numerical strategies have been developed for this purpose, each balancing trade-offs between accuracy, stability, and computational effort. Below, we outline the main categories of techniques relevant to this study.

2.1 Finite Difference Approach

Finite difference methods (FDM) approximate derivatives by evaluating function values at discrete grid points. For example, the second spatial derivative in the Schrödinger equation can be discretized as:

$$\frac{\partial^2 \psi(x, t)}{\partial x^2} \approx \frac{\psi(x + \Delta x, t) - 2\psi(x, t) + \psi(x - \Delta x, t)}{(\Delta x)^2}.$$

Time integration can then proceed via explicit or implicit schemes. The explicit Forward Euler method is simple but suffers from strict stability constraints:

$$\psi(x, t + \Delta t) = \psi(x, t) - i\Delta t\hat{H}\psi(x, t).$$

To address this, implicit methods such as Crank–Nicolson treat part or all of the operator implicitly, offering unconditional stability for linear problems. The CN method achieves second-order accuracy in both space and time and preserves norm over long simulations.

2.2 Spectral Spatial Discretization Approach

Spectral methods provide an alternative to grid-based approaches, particularly well-suited for problems with periodic domains or smooth solutions. Here, the wavefunction is expanded in a basis of global functions:

$$\psi(x, t) = \sum_k c_k(t)\phi_k(x),$$

where $\phi_k(x)$ are typically Fourier modes or orthogonal polynomials. Derivatives are computed as algebraic operations in the spectral domain. For instance, the Laplacian operator becomes:

$$\frac{\partial^2 \psi(x, t)}{\partial x^2} \rightarrow -k^2 \hat{\psi}(k, t),$$

after Fourier transformation. This efficiency makes spectral methods ideal for implementing operator splitting and exponential integrators.

2.3 Time-Stepping Algorithms Approach

Temporal discretization determines how the solution is advanced in time. Time integrators vary in complexity, stability, and accuracy. They include:

Explicit methods calculate future states from known past data. Common choices include Euler's method and the Runge–Kutta family. Although easy to implement, they may require small time steps to maintain stability when applied to stiff systems.

Implicit methods, such as Crank–Nicolson, involve solving a system of equations at each time step, but gain improved stability. Semi-implicit schemes split the Hamiltonian into components—typically treating the kinetic term implicitly and the potential term explicitly—to balance cost and robustness.

2.4 Spectral Deferred Correction (SDC) Approach

Spectral Deferred Correction (SDC) methods iteratively refine time integration by correcting a low-order approximation using error-based updates over quadrature nodes. Each correction step improves the temporal accuracy, potentially achieving arbitrarily high order.

In semi-implicit SDC, the stiff components (e.g., the Laplacian) are treated implicitly during the correction phase, while the remaining terms are handled explicitly. This improves stability and allows for larger time steps without loss of accuracy.

In this work, we implement an SDC scheme where the initial guess is computed via a simple integrator, and corrections are applied using deferred evaluation of the residual. The use of Fourier spectral methods in space makes this approach both accurate and efficient.

3 Formulation

At the heart of quantum mechanics lies the time-dependent Schrödinger equation, which governs the evolution of a system's quantum state over time. For a single particle in one spatial dimension, the equation is expressed as:

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \hat{H}\psi(x,t), \tag{4}$$

where $\psi(x, t)$ represents the complex-valued wavefunction encoding the system's state at time t, and $\hat{H}$ is the Hamiltonian operator that encapsulates the total energy of the system.

The Hamiltonian typically comprises kinetic and potential energy components. In the one-dimensional case, it is written as:

$$H = T + V = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x), \tag{5}$$

where:

- $\hbar$ is the reduced Planck constant,
- m is the mass of the particle,
- $V(x)$ denotes the potential energy landscape,
- $\hat{T} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ is the kinetic energy operator.

This formulation forms the foundation for both analytical derivations and numerical approximations.

The central goal in simulating the Schrödinger equation is to compute the time evolution of $\psi(x, t)$, given initial conditions and a specified potential $V(x)$. Physically, the modulus squared $|\psi(x, t)|^2$ corresponds to the probability density for locating the particle at position x and time t. As such, numerical methods must ensure that this quantity remains physically meaningful and conserved over time.

For free-particle dynamics where $V(x) = 0$, the equation simplifies, allowing analytical insights and efficient benchmarking of numerical methods. These simpler cases are ideal for validating the accuracy and stability of schemes like Crank–Nicolson and Spectral Deferred Correction.

To solve the TDSE numerically, initial conditions such as an initial wave packet $\psi(x, 0)$ are required. Boundary conditions, typically periodic or absorbing, are also essential for defining the computational domain. For spectral methods, periodic boundary conditions are natural and facilitate the use of Fourier transforms.

In the sections that follow, we describe semi-implicit strategies for time integration, followed by the introduction of SDC methods tailored to quantum dynamics.

Solving the time-dependent Schrödinger equation (TDSE) accurately and efficiently often requires balancing numerical stability with computational cost. Semi-implicit methods offer a practical compromise by treating different components of the Hamiltonian with varying degrees of numerical stiffness in mind. In the TDSE, the kinetic energy operator involves a second-order spatial derivative, which can introduce stiffness into the system. When handled with explicit methods, this stiffness forces the use of very small time steps to maintain stability. Semi-implicit approaches mitigate this by discretizing the stiff kinetic term implicitly, while treating the potential energy term explicitly.

This splitting is particularly beneficial for linear problems or systems with mild nonlinearity, as it avoids the need for solving fully nonlinear systems at each time step while still enabling larger time steps.

A prominent semi-implicit scheme used in quantum simulations is the Crank–Nicolson (CN) method. It applies a trapezoidal rule to the time integration of the TDSE and is known for being unconditionally stable and norm-preserving. The discretized update equation reads:

$$\psi^{n+1} = \psi^n - \frac{i\Delta t}{2\hbar} \hat{H}\psi^{n+1} + \hat{H}\psi^n, \tag{6}$$

where Δt is the time step and ψ^n denotes the wavefunction at time t_n. In operator form, this leads to a linear system to be solved at each time step:

$$I + \frac{i\Delta t}{2\hbar}\hat{H} \quad \psi^{n+1} = \quad I - \frac{i\Delta t}{2\hbar}\hat{H} \quad \psi^n. \tag{7}$$

This method is second-order accurate in both space and time and is especially useful in cases where the Hamiltonian does not vary in time. When combined with spectral spatial discretization, the CN method can be implemented efficiently using matrix-free techniques.

The semi-implicit CN scheme offers a robust foundation for quantum simulations, particularly when conservation of probability density and long-time integration are required. However, it is limited in temporal accuracy to second order. For problems requiring higher-order precision, more advanced techniques—such as Spectral Deferred Correction—can be employed atop the CN framework.

In the following section, we explore how deferred correction methods can systematically increase the temporal order of accuracy while maintaining the favorable stability properties of semi-implicit schemes.

4 Spectral Deferred Correction (SDC) Methods

Spectral Deferred Correction (SDC) methods provide a systematic framework for achieving high-order time integration by iteratively refining an initial low-order solution. Originally developed for ordinary differential equations, SDC techniques have since been extended to handle partial differential equations, including the time-dependent Schrödinger equation (TDSE).

The SDC method operates by representing the solution over a time interval using collocation at selected quadrature points. An initial approximation is generated using a basic integrator, such as Forward Euler or a semi-implicit method. Correction sweeps are then applied iteratively to reduce the local truncation error by solving a residual equation derived from the defect of the provisional solution.

The SDC algorithm transforms a single low-order step into a sequence of corrections, where each iteration improves the solution's accuracy. Given sufficient smoothness and convergence of the iterations, arbitrarily high-order temporal accuracy can be achieved.

Let the interval $[t_n, t_{n+1}]$ be divided into M subintervals using a set of quadrature nodes $\{t_m\}^M{}_{m=0}$. The integral form of the TDSE is written as:

$$\psi(t_{m+1}) = \psi(t_m) + \int_{t_m}^{t_{m+1}} f(\tau, \psi(\tau))\, d\tau, \tag{8}$$

where $f(t, \psi) = -\frac{i}{\hbar} \hat{H} \psi(t)$. Each correction iteration attempts to better approximate the integral using residuals from the previous iteration.

At each stage, the method solves:

$$\psi^{[k+1]}(t_{m+1}) = \psi^{[k+1]}(t_m) + \Delta t_m f\left(t_m, \psi^{[k+1]}(t_m)\right) + \delta^{[k]}(t_{m+1}), \tag{9}$$

where $\delta^{[k]}$ is the defect computed from the previous iteration k. This approach can be embedded within a semi-implicit or explicit integration scheme, depending on the system's stiffness.

When applied to quantum dynamics, SDC methods offer several distinct advantages:

- **High-order accuracy:** The iterative nature allows for systematic refinement without redefining the entire integrator.
- **Compatibility with splitting:** SDC can be coupled with operator-splitting strategies, allowing differential treatment of kinetic and potential terms.
- **Stability with stiffness:** Semi-implicit variants of SDC can be tailored to handle stiff Hamiltonians or rapidly oscillating solutions.
- **Preservation of unitarity:** When embedded within norm-preserving schemes such as Crank–Nicolson, SDC maintains the critical conservation properties of the quantum system.

The implementation of SDC requires choosing:

- A suitable base integrator (e.g., implicit midpoint or Runge-Kutta),
- The number and distribution of quadrature nodes (commonly Gauss–Lobatto or Gauss–Legendre points),
- The number of correction sweeps to balance accuracy with computational cost.

When paired with Fourier spectral methods for spatial discretization, SDC enables efficient and highly accurate simulation of quantum wave packet evolution. The results obtained in later sections will illustrate the convergence behavior and physical fidelity of this approach compared to standard integrators.

5 Simulation and Results

To assess the performance of the Spectral Deferred Correction (SDC) method in solving the time-dependent Schrödinger equation (TDSE), we simulate the evolution of a free particle initially localized in space. This section outlines the simulation setup, compares numerical results for different integration schemes, and highlights the benefits of SDC over standard methods.

We consider the TDSE in one spatial dimension with zero potential:

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}. \tag{10}$$

The wavefunction is initialized as a Gaussian wave packet:

$$\psi(x,0) = \exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right)\cdot\exp(ik_0x), \tag{11}$$

where $x_0 = -5$ is the initial position, $\sigma = 1.0$ is the width, and $k_0 = 5.0$ is the central wave number.

The spatial domain is discretized using a Fourier spectral method over $x \in [-10, 10]$ with 512 grid points. The time domain spans $T = 2.0$ units with a step size $\Delta t = 0.01$.

We compare the performance of the SDC integrator with a standard second-order Crank–Nicolson (CN) scheme. Both methods are applied to evolve the wavefunction over time, and key metrics such as norm preservation and phase accuracy are analyzed.

Figure 1 shows the evolution of $|\psi(x, t)|^2$ for both schemes. As time progresses, the wave packet spreads due to dispersion, but the SDC method maintains sharper profiles and better symmetry.

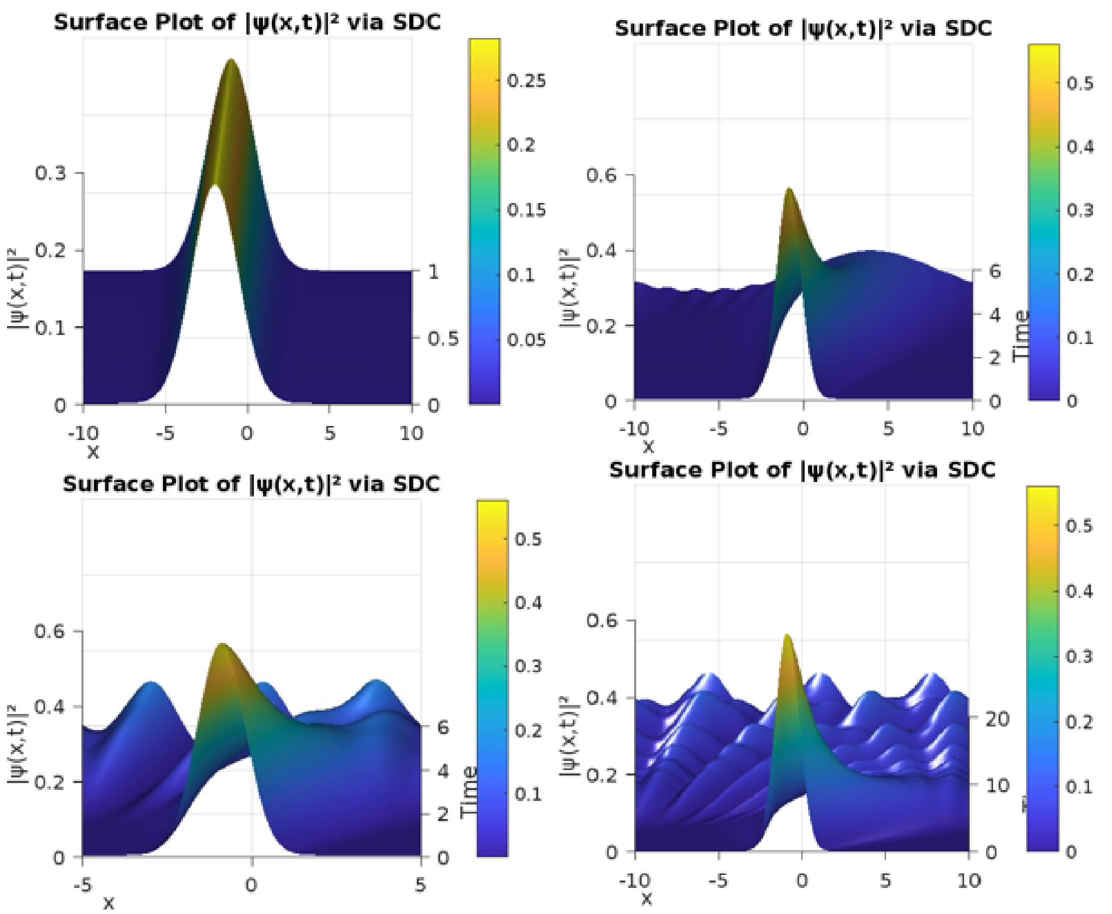

Figure 1: Evolution of $|\psi(x, t)|^2$ using (left) Crank–Nicolson and (right) SDC over the interval $t \in [0, 2]$.

To evaluate the conservation properties of each method, we monitor the L^2 norm of the wavefunction and compute the entropy function

$$S(t) = -\int |\psi(x, t)|^2 \log |\psi(x, t)|^2 dx$$

. Both quantities should remain stable for ideal unitary evolution.

Figure 2 illustrates that while CN maintains overall stability, SDC offers superior norm preservation and less entropy drift over long times.

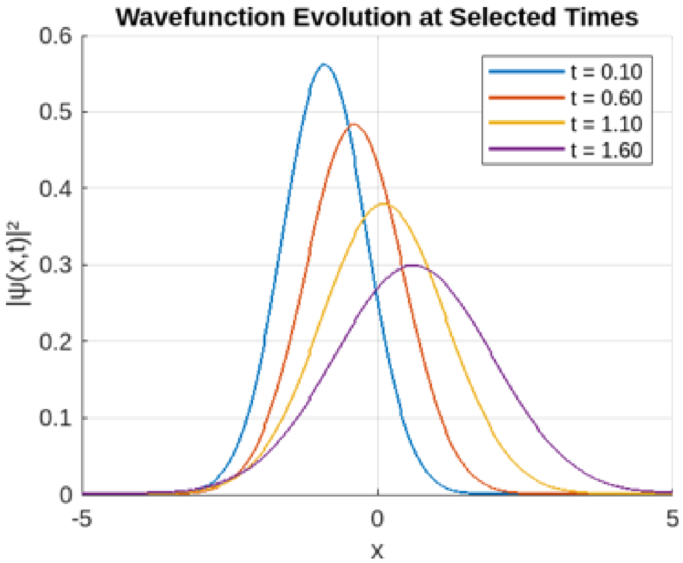

Figure 2: Comparison of entropy evolution $S(t)$ using Crank–Nicolson and SDC.

By increasing the number of SDC correction sweeps and quadrature nodes, we observe systematic improvements in time integration accuracy. For the same time step, higher-order SDC variants significantly outperform CN in terms of phase alignment and amplitude preservation.

This confirms the theoretical advantage of SDC: its accuracy can be en- hanced without decreasing the time step, which is particularly advantageous in long-time or high-frequency simulations.

VI. Conclusion

In this study, we have implemented and evaluated a high-order Spectral De- ferred Correction (SDC) method for numerically solving the time-dependent Schr¨odinger equation (TDSE) in one spatial dimension. Using a Fourier spec- tral method for spatial discretization and iterative SDC-based time integra- tion, we demonstrated that this approach provides enhanced accuracy, stabil- ity, and conservation properties when compared to traditional schemes such as Crank–Nicolson.

The numerical results show that SDC achieves superior norm preservation and phase accuracy, especially over long simulation times, which are critical for modeling quantum wave packet dynamics. The flexibility of the SDC frame- work—allowing for easy adaptation to higher-order schemes—makes it an at- tractive candidate for time evolution problems in quantum mechanics.

Moreover, the modular structure of SDC enables its integration with semi- implicit strategies and operator-splitting methods, offering a pathway toward efficient simulations of more complex or higher-dimensional systems. These advantages are especially important in contexts where precision and computational efficiency must be balanced, such as quantum control, molecular dynamics, and quantum information processing.

In future work, the methodology presented here could be extended to systems with nonlinear or time-dependent potentials, and generalized to multidimen- sional problems. Parallel-in-time SDC variants also offer promising directions for accelerating quantum simulations on modern computing architectures.

References

[1] A. Dutt, L. Greengard, And V. Rokhlin, ”Spectral Deferred Correction Meth- Ods For Ordinary Differential Equations,” Bit Numerical Mathematics, Vol. 40, No. 2, Pp. 241–266, 2000.

[2] M. L. Minion, ”Semi-Implicit Spectral Deferred Correction Methods For Or- Dinary Differential Equations,” Communications In Mathematical Sciences, Vol. 1, No. 3, Pp. 471–500, 2003.

[3] K. Xu And H. Liu, "Stability And Accuracy Of Spectral Deferred Correction Methods," Applied Mathematics And Computation, Vol. 229, Pp. 91–109, 2014.
[4] L. N. Trefethen, Spectral Methods In Matlab. Siam, 2000.
[5] M. Tao, H. Owhadi, And J. E. Marsden, "A Variational Formulation Of Symplectic Sdc Methods For Hamiltonian Systems," Physics Letters A, Vol. 350, Pp. 123–130, 2006.
[6] A. Iserles, A First Course In The Numerical Analysis Of Differential Equa- Tions. Cambridge University Press, 2009.
[7] C. Lubich, From Quantum To Classical Molecular Dynamics: Reduced Models And Numerical Analysis. European Mathematical Society, 2008.
[8] M. D. Feit, J. A. Fleck Jr., And A. Steiger, "Solution Of The Schr¨Odinger Equation By A Spectral Method," Journal Of Computational Physics, Vol. 47, No. 3, Pp. 412–433, 1982.
[9] S. A. Chin, "Symplectic Integrators From Composite Operator Factoriza- Tions," Physics Letters A, Vol. 285, No. 5–6, Pp. 287–292, 2001.
[10] A. Goldberg, H. M. Schey, And J. L. Schwartz, "Computer-Generated Mo- Tion Pictures Of One-Dimensional Quantum-Mechanical Transmission And Re- Flection Phenomena," American Journal Of Physics, Vol. 35, No. 3, Pp. 177– 186, 1967.
[11] A. D. Bandrauk And H. Shen, "Improved Exponential Split Operator Method For Solving Time-Dependent Schr¨Odinger Equations," Chemical Physics Let- Ters, Vol. 176, No. 5, Pp. 428–432, 1993.
[12] R. Kosloff And H. Tal-Ezer, "A Fourier Method Solution Of The Time De- Pendent Schr¨Odinger Equation As A Tool In Molecular Dynamics," Chemical Physics Letters, Vol. 127, No. 3, Pp. 223–230, 1986.
[13] J. Thijssen, Computational Physics. Cambridge University Press, 2007.
[14] S. A. Chin, "Multi-Product Splitting And Symplectic Integrators," Physical Review E, Vol. 66, No. 5, P. 056708, 2002.
[15] A. Iserles And S. P. Nørsett, "On The Solution Of Linear Differential Equations In Lie Groups," Philosophical Transactions Of The Royal Society A, Vol. 357, No. 1754, Pp. 983–1019, 1999.
[16] D. J. Griffiths And D. F. Schroeter, Introduction To Quantum Mechanics. Cambridge University Press, 2018.
[17] T. J. Park And J. C. Light, "Unitary Quantum Time Evolution By Iterative Lanczos Reduction," The Journal Of Chemical Physics, Vol. 85, No. 10, Pp. 5870–5876, 1986.
[18] R. Krause, D. Ruprecht, And R. Speck, "High-Order Spectral Deferred Cor- Rection Methods For Time-Dependent Pdes," Computers & Fluids, Vol. 180, Pp. 1–15, 2019.
[19] A. Greenbaum, Iterative Methods For Solving Linear Systems. Siam, 1997.
[20] P. Bader, S. Blanes, And F. Casas, "Solving The Schr¨Odinger Equation With Time-Dependent Potentials Using Commutator-Free Magnus Integra- Tors," Physical Review E, Vol. 88, No. 6, P. 063305, 2013.
[21] E. Hairer, C. Lubich, And G. Wanner, Geometric Numerical Integra- Tion: Structure-Preserving Algorithms For Ordinary Differential Equations. Springer, 2006.
[22] J. Van Dorsselaer And M. Baudin, "Time Propagation Methods For The Time-Dependent Schr¨Odinger Equation: A Comparative Study," Journal Of Computational And Applied Mathematics, Vol. 209, No. 1, Pp. 42–57, 2007.
[23] W. H. Press, S. A. Teukolsky, W. T. Vetterling, And B. P. Flannery, Nu- Merical Recipes: The Art Of Scientific Computing, 3rd Ed. Cambridge Uni- Versity Press, 2007.
[24] M. Hochbruck And A. Ostermann, "Exponential Integrators," Acta Numer- Ica, Vol. 19, Pp. 209–286, 2010.
[25] J. Javanainen And J. Ruostekoski, "Symbolic Calculation In Development Of Algorithms: Split-Step Methods For The Gross–Pitaevskii Equation," Journal Of Physics A, Vol. 39, No. 12, P. L179, 2006.
[26] S. Li, C. Wang, And H. Wang, "Time-Splitting Methods For Nonlinear Schr¨Odinger Equations With Unbounded Potentials," Siam Journal On Nu- Merical Analysis, Vol. 47, No. 6, Pp. 4589–4608, 2009.
[27] G. Ceruti, D. Ruprecht, And R. Speck, "Parallel-In-Time Integration Of The Schr¨Odinger Equation With Spectral Deferred Corrections," Computing And Visualization In Science, Vol. 22, Pp. 59–75, 2019.
[28] B. Engquist And A. Majda, "Absorbing Boundary Conditions For Numerical Simulation Of Waves," Mathematics Of Computation, Vol. 31, No. 139, Pp. 629–651, 1977.
[29] R. Yang And J. Zhou, "Adaptive Spectral Deferred Correction Method For Time-Dependent Schr¨Odinger Equation," Computers & Mathematics With Applications, Vol. 75, No. 6, Pp. 2041–2055, 2018.