A generalized finite-difference time-domain quantum method for the $N$-body interacting Hamiltonian

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ABSTRACT

The Quantum Finite-Difference Time-Domain (FDTD-Q) method is a numerical method for solving the time evolution of the Schrödinger equation. It can be applied to systems of interacting particles, allowing for realistic simulations of quantum mechanics of various experimental systems. One of the drawbacks of the method is that divergences in the numerical evolution occur rather easily in the presence of interactions, which necessitates a large number of evolution steps or imaginary time evolution. We present a generalized (GFDTD-Q) method for solving the time-dependent Schrödinger equation including interactions between the particles. The new scheme provides a more relaxed condition for stability when the finite difference approximations for spatial derivatives are employed, as compared with the original FDTD-Q scheme. We demonstrate our scheme by simulating the time evolution of a two-particle interaction Hamiltonian. Our results show that the generalized method allows for stable time evolutions, in contrast to the original FDTD-Q scheme which produces a divergent solution.

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1. Introduction

Recent advances in the experimental techniques of quantum information technology have introduced the need for performing more realistic simulations of quantum mechanical systems. For example, ultracold atoms may be trapped in optical lattices realizing a Mott insulator state where one atom is trapped on each lattice site [1]. In semiconductor systems, quantum dots consisting of single electrons may be positioned in close proximity permitting the realization of simple qubit operations [2]. In addition, ion traps offer the possibility of controlling a few trapped ion systems due to the combination of Paul traps and their mutual Coulomb repulsion [3]. When designing such systems, simulations must include not only the qualitative features of the problem, but also a detailed modeling of the experimental conditions. This is often required in order to achieve precision control. Such systems also require an extension beyond a single particle problem to a several particle interaction model. Moreover, for quantum information processing applications, the effect of control in the time domain is also necessary. For example, this may occur due to gate operations being performed on qubits. The combination of these factors places rather large demands on the numerical simulation, in terms of the computational overhead and the stability of the algorithm being used to perform the simulation.

There are many numerical methods (finite-difference [4–23], spectral [24,25], and integration [26–29]) for solving the linear time-dependent Schrödinger equation. In particular, the finite-difference time-domain (FDTD) method [14,15,22], which is often employed in simulations of electromagnetic fields, was developed to solve the time-dependent Schrödinger equation. The application of the FDTD technique for the analysis of quantum devices is named the FDTD-Q (quantum). However, the FDTD-Q method requires a very restricted stability condition in order to prevent the numerical solution from diverging [5,13]. In this article, we present a new generalized FDTD-Q scheme for solving the time-dependent Schrödinger equation for studying the $N$-body interacting Hamiltonian. The new scheme is not only explicit and simple for computation, but also provides a more relaxed condition for stability when the fourth-order finite difference approximations for spatial derivatives are employed, as compared with the original FDTD-Q scheme. This will allow us to employ a larger time step in the computation, which is particularly important for quantum simulations. We have managed to produce a convergent solution with a greatly reduced number of iterations in comparison to the standard FDTD-Q scheme. The Generalized Finite-Difference Time-Domain Quantum (GFDTD-Q) method is used to analyze the two-particle interaction Hamiltonian during which the original FDTD-Q scheme produces a divergent solution.
The contents of this paper are organized as follows. In Section 2, we give a brief summary of the N-body interacting Hamiltonian that is simulated. For example, in Section 3, a description of the GFDTD-Q method will be given which demonstrates the improved scheme for two particles in a two dimensional space. The stability of the algorithm is examined in Section 4. Finally, a numerical example will be given pertaining to a two-particle system at a two-site optical lattice geometry in Section 5. In Section 6, we summarize our findings and conclude results.

2. Schrödinger equation

The N-body interacting Hamiltonian is

\[ \hat{H} = \sum_{i=1}^{N} \left[ -\frac{\hbar^2}{2m_i} \nabla_i^2 + V_i(r_i) \right] + \sum_{j<k} V_{j,k}(r_j, r_k), \tag{1} \]

where \( m_i \) is the mass of each individual particle, \( \hbar = 1.054 \times 10^{-34} \) J·s is Planck’s constant. Here, \( V_i \) is the single-body potential for the \( j \)-th particle which depends on space \( r_j \), and \( V_{j,k} \) represents the Coulombic interaction potential between the \( j \)-th and \( k \)-th particles, which depend on space \( r_j \) and \( r_k \). This is typically a function of \(|r_j - r_k|\). Consequently, the quantum behavior of each particle in an N-body system can be expressed by a time-dependent Schrödinger equation as

\[ \hbar \frac{\partial \psi(t)}{\partial t} = \hat{H} \psi(t), \tag{2} \]

where \( \psi(t) \) is a wave function and \( i = \sqrt{-1} \). If we consider only two particles in the x-z plane, then the above equation can be written as

\[ \hbar \frac{\partial \psi(x_1, z_1, x_2, z_2, t)}{\partial t} = \left[ -\frac{\hbar^2}{2m_1} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial z_1^2} \right) - \frac{\hbar^2}{2m_2} \left( \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial z_2^2} \right) \right] \psi(x_1, z_1, x_2, z_2, t) + \left[ V_1(x_1) + V_2(x_2) + V_{1,2}(x_1, z_1, x_2, z_2) \right] \psi(x_1, z_1, x_2, z_2, t). \tag{3} \]

The solution of the time-dependent Schrödinger equation can be written as a linear superposition of stationary states with time dependence given by the phase factor \( \exp(-iE_n t / \hbar) \), with \( E_n \)signifying the nth energy level of the quantum system.

We may also consider an imaginary time evolution, where we replace time \( t \) with \(-i\tau\). This will reveal a solution as a sum of decay amplitudes given by the form \( \exp(-iE_n \tau / \hbar) \). Evolved for sufficient imaginary time, one can obtain ground state energy \( E_{GS} \) and ground state wave function \( \psi_{GS} \) of the quantum system, independent of the initial state prepared. The Schrödinger equation in imaginary time is

\[ -\hbar \frac{\partial \psi(r_1, r_2, \ldots, r_N, \tau)}{\partial \tau} = \hat{H} \psi(r_1, r_2, \ldots, r_N, \tau). \tag{4} \]

In order to consider a system of interacting quantum particles and analyze their behavior under the FDTD algorithms, we follow the suggestions in [1,6] and choose the potential in numerical simulations to be

\[ V_j(x_j) = V \cos \left( \frac{2\pi x_j}{L} \right), \quad j = 1, 2. \tag{5} \]

It is only modulated in the x-direction and the Coulombic interaction potential has the following form with \( x_1 \neq x_2 \) and \( z_1 \neq z_2 \)

\[ V_{1,2}(x_1, z_1, x_2, z_2) = \frac{e^2}{4\pi \varepsilon_0 \varepsilon_0} \frac{1}{\sqrt{(x_1 - x_2)^2 + (z_1 - z_2)^2}}, \tag{6} \]

where \( e \) is the elementary charge, \( \varepsilon_0 \) is the permittivity of free space, and \( \varepsilon_i \) is the relative permittivity. Here, we assume that both particles are electrons with the same mass \( m_1 = m_2 = m^*_e \) and anti-parallel spins (↑, ↓). The spin component of the system’s wave function is also assumed to be anti-symmetric. Due to the fact that electrons are Fermionic particles (Fermions), we employ the N-body interacting Hamiltonian in this study. It should be pointed out that the Coulomb interaction, Eq. (6), is a fundamental form of interaction which affects all types of charged particles in a variety of systems, ranging from atoms to solid state systems such as semiconductors and lattice models. Furthermore, the long-ranged nature of the Coulomb interaction makes the simulation more challenging since the interaction cannot be neglected even when the particles are separated by large distances.

3. Generalized FDTD-Q scheme

To develop the GFDTD-Q scheme, the wave function \( \psi(x_1, x_2, z_1, z_2, t) \) is first split into real \( \psi_{\text{real}} \) and imaginary \( \psi_{\text{imag}} \) components. Substituting them into Eq. (3) results in the following coupled set of equations:

\[ \frac{\partial \psi_{\text{real}}(x_1, x_2, z_1, z_2, t)}{\partial t} = \left[ \frac{h}{2m_1} \nabla_1^2 + \frac{h}{2m_2} \nabla_2^2 - V_1(x_1) - V_2(x_2) - V_{1,2}(x_1, z_1, x_2, z_2) \right] \psi_{\text{real}}(x_1, x_2, z_1, z_2, t), \tag{7} \]

\[ \frac{\partial \psi_{\text{imag}}(x_1, x_2, z_1, z_2, t)}{\partial t} = \left[ \frac{h}{2m_1} \nabla_1^2 + \frac{h}{2m_2} \nabla_2^2 - V_1(x_1) - V_2(x_2) - V_{1,2}(x_1, z_1, x_2, z_2) \right] \psi_{\text{imag}}(x_1, x_2, z_1, z_2, t), \tag{8} \]

where \( \nabla_1^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial z_1^2} \) and \( \nabla_2^2 = \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial z_2^2} \). Here, we assume that \( \psi_{\text{real}} \) and \( \psi_{\text{imag}} \) are sufficiently smooth functions which vanish for large enough \(|x|\) and \(|z|\). Using the Taylor series method to expand \( \psi_{\text{real}}(x_1, x_2, z_1, z_2, t_n) \) and \( \psi_{\text{imag}}(x_1, x_2, z_1, z_2, t_n) \) at \( t = t_n - \frac{\Delta t}{2} = \left(n - \frac{1}{2}\right) \Delta t \) gives:

\[ \psi_{\text{real}}(x_1, x_2, z_1, z_2, t_n) = \psi_{\text{real}}(x_1, x_2, z_1, z_2, t_n - \frac{\Delta t}{2}) + 2 \sum_{p=0}^{\infty} \frac{(\Delta t/2)^{2p+1}}{(2p+1)!} \psi_{\text{real}}(x_1, x_2, z_1, z_2, t_n - \frac{\Delta t}{2}) \frac{d^{2p+1}}{dt^{2p+1}}, \tag{9} \]

where \( \Delta t \) is the time step and \( n \) is the time level. We evaluate those derivatives in Eq. (9) by using Eqs. (7)–(8) repeatedly:

\[ \frac{\partial \psi_{\text{real}}(x_1, x_2, z_1, z_2, t_n - \frac{\Delta t}{2})}{\partial t} = \left[ \frac{h}{2m_1} \nabla_1^2 - \frac{h}{2m_2} \nabla_2^2 + V_1 + V_2 + V_{1,2} \right] \psi_{\text{imag}}(x_1, x_2, z_1, z_2, t_n - \frac{\Delta t}{2}), \tag{10a} \]
\[ \frac{\partial^2 \psi_{\text{real}}(x_1, x_2, z_1, z_2, t_{n-\frac{1}{2}})}{\partial t^2} = -\left( \frac{h}{2m_1} \nabla^2_{\text{real}} + \frac{h}{2m_2} \nabla^2_{\text{imag}} - \frac{V_1 + V_2 + V_{1,2}}{h} \right) \]

\[ \times \psi_{\text{imag}}(x_1, x_2, z_1, z_2, t_{n-\frac{1}{2}}) \]

and so on. Substituting Eq. (10) into Eq. (9) reveals

\[
\psi_{\text{real}}(x_1, x_2, z_1, z_2, t_n) = \psi_{\text{real}}(x_1, x_2, z_1, z_2, t_{n-1}) + 2 \sum_{p=0}^{\infty} \left( \frac{\Delta t}{2} \right)^{2p+1} \frac{(-1)^{p+1}}{(2p+1)!} \left( \frac{h}{2m_1} \nabla^2_{\text{real}} + \frac{h}{2m_2} \nabla^2_{\text{imag}} - \frac{V_1 + V_2 + V_{1,2}}{h} \right)^{2p+1} \psi_{\text{imag}}(x_1, x_2, z_1, z_2, t_{n-\frac{1}{2}}) \]  

Similarly, we employ the Taylor series method to expand \( \psi_{\text{imag}}(x_1, x_2, z_1, z_2, t_{n-\frac{1}{2}}) \) and \( \psi_{\text{imag}}(x_1, x_2, z_1, z_2, t_{n-\frac{1}{2}}) \) at \( t = t_n \), and then use Eqs. (7)–(8) repeatedly to evaluate the related derivatives. This gives

\[
\psi_{\text{imag}}(x_1, x_2, z_1, z_2, t_{n-\frac{1}{2}}) = \psi_{\text{imag}}(x_1, x_2, z_1, z_2, t_{n-\frac{1}{2}}) + 2 \sum_{p=0}^{\infty} \left( \frac{\Delta t}{2} \right)^{2p+1} \frac{(-1)^p}{(2p+1)!} \left( \frac{h}{2m_1} \nabla^2_{\text{imag}} + \frac{h}{2m_2} \nabla^2_{\text{real}} - \frac{V_1 + V_2 + V_{1,2}}{h} \right)^{2p+1} \psi_{\text{real}}(x_1, x_2, z_1, z_2, t_n) \]  

We denote \( \psi_{\text{real}}^{n+1}(k_{x1}, k_{x2}, k_{z1}, k_{z2}) \) and \( \psi_{\text{imag}}^{n+1}(k_{x1}, k_{x2}, k_{z1}, k_{z2}) \) as the approximations of \( \psi_{\text{real}}(k_{x1}\Delta x, k_{x2}\Delta z, k_{z1}\Delta x, k_{z2}\Delta z, t_{n-\frac{1}{2}}) \) and \( \psi_{\text{imag}}(k_{x1}\Delta x, k_{x2}\Delta z, k_{z1}\Delta x, k_{z2}\Delta z, t_{n-\frac{1}{2}}) \), respectively. Here, \( k_{x1}, k_{x2}, k_{z1}, k_{z2} \) are integers and \( \Delta x, \Delta z \) are grid sizes in the \( x \) and \( z \) directions, respectively. Using some higher-order accurate finite difference operators for \( \nabla^2_{\text{real}} \) and \( \nabla^2_{\text{imag}} \), such as the fourth-order central difference operator \( \frac{1}{\Delta x^2} D_x^1 + \frac{1}{\Delta z^2} D_z^1 \), as follows:

\[
\nabla^2_{\text{real}} \psi_{\text{real}}^{n}(k_{x1}, k_{x2}, k_{z1}, k_{z2}) 
\approx \frac{1}{\Delta x^2} D_x^1 \psi_{\text{real}}^{n}(k_{x1}, k_{x2}, k_{z1}, k_{z2}) + 16 \psi_{\text{real}}^{n}(k_{x1} + 1, k_{x2}, k_{z1}, k_{z2}) - 30 \psi_{\text{real}}^{n}(k_{x1}, k_{x2} + 1, k_{z1}, k_{z2}) + 16 \psi_{\text{real}}^{n}(k_{x1} - 1, k_{x2}, k_{z1}, k_{z2}) \]

and similar finite difference approximations are made for \( \nabla^2_{\text{imag}} \psi_{\text{imag}}^{n+\frac{1}{2}}(k_{x1}, k_{x2}, k_{z1}, k_{z2}) \), we obtain from Eq. (11), by truncating up to the \( P \) term, a generalized higher-order FDTD-Q scheme for solving the time-dependent Schrödinger equation for studying two interacting particles in real time as follows:

\[
\psi_{\text{real}}^{n+1}(k_{x1}, k_{x2}, k_{z1}, k_{z2}) = \psi_{\text{real}}^{n}(k_{x1}, k_{x2}, k_{z1}, k_{z2}) + 2 \sum_{p=0}^{P} \left( \frac{(-1)^{p+1}}{(2p+1)!} \left( \frac{h}{4m_1} (r_x D_x^1 + r_z D_z^1) + \frac{h}{4m_2} (r_x D_x^2 + r_z D_z^2) \right) \right)^{2p+1} \times \psi_{\text{imag}}^{n+\frac{1}{2}}(k_{x1}, k_{x2}, k_{z1}, k_{z2}) \]  

\[
\psi_{\text{imag}}^{n+\frac{1}{2}}(k_{x1}, k_{x2}, k_{z1}, k_{z2}) = \psi_{\text{imag}}^{n}(k_{x1}, k_{x2}, k_{z1}, k_{z2}) + 2 \sum_{p=0}^{P} \left( \frac{(-1)^p}{(2p+1)!} \left( \frac{h}{4m_1} (r_x D_x^1 + r_z D_z^1) + \frac{h}{4m_2} (r_x D_x^2 + r_z D_z^2) \right) \right)^{2p+1} \times \psi_{\text{real}}^{n}(k_{x1}, k_{x2}, k_{z1}, k_{z2}) \]  

where \( r_x = \frac{\Delta t}{\Delta x^2} \) and \( r_z = \frac{\Delta t}{\Delta z^2} \), and the truncation error is the order of \((\Delta t)^{2p+1} + (\Delta x)^4 + (\Delta z)^4\). It should be pointed out that for the case where the potential \( V \) is dependent on both temporal and spatial variables, the derivatives are similar to those in Eq. (14) except that the product rule of derivative with respect to \( t \) should be used. It can be seen that if \( P = 0 \), the above generalized FDTD-Q scheme will reduce to the original FDTD-Q scheme.  

4. Stability analysis

We now analyze the stability of the GFDTD-Q scheme using a von Neumann analysis [30], assuming that \( V_1, V_2 \) and \( V_{1,2} \) are constants for simplicity. We let

\[
\psi_{\text{real}}^{n}(k_{x1}, k_{x2}, k_{z1}, k_{z2}) = \psi_{\text{real}}^{n}(k_{x1}\beta_{11} k_{x2}\beta_{12} k_{z1}\Delta x + k_{x2}\beta_{12} k_{z2}\Delta z, k_{z1}\Delta x + k_{z2}\beta_{12} k_{z2}\Delta z), \]

\[
\psi_{\text{imag}}^{n}(k_{x1}, k_{x2}, k_{z1}, k_{z2}) = \psi_{\text{imag}}^{n}(k_{x1}\beta_{11} k_{x2}\beta_{12} k_{z1}\Delta x + k_{x2}\beta_{12} k_{z1}\Delta x + k_{z2}\beta_{12} k_{z2}\Delta z), \]

Substituting them into \((r_x D_x^1 + r_z D_z^1)\psi_{\text{real}}^{n}(k_{x1}, k_{x2}, k_{z1}, k_{z2})\) gives

\[
(r_x D_x^1 + r_z D_z^1)\psi_{\text{real}}^{n}(k_{x1}, k_{x2}, k_{z1}, k_{z2}) = -c_1 \psi_{\text{real}}^{n}(k_{x1}\beta_{11} k_{x2}\beta_{12} k_{z1}\Delta x + k_{x2}\beta_{12} k_{z2}\Delta z, k_{z1}\Delta x + k_{z2}\beta_{12} k_{z2}\Delta z), \]  

(16a)
\[ (r_x D_x^2 + r_y D_y^2)^{\lambda}_{\text{imag}} (k_1, k_2, k_2, k_2) \]

where

\[ c_1 = \frac{4}{3} \left[ r_x \sin^2 \frac{\beta_{1x} \Delta x}{2} + r_y \sin^2 \frac{\beta_{1y} \Delta y}{2} \right]. \]

Similarly, for the real part,

\[ (r_x D_x^2 + r_y D_y^2)^{\lambda}_{\text{real}} (k_1, k_1, k_2, k_2) \]

\[ \lambda \text{real} = \lambda_{\text{real}} + 2 \sum_{p=0}^{\infty} \frac{(-1)^p}{(2p+1)!} \left[ \frac{h}{4m_1} c_1 + \frac{h}{4m_2} c_2 \right] \left( \frac{\Delta t}{2h} (V_1 + V_2 + V_{1.2}) \right)^{2p+1}. \]

And so on. Substituting Eq. (15) into Eq. (14), using the above properties, and then deleting the common factor \( e^{i(k_1 x_1 + k_2 x_2 + k_1 \Delta x + k_2 \Delta y)} \), we obtain:

\[ c_2 = \frac{4}{3} \left[ r_x \sin^2 \frac{\beta_{2x} \Delta x}{2} + r_y \sin^2 \frac{\beta_{2y} \Delta y}{2} \right]. \]

Moreover, we have

\[ (r_x D_x^2 + r_y D_y^2)^{\lambda}_{\text{imag}} (k_1, k_1, k_2, k_2) \]

\[ \lambda \text{imag} = \lambda_{\text{imag}} + 2 \sum_{p=0}^{\infty} \frac{(-1)^p}{(2p+1)!} \left[ \frac{h}{4m_1} c_1 + \frac{h}{4m_2} c_2 \right] \left( \frac{\Delta t}{2h} (V_1 + V_2 + V_{1.2}) \right)^{2p+1}. \]

Since Eq. (19a) is true for any time level \( n \), we change \( n \) in Eq. (19a) to \( n + 1 \) as follows:

\[ (r_x D_x^2 + r_y D_y^2)^{\lambda}_{\text{real}} (k_1, k_2, k_2, k_2) \]

\[ \lambda \text{real} = (2 - \alpha^2) \lambda_{\text{real}} + 1 = 0, \]

where

\[ \alpha = 2 \sum_{p=0}^{\infty} \frac{(-1)^{p-1}}{(2p+1)!} \left( \frac{h}{4m_1} c_1 + \frac{h}{4m_2} c_2 + \frac{\Delta t}{2h} (V_1 + V_2 + V_{1.2}) \right)^{2p+1}. \]

Using the fact that for a quadratic equation \( x^2 + 8x + C = 0 \), the solution satisfies \(|x| \leq 1\) if and only if \(|B| \leq 1 + |C|\) and \(|C| \leq 1\), we obtain from Eq. (20) that \( |\lambda_{\text{real}}| \leq 1\) if and only if \(|\alpha| \leq 2\). By the von Neumann analysis, we conclude that the generalized FDTD-Q scheme is stable if \(|\alpha| \leq 2\), i.e.,

\[ \frac{p}{(2p+1)!} \left[ \frac{h}{4m_1} c_1 + \frac{h}{4m_2} c_2 \right] \left( \frac{\Delta t}{2h} (V_1 + V_2 + V_{1.2}) \right)^{2p+1} + \leq 1. \]

It can be seen that

\[ \lim_{P \to \infty} \sum_{p=0}^{P} \frac{(-1)^p}{(2p+1)!} \left[ \frac{h}{4m_1} c_1 + \frac{h}{4m_2} c_2 \right] \left( \frac{\Delta t}{2h} (V_1 + V_2 + V_{1.2}) \right)^{2p+1} \]

\[ \leq 1. \]

implying that, when \( P \to \infty \), Eq. (21) is automatically satisfied, and hence the scheme with \( P \to \infty \) is unconditionally stable. However, we cannot choose \( P = \infty \), and, therefore, the generalized FDTD-Q scheme should be imposed on the condition in Eq. (21). Noting that the condition in Eq. (21) gives only \(|\lambda_{\text{real}}| \leq 1\) and does not indicate whether or not there is a double root with \(|\lambda_{\text{real}}| = 1\) in Eq. (20) (for this case, the numerical solution may still be divergent), we choose the maximum value of \( \frac{\sin^2 \frac{\beta_{1x} \Delta x}{2}}{2} \) and \( \max_{x_1, x_2, y_2, k_2} (|V_1| + |V_2| + |V_{1.2}|) \) for the no constant case and obtain

\[ \left| \sum_{p=0}^{P} \frac{(-1)^p}{(2p+1)!} \left[ \left( \frac{4h}{3m_1} + \frac{4h}{3m_2} \right) (r_x + r_y) \right] \left( \frac{\Delta t}{2h} (V_1 + V_2 + V_{1.2}) \right)^{2p+1} \right| \leq c < 1. \]

Theorem 1. The generalized FDTD-Q scheme, Eq. (14), is stable if the condition, Eq. (23), is satisfied.

It can be seen from Eq. (14) that the values of \((r_x D_x^2 + r_y D_y^2)^{\lambda_{\text{imag}} + 1/2} \psi_\text{imag} \) and \((r_x D_x^2 + r_y D_y^2)^{\lambda_{\text{real}} + 1/2} \psi_\text{real} \) need to be calculated, and this may be very tedious for large integer values of \( P \). For this case, one may use Eq. (13) (with both sides multiplied by \( \Delta t \)) recursively to obtain an approximation for \((r_x D_x^2 + r_y D_y^2)^{2p+1} \psi_\text{real} \). The idea is, for instance, once the values of \((r_x D_x^2 + r_y D_y^2)^{\lambda_{\text{real}} + 1/2} \psi_\text{real} \) for all \( k_x \) and \( k_y \) are calculated by Eq. (13), we replace those \( \psi_\text{real} \) on the right-hand-side of Eq. (13) by \((r_x D_x^2 + r_y D_y^2)^{\lambda_{\text{imag}} + 1/2} \psi_\text{imag} \) to obtain \((r_x D_x^2 + r_y D_y^2)^{\lambda_{\text{imag}} + 1/2} \psi_\text{imag} \) for all \( k_x \) and \( k_y \) and continue the procedure until \((r_x D_x^2 + r_y D_y^2)^{2p+1} \psi_\text{real} \) for all \( k_x \) and \( k_y \) are calculated. For this reason, one may choose \( P \) to be a small integer for simplicity of computation.

5. Numerical example

We considered two electrons trapped in a two-dimensional infinite potential well, where the particles are confined to the area \( D = \{(x, y) | 0 < x < L_x, 0 < y < L_y\} \) in the \( x-y \) plane. We assumed that both electrons are in the initial ground state [6], where the initial ground state energy is given by \( E_0 = \frac{\pi^2 \hbar^2}{2m} \left( \frac{1}{L_x^2} + \frac{1}{L_y^2} \right) \) and the wave function of the system is \( \psi_0(x_1, x_2) = \frac{1}{L_x L_y} \sin \left( \frac{n_1 \pi x_1}{L_x} \right) \sin \left( \frac{n_2 \pi x_2}{L_y} \right) \). As \( V_1 \) and \( V_2 \) in Eq. (3) are increased, both electrons localize on their respective optical lattice site. This occurs when \( V_1, 2 \) in Eq. (6) is equal to zero. When \( V_1, 2 \) in Eq. (6) is much larger than zero, each electron is in a superposition of left and right on site states. In this state, quantum tunneling is probable. In the two-site geometry, the ground state of a single electron is expressed by two basic states \( |l \rangle \) and \( |r \rangle \), or their superposition.
mostly found on the left site \((0 \leq x \leq L_x/2)\). Conversely, the \(|R⟩\) state corresponds to where the electron is mostly found on the right site \((L_x/2 \leq x \leq L_x)\). The ground state of the two-electron system with no interaction potential is
\[
|Ψ⟩_{V, L, R} = \frac{1}{\sqrt{2}} (|L⟩ + |R⟩) \otimes \frac{1}{\sqrt{2}} (|L⟩ + |R⟩) _2
\]
where \(\otimes\) is a tensor-product, \(|LL⟩ = |L⟩_1 \otimes |L⟩_2\), \(|LR⟩ = |L⟩_1 \otimes |R⟩_2\), and \(|RR⟩ = |R⟩_1 \otimes |R⟩_2\). On the other hand, the ground state of the system with large particle repulsion is
\[
|Ψ⟩_{V, L, R} = \frac{1}{\sqrt{2}} (|LR⟩ + |RL⟩),
\]
which results from \(|LL⟩ + |RR⟩\) giving a higher interaction energy.

We employed the GFDTD-Q scheme with \(P = 2\) in Eq. (14) and the FDTD-Q scheme, respectively, to study the regime with a strong particle interaction, corresponding to a Mott insulator quantum phase. Parameters \(k_{s1}, k_{s2} \in \{k|x| = 0, 1, \ldots, N_x\}\) and \(k_{s1}, k_{s2} \in \{k|x| = 0, 1, \ldots, N_x\}\) correspond to \(x_1, x_2, z_1, \) and \(z_2\) respectively, such that \(N_x \Delta x = L_x, N_z \Delta z = L_z\) as listed in Table 1.

In our computation, the discretized initial values were set to be
\[
\psi^{|real|}(k_{s1}, k_{s2}) = \frac{4}{L_x L_z} \sin \left( \frac{\pi k_{s1}}{N_x} \right) \sin \left( \frac{\pi k_{s2}}{N_z} \right) \times \sin \left( \frac{\pi k_{s2}}{N_z} \right) \sin \left( \frac{\pi k_{s2}}{N_z} \right),
\]
\[
\psi^{|imag|}(k_{s1}, k_{s2}) = -\psi^{|real|}(k_{s1}, k_{s2}) \sin \left( \frac{E_{c5} \Delta t}{\hbar} \right).
\]

We used the following values for parameters [6]: \(h = 1.054 \times 10^{-34} \) [J-s], \(\epsilon_v = 13.1, \epsilon_0 = 8.854187817 \times 10^{-12} \) [F-m⁻¹], and \(e = 1.602177 \times 10^{-19} \) [C], and \(m_1 = m_2 = m = 0.067 \) [kg] × 9.1 \times 10⁻³¹ [kg]. When the index satisfies \((k_{s1}, k_{s2}) = (k_{s2}, k_{s1})\), in which the Coulomb potential diverges, the wave function is set to zero as \(\psi^{|real|}(k_{s1}, k_{s2}) = \psi^{|imag|}(k_{s1}, k_{s2}) = 0\).

Figs. 1–5 demonstrate our results. Fig. 1 illustrates that the probability density distribution of the initial state is spread with even phase coherence over the entire lattice. After the electrons are released from the potential energies, solutions are given. Fig. 1 shows the initial state as given by Eq. (24). As the lattice potential is increased in time, electrons localize on their respective lattice sites. The ground state of the two-electron interaction is calculated in imaginary time by using a similar GFDTD-Q scheme for Eq. (4) as follows:
\[
\psi^{|real|}(k_{s1}, k_{s2}) = \psi^{|imag|}(k_{s1}, k_{s2})
\]
\[
-2 \sum_{p=0}^{p} \frac{1}{(2p + 1)!} \left[ \frac{\hbar}{4m_1} (r_x D_x^2 + r_y D_y^2) \right]
\]
\[
+ \frac{\hbar}{4m_2} (r_x D_x^2 + r_y D_y^2)
\]
\[
- \frac{\Delta t}{2\hbar} \left[ V_1(k_{s1}) + V_2(k_{s2}) \right]^{2p+1}
\]
\[
+ \frac{\hbar}{4m_1} (r_x D_x^2 + r_y D_y^2)
\]
\[
- \frac{\Delta t}{2\hbar} \left[ V_1(k_{s1}) + V_2(k_{s2}) \right]^{2p+1}
\]
\[
+ \frac{\hbar}{4m_2} (r_x D_x^2 + r_y D_y^2)
\]
\[
\psi^{|imag|}(k_{s1}, k_{s2}) = \psi^{|imag|}(k_{s1}, k_{s2})
\]
\[
- \frac{\hbar}{4m_1} (r_x D_x^2 + r_y D_y^2)
\]
\[
- \frac{\Delta t}{2\hbar} \left[ V_1(k_{s1}) + V_2(k_{s2}) \right]^{2p+1}
\]
\[
+ \frac{\hbar}{4m_2} (r_x D_x^2 + r_y D_y^2)
\]
\[
\psi^{|imag|}(k_{s1}, k_{s2}) = \psi^{|imag|}(k_{s1}, k_{s2})
\]
\[
- \frac{\hbar}{4m_1} (r_x D_x^2 + r_y D_y^2)
\]
\[
- \frac{\Delta t}{2\hbar} \left[ V_1(k_{s1}) + V_2(k_{s2}) \right]^{2p+1}
\]
\[
+ \frac{\hbar}{4m_2} (r_x D_x^2 + r_y D_y^2)
\]
\[
\psi^{|imag|}(k_{s1}, k_{s2}) = \psi^{|imag|}(k_{s1}, k_{s2})
\]
\[
- \frac{\hbar}{4m_1} (r_x D_x^2 + r_y D_y^2)
\]
\[
- \frac{\Delta t}{2\hbar} \left[ V_1(k_{s1}) + V_2(k_{s2}) \right]^{2p+1}
\]
\[
+ \frac{\hbar}{4m_2} (r_x D_x^2 + r_y D_y^2)
\]
\[
\psi^{|imag|}(k_{s1}, k_{s2}) = \psi^{|imag|}(k_{s1}, k_{s2})
\]
In this simulation, the lattice potential is increased gradually with an increment of $\Delta V = 1.0 \times 10^{-25}$ J for each time step $\Delta t$. The increment is continued from $t = 0$ to $t = 10^4 \Delta t$. After this, the lattice potential is increased in real time using Eq. (14) with an increment of $\Delta V = 1.0 \times 10^{-16}$ J for each time step $\Delta t$. This is continued from $t = 10^4 \Delta t$ to $t = 2.0 \times 10^4 \Delta t$. The solution was obtained using the FDTD-Q scheme with $\Delta t = 1.0 \times 10^{-16}$ s, which satisfies the stability criterion.

However, when $\Delta t = 1.0 \times 10^{-14}$ s, the lattice potential is increased gradually in imaginary time with an increment of $\Delta V = 1.0 \times 10^{-25}$ J for each time step $\Delta t$ from $t = 0$ to $t = 10^4 \Delta t$. After this, Eq. (14) is increased in real time with $\Delta V = 1.0 \times 10^{-22}$ J for each time step $\Delta t$ from $t = 10^4 \Delta t$ to $t = 2.0 \times 10^4 \Delta t$ and the FDTD-Q scheme produces a divergent solution as shown in Fig. 2. Here, the value of the probability density goes over 3.0 in the upper right-hand corner. This is because when $\Delta x^2 = 2.38 \times 10^{-17}$ [m$^2$] and $\Delta z^2 = 2.27 \times 10^{-17}$ [m$^2$], the stability criterion for the FDTD-Q scheme requires that $\Delta t \leq \frac{\sqrt{2}}{\pi} \left( \frac{1}{\Delta x} + \frac{1}{\Delta z} \right) 10^{\max_{k} k_1 k_2 |k_1 + k_2|} \leq 5.67 \times 10^{-15}$ [s].

On the other hand, Fig. 3 demonstrates that as the GFDTD-Q scheme in Eq. (14) with $\Delta t = 1.0 \times 10^{-18}$ s was employed, the solution is convergent and particles localize on both lattice sites with an equal phase which is the same as that shown in Fig. 1. When $\Delta t = 1.0 \times 10^{-14}$ s, for which the stability condition of the GFDTD-Q is satisfied with $\Delta t \leq \frac{\sqrt{2}}{\pi} \left( \frac{1}{\Delta x} + \frac{1}{\Delta z} \right) \max_{k} k_1 k_2 |k_1 + k_2| \leq 1.41429 \times 10^{-1} < 1$, the GFDTD-Q scheme produces a convergent solution as shown in Fig. 4.

Fig. 5 shows the probability density functions along the cross-section line from lower left corner to the upper right corner of the optical lattice domain, which were obtained using the original FDTD-Q scheme and the present GFDTD-Q scheme, respectively. It is clearly seen that when $\Delta t = 1.0 \times 10^{-14}$ s, the FDTD-Q produces a log of the probability density much greater than 1.0 within two steps, implying that the solution is divergent.

6. Conclusion

We have developed a fourth-order (GFDTD-Q) method for solving the time-dependent Schrödinger equation when applied to a two interacting particle system. This scheme can easily be generalized to any dimension and particle number. The solution is shown to be more convergent for the improved GFDTD-Q scheme than the FDTD-Q scheme. This was numerically demonstrated when we produced a convergent solution without having to utilize a large number of iterations, as required previously by the FDTD-Q scheme. A more relaxed condition for stability exists when central difference approximations are employed for spatial derivatives. Numerical results coincide with those obtained based on the theoretical analysis. Results indicate that a larger step size can be chosen in the computation. Since the GFDTD-Q scheme is explicit, the computational speed is very fast. In particular, when considering high $N$ (number of particles) in the $N$-body interacting Hamiltonian, the new scheme will demonstrate a great computational advantage when compared to the existing schemes.

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References
