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Application of Finite Difference Time Domain Method to Gross-Pitaevskii Equation

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Abstract. In this paper, the finite difference time domain (FDTD) method is applied to solve the Gross-Pitaevskii (GP) equation. A simple procedure to include the non-linear term of the GP equation in the FDTD algorithm is given and discussed. For validation of the FDTD method, ground state, excited state wavefunctions and energies are computed for various trap potentials and compared to results from other numerical methods. The FDTD method is shown to be suitable and accurate for solving the GP equation.

INTRODUCTION

A quantum system consists of identical bosonic particles trapped in a potential well is known as a Bose-Einstein condensate (BEC)[1]. At very low temperature, due their bosonic properties, the particles behave as a single particle and all of the particles have the same quantum ground state[1]. The properties of BEC system is governed by the Schrödinger equation with interacting potentials between particles. However, the Schrödinger equation for many body systems is hard to be solved. Instead of that, one generally uses the Hartree-Fock approximation and pseudopotential interaction model of the BEC system which then leads to the Gross-Pitaevskii (GP) equation [2][3].

The GP equation is a nonlinear partial differential equation and it does not have any analytical solutions. Various numerical methods used previously for solving the GP equation are, for examples, finite difference [4][5], split-step Crank-Nicolson [6]-[10] and Fourier spectral [11][12] methods. A numerical method known as the finite difference time domain (FDTD) method has been applied to obtain solutions of the Schrödinger equation for various systems [13]-[16]. In this paper, the FDTD method for a one dimensional GP equation is presented. Due to the simplicity in the numerical algorithm, the FDTD method can be further extended to two and three dimensions without significant problems.

This paper is organized as follows: the next section explains the theory of the FDTD method and how the GP equation can be solved numerically, then followed by results and discussions. The final section gives conclusions of our findings.

METHOD

The one-dimensional time-independent Gross-Pitakevskii equation is given by

$$\hat{H}\psi(x)=\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)+g\left|\psi(x)\right|^2\right]\psi(x)=E\psi(x) \tag{1}$$

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where the nonlinear parameter $g = 4\pi\hbar^2 a_S / m$ is dependent on the scattering length a_S and m is the mass of a boson particle. The wavefunction $\psi(x,t)$ must also satisfy a normalization condition, $\int |\psi(x,t)|^2 \, dx = N$, where N is the number of boson particles.

Following Sudiarta and Geldart[13], the ground state of GP equation can be obtained by simulating an evolution of the wavefunction $\psi(x,t)$ using a diffusion equation given by

$$\frac{\partial \psi(x,t)}{\partial t} = -\frac{1}{\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) + g|\psi(x,t)|^2 \right]\psi(x,t) \tag{2}$$

After a long enough of simulation time, the wavefunction decays and approaches to an unnormalized GP ground state wavefunction.

$$\lim_{t\to\infty} \psi(x,t) = A\psi_0(x) \tag{3}$$

with A is a very small multiplicative constant. This constant is not important and can be ignored because the wavefunction can be renormalized after the convergence of the ground state wavefunction has been reached.

The excited states are then obtained using a similar procedure as for obtaining the ground state with an additional condition such that the wavefunction $\psi(x,t)$ is orthogonal to lower energy wavefunctions. For simplicity in computation, the initial wavefunction to begin the simulation is taken to be the infinite square well wavefunctions as given as the following equation

$$\psi_k(x, t=0) = \sqrt{\frac{2}{L}} \sin\frac{k\pi x}{L} \tag{4}$$

For computation, units of the spatial and temporal variables are chosen such that $m = 1$ and $\hbar = 1$. Equation (2) becomes

$$\frac{\partial \psi(x,t)}{\partial t} = \left[\frac{1}{2}\frac{\partial^2}{\partial x^2} - V(x) - g|\psi(x,t)|^2 \right]\psi(x,t) \tag{5}$$

where $g = 4\pi a_S$.

To perform the simulation using Eq. (5), the finite difference time domain (FDTD) scheme is used. The spatial and temporal variables are descretized into grids using spatial and temporal intervals of Δx and Δt. For a numerical algorithm, a notation of $\psi^n(i) \equiv \psi(i\Delta x, n\Delta t)$ is used. Following a numerical derivation as in Sudiarta and Geldart[13], an iterative numerical equation used to evolve the wavefunction is

$$\psi^{n+1}(i) = a(i)\psi^n(i) + b(i)\left[\psi^n(i-1) - 2\psi^n(i) + \psi^n(i+1)\right] + c(i)\psi^n(i) \tag{6}$$

with the coefficients given by

$$a(i) = \left[1 - \tfrac{1}{2}\Delta t V(i)\right]\left[1 + \tfrac{1}{2}\Delta t V(i)\right]^{-1} \tag{7}$$

$$b(i) = \left[\frac{\Delta t}{2(\Delta x)^2}\right]\left[1 + \tfrac{1}{2}\Delta t V(i)\right]^{-1} \tag{8}$$

$$c(i) = \Delta t g \left|\phi^n(i)\right|^2 \left[1 + \tfrac{1}{2}\Delta t V(i)\right]^{-1} \tag{9}$$

and $\phi^n(i)$ is obtained from the wavefunction and normalized to the number of boson particles. In this case, $\phi^n(i)$ is given by

$$\phi^n(i) = \psi^n(i)\sqrt{N}\left[\Delta x \sum_i \left|\psi^n(i)\right|^2\right]^{-1/2} \tag{10}$$

In order to have a stable numerical iteration, the temporal interval Δt is chosen to satisfy the following stability conditions.

$$\left|\Delta t g \left|\phi^n(i)\right|^2 \left[1 + \tfrac{1}{2}\Delta t V(i)\right]^{-1}\right| < 1 \quad \text{and} \quad \left|\left[\frac{\Delta t}{2(\Delta x)^2}\right]\left[1 + \tfrac{1}{2}\Delta t V(i)\right]^{-1}\right| < 1 \tag{11}$$

The energy of the system is computed numerically from the wavefunction using trapezoidal integration formula as given by

$$E = \left[\sum_i \psi(i)\left[\hat{H}\psi(i)\right]\right]\left[\sum_i \left|\psi(i)\right|^2\right]^{-1} \tag{12}$$

For comparison of the FDTD results, the wave function for bosons in a potential trap using Thomas Fermi approximation is given by the following equation.

$$\psi(x) = \sqrt{\frac{E_0 - V(x)}{g}} \tag{13}$$

where E_0 is the ground state energy of the BEC system.

RESULT AND DISCUSSION

To verify our numerical FDTD method for the GP equation, three cases are considered which are: bosons in (1) a box potential, (2) a harmonic potential and (3) a linear gravitational potential. The linear trap is included in order to show that the FDTD method can be used for any potential well. To simplify computations and comparisons, for all results given in this paper the scattering length $a_S = 1$ is used. This means that the value of the nonlinear coefficient $g = 4\pi$.

Numerical results of eigen energies for N bosons in a one dimensional box potential are shown in Fig. 1. Three eigen wavefunctions for N = 10 for bosons in the 1D box potential and the harmonic potential are given in Fig. 2 and 3. The numerical energies are shown to be in good agreement with the results obtained from digitization of a figure in[4]. For the wavefunctions in Fig. 2 and 3 are qualitatively in agreement with results found in [4]. A quantitative comparison of our results with[4] for the wavefunctions are difficult to do due to different numerical parameters and different graphical presentation are used.

To show that the FDTD method produces accurate results, comparisons FDTD results with Thomas-Fermi (TF) wavefunctions are given in Fig. 4 and 5. The FDTD results are in agreement with the TF results.

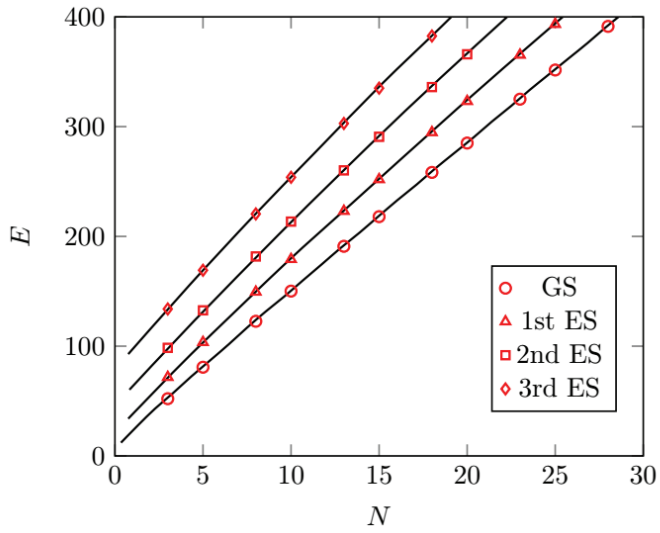

FIGURE 1. Eigen energies of the ground state (GS) and the first three excited states (ES) as a function of N particles in a one dimensional box potential with a side length of 1.0. The symbols for numerical FDTD results and the lines are obtained from digitization results of a figure in Ref. [4] using Engauge Digitizer [17]. The FDTD parameters used are $\Delta x = 0.1$, $\Delta t = (\Delta x)^2 / 10$, and the length of the computational domain is 1.0.

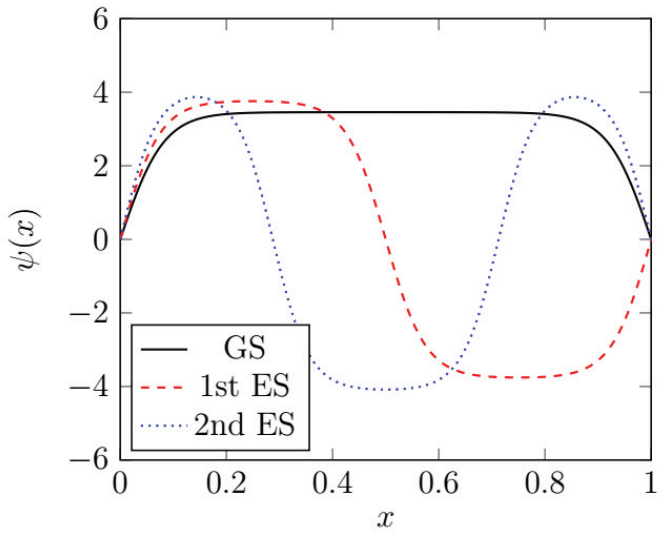

FIGURE 2. Wavefunctions for the ground state (GS), first and second excited states (ES) with $N = 10$ particles in a one dimensional box potential with a side length of 1.0. The FDTD parameters used are the same as in Fig.1.

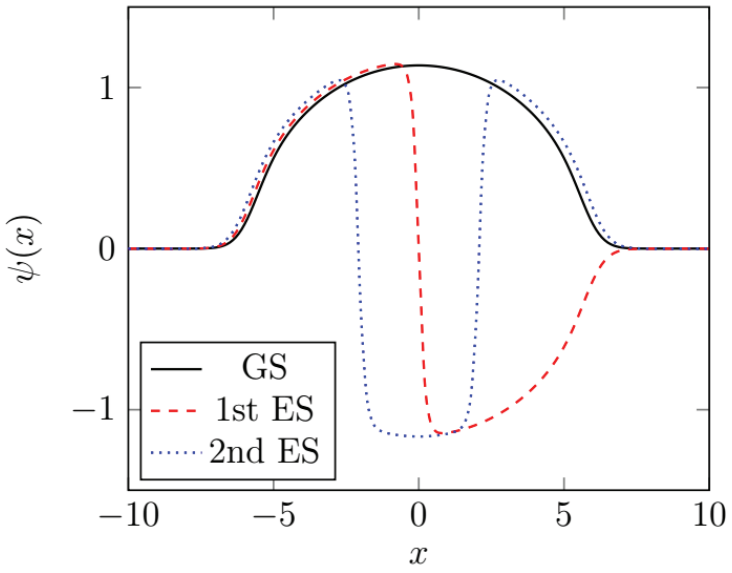

FIGURE 3. The ground state (GS) and the first two excited state (ES) wavefunctions for N = 10 bosons in a one dimensional harmonic potential $V(x) = \frac{1}{2}x^2$. The FDTD parameters are $\Delta x = 0.2$ and

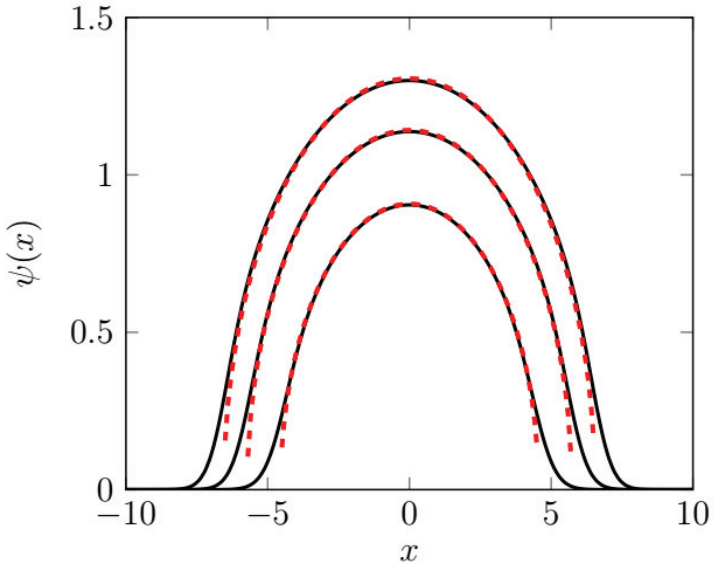

FIGURE 4. Ground state wavefunctions for N = 5, 10, 15 bosons (from bottom to top solid black curves) in a one dimensional harmonic potential $V(x) = \frac{1}{2}x^2$. Wave functions using the Thomas Fermi approximation are given by red dashed curves. The FDTD parameters used are $\Delta x = 0.2$, $\Delta t = (\Delta x)^2 / 20$, and the computational length is 20.

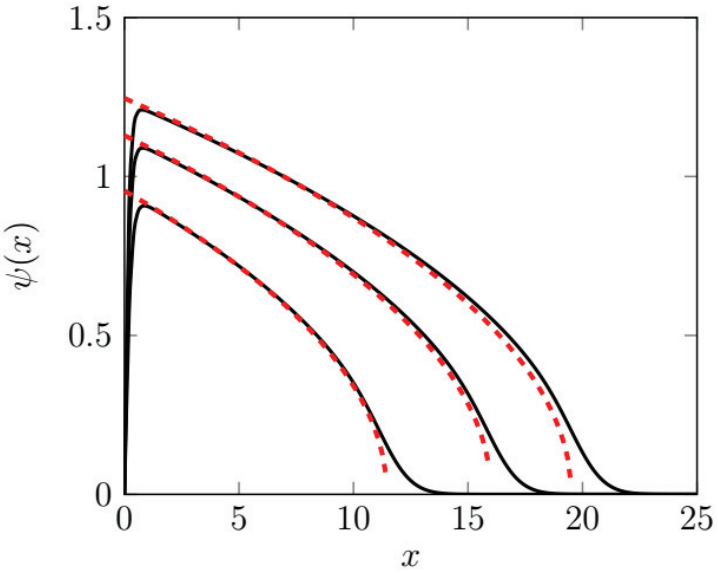

FIGURE 5. The same as in Fig. 4 except that this is for a linear potential given $V(x) = \mathrm{x}$ for $x > 0$ and $V(x) = \infty$ for $x \leq 0$. The FDTD parameters used are $\Delta x = 0.2$, $\Delta t = (\Delta x)^2 / 20$ and the computational length is 40.

CONCLUSION

The finite difference time domain (FDTD) method has been applied to determine eigen energies and wavefunctions of the Gross-Pitaevskii (GP) equation for three types of potentials. The numerical FDTD results are found to be in an good agreement with other results and Thomas-Fermi approximation. Due to the finite difference scheme is used, the numerical FDTD algorithm can be extended to be applied for two and three dimensional systems.

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