Bose-Einstein Condensation Dynamics from the Numerical Solution of the Gross-Pitaevskii Equation by the Pseudospectral Method

Paulsamy Muruganandam and Sadhan K. Adhikari

Abstract—We study certain stationary and time-evolution problems of trapped Bose-Einstein condensates of weakly interacting alkali atoms described by a nonlinear Gross-Pitaevskii (GP) equation. We suggest a pseudospectral method involving Laguerre polynomials to solve the time dependent GP for a spherically symmetric trap potential. The radial wavefunction and energy values have been calculated for different nonlinearities. Further, we study the effect of suddenly changing the interatomic scattering length or harmonic oscillator trap potential in the condensate. We also investigate the frequency of oscillation due to the variation in the strength of nonlinearity.

Keywords—Bose-Einstein condensation, Pseudospectral method

I. INTRODUCTION

The experimental realization of Bose-Einstein condensates (BECs) in dilute weakly-interacting trapped bosonic atoms at ultra-low temperature initiated intense theoretical effort to describe the properties of the condensate. The properties of a condensate at zero temperature are usually described by the time-dependent, nonlinear, mean-field Gross-Pitaevskii (GP) equation. The effect of the interatomic interaction (few-body correlation) leads to a nonlinear term in the GP equation which complicates the solution procedure. Although there have been previous studies of the solution of the GP equation for stationary or time-independent problems, virtually all time-dependent studies in realistic cases, e.g., in three space dimensions, have employed approximate approaches rather than exact numerical solution of the GP equation.

A numerical study of the time-dependent GP equation is of interest, as this can provide solution to many stationary and time-evolution problems. The time-independent GP equation yields only the solution of stationary problems. As our principal interest is in time evolution problems, we shall only consider the time-dependent GP equation in this paper.

Here we propose a pseudospectral time-iteration method for the solution of the three-dimensional GP equation with spherically symmetric trap. In the pseudospectral method the unknown wave function is expanded in terms interpolating polynomials. When this expansion is substituted into the GP equation, we get a set of coupled ordinary differential equations (ODEs) in time which is solved by a fourth-order adaptive step-size controlled Runge-Kutta method using successive time iteration. Reinhardt and Clark have employed pseudospectral methods for the solution of the GP equation, where a variable step forth order Runge-Kutta time propagator was used, as in the present work. A pseudospectral Fourier-sine basis was used for finite traps, and a corresponding complex pseudospectral basis was used for systems with periodic boundary conditions.

Such a pseudospectral method is used in [5] with Hermite polynomials as the interpolant for the case of completely anisotropic trap potential. However, when the system has radial or axial symmetry the three dimensional problem reduces to one or two dimensions. In such situations, it will be more advantageous to employ the integration in reduced dimensions as it saves considerable amount of computer memory and time. In this paper we considered the GP equation for spherically symmetric trap potential.

In section II, we describe briefly the three-dimensional, time-dependent GP equation with spherically symmetric trap. The pseudospectral method is described in section III. In section IV we report the numerical results for the wave function and energy for different nonlinearities as well as an account of our study on the effect of sudden changes in the interatomic scattering length or harmonic oscillator trap potential in the condensate. An analysis on the frequency of oscillation with respect to variation of the strength of nonlinearity is also reported. Finally, in section V we present our conclusions.

II. NONLINEAR GROSS-PITADEVSKII EQUATION

At zero temperature, the time-dependent Bose-Einstein condensate wave function \( \Psi(r; \tau) \) at position \( r \) and time \( \tau \) may be described by the following mean-field nonlinear GP equation

\[
-\frac{\hbar^2 \nabla^2}{2m} + V(r) + gN_0|\Psi(r; \tau)|^2 - i\hbar \frac{\partial}{\partial \tau} \Psi(r; \tau) = 0.
\]

Here \( m \) is the mass and \( N_0 \) the number of atoms in the condensate, \( g = 4\pi\hbar^2 a/m \) the strength of interatomic interaction, with \( a \) the atomic scattering length. The normalization condition of the wave function is \( \int d^3r |\Psi(r; \tau)|^2 = 1 \).

The three-dimensional trap potential is given by \( V(r) = \frac{1}{2}m(\omega_x^2x^2 + \omega_y^2y^2 + \omega_z^2z^2) \), where \( \omega_x \equiv \omega_0, \omega_y \), and \( \omega_z \) are the angular frequencies in the \( x, y \) and \( z \) directions, respectively, and \( r \equiv (x, y, z) \) is the radial vector.

A. Spherically Symmetric Case

In the spherically symmetric trap, i.e., \( \omega_x = \omega_y = \omega_z \equiv \omega_0 \) the trap potential is given by \( V(r) = \frac{1}{2}m\omega_0^2r^2 \), where \( \omega_0 \) is the harmonic oscillator frequency.
the angular frequency and \( \hat{r} \) the radial distance. The wave function can be written as \( \Psi(r; \tau) = \psi(\hat{r}, \tau) \). After a transformation of variables to dimensionless quantities defined by \( r = \sqrt{2r/l}, t = \tau \omega_0, l \equiv \sqrt{(h/m \omega_0)} \) and \( \phi(r, t) \equiv \varphi(r, t)/r = \psi(\hat{r}, \tau)(4\pi l^3)^{1/2} \), the GP equation in this case becomes

\[
\left[ -\frac{\partial^2}{\partial r^2} + \frac{r^2}{4} + N \left( \frac{\varphi(r, t)}{r} \right)^2 - i \frac{\partial}{\partial t} \right] \varphi(r, t) = 0, \tag{2}
\]

where \( N = N_0 a/l \). The normalization condition for the wave function is

\[
\int_0^\infty |\varphi(r, t)|^2 \, dr = 2\sqrt{2}. \tag{3}
\]

III. Pseudospectral Runge-Kutta (PSRK) method

The main idea of this method is that the spatial differentiation operators in equation \( (2) \) are replaced by appropriate differential matrices which are derived from spectral or pseudospectral collocation. Then the time integration is carried out by any ordinary differential equation (ODE) solver.

In the pseudospectral approximation, an unknown function \( f(x) \) is expanded in terms of weighted interpolants of the form \( \{x_j\}_{j=0}^n \),

\[
f(x) \approx p_n(x) = \sum_{j=0}^n \frac{\alpha(x)}{\alpha(x_j)} \xi_j(x)f_j. \tag{4}
\]

Here \( \{x_j\}_{j=0}^n \) is a set of distinct interpolation nodes, \( f_j = f(x_j) \), \( \alpha(x) \) is a weight function, the interpolating functions \( \{\xi_j(x)\}_{j=0}^n \) satisfy \( \xi_k(x_k) = \delta_{jk} \) (the Kronecker delta) and involve orthogonal polynomials of degree \( n \), so that \( f(x_k) = p_n(x_k) \), \( k = 0, 1, \ldots, n \). One could use orthogonal polynomials such as, Chebyshev, Hermite, Laguerre and Legendre as the interpolant. Even non-polynomial interpolants like Fourier (spectral) expansion of the function in terms of periodic cosine and sine functions can be used in the case of periodic boundary. The choice of interpolant depends on the domain and nature of boundary conditions.

Differentiating \( m \) times, the \( m \)th derivative of \( f(x) \) at the nodes is given by,

\[
f^{(m)}(x) \approx \sum_{j=0}^n \frac{d^m}{dx^m} \left[ \frac{\alpha(x)}{\alpha(x_j)} \xi_j(x) \right]_{x=x_k} f_j, \tag{5}
\]

with \( k = 1, \ldots, n \). Here the derivative operator is represented by \( D^{(m)} \) which is the differentiation matrix with elements,

\[
D^{(m)}_{k,j} = \frac{d^m}{dx^m} \left[ \frac{\alpha(x)}{\alpha(x_j)} \xi_j(x) \right]_{x=x_k}. \tag{6}
\]

Thus, the numerical differentiation of the function \( f(x) \), \( f^{(m)} = D^{(m)} f \) is performed as the matrix-vector product where \( f \) and \( f^{(m)} \) are the vectors of the function and its derivative values evaluated at the nodes.

In the present work we consider Laguerre polynomials \( L_n(x) \) as the interpolating functions with the weight function \( \alpha(x) = e^{-\frac{\hat{r}^2}{2}} \). The reason behind the choice of Laguerre polynomials is that they are well defined in the interval \( x \in [0, \infty) \) and satisfy the boundary conditions of the wave function of the GP equation \( (7) \). The choice \( x = \hat{r}^2 \) gives exact eigenfunctions of the GP equation \( (2) \) when the nonlinearity term \( N = 0 \). Actually, the associated Laguerre polynomials are more appropriate as they are the radial eigenfunctions of linearized GP equations. However, from a numerical point of view the use of both of the polynomials yield more or less the same result. Also it has not been known whether there is a significant advantage of improvement in the results by considering associated Laguerre polynomials \( (2) \).

Consequently, the partial differential equation \( (2) \) is reduced to a set of coupled ODEs in the time variable \( t \) involving \( \xi_j, j = 0, 1, \ldots, n \). In this way we obtain a set of ODEs by collocating the original equations on a suitable set of points (the roots of some Laguerre polynomials).

For solving the set of ODEs we use the adaptive step-size control based on the embedded Runge-Kutta formulas due to Fehlberg \( (3) \), which gives a definite clue about how to modify the step size in order to achieve a desired accuracy in a controlled way. For orders \( M \) higher than four of the Runge-Kutta formula, evaluation of more than \( M \) functions (though never more than \( M + 2 \)) is required. This makes the classic fourth order method requiring the evaluation of four functions more economic. Fehlberg suggested a fourth-order and a fifth-order method each requiring the evaluation of six functions. The difference between the results of these two gives the error \( \delta \) in the fourth-order method with a step size \( h \), where \( \delta \) scales as \( h^5 : \delta \propto h^5 \). This scaling immediately gives the factor by which the step size \( h \) should be reduced, so that a desired \( \delta \) can be obtained. The detailed fourth-order and fifth-order Runge-Kutta formulas of Fehlberg are given in \( (3) \). We use these formulas with the constants given by Cash and Karp also tabulated in \( (3) \). For the present problem we find that the use of Cash-Karp constants in the Fehlberg formulas leads to more accurate results than the original constants due to Fehlberg.

Using the differentiation matrix \( (6) \), the GP equation is discretized. The grid points are the roots of the Laguerre polynomial \( L_n(x_j) = 0 \). However, the actual \( x_j \) values employed are obtained by scaling these roots by a constant factor so that most of the roots fall in the region where the condensate wave function is sizable and only a few points are located in the region where the wave function is negligible. In the present paper, all the numerical simulations have been carried out with \( n = 31 \) grid points.

IV. Numerical simulation

A. Wavefunction and energy

Once the GP equation \( (3) \) is reduced to a set of coupled ODEs, the time integration is carried out with an initial seed wavefunction. We use the solution corresponding to the linearized GP equation as the seed. The final wavefunction is obtained by adding the nonlinear terms in small steps until the desired nonlinearity is achieved. Then the stationary wave function \( \phi \) and the parametric energy \( \mu \) (the chemical potential) can be extracted from the evolution of the time-dependent GP equation over a macroscopic interval of time \( (8) \).

First, we are interested to calculate the wavefunction and energy.
ergy with different nonlinearity strengths. For this purpose, we numerically integrate equation (2) with the following normalized analytic solution,

\[ \phi(r) = \left( \frac{2}{\pi^2} \right) r \exp \left( -\frac{r^2}{4} \right). \]  

(7)

The above \( \phi(r) \) corresponds to the ground state of (2) for spherical symmetry with the coefficient of the nonlinear term set to zero. During the integration the coefficient of the nonlinear term is increased from 0 at each step by \( \delta_\alpha = 0.001 \) until the final value of nonlinearity \( N \) is attained at a time called time \( t = 0 \). This corresponds to the final solution and this solution is found to be stable. The norm of the wavefunction is conserved during the integration. However, it is of advantage to reinforce numerically the proper normalization of the wave function given by (3) after finite number of RK steps in order to improve the precision of the result. As the grid points are the corresponding Laguerre roots, the integral in (3) can easily be evaluated by appropriate Gauss-Laguerre formula. Figure 1 depicts the radial wavefunction of the condensate for different nonlinearity strengths. The stationary wavefunction has trivial time dependence \( \phi(r, t) = \phi(r) \exp(-i\mu t) \). Thus, the parametric energy \( \mu \) (chemical potential) can be extracted from the evolution of the GP equation over a macroscopic interval of time. In Table I we present the chemical potential of several BECs with different number of atoms for the spherically symmetric trap potential. The typical value of the harmonic trap frequency is \( \omega_0 = 87 \text{ rad/s} \) and scattering length is \( a = 52 a_0 \) (for Na) where \( a \) is the Bohr radius. The energy values calculated here for different nonlinearity strengths are compared reasonably well with the results of Schneider and Feder by time-independent approach.

B. Time evolution

Next we consider certain time-evolution problems which can be tackled more effectively with the present pseudospectral method. From the experimental point of view, it is of great interest to study the effects of changing (i) the trap potential and (ii) the atomic scattering length. The former can be achieved in the laboratory by changing the magnetic field responsible for trapping while it has been possible to modify the scattering length in a controlled fashion by exploiting a Feshbach resonance. In this paper we restrict ourselves to the study on the effect of suddenly changing both the trap potential as well as the atomic scattering length.

B.1 Effect of changing trap potential and scattering length

As said above, one can increase or reduce suddenly the strength of the nonlinear term through a change of the scattering length in this fashion and study the oscillation of the condensate thereafter. In both these cases one observes the time evolution of the root mean square (rms) radius \( \langle r \rangle_{\text{rms}} \) of the condensate. For the time evolution study we consider a previously formed condensate with finite number of atoms, for example, \( N_0 = 16384 \) prepared at \( t = 0 \) as in the study of the stationary problem. We then inflict the four following changes in the system. At \( t = 0 \) we (a) increase or (b) decrease suddenly the coefficient of the harmonic oscillator \( r^2/4 \) term in (2) by a factor of 2. Next at \( t = 0 \) we (c) increase or (d) decrease suddenly the coefficient of the nonlinear term \( N \) in (2) by a factor of 2.

When the harmonic oscillator term is doubled or the nonlinearity halved, the system is compressed and the rms radius oscillates between its initial value and a smaller final value. When the harmonic oscillator term is halved or the nonlinearity doubled, the system expands and the rms radius oscillates between its initial value and a larger final value.

We have calculated the frequency of oscillation of the rms radius in all the four cases considered above. These frequencies are calculated as, for the (a), (b), (c), and (d) cases above, 0.4834, 0.2441, 0.3467, and 0.3418, (in units of \( \omega_0^{-1} \)) respectively. Here the time is measured in units of \( \omega_0^{-1} = 1 \) and hence the trap frequency corresponding to (2) is \( \nu_0 = 1/(2\pi) \). The frequency of oscillation was two times the existing harmonic oscillator frequency for nonlinearity \( N = 0 \). As the frequencies are increased and reduced by \( \sqrt{2} \) in cases (a) and (b), two times the existing frequency for (a) is \( 2\nu = \sqrt{2}/\pi \approx 0.45 \) and for (b) is \( 2\nu = 1/(\sqrt{2}\pi) \approx 0.23 \). In case of (c) and (d) the frequency is unchanged and \( 2\nu = 1/\pi \approx 0.32 \). These numbers compare well with the respective above results.

We also found that these frequencies are in good agreement with those calculated using finite difference scheme. There are differences when comparing these frequencies with the corresponding harmonic trap frequencies, the reason for which is due to the presence of nonlinearity in the system. We study the

![Figure 1](image-url)

**Figure 1**

**Figure showing the radial wavefunctions of the condensate for different number of atoms** \( N_0 = 2^q \).

| \( N_0 \) | \( N \) | \( \mu \) | \( N_0 \) | \( N \) | \( \mu \) |
|---|---|---|---|---|---|
| 1024 | 0.50 | 1.824 | 2048 | 1.00 | 2.065 |
| 4096 | 1.98 | 2.429 | 8192 | 3.97 | 2.969 |
| 16384 | 7.93 | 3.722 | 32768 | 15.86 | 5.748 |
| 65536 | 31.72 | 6.155 | 131072 | 63.44 | 8.041 |


frequency of oscillation as a function of nonlinearity in the following.

B.2 Frequency of oscillation of the condensate

Having studied various time independent as well as time dependent problems, we further investigate the frequency of oscillation of the condensate due to a variation of nonlinearity. When the nonlinear term is added in sufficiently large steps during the preparation of the condensate numerically, a breathing type oscillation with some frequency, $\nu$ occurs which is determined solely by the final nonlinearity. This frequency can be extracted by exploiting the Fourier transform on the time series of the mean distance, $\langle r \rangle_{\text{rms}}$ from numerical simulation. We express the final nonlinearity in terms of the final value of $N_0$.

We found that the frequency of oscillation increases as the final number of atoms is increased and it saturate to a final value $0.354$ when $N_0 > 2^{16} \approx 7 \times 10^4$. Figure 2 shows the frequency of oscillation $\nu$ as a function of nonlinearity in the condensate. By fitting the numerical data for the frequencies, the frequency of oscillation as a function of final $N_0$ can be represented by the following relation,

$$\nu(N_0) = \nu_0 + \frac{1}{b} \exp \left( -\frac{1}{c} N_0 \right).$$

The parameters are calculated as $\nu_0 = 0.3536$, $b = -28.6858$, $c = 227.26$ and $\gamma = 0.6202$.

V. SUMMARY AND CONCLUSIONS

We propose the use of pseudospectral method to solve time dependent nonlinear Gross-Pitaevskii equation describing Bose-Einstein condensation in spherically symmetric trap potential. In particular, we emphasize on the advantages of using Laguerre polynomial interpolation for the spatial differentiation operator and we study both stationary as well as time evolution problems. In the stationary problem, the radial wavefunction and the ground state energy are calculated by solving the GP equation for different nonlinearity strengths which determines the number of atoms in the condensate. We noted that the energy values are calculated more accurately with very few number of discretization points (nodes). For the time evolution problem, first we study the effect of sudden changes in the interatomic scattering length or harmonic oscillator trap potential in the condensate. We have also made an analysis on the variation of frequency of oscillation as a function of the strength of nonlinearity.

This paper summarizes our attempts to understand certain dynamical aspects of Bose-Einstein condensation as a nonlinear dynamical system. We found that the present approach based on pseudospectral differentiation matrices for solving Gross-Pitaevskii equation is more effective when compared to finite-difference schemes. Though, we are solving the problem effectively in one-dimension because of the spherically symmetric trap, the anisotropic problems can be easily tackled with similar approach [5].

ACKNOWLEDGMENTS

The work of PM is supported by DST, Govt. of India and SKA acknowledges CNPq of Brasil.

REFERENCES

[1] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, “Theory of Bose-Einstein condensation in trapped gases,” Rev. Mod. Phys., vol. 71, pp. 463, 1999.
[2] J. A. C. Weideman and S. C. Reddy, “A Matlab Differentiation Matrix Suite,” ACM Transactions on Math Software, vol. 26, pp. 465, 2000.
[3] W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, Numerical Recipes in Fortran 77: The Art of Scientific Computing, Cambridge University Press, Cambridge, 1993.
[4] W. P. Reinhardt and C. W. Clark, “Soliton dynamics in the collisions of Bose-Einstein condensates: an analogue of the Josephson effect,” J. Phys. B: At. Mol. Opt. Phys., vol. 30, pp. L785, 1997.
[5] P. Muruganandam and S. K. Adhikari, “Bose-Einstein condensation dynamics in three dimensions by the pseudospectral and finite-difference methods,” J. Phys. B: At. Mol. Opt. Phys., vol. 36, no. 12, pp. 2501, 2003.
[6] B. Fornberg, A Practical Guide to Pseudospectral Methods, Cambridge University Press, Cambridge, 1996.
[7] M. Edwards and K. Burnett, “Numerical solution of the nonlinear Schrödinger equation for small samples of trapped neutral atoms,” Phys. Rev. A, vol. 51, pp. 4704, 1995.
[8] S. K. Adhikari, “Numerical study of the coupled time-dependent Gross-Pitaevskii equation: Application to Bose-Einstein condensation,” Phys. Rev. E, vol. 65, pp. 056704, 2001.
[9] B. L. Schneider and D. L. Feder, “Numerical approach to the ground and excited state of a Bose-Einstein condensed gas confined in a completely anisotropic trap,” Phys. Rev. A, vol. 59, pp. 2232, 1999.
[10] S. Inouye, M. R. Andrews, J. Stenger, H.-J. Miesner, D. M. Stamper-Kurn, and W. Ketterle, “Observation of Feshbach resonances in a Bose-Einstein condensate,” Nature, vol. 392, pp. 151, Mar. 1998.
[11] S. K. Adhikari and P. Muruganandam, “Bose-Einstein condensation dynamics from the numerical solution of the Gross-Pitaevskii equation,” J. Phys. B: At. Mol. Opt. Phys., vol. 35, no. 12, pp. 2831, 2002.