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The numerical method for computing the ground state of the two-component dipolar Bose-Einstein condensate

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Abstract

A two-component Bose-Einstein condensate described by two coupled Gross-Pitaevskii (GP) equations in three dimensions is considered, where one equation has dipole-dipole interactions while the other one has only the usual s -wave contact interaction, in a harmonic trap. The singularity in the dipole-dipole interactions brings significant difficulties both in mathematical analysis and in numerical simulations. The backward Euler method in time and the sine spectral method in space are proposed to compute the ground states. Numerical results are given to show the efficiency of this method.

Keywords: Bose-Einstein condensate; Gross-Pitaevskii equation; dipolar interaction; ground state; spectral method

1 Introduction

Since 1995, the Bose-Einstein condensation (BEC) of ultra-cold atomic and molecular gases has attracted much attention both theoretically and experimentally. Most of the properties of these trapped quantum gases are governed by the interactions between particles in the condensate [1]. Over the past decade, there has been an investigation for realizing a new kind of quantum gases with the dipolar interaction, acting between particles having a permanent magnetic or electric dipole moment. The experimental realization of a BEC of ^{52}Cr atoms [2, 3] at the University of Stuttgart in 2005 gave new impetus to the theoretical and numerical investigations on these novel dipolar quantum gases at low temperature. Recently more detailed and controlled experimental results have been obtained, illustrating the effects of phase separation in a multi-component BEC [4–6]. In these papers, the studies of the binary condensates were limited to the case of s -wave interactions, while recently the dipolar BEC has drawn a great deal of attention.

In this work, a numerical method for computing the ground state of the two-component dipolar BEC is considered, where one equation has dipole-dipole interactions and the other has only the usual s -wave contact interaction. However, since the dipole-dipole interactions are long range, anisotropic and partially attractive, and the computational cost in three dimensions is high, the nontrivial task of achieving and controlling the dipolar BEC is thus particularly challenging.

The two-component dipolar BEC, confined in a cylindrical trap, is described by two coupled Gross-Pitaevskii equations. As far as the dipolar interaction is concerned, a con-

volution term is introduced [7–9] to modify the classical Gross-Pitaevskii equation, which results in the following differential-integral equations (1). Since the transition metal has a magnetic dipole interaction while the alkali metal has not, we take into account this factor in this system. We take Cr as component 1 and Rb as component 2 [10]. Then the GP equations for this system can be written as

$$\begin{cases} i\hbar \frac{\partial \varphi_1(\vec{r}, t)}{\partial t} = [-\frac{\hbar^2}{2m_1} \nabla^2 + V_1 + U_1|\varphi_1|^2 + U_{12}|\varphi_2|^2 + V_{\text{dip}}^*|\varphi_1|^2]\varphi_1, \\ i\hbar \frac{\partial \varphi_2(\vec{r}, t)}{\partial t} = [-\frac{\hbar^2}{2m_2} \nabla^2 + V_2 + U_2|\varphi_2|^2 + U_{12}|\varphi_1|^2]\varphi_2, \end{cases} \quad (1)$$

where φ_1, φ_2 are the wave functions of component 1 and 2, respectively. The inter-atomic and inter-component s -wave scattering interactions are described by U_j ($j = 1, 2$) and U_{12} , respectively, with the following expressions [11]:

$$U_j = \frac{4\pi \hbar^2 a_j}{m_j}, \quad U_{12} = \frac{2\pi \hbar^2 a_{12}}{m_1 m_2 / (m_1 + m_2)} \quad (j = 1, 2),$$

where a_j is the scattering length of component j and a_{12} is that between component 1 and 2. Here \hbar is the Planck constant, m_j is the mass of the atom of component j , and V_j ($j = 1, 2$) is the external trapping potential confining the gas. Generally, it is harmonic, that is, $V_j(\vec{r}) = \frac{m_j}{2}(\omega_{jx}^2 x^2 + \omega_{jy}^2 y^2 + \omega_{jz}^2 z^2)$ with ω_{jp} ($p = x, y, z$) represents the trap frequency in x, y, z directions, respectively. The local mean-field $U_j|\varphi_j|^2$ represents the s -wave interaction. V_{dip} is the long-range isotropic dipolar interaction potential between two dipoles, and it is defined by

$$V_{\text{dip}} = \frac{\mu_0 \mu_{\text{dip}}^2}{4\pi} \cdot \frac{1 - 3(\vec{r} \cdot \vec{n})^2 / |\vec{r}|^2}{|\vec{r}|^3} = \frac{\mu_0 \mu_{\text{dip}}^2}{4\pi} \cdot \frac{1 - 3 \cos^2 \theta}{|\vec{r}|^3},$$

where θ is the angle between the polarization axis \vec{n} and the relative of two atoms (*i.e.*, $\cos \theta = \vec{n} \cdot \vec{r}/r$, $r = |\vec{r}| = \sqrt{x^2 + y^2 + z^2}$). The wave function $\varphi_i(x, t)$ is normalized according to $\|\varphi_i\|^2 = \int_{R^3} |\varphi_i(\vec{r}, t)|^2 d\vec{r} = N_i$ ($i = 1, 2$), where N_i is the number of the atoms in the dipolar BEC.

This paper is organized as follows. In Section 2, a numerical method for computing ground states is presented. In Section 3, numerical results are reported to verify the efficiency of this numerical method. Finally, some concluding remarks are drawn in Section 4.

2 Numerical method for computing the ground states

System (1) can be made dimensionless and simplified by adopting a unit system, where the units for length, time and energy are given by $a_0, 1/\omega_0$, and $\hbar\omega_0$, respectively, with $a_0 = \sqrt{\frac{\hbar}{m_1\omega_0}}$, $\omega_0 = \min\{\omega_{jx}, \omega_{jy}, \omega_{jz}\}$ [12]. By introducing the dimensionless variables $t' = \frac{t}{\omega_0}$, $\vec{r}' = \vec{r}/a_0$, $\varphi'_j = a_0^{3/2}\varphi_j$, we obtain the dimensionless GP equations in 3D from (1) as follows:

$$\begin{cases} i \frac{\partial \varphi'_1}{\partial t'} = [-\frac{1}{2} \nabla'^2 + V'_1 + \beta_{11}|\varphi'_1|^2 + \beta_{12}|\varphi'_2|^2 + \lambda(V_{\text{dip}}^*|\varphi'_1|^2)]\varphi'_1, \\ i \frac{\partial \varphi'_2}{\partial t'} = [-\frac{1}{2} \nabla'^2 + a_m V'_2 + \beta_{21}|\varphi'_1|^2 + \beta_{22}|\varphi'_2|^2]\varphi'_2, \end{cases} \quad (2)$$

where $\beta_{11} = 4\pi a_1 N_1$, $\beta_{12} = \frac{1+a_m}{a_m} 2\pi a_{12} N_2$, $\beta_{21} = \frac{1+a_m}{a_m} 2\pi a_{12} N_1$, $\beta_{22} = \frac{4\pi a_2}{a_m} N_2$, $a_m = \frac{m_2}{m_1}$, $\lambda = \frac{m_1 N_1 \mu_0 \mu_{\text{dip}}^2}{3\hbar^2 a_0}$, $V_{\text{dip}} = \frac{3}{4\pi} \cdot \frac{1-3\cos^2 \theta}{r^3}$. In addition the wave functions in (2) satisfy $\int_{R^3} |\varphi'_1|^2 = 1$,

$\int_{R^3} |\varphi_2'|^2 = 1$. By using the following formula [13]

$$\frac{1}{r^3} \left(1 - \frac{3(\vec{n} \cdot \vec{r})^2}{r^2} \right) = -\frac{3}{4\pi} \delta(\vec{r}) - \partial_{nm} \left(\frac{1}{r} \right), \tag{3}$$

where $\delta(\vec{r})$ is the Dirac delta function and $\partial_{nm} = \vec{n} \cdot \nabla(\vec{n} \cdot \nabla)$, we can get

$$V_{\text{dip}}^* |\varphi_1'|^2 = -|\varphi_1'|^2 - 3\partial_{nm}(\xi), \tag{4}$$

where

$$\xi(\vec{r}, t) = \frac{1}{4\pi} \int_{R^3} \frac{1}{|\vec{r} - \vec{r}'|} \cdot |\varphi_1'(\vec{r}', t)|^2 d\vec{r}'. \tag{5}$$

And it is easy to see

$$\nabla^2 \xi = -|\varphi_1'(\vec{r}, t)|^2. \tag{6}$$

Plugging (4) into (2) and noticing (5) and (6), we can reformulate GPE (2) into the Schrödinger-Poisson type system

$$\begin{cases} i \frac{\partial \varphi_1}{\partial t} = [-\frac{1}{2} \nabla^2 + V_1 + (\beta_{11} - \lambda)|\varphi_1|^2 + \beta_{12}|\varphi_2|^2 - 3\lambda\partial_{nm}(\xi)]\varphi_1, \\ i \frac{\partial \varphi_2}{\partial t} = [-\frac{1}{2} \nabla^2 + V_2 + \beta_{21}|\varphi_1|^2 + \beta_{22}|\varphi_2|^2]\varphi_2, \\ \nabla^2 \xi = -|\varphi_1(\vec{r}, t)|^2, \end{cases}$$

by removing the symbol “’” in (2)-(6) to simplify the denotation. In practical computation, the whole space problem is usually truncated into a bounded computational domain $\Omega = [a, b] \times [c, d] \times [e, f]$ with the homogeneous Dirichlet boundary condition. Let

$$\begin{aligned} \Omega_{MKL} &= \{(j, k, l) | j = 1, 2, \dots, M-1, k = 1, 2, \dots, K-1, l = 1, 2, \dots, L-1\}, \\ \Omega_{MKL}^0 &= \{(j, k, l) | j = 0, 1, \dots, M, k = 0, 1, \dots, K, l = 0, 1, \dots, L\}. \end{aligned}$$

Choose the spatial mesh size as $h_x = \frac{b-a}{M}$, $h_y = \frac{d-c}{K}$, $h_z = \frac{f-e}{L}$, and define $x_j = a + jh_x$, $y_k = c + kh_y$, $z_l = e + lh_z$, $(j, k, l) \in \Omega_{MKL}^0$. Then denote the space $Y_{MKL} = \text{span}\{\phi_{pqs}(\vec{r}), (p, q, s) \in \Omega_{MKL}\}$ with

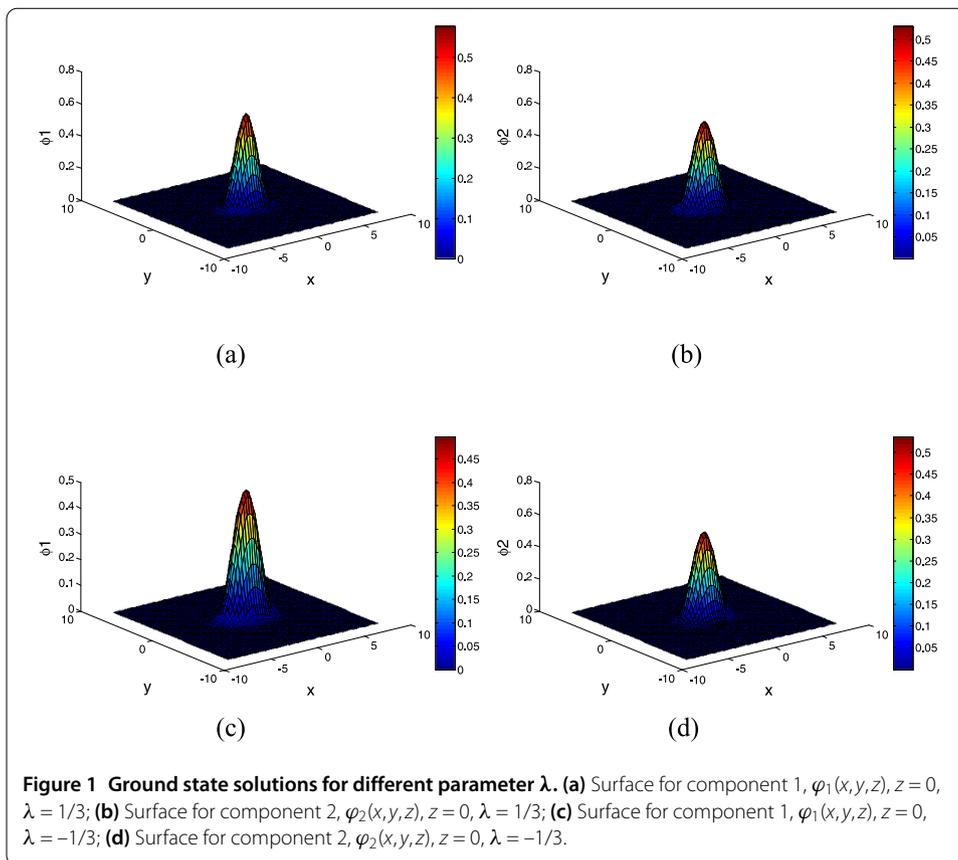
$$\phi_{pqs}(r) = \sin(u_p(x-a)) \sin(u_q(y-c)) \sin(u_s(z-e)),$$

where $u_p = \frac{p\pi}{b-a}$, $u_q = \frac{q\pi}{d-c}$, $u_s = \frac{s\pi}{f-e}$.

To compute the ground state, an imaginary time method is adopted [14]. That is,

$$\begin{cases} \frac{\partial \varphi_1}{\partial t} = [\frac{1}{2} \nabla^2 - V_1 - (\beta_{11} - \lambda)|\varphi_1|^2 - \beta_{12}|\varphi_2|^2 + 3\lambda\partial_{nm}(\xi)]\varphi_1, \\ \frac{\partial \varphi_2}{\partial t} = [\frac{1}{2} \nabla^2 - V_2 - \beta_{21}|\varphi_1|^2 - \beta_{22}|\varphi_2|^2]\varphi_2, \\ \nabla^2 \xi = -|\varphi_1(\vec{r}, t)|^2. \end{cases}$$

We use the backward Euler method for time discretization and the sine-pseudospectral method for spatial derivatives. Then we obtain the following equations in a three-



dimensional space. If we assume that

$$\begin{aligned} \varphi_1(r, t_{n+1}) &= \varphi_1^{n+1}(r) = \sum_{p=1}^{M-1} \sum_{q=1}^{K-1} \sum_{s=1}^{L-1} \alpha_{pqs} \phi_{pqs} \quad \text{and} \\ \varphi_2(r, t_{n+1}) &= \varphi_2^{n+1}(r) = \sum_{p=1}^{M-1} \sum_{q=1}^{K-1} \sum_{s=1}^{L-1} \alpha'_{pqs} \phi_{pqs}. \end{aligned}$$

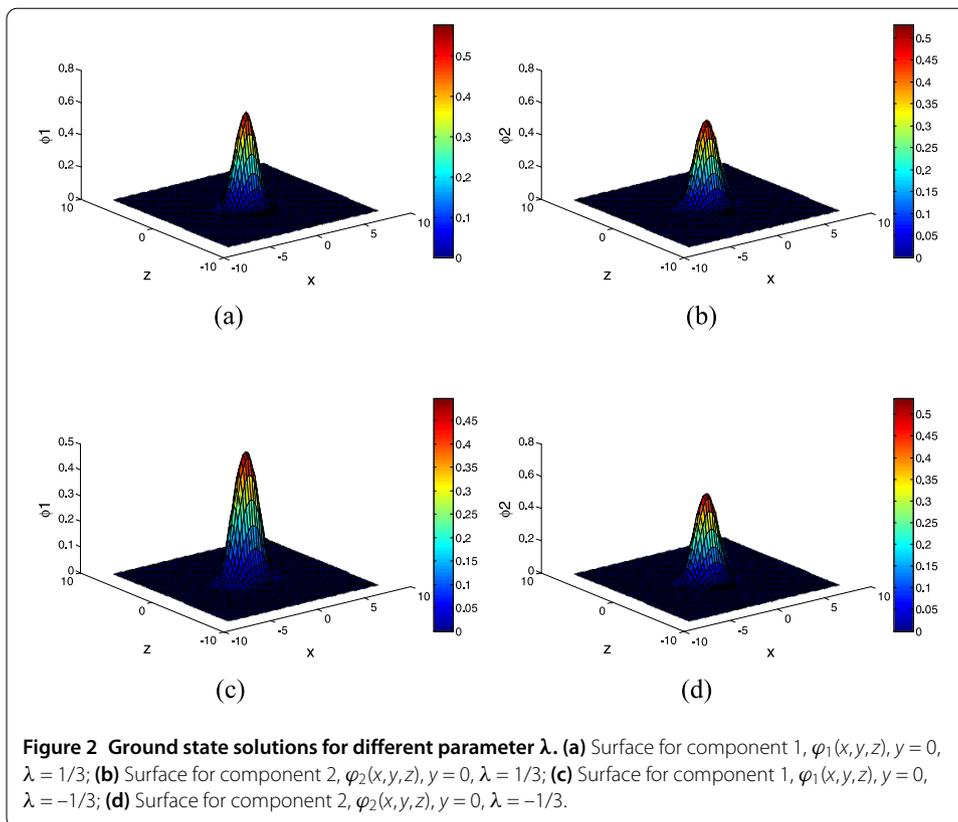
$$\begin{cases} \frac{\varphi_{1jkl}^* - \varphi_{1jkl}^n}{\Delta t} = \frac{1}{2} \nabla_h^2 \varphi_{1jkl}^* - [V(x_j, y_k, z_l) + (\beta_{11} - \lambda) |\varphi_{1jkl}^n|^2 \\ \quad + \beta_{12} |\varphi_{2jkl}^n|^2 - 3\lambda \partial_{nn} \xi^n |_{jkl}] \varphi_{1jkl}^* \\ \frac{\varphi_{2jkl}^* - \varphi_{2jkl}^n}{\Delta t} = \frac{1}{2} \nabla_h^2 \varphi_{2jkl}^* - [V(x_j, y_k, z_l) \\ \quad + \beta_{21} |\varphi_{2jkl}^n|^2 + \beta_{22} |\varphi_{1jkl}^n|^2] \varphi_{2jkl}^* \\ \nabla^2 \xi = -|\varphi_1(\vec{r}, t)|^2, \end{cases} \quad t_n \leq t \leq t_{n+1}, \quad (7)$$

with boundary conditions

$$\begin{aligned} \varphi_{10kl}^* &= \varphi_{1Mkl}^* = \varphi_{1j0l}^* = \varphi_{1jkl}^* = \varphi_{1jk0}^* = \varphi_{1jkl}^* = 0, \quad (j, k, l) \in \Omega_{MKL}^0, \\ \varphi_{20kl}^* &= \varphi_{2Mkl}^* = \varphi_{2j0l}^* = \varphi_{2jkl}^* = \varphi_{2jk0}^* = \varphi_{2jkl}^* = 0, \quad (j, k, l) \in \Omega_{MKL}^0, \end{aligned}$$

and initial conditions

$$\varphi_{1jkl}^0 = \varphi_{1,0}(x_j, y_k, z_l), \quad \varphi_{2jkl}^0 = \varphi_{2,0}(x_j, y_k, z_l), \quad (j, k, l) \in \Omega_{MKL}^0,$$



$$\varphi_{1jkl}^{n+1} = \frac{\varphi_{1jkl}^*}{\|\varphi_1^*\|}, \quad \varphi_{2jkl}^{n+1} = \frac{\varphi_{2jkl}^*}{\|\varphi_2^*\|}, \quad (j, k, l) \in \Omega_{MKL},$$

where $\|\varphi_1^*\|^2 = h_x h_y h_z \sum_{j=1}^{M-1} \sum_{k=1}^{K-1} \sum_{l=1}^{L-1} |\varphi_{1jkl}^*|^2$, $\|\varphi_2^*\|^2 = h_x h_y h_z \sum_{j=1}^{M-1} \sum_{k=1}^{K-1} \sum_{l=1}^{L-1} |\varphi_{2jkl}^*|^2$; $\nabla_h^2 \varphi^n$ and $\partial_{nn} \xi^n$ are sine pseudo-spectral approximations of $\nabla^2 \varphi$ and $\partial_{nn} \xi$ at time $t = t_n$, respectively, defined for $(p, q, s) \in \Omega_{MKL}$ as

$$\begin{aligned} \nabla^2 \varphi_1^{n+1}(r)|_{jkl} &= - \sum_{pqs} (u_p^2 + u_q^2 + u_s^2) \alpha_{pqs} \sin\left(\frac{jp\pi}{M}\right) \sin\left(\frac{kq\pi}{K}\right) \sin\left(\frac{ls\pi}{L}\right), \\ \nabla^2 \varphi_2^{n+1}(r)|_{jkl} &= - \sum_{pqs} (u_p^2 + u_q^2 + u_s^2) \alpha'_{pqs} \sin\left(\frac{jp\pi}{M}\right) \sin\left(\frac{kq\pi}{K}\right) \sin\left(\frac{ls\pi}{L}\right), \\ \partial_{nn} \xi^n(r)|_{jkl} &= - \sum_{pqs} (u_p^2 + u_q^2 + u_s^2) \beta_{pqs} \sin\left(\frac{jp\pi}{M}\right) \sin\left(\frac{kq\pi}{K}\right) \sin\left(\frac{ls\pi}{L}\right) = - |\varphi_{1pqs}(r)|^2. \end{aligned}$$

The discrete sine transform coefficients of the vector $\phi_{pqs}(r)|_{(x_j, y_k, z_l)}$ for $(p, q, s) \in \Omega_{MKL}$ are

$$\begin{aligned} \alpha_{pqs} &= \frac{8}{MKL} \sum_{j=1}^{M-1} \sum_{k=1}^{K-1} \sum_{l=1}^{L-1} \varphi_{1jkl}^{n+1} \sin\left(\frac{jp\pi}{M}\right) \sin\left(\frac{kq\pi}{K}\right) \sin\left(\frac{ls\pi}{L}\right), \\ \alpha'_{pqs} &= \frac{8}{MKL} \sum_{j=1}^{M-1} \sum_{k=1}^{K-1} \sum_{l=1}^{L-1} \varphi_{2jkl}^{n+1} \sin\left(\frac{jp\pi}{M}\right) \sin\left(\frac{kq\pi}{K}\right) \sin\left(\frac{ls\pi}{L}\right), \end{aligned}$$

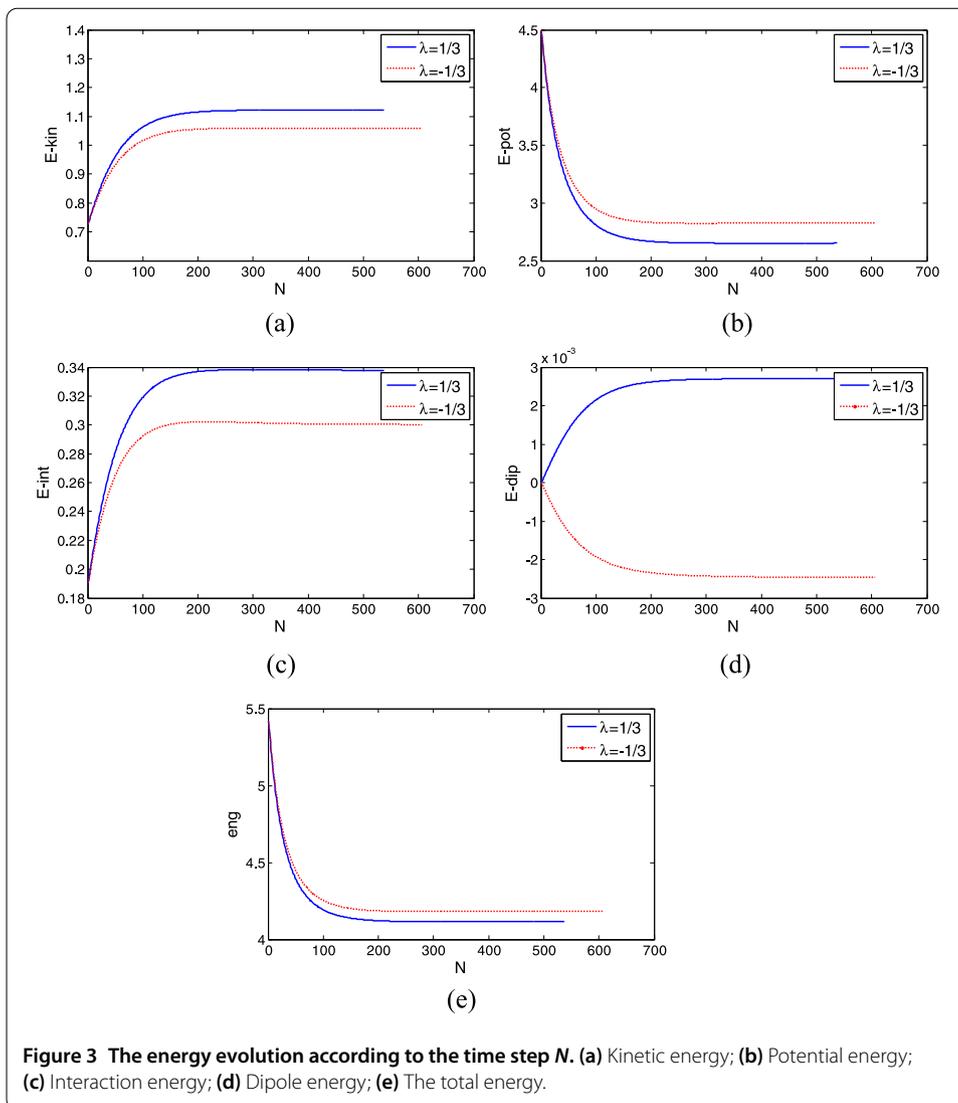


Figure 3 The energy evolution according to the time step N . (a) Kinetic energy; (b) Potential energy; (c) Interaction energy; (d) Dipole energy; (e) The total energy.

$$\beta_{pqs} = \frac{1}{u_p^2 + u_q^2 + u_s^2} \frac{8}{MKL} \sum_{j=1}^{M-1} \sum_{k=1}^{K-1} \sum_{l=1}^{L-1} |\varphi_{1jkl}^{n+1}|^2 \sin\left(\frac{jp\pi}{M}\right) \sin\left(\frac{kq\pi}{K}\right) \sin\left(\frac{ls\pi}{L}\right).$$

Linear system (7) can be iteratively solved in a phase space very efficiently via discrete sine transform under the conditions $\max_{j,k,l} |\varphi_{1jkl}^{n+1} - \varphi_{1jkl}^n| < 10^{-6}$ and $\max_{j,k,l} |\varphi_{2jkl}^{n+1} - \varphi_{2jkl}^n| < 10^{-6}$.

3 Numerical results

Example 1 Consider the ground state of the BEC with $V(r) = \frac{1}{2}(x^2 + 2y^2 + 2z^2)$. The initial condition is given as follows:

$$\begin{cases} \varphi_{1,0} = \varphi_1(x, y, z, 0) = \pi^{-3/4} \gamma_x^{1/2} \gamma_z^{1/4} e^{-\frac{1}{2}(\gamma_x(x^2+y^2)+\gamma_z z^2)}, \\ \varphi_{2,0} = \varphi_2(x, y, z, 0) = \pi^{-3/4} \gamma_x^{1/2} \gamma_z^{1/4} e^{-\frac{1}{2}(\gamma_x(x^2+y^2)+\gamma_z z^2)}, \end{cases} \quad (x, y, z) \in R^3.$$

Here, $\gamma_x = \frac{\omega_x}{2\omega_0}$, $\gamma_z = \frac{\omega_z}{2\omega_0}$, $\omega_0 = \min\{\omega_{jx}, \omega_{jy}, \omega_{jz}\}$. We solve this system on $[-8, 8]^3$ with $h_x = h_y = h_z = 1/4$ and $\Delta t = 0.005$.

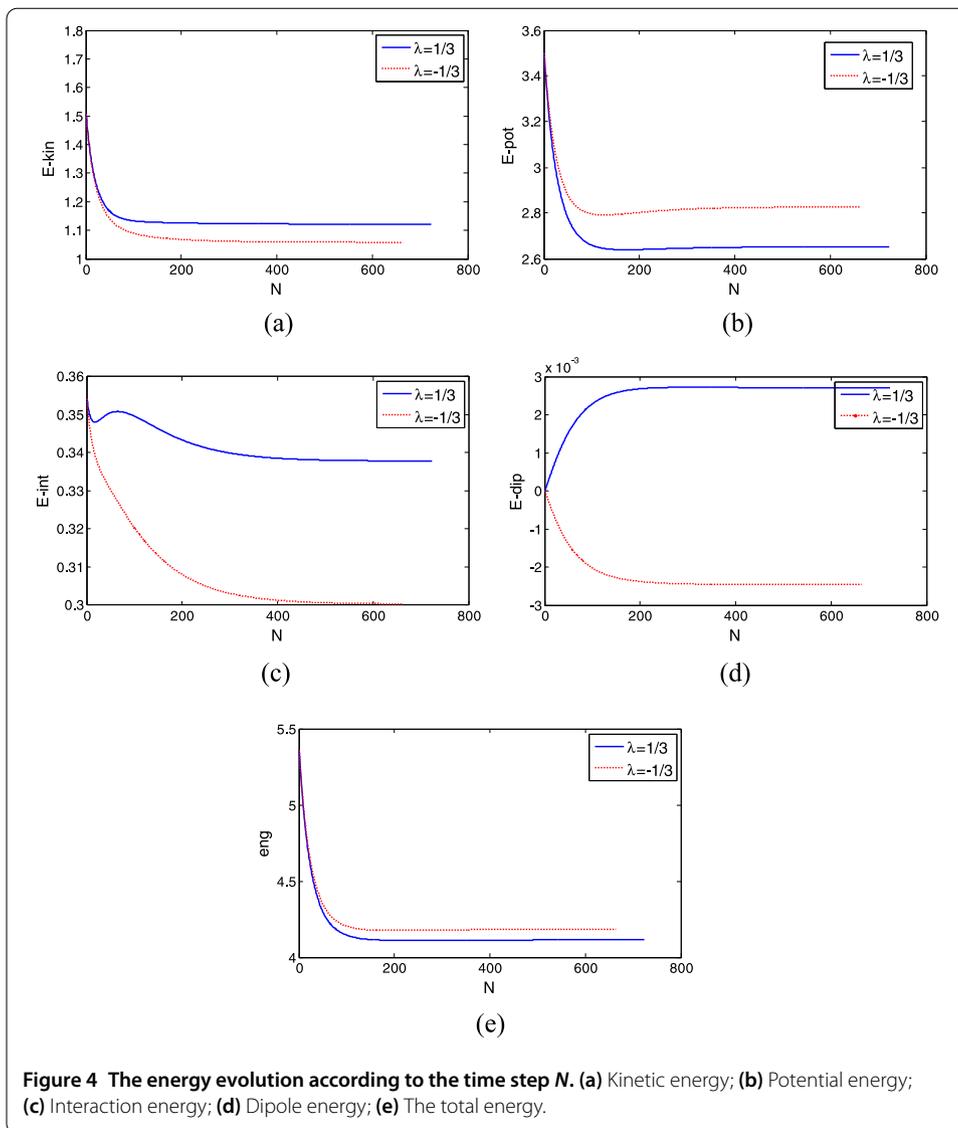


Figure 1 shows the results for the case of $\gamma_x = \gamma_z = 1$.

Example 2 Solve the ground state problem for a dipolar BEC with $V(r) = \frac{1}{2}(x^2 + 2y^2 + 2z^2)$. The initial condition is

$$\begin{cases} \varphi_{1,0} = \varphi_1(x, y, z, 0) = \pi^{-3/4} \gamma_x^{1/4} \gamma_y^{1/4} \gamma_z^{1/4} e^{-\frac{1}{2}(\gamma_x x^2 + \gamma_y y^2 + \gamma_z z^2)}, \\ \varphi_{2,0} = \varphi_2(x, y, z, 0) = \pi^{-3/4} \gamma_x^{1/4} \gamma_y^{1/4} \gamma_z^{1/4} e^{-\frac{1}{2}(\gamma_x x^2 + \gamma_y y^2 + \gamma_z z^2)}, \end{cases} \quad (x, y, z) \in \mathbb{R}^3.$$

Figure 2 shows the results for the case of $\gamma_x = 2, \gamma_y = 8, \gamma_z = 1$.

4 Conclusion

An efficient numerical method is presented for computing the ground states of dipolar Bose-Einstein condensates based on two coupled three-dimensional Gross-Pitaevskii equations, where one equation has a dipole-dipole interaction potential and the other one has only the usual s -wave contact interaction. Using equality (3), we can reformulate the

GPE for dipolar BEC into a Gross-Pitaevskii-Poisson type system. Numerical examples are given to show the efficiency of our method. In all cases, total energy decreases (Figure 3 and Figure 4). The results agree with the previous work [15]. Numerical results are given to demonstrate the efficiency of our numerical method. And dynamics will be the latter part of our work to be carried out.

Competing interests

The authors declare that they have no competing interests.

Authors' contributions

SQL established the scheme, performed the numerical examples in Section 3 and drafted the manuscript. XGL designed the study. DYH established the model and helped to inspect the manuscript. All authors read and approved the final manuscript.

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