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Spectral collocation and a two-level continuation scheme for dipolar Bose–Einstein condensates

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ABSTRACT

We exploit the high accuracy of spectral collocation methods in the context of a two-level continuation scheme for computing ground state solutions of dipolar Bose–Einstein condensates (BEC), where the first kind Chebyshev polynomials and Fourier sine functions are used as the basis functions for the trial function space. The governing Gross–Pitaevskii equation (or Schrödinger equation) can be reformulated as a Schrödinger–Poisson (SP) type system [13]. The two-level continuation scheme is developed for tracing the first solution curves of the SP system, which in turn provide an appropriate initial guess for the Newton method to compute ground state solutions for 3D dipolar BEC. Extensive numerical experiments on 3D dipolar BEC and dipolar BEC in optical lattices are reported.

1. Introduction

In past years, a successful experimental result has been obtained on dipolar Bose–Einstein condensates (BECs), where a BEC of ^{52}Cr atoms has been realized [1]. The achievement allows experimental investigations of the unique properties of dipolar BEC. The experimental breakthrough on cooling and trapping of molecules [2], on photoassociation [3], and on Feshbach resonances of binary mixtures [4] have opened up new research areas in the atomic physics community [5–11].

The 3D dipolar BEC at zero temperature trapped in a harmonic potential $V(\mathbf{x}) = \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$ is well described by the macroscopic wave function $\psi(\mathbf{x},t)$ whose evolution is governed by the Gross–Pitaevskii equation (GPE) [5,12]

$$\mathbf{i}\hbar\partial_t\psi(\mathbf{x},t) = \left[-\frac{\hbar^2}{2m}\Delta + V(\mathbf{x}) + U_0\left|\psi(\mathbf{x},t)\right|^2 + V_{\mathrm{dip}}(\mathbf{x}) * \left|\psi(\mathbf{x},t)\right|^2\right]\psi(\mathbf{x},t), \quad \mathbf{x}\in\mathbb{R}^3,\ t>0, \tag{1.1}$$

where $\hbar$ is the Planck constant, t is the time variable, $\mathbf{x} = (x, y, z)^T \in \mathbb{R}^3$, m is the mass of a dipolar particle, ω_x, ω_y, and ω_z are the trap frequencies in the x-, y-, and z-direction, respectively. The parameter $U_0 = \frac{4\pi\hbar^2 a_s}{m}$ denotes local (or short-range) interaction between dipoles in the condensates with a_s the s-wave scattering length, V_{dip} denotes the long-range dipolar interaction between two dipoles which is given by

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$$V_{\mathrm{dip}}(\mathbf{x}) = \frac{\mu_0\mu_{\mathrm{dip}}^2}{4\pi}\frac{1-3(\mathbf{x}\cdot\mathbf{n})^2/|\mathbf{x}|^2}{|\mathbf{x}|^3} = \frac{\mu_0\mu_{\mathrm{dip}}^2}{4\pi}\frac{1-3\cos^2\theta}{|\mathbf{x}|^3}, \quad \mathbf{x}\in\mathbb{R}^3, \tag{1.2}$$

where μ_0 is the vacuum magnetic permeability, μ_{dip} is the permanent magnetic dipole moment (e.g., $\mu_{\mathrm{dip}} = 6\mu_B$ for ^{52}Cr with μ_B being the Bohr magneton), $\mathbf{n} = (n_1, n_2, n_3)^T \in \mathbb{R}^3$ is the dipole axis (or dipole moment) with $\|\mathbf{n}\|_2 = 1$, and θ is the angle between the dipole axis $\mathbf{n}$ and position vector $\mathbf{x}$. The wave function ψ is normalized according to

$$\|\psi\|^2 := \int_{\mathbb{R}^3} \left|\psi(\mathbf{x},t)\right|^2 d\mathbf{x} = M, \tag{1.3}$$

where M is the total number of dipolar particles in the dipolar BEC.

By introducing the dimensionless variables [13], $t \to \frac{t}{\omega_0}$ with $\omega_0 = \min\{\omega_x, \omega_y, \omega_z\}$, $\mathbf{x} \to a_0\mathbf{x}$ with $a_0 = \sqrt{\hbar/m\omega_0}$, $\psi \to \frac{\sqrt{M}\psi}{a_0^{3/2}}$, Eqs. (1.1) and (1.3) are expressed as

$$\mathbf{i}\partial_t\psi(\mathbf{x},t) = \left[-\frac{1}{2}\Delta + V(\mathbf{x}) + \beta\left|\psi(\mathbf{x},t)\right|^2 + \lambda\left(U_{\mathrm{dip}}(\mathbf{x}) * \left|\psi(\mathbf{x},t)\right|^2\right)\right]\psi(\mathbf{x},t), \quad \mathbf{x}\in\mathbb{R}^3,\ t>0, \tag{1.4}$$

$$\|\psi\|^2 = \int_{\mathbb{R}^3} \left|\psi(\mathbf{x},t)\right|^2 d\mathbf{x} = 1, \tag{1.5}$$

where $V(\mathbf{x}) = \frac{1}{2}(\gamma_x^2x^2 + \gamma_y^2y^2 + \gamma_z^2z^2)$ is the dimensionless harmonic trapping potential with $\gamma_x = \omega_x/\omega_0$, $\gamma_y = \omega_y/\omega_0$, and $\gamma_z = \omega_z/\omega_0$, $\beta = \frac{MU_0}{\hbar\omega_0 a_0^3} = \frac{4\pi a_s M}{a_0}$, $\lambda = \frac{mM\mu_0\mu_{\mathrm{dip}}^2}{3\hbar^2 a_0}$, and the dimensionless long-range dipolar interaction potential U_{dip} is given as

$$U_{\mathrm{dip}}(\mathbf{x}) = \frac{3}{4\pi}\frac{1-3(\mathbf{x}\cdot\mathbf{n})^2/|\mathbf{x}|^2}{|\mathbf{x}|^3} = \frac{3}{4\pi}\frac{1-3\cos^2\theta}{|\mathbf{x}|^3}, \quad \mathbf{x}\in\mathbb{R}^3. \tag{1.6}$$

Recently, Bao et al. [13] decoupled the two-body dipolar interaction potential into short-range (or local) and long-range interactions (or repulsive and attractive interactions), and transformed Eq. (1.4) into a Gross–Pitaevskii–Poisson or Schrödinger–Poisson (SP) type system of the following form

$$\mathbf{i}\partial_t\psi(\mathbf{x},t) = \left[-\frac{1}{2}\Delta + V(\mathbf{x}) + (\beta-\lambda)\left|\psi(\mathbf{x},t)\right|^2 - 3\lambda\widetilde{\varphi}(\mathbf{x},t)\right]\psi(\mathbf{x},t), \quad \mathbf{x}\in\mathbb{R}^3,\ t>0, \tag{1.7}$$

$$\begin{cases} -\Delta\varphi(\mathbf{x},t) = \left|\psi(\mathbf{x},t)\right|^2, & \lim\limits_{|\mathbf{x}|\to\infty}\varphi(\mathbf{x},t) = 0, \\ \widetilde{\varphi}(\mathbf{x},t) = \partial_{\mathbf{nn}}\varphi(\mathbf{x},t), \end{cases} \tag{1.8}$$

where $\partial_{\mathbf{n}} = \mathbf{n}\cdot\nabla = n_1\partial_x + n_2\partial_y + n_3\partial_z$, $\partial_{\mathbf{nn}} = \partial_{\mathbf{n}}(\partial_{\mathbf{n}})$. The decoupled short-range and long-range interactions of the dipolar interaction potential are attractive and repulsive, respectively, when $\lambda > 0$; and are repulsive and attractive, respectively, when $\lambda < 0$. Moreover, the total energy per particle is

$$E(\psi) = E_{\mathrm{kin}}(\psi) + E_{\mathrm{pot}}(\psi) + E_{\mathrm{int}}(\psi) + E_{\mathrm{dip}}(\psi), \tag{1.9}$$

where

$$E_{\mathrm{kin}}(\psi) = \frac{1}{2}\int_{\mathbb{R}^3} |\nabla\psi|^2\, d\mathbf{x}, \qquad E_{\mathrm{pot}}(\psi) = \int_{\mathbb{R}^3} V(\mathbf{x})|\psi|^2\, d\mathbf{x},$$

$$E_{\mathrm{int}}(\psi) = \frac{\beta}{2}\int_{\mathbb{R}^3} |\psi|^4\, d\mathbf{x}, \qquad E_{\mathrm{dip}}(\psi) = \frac{\lambda}{2}\int_{\mathbb{R}^3} \left(-|\psi|^4 + 3|\partial_{\mathbf{n}}\nabla\varphi|^2\right) d\mathbf{x},$$

are kinetic, potential, interaction, and dipolar energies, respectively. Substituting the formula [14]

$$\psi(\mathbf{x},t) = e^{-\mathbf{i}\mu t}\phi(\mathbf{x}), \quad \mathbf{x}\in\mathbb{R}^3,\ t\geqslant 0, \tag{1.10}$$

into Eqs. (1.7)–(1.8) and the constraint (1.5), we obtain the nonlinear eigenvalue problem