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Accurate and Efficient Numerical Methods for Computing Ground States and Dynamics of Dipolar Bose-Einstein Condensates via the Nonuniform FFT

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Abstract. We propose efficient and accurate numerical methods for computing the ground state and dynamics of the dipolar Bose-Einstein condensates utilising a newly developed dipole-dipole interaction (DDI) solver that is implemented with the non-uniform fast Fourier transform (NUFFT) algorithm. We begin with the three-dimensional (3D) Gross-Pitaevskii equation (GPE) with a DDI term and present the corresponding two-dimensional (2D) model under a strongly anisotropic confining potential. Different from existing methods, the NUFFT based DDI solver removes the singularity by adopting the spherical/polar coordinates in the Fourier space in 3D/2D, respectively, thus it can achieve spectral accuracy in space and simultaneously maintain high efficiency by making full use of FFT and NUFFT whenever it is necessary and/or needed. Then, we incorporate this solver into existing successful methods for computing the ground state and dynamics of GPE with a DDI for dipolar BEC. Extensive numerical comparisons with existing methods are carried out for computing the DDI, ground states and dynamics of the dipolar BEC. Numerical results show that our new methods outperform existing methods in terms of both accuracy and efficiency.

AMS subject classifications: 35Q40, 35Q41, 35Q55, 65M70, 65T40, 65T50, 81-08

Key words: Dipolar BEC, dipole-dipole interaction, NUFFT, ground state, dynamics, collapse.

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1 Introduction

Since its first experimental creation in 1995 [4, 20, 23], the Bose-Einstein condensation (BEC) has provided an incredible glimpse into the macroscopic quantum world and opened a new era in atomic and molecular physics as well as condensated matter physics. It regains vast interests and has been extensively studied both experimentally and theoretically [3,17,19,24,36,40,44]. At early stage, experiments mainly realize BECs of ultracold atomic gases whose properties are mainly governed by the isotropic and short-range interatomic interactions [44]. However, recent experimental developments on Feshbach resonances [33], on cooling and trapping molecules [41, 47] and on precision measurements and control [45, 49] allow one to realize BECs of quantum gases with different, richer interactions and gain even more interesting properties. In particular, the successful realization of BECs of dipolar quantum gases with long-range and anisotropic dipolar interaction, e.g., ^{52}Cr [26], ^{164}Dy [38] and ^{168}Er [2], has spurred great interests in the unique properties of degenerate dipolar quantum gases and stimulated enthusiasm in studying both the ground state [7,8,30,46,50] and dynamics [13,14,22,28,35,43] of dipolar BECs.

At temperatures T much smaller than the critical temperature T_c, the properties of BEC with long-range dipole-dipole interactions (DDI) are well described by the macroscopic complex-valued wave function $\psi=\psi(\mathbf{x},t)$ whose evolution is governed by the celebrating three-dimensional (3D) Gross-Pitaevskii equation (GPE) with a DDI term. Moreover, the 3D GPE can be reduced to an effective two-dimensional (2D) version if the external trapping potential is strongly confined in the z-direction [8,21]. In a unified way, the dimensionless GPE with a DDI term in d-dimensions ($d=2$ or 3) for modeling a dipolar BEC reads as [6,7,14,25,35,50]:

$$i\partial_t\psi(\mathbf{x},t)=\left[-\frac{1}{2}\nabla^2+V(\mathbf{x})+\beta|\psi|^2+\lambda\Phi(\mathbf{x},t)\right]\psi(\mathbf{x},t),\quad \mathbf{x}\in\mathbb{R}^d,\quad t>0, \tag{1.1}$$

$$\Phi(\mathbf{x},t)=\left(U_{\rm dip}*|\psi|^2\right)(\mathbf{x},t),\qquad \mathbf{x}\in\mathbb{R}^d,\quad t\geq 0, \tag{1.2}$$

$$\psi(\mathbf{x},t=0)=\psi_0(\mathbf{x}),\qquad \mathbf{x}\in\mathbb{R}^d, \tag{1.3}$$

where t is time, $\mathbf{x}=(x,y)^T\in\mathbb{R}^2$ or $\mathbf{x}=(x,y,z)^T\in\mathbb{R}^3$, $*$ represents the convolution operator with respect to spatial variable. The dimensionless constant β describes the strength of the short-range two-body interactions in a condensate (positive for repulsive interaction, and resp. negative for attractive interaction), while $V(\mathbf{x})$ is a given real-valued external trapping potential which is determined by the type of system under investigation. In most BEC experiments, a harmonic potential is chosen to trap the condensate, i.e.,

$$V(\mathbf{x})=\frac{1}{2}\begin{cases}\gamma_x^2x^2+\gamma_y^2y^2, & d=2,\\ \gamma_x^2x^2+\gamma_y^2y^2+\gamma_z^2z^2, & d=3,\end{cases} \tag{1.4}$$

where $\gamma_x>0$, $\gamma_y>0$ and $\gamma_z>0$ are dimensionless constants proportional to the trapping frequencies in x-, y- and z-direction, respectively. Moreover, λ is a dimensionless constant