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A Preconditioned Conjugated Gradient Method for Computing Ground States of Rotating Dipolar Bose-Einstein Condensates via Kernel Truncation Method for Dipole-Dipole Interaction Evaluation

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Dedicated to Professor Houde Han on the occasion of his 80th birthday

Abstract. In this paper, we propose an efficient and accurate method to compute the ground state of 2D/3D rotating dipolar BEC by incorporating the Kernel Truncation Method (KTM) for Dipole-Dipole Interaction (DDI) evaluation into the newly-developed Preconditioned Conjugate Gradient (PCG) method [9]. Adaptation details of KTM and PCG, including multidimensional discrete convolution acceleration for KTM, choice of the preconditioners in PCG, are provided. The performance of our method is confirmed with extensive numerical tests, with emphasis on spectral accuracy of KTM and efficiency of ground state computation with PCG. Application of our method shows some interesting vortex lattice patterns in 2D and 3D respectively.

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

Key words: Rotating dipolar BEC, Dipole-Dipole Interaction, Preconditioned Conjugate Gradient method, Kernel Truncation Method, ground state.

1 Introduction

The successful realization of Bose-Einstein condensates of gases of ^{52}Cr [35], ^{164}Dy [39] and ^{168}Er [3] provides the possibility to study and probe novel interesting phenomenon

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with dipolar quantum gas. Different from the early BECs of ultra cold atomic gases whose properties are mainly governed by isotropic and short-range interatomic interactions [48], in dipolar BEC, the magnetic/electric dipole-dipole interatomic interaction is anisotropic and long-range, and it brings in unique phenomena, such as roton-maxon spectrum [42, 49], vortex lattice patterns [45], and the self-bound droplet state [32, 52]. There is everlasting enthusiasm in studying both the ground state [6, 8, 12, 13, 29, 38, 51, 56–58] and dynamics [18, 24, 36, 43, 47] 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 $\psi(\mathbf{x},t)$ 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 [13, 22]. 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 [11, 12, 18, 33, 57]:

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

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

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

where t is the time variable, $\mathbf{x}=(x,y)^T\in\mathbb{R}^2$ or $\mathbf{x}=(x,y,z)^T\in\mathbb{R}^3$, $*$ represents the convolution operator with respect to the spatial variable, $L_z=-i(x\partial_y-y\partial_x)=-i\partial_\theta$ is the z-component of the angular momentum and ω represents the rotating frequency. 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), $V(\mathbf{x})$ 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 constant characterizing the strength of DDI and $U_{\rm dip}(\mathbf{x})$ is the long-range DDI potential. In 3D, $U_{\rm dip}(\mathbf{x})$ reads as

$$U_{\rm dip}(\mathbf{x})=\frac{3}{4\pi|\mathbf{x}|^3}\left[1-\frac{3(\mathbf{x}\cdot\boldsymbol{n})^2}{|\mathbf{x}|^2}\right]=-\delta(\mathbf{x})-3\partial_{\boldsymbol{nn}}\left(\frac{1}{4\pi|\mathbf{x}|}\right),\quad \mathbf{x}\in\mathbb{R}^3, \tag{1.5}$$

with $\boldsymbol{n}=(n_1,n_2,n_3)^T$ a given unit vector, i.e., $|\boldsymbol{n}(t)|=\sqrt{n_1^2+n_2^2+n_3^2}=1$, representing the dipole axis (or dipole moment), $\partial_{\boldsymbol{n}}=\boldsymbol{n}\cdot\nabla$ and $\partial_{\boldsymbol{nn}}=\partial_{\boldsymbol{n}}(\partial_{\boldsymbol{n}})$, while in 2D, it is defined