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# A combined discontinuous Galerkin method for the dipolar Bose–Einstein condensation ☆

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ABSTRACT

In this work, a combined discontinuous Galerkin (DG) method, which is a hybridized mixed discontinuous Galerkin (HMDG) method combined with the direct discontinuous Galerkin (DDG) method, is proposed to compute ground states and dynamics of dipolar Bose–Einstein condensates (BECs) described by a multi-dimensional Gross–Pitaevskii equation (GPE) coupled with a first-order velocity system. Due to the adaption of the first-order velocity system instead of dipolar interactions, the proposed combined DG method avoids to evaluate integrals with high singularity. Additionally, this method keeps the conservation of the particle number. The Krylov semi-implicit method is applied to the time discretization. Finally, numerical examples are presented to demonstrate the accuracy and capability of the proposed method.



## 1. Introduction

The first dilute atomic Bose–Einstein condensate (BEC) was created by Eric Cornell, Carl Wieman, and coworkers in 1995 [1], and then a great revolution was launched in the field of ultracold atomic physics. In 2005, the dipolar BEC of $^{52}$Cr was observed at Stuttgart University [18,27]. This dramatic experimental breakthrough has stimulated strongly the theoretical and numerical investigations. It is known that the degenerate quantum gases are usually dominated by *s*-wave contact interaction which is isotropic and short range, while dipolar quantum gases are governed by the *d*-wave symmetry of dipole–dipole interaction which is anisotropic and long range. Although it has become apparent that the contact interactions between the condensed atoms govern most of the observed phenomena, this long-range difference gives rise to novel properties. In fact, the long-range nature of dipolar interactions means that the GPE which governs the BEC is not only nonlinear but also nonlocal.

When the temperature $T$ is much smaller than the critical temperature, the dipolar BEC in the mean field theory is well described by the macroscopic wave function $\psi(\mathbf{x}, t)$, whose evolution is governed by the following GPE [5,31]:

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

with initial data, where $\hbar$ is the Planck constant, $m$ is the mass of the atom and $V(\mathbf{x})$ is the external trapping potential which is generally harmonic, that is, $V(\mathbf{x})=\frac{m}{2}(\omega_1^2x^2+\omega_2^2y^2+\omega_3^2z^2)$ with $\omega_i$ $(i=1,2,3)$ represent the trap frequencies in $x$, $y$, $z$ directions, respectively. $U_0=4\pi\hbar^2a_s/m$, with the $s$-wave scattering length $a_s$, is a dimensionless constant describing the local interaction between dipoles in the condensate, and it is positive for repulsive interaction and negative for attractive interaction, respectively, by Feshbach resonance. Let $\mathbf{l}=(l_1,l_2,l_3)$ be the unit vector on the polarization axis, then $V_{dip}(\mathbf{x})$ denotes the long-range anisotropic dipolar interaction potential defined by

$$V_{dip}(\mathbf{x})=\frac{C_{dd}}{4\pi}\frac{1-3\cos^2\theta}{|\mathbf{x}|^3},\quad \mathbf{x}\in\mathbb{R}^3, \tag{1.2}$$

where $\theta$ is the angle between the polarization axis $\mathbf{l}$ and the vector $\mathbf{x}$, i.e., $\cos\theta=\frac{\mathbf{l}\cdot\mathbf{x}}{|\mathbf{x}|}$. For magnetic dipoles, we have $C_{dd}=\mu_0\mu_d^2$, where $\mu_0$ is the magnetic vacuum permeability and $\mu_d$ is the dipole moment. For electric dipoles, we have $C_{dd}=d^2/\mu_0$, where $\mu_0$ is the vacuum permittivity and $d$ is the electric dipole moment. The amplitude and the sign of $C_{dd}$ are usually dependent on the rotation of the polarization axis. The wave function $\psi(\mathbf{x},t)$ is normalized to

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

where $N$ is the number of the atoms in the dipolar BEC. After the dimensionless transformation, that is, by letting $\mathbf{x}=a_0\tilde{\mathbf{x}}$, $t=\frac{\tilde{t}}{\omega_0}$, $\psi=\frac{\sqrt{N}\tilde{\psi}}{a_0^{3/2}}$, where $\omega_0=\min\{\omega_1,\omega_2,\omega_3\}$, $a_0=\sqrt{\frac{\hbar}{m\omega_0}}$, we can get

$$i\tilde{\psi}_{\tilde{t}}=-\frac{1}{2}\tilde{\nabla}^2\tilde{\psi}+\frac{1}{2}\left(\gamma_1^2\tilde{x}^2+\gamma_2^2\tilde{y}^2+\gamma_3^2\tilde{z}^2\right)\tilde{\psi}+\beta|\tilde{\psi}|^2\tilde{\psi}+\lambda\left(U_{dip}*|\tilde{\psi}|^2\right)\tilde{\psi}$$

with $\beta=\frac{U_0N}{\hbar\omega_0a_0^3}=\frac{4\pi a_sN}{a_0}$, $\lambda=\frac{mN}{a_0\hbar^2}$, $\gamma_i=\frac{\omega_i}{\omega_0}$ $(i=1,2,3)$ and $U_{dip}=\frac{C_{dd}}{4\pi}\frac{1-3\cos^2\theta}{|\tilde{\mathbf{x}}|^3}$. It is easy to see that $\lambda=\beta/U_0$. To simplify the notation, we remove the tildes from the variables in the above equation, and get the following dimensionless nonlocal GPE:

$$i\psi_t(\mathbf{x},t)=\left(-\frac{1}{2}\nabla^2+V(\mathbf{x})+\beta\left|\psi(\mathbf{x},t)\right|^2+\lambda\,U_{dip}*\left|\psi(\mathbf{x},t)\right|^2\right)\psi(\mathbf{x},t) \tag{1.3}$$

with the constraint of $\|\psi(\mathbf{x},t)\|=1$, where $V(\mathbf{x})=\frac{1}{2}(\gamma_1^2x^2+\gamma_2^2y^2+\gamma_3^2z^2)$, and

$$U_{dip}=\frac{C_{dd}}{4\pi}\frac{1-3\cos^2\theta}{|\mathbf{x}|^3}.$$

It is well known that (1.3) possesses the conservations of the particle number and the total energy, i.e.

$$\int_{\mathbb{R}^3}\left|\psi(\mathbf{x},t)\right|^2d\mathbf{x}\equiv\int_{\mathbb{R}^3}\left|\psi(\mathbf{x},0)\right|^2d\mathbf{x}=1 \tag{1.4}$$

and

$$\begin{aligned}E\big(\psi(\mathbf{x},t)\big)&=\frac{1}{2}\int_{\mathbb{R}^3}|\nabla\psi|^2d\mathbf{x}+\int_{\mathbb{R}^3}V(\mathbf{x})|\psi|^2d\mathbf{x}+\frac{\beta}{2}\int_{\mathbb{R}^3}|\psi|^4d\mathbf{x}+\frac{\lambda}{2}\int_{\mathbb{R}^3}\left(U_{dip}*|\psi|^2\right)|\psi|^2d\mathbf{x}\\&\equiv E\big(\psi(\mathbf{x},0)\big).\end{aligned} \tag{1.5}$$

The theoretical study of dipolar BECs including ground states and dynamics as well as quantized vortices has been carried out in recent years based on (1.1). We refer [2,11,19,20,24,32] for physical study. In mathematical aspect, existence and uniqueness as well as the possible blow-up of solutions were studied in [3]. If there is no dipolar interaction, i.e. $\lambda=0$, (1.3) becomes the BEC with alkali atoms and for such case many numerical methods were developed, for example, the local discontinuous Galerkin (LDG) method [29] for the nonlinear Schrödinger equation and the spectral method [4,7,8,16] for the dynamic quantum evolution. When $\lambda\neq0$, (1.3) is difficult to be solved numerically because of the presence of the high singularity of the dipolar interaction via the convolution term. To overcome this difficulty, the dipolar interaction potential is split into short and long-range interactions [5,28] and thus the following equivalent Gross–Pitaevskii–Poisson (GPP) type system is considered:

$$i\psi_t(\mathbf{x},t)=\left[-\frac{1}{2}\nabla^2+V(\mathbf{x})+(\beta-\lambda)\left|\psi(\mathbf{x},t)\right|^2-3\lambda\partial_{\mathbf{ll}}\big(\omega(\mathbf{x},t)\big)\right]\psi(\mathbf{x},t), \tag{1.6}$$

$$\nabla^2\omega(\mathbf{x},t)=-|\psi|^2, \tag{1.7}$$