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A robust and efficient numerical method to compute the dynamics of the rotating two-component dipolar Bose–Einstein condensates

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ABSTRACT

We present a robust and efficient numerical method to compute the dynamics of the rotating two-component dipolar Bose–Einstein condensates (BEC). Using the rotating Lagrangian coordinates transform (Bao et al., 2013), we reformulate the original coupled Gross–Pitaevskii equations (CGPE) into new equations where the rotating term vanishes and the potential becomes time-dependent. A time-splitting Fourier pseudospectral method is proposed to numerically solve the new equations where the nonlocal Dipole–Dipole Interactions (DDI) are computed by a newly-developed Gaussian-sum (GauSum) solver (Exl et al., 2016) which helps achieve spectral accuracy in space within $O(N \log N)$ operations (N is the total number of grid points). The new method is spectrally accurate in space and second order accurate in time — these accuracies are confirmed numerically. Dynamical properties of some physical quantities, including the total mass, energy, center of mass and angular momentum expectation, are presented and confirmed numerically. Interesting dynamical phenomena that are peculiar to the rotating two-component dipolar BECs, such as dynamics of center of mass, quantized vortex lattices dynamics and the collapse dynamics in 3D, are presented.

1. Introduction

The Bose–Einstein condensation (BEC) yields most interesting state-of-the-art experiments for relatively large quantum systems and has been extensively studied since its first experimental realization in 1995 [1–3]. A subsequent achievement of quantum vortices in rotating BECs [4–6] broadens the attention to explore vortex states and their dynamics associated with superfluidity. Initially, the experiments/simulations were limited to the case of short-range interatomic interactions [7]. Recently, considerable attention has been drawn to systems with long-range dipole–dipole interactions (DDIs) in ultracold physics [8]. For heteronuclear molecules, DDIs come from their electric dipole moments [9]. In a state with a well-defined angular momentum, molecules do not have a dipole moment. Nevertheless, dipolar moments can be induced when molecules are polarized via an external electric field. For atoms, dipolar interactions arise from their magnetic moments and become significant for large electronic spin. Recent experiments on dipolar BECs of Cr atoms and others [10–12] demonstrated very well for such interactions and has spurred new impetus in the study of dipolar BECs.

Due to the presence of anisotropic DDI, vortices in rotating dipolar BECs exhibit novel properties and richer phenomena [13–16]. On the other hand, thanks to the development of trapping techniques, binary condensates are also realized [17–19] and provide an ideal system for studying phase transitions and coexistence of different phases [20–22]. Far from being a trivial extension of the single-component BEC, the physics of a dipolar mixture may feature different and remarkable properties, such as the domain walls, vortons and square vortex lattices [18,19,23].

Very recently, the vortices of rotating two-component dipolar BECs under different trapping potentials have been investigated in several studies by physicists [22–26]. At temperatures T much smaller than the critical temperature T_c, the properties of rotating two-component dipolar BECs are well described by the macroscopic complex-valued wave function $\Psi = (\psi_1(\mathbf{x}, t), \psi_2(\mathbf{x}, t))^T$ calculated from the three-dimensional (3D) Coupled Gross–Pitaevskii Equations (CGPE) with DDI term. Moreover, the 3D CGPE can be reduced to an effective two-dimensional (2D) equation if the external potential is highly anisotropic, i.e. much stronger in $z-$direction [27,28]. In a unified way, the $d-$dimensional ($d = 2$ or 3) dimensionless CGPE with DDI term

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reads as [23,25,26,29,30]:

$$i\partial_t \psi_j(\mathbf{x},t) = \Big[-\frac{1}{2}\nabla^2 + V_j(\mathbf{x}) - \Omega L_z + \sum_{k=1}^{2}\big(\beta_{jk}|\psi_k|^2 + \lambda_{jk}\,\Phi_k(\mathbf{x},t)\big)\Big]\psi_j(\mathbf{x},t), \tag{1.1}$$

$$\Phi_j(\mathbf{x},t) = U_{\rm dip} * |\psi_j|^2, \qquad \psi_j(\mathbf{x},t=0) = \psi_j^0(\mathbf{x}), \quad j = 1,\ 2, \quad \mathbf{x}\in\mathbb{R}^d, \quad t \ge 0. \tag{1.2}$$

Here, Φ_j is defined as a convolution of the kernel $U_{\rm dip}$ with the density $|\psi_j|^2$ where $*$ denotes the convolution operator, t denotes time, $\mathbf{x} = (x,y,z)^T \in \mathbb{R}^3$ and/or $\mathbf{x} = (x,y)^T \in \mathbb{R}^2$ is the Cartesian coordinate vector. The constant β_{jk} describes the strength of the short-range interactions in a condensate (positive/negative for repulsive/attractive interaction), $L_z = -i(x\partial_y - y\partial_x) = -i\partial_\theta$ is the z-component of the angular momentum and Ω represents the rotating frequency. $V_j(\mathbf{x})$ $(j = 1, 2)$ is a given real-valued external trapping potential determined by the type of system under investigation. In most BEC experiments, a harmonic potential is chosen to trap the condensates, i.e. for $j = 1, 2$

$$V_j(\mathbf{x}) = \frac{1}{2}\begin{cases}\gamma_{x,j}^2x^2 + \gamma_{y,j}^2y^2, & d = 2,\\ \gamma_{x,j}^2x^2 + \gamma_{y,j}^2y^2 + \gamma_{z,j}^2z^2, & d = 3,\end{cases} \tag{1.3}$$

where $\gamma_{v,j}$ $(v = x, y, z)$ are dimensionless constants representing the trapping frequencies in v-direction. Moreover, λ_{ij} $(i, j = 1, 2)$ 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

$$U_{\rm dip}(\mathbf{x}) = \frac{3}{4\pi|\mathbf{x}|^3}\left[1 - \frac{3(\mathbf{x}\cdot\mathbf{n})^2}{|\mathbf{x}|^2}\right] = -\delta(\mathbf{x}) - 3\,\partial_{\mathbf{nn}}\left(\frac{1}{4\pi|\mathbf{x}|}\right), \quad \mathbf{x}\in\mathbb{R}^3, \tag{1.4}$$

with $\mathbf{n} = (n_1, n_2, n_3)^T$, a given unit vector i.e. $|\mathbf{n}(t)| = \sqrt{n_1^2 + n_2^2 + n_3^2} = 1$, representing the dipole axis (or dipole moment), $\partial_{\mathbf{n}} = \mathbf{n}\cdot\nabla$ and $\partial_{\mathbf{nn}} = \partial_{\mathbf{n}}(\partial_{\mathbf{n}})$. While in 2D, it is defined as [27,31]

$$U_{\rm dip}(\mathbf{x}) = -\frac{3}{2}\left(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\nabla_\perp^2\right)\left(\frac{1}{2\pi|\mathbf{x}|}\right), \quad \mathbf{x}\in\mathbb{R}^2, \tag{1.5}$$

where $\nabla_\perp = (\partial_x, \partial_y)^T$, $\mathbf{n}_\perp = (n_1, n_2)^T$, $\partial_{\mathbf{n}_\perp} = \mathbf{n}_\perp\cdot\nabla_\perp$ and $\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} = \partial_{\mathbf{n}_\perp}(\partial_{\mathbf{n}_\perp})$. In fact, for smooth densities, the DDI potential can be reformulated via the Coulomb potential whose convolution kernel is $U_{\rm cou}(\mathbf{x}) = \frac{1}{2^{d-1}|\mathbf{x}|}$. To be precise, the 3D DDI potential (1.4) is reformulated as follows

$$\Phi_j(\mathbf{x}) = -\rho_j - 3\,\partial_{\mathbf{n}}\partial_{\mathbf{n}}\left(\frac{1}{4\pi|\mathbf{x}|} * \rho_j\right) = -\rho_j - 3\,\frac{1}{4\pi|\mathbf{x}|} * (\partial_{\mathbf{n}}\partial_{\mathbf{n}}\rho_j), \quad \mathbf{x}\in\mathbb{R}^3, \tag{1.6}$$

while the 2D DDI (1.5) is rewritten as

$$\Phi_j(\mathbf{x}) = -\frac{3}{2}\,\frac{1}{2\pi|\mathbf{x}|} * \left[\left(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\nabla_\perp^2\right)\rho_j\right], \quad \mathbf{x}\in\mathbb{R}^2. \tag{1.7}$$

The time dependent CGPE in (1.1)–(1.2) conserve two important quantities: the total *mass* (or *normalization*) of the wave function

$$\mathcal{N}(t) := \|\Psi(\mathbf{x},t)\|^2 = \mathcal{N}_1(t) + \mathcal{N}_2(t) \equiv \|\Psi(\mathbf{x},0)\|^2 = 1, \tag{1.8}$$

where $\mathcal{N}_j(t)$ is the mass of the jth component at time $t \ge 0$, which reads as

$$\mathcal{N}_j(t) := \int_{\mathbb{R}^d} |\psi_j(\mathbf{x},t)|^2 d\mathbf{x} \equiv \mathcal{N}_j(0), \quad j = 1, 2,\ t \ge 0, \tag{1.9}$$

and the *energy per particle*

$$\begin{aligned}\mathcal{E}(\Psi(\cdot,t)) = \int_{\mathbb{R}^d}\Big[\sum_{j=1}^{2}\Big(&\frac{1}{2}|\nabla\psi_j|^2 + V_j(\mathbf{x})|\psi_j|^2 + \frac{\beta_{ij}}{2}|\psi_j|^4 \\ &+ \frac{\lambda_{ij}}{2}\Phi_j|\psi_j|^2 - \Omega\,\psi_j^* L_z\psi_j\Big) \\ &+ \frac{1}{2}(\beta_{12}+\beta_{21})|\psi_1|^2|\psi_2|^2 \\ &+ \frac{1}{4}(\lambda_{12}+\lambda_{21})(\Phi_1|\psi_2|^2 + \Phi_2|\psi_1|^2)\Big]d\mathbf{x} \\ \equiv\ &\mathcal{E}(\Psi(\cdot,0)), \qquad t \ge 0.\end{aligned} \tag{1.10}$$

There have been extensive mathematical and numerical studies on the single-component dipolar BEC; we refer the reader to [28,30–37]. For the rotating two-component BEC without DDI, dynamics and stationary states have been studied in [38,39] and [40–42], respectively. Recently, there is growing interest from physicists for studying the properties of (non)-rotating two-component BEC with DDI [20–26,29,43]. However, up to now, there are few numerical studies on the rotating two-component BEC with DDI based on the CGPE (1.1)–(1.2). In this paper, we give an exhaustive mathematical study of new efficient numerical methods of the rotating two-component dipolar BECs.

To compute the dynamics, the main difficulties lie in the nonlocal DDI evaluation and proper treatment of the rotation term. As is shown before, the DDI can be computed via the Coulomb potential. On bounded rectangular domains with Dirichlet boundary conditions, the Discrete Sine Transform (DST) method applies directly [28,30]. However, the DST method requires a quite large computation domain in order to achieve a satisfactory accuracy. In 2014, Jiang et al. [44] proposed a NonUniform Fast Fourier Transform (NUFFT) solver by adopting the polar/spherical coordinates in the Fourier domain, we refer to [32,45] for extensions and applications in the context of Nonlinear Schrödinger equation (NLSE). Recently, using an accurate Gaussian-summation approximation of the convolution kernel, Zhang et al. [51] introduced an even more efficient and accurate method, which we shall refer to as GauSum solver hereafter. Both NUFFT and GauSum solver are fast algorithms with a complexity of $O(N\log N)$ where N is the total number of grid points. Compared with the NUFFT solver, the GauSum solver is 3–5 times faster, thus it is the state-of-the-art method for applications [46]. For the rotation term, Bao et al. [47] developed a rotating Lagrangian coordinates transformation method to reformulate the rotating term into a time-dependent trapping potential, and this method allows for the implementation of high order time marching schemes [48–50]. Note that in Eulerian coordinates, additional efforts have to be made for the rotational term. In the literature, to discretize the rotational term, popular approaches either introduce ADI technique or use polar/spherical coordinate. The former method introduces extra splitting error and is complicated to be extended to higher order time marching schemes, while the later imposes artificial boundary at the origin point $r = 0$ and the radial direction is discretized by lower order schemes, for example finite difference method (FDM) and finite element method (FEM).

The main objectives of this paper are threefold.

1. Using the rotating Lagrangian coordinates transform [47], we reformulate the original CGPE into new equations without rotating term. Then we develop a robust and efficient numerical method to compute dynamics of the new equations by incorporating the GauSum solver [51], which is designed to compute the nonlocal DDI, into an adapted version of the time-splitting Fourier pseudospectral method. Detailed numerical results are presented that confirm the spectral accuracy in space and second order temporal accuracy of the proposed method in 2D and 3D respectively.

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