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A normalized gradient flow method with attractive–repulsive splitting for computing ground states of Bose–Einstein condensates with higher-order interaction

Xinran Ruan

Department of Mathematics, National University of Singapore, Singapore 119076, Singapore

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ABSTRACT

In this paper, we generalize the normalized gradient flow method to compute the ground states of Bose–Einstein condensates (BEC) with higher order interactions (HOI), which is modeled via the modified Gross–Pitaevskii equation (MGPE). Schemes constructed in naive ways suffer from severe stability problems due to the high restrictions on time steps. To build an efficient and stable scheme, we split the HOI term into two parts with each part treated separately. The part corresponding to a repulsive/positive energy is treated semi-implicitly while the one corresponding to an attractive/negative energy is treated fully explicitly. Based on the splitting, we construct the BEFD-splitting and BESP-splitting schemes. A variety of numerical experiments show that the splitting will improve the stability of the schemes significantly. Besides, we will show that the methods can be applied to multidimensional problems and to the computation of the first excited state as well.

1. Introduction

The Bose–Einstein condensate (BEC), which is a many body system with low density and low temperature, has drawn great attention since its first experimental realization in 1995 [1,18,26] as it offers a way to measure the microscopic quantum mechanical properties in a macroscopic scale. The Gross–Pitaevskii equation (GPE), which is a mean field approximation by approximating the interaction between particles by an external pseudo-potential [30,32,33,35,36], has gained considerable research interest due to its simplicity and effectiveness in describing Bose–Einstein condensates (BEC). One key assumption in deriving GPE is that the interaction between particles can be well approximated by the binary interaction in the form

$$V_{\text{int}}(\mathbf{x}_1 - \mathbf{x}_2) = g_0\delta(\mathbf{x}_1 - \mathbf{x}_2), \quad \mathbf{x}_1, \mathbf{x}_2 \in \mathbb{R}^3, \tag{1.1}$$

where $\delta(\cdot)$ is the Dirac delta function and $g_0 = \frac{4\pi\hbar^2 a_s}{m}$ is the contact interaction strength with a_s being the s-wave scattering length, $\hbar$ being the reduced Planck constant and m being the mass of the particle [32]. The theory has shown excellent agreement with most experiments. However, the validity of the approximation needs to be carefully examined in certain cases, such as in the experiments which take advantage of the Feshbach resonances in cold atomic collision [47]. In such

E-mail address: a0103426@u.nus.edu.

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cases, higher order interaction (HOI) (or effective range expansion) as a correction to the Dirac delta function has to be taken into account. In [23,27], the higher order interaction correction is analyzed and a new binary interaction is derived as

$$V_{\text{int}}(\mathbf{z}) = g_0\left[\delta(\mathbf{z}) + g_1\left(\delta(\mathbf{z})\nabla_{\mathbf{z}}^2 + \nabla_{\mathbf{z}}^2\delta(\mathbf{z})\right)\right], \tag{1.2}$$

where g_0 is defined as before, $\mathbf{z} = \mathbf{x}_1 - \mathbf{x}_2 \in \mathbb{R}^3$ and the HOI correction is given by the parameter $g_1 = \frac{a_s^2}{3} - \frac{a_s r_e}{2}$ with r_e being the effective range of the two-body interaction. When $r_e = \frac{2}{3}a_s$, it is for the hard sphere potential and reduces back to the classical case. In certain cases, g_1 can be extremely large [47] and, therefore, the HOI can no longer be ignored. With this new choice of the binary interaction (1.2), the modified Gross–Pitaveskii equation (MGPE) [29,28,23,37,41] is derived as

$$i\hbar\partial_t\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + Ng_0\left(|\psi|^2 + g_1\nabla^2|\psi|^2\right)\right]\psi,\ t \geq 0,\ \mathbf{x} \in \mathbb{R}^3 \tag{1.3}$$

where N is the number of particles, $V(\mathbf{x})$ is a real-valued external trapping potential and $\|\psi(\mathbf{x},t)\| := \sqrt{\int_{\mathbb{R}^d}|\psi(\mathbf{x},t)|^2\,d\mathbf{x}} = 1$.

In experiments, the confinement induced by the external potential might be strong in one or two directions. As a result, the BEC in 3D could be well described by the MGPE in 2D or 1D, respectively, by performing a proper dimension reduction [37,13,38]. Finally, we get the dimensionless modified GPE (MGPE) in d-dimensions ($d = 1, 2, 3$) as

$$i\partial_t\psi = \left[-\frac{1}{2}\Delta + V(\mathbf{x}) + \beta|\psi|^2 - \delta\Delta(|\psi|^2)\right]\psi, \quad t \geq 0,\ \mathbf{x} \in \mathbb{R}^d, \tag{1.4}$$

with energy

$$E(\psi(\cdot,t)) := \int_{\mathbb{R}^d}\left[\frac{1}{2}|\nabla\psi|^2 + V(\mathbf{x})|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{\delta}{2}|\nabla|\psi|^2|^2\right]d\mathbf{x}. \tag{1.5}$$

It is easy to check that the L_2-norm and the energy are conserved, i.e.

$$\|\psi(\cdot,t)\| \equiv \|\psi(\cdot,0)\|, \quad E(\psi(\cdot,t)) \equiv E(\psi(\cdot,0)). \tag{1.6}$$

A fundamental problem in studying BEC is to find its stationary states, especially the ground state which is the stationary state with the lowest energy. Mathematically speaking, the ground state $\phi_g^{\beta,\delta} := \phi_g^{\beta,\delta}(\mathbf{x})$ of the MGPE (1.4) is defined as the minimizer of the energy functional (1.5) under the normalization constraint, i.e.

$$\phi_g^{\beta,\delta} := \arg\min_{\phi\in S} E(\phi), \tag{1.7}$$

where S is defined as

$$S := \{\phi \mid \|\phi\| = 1, \quad E(\phi) < \infty\}. \tag{1.8}$$

$E_g^{\beta,\delta} := E(\phi_g^{\beta,\delta})$ is called the ground state energy. The Lagrangian of the problem (1.7) implies that the ground state $\phi_g^{\beta,\delta}$ satisfies the following nonlinear eigenvalue problem

$$\mu\phi = \left[-\frac{1}{2}\Delta + V(\mathbf{x}) + \beta|\phi|^2 - \delta\Delta(|\phi|^2)\right]\phi, \tag{1.9}$$

where the corresponding eigenvalue (also named chemical potential) μ can be computed as

$$\mu = \int_{\mathbb{R}^d}\left[\frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \beta|\phi|^4 + \delta\left|\nabla|\phi|^2\right|^2\right]d\mathbf{x}. \tag{1.10}$$

It is worth noticing that, when $\delta \neq 0$, the ground state exists if and only if $\delta > 0$ [10]. And the ground state can be chosen to be nonnegative. Furthermore, the ground state is unique if we have both $\beta > 0$ and $\delta > 0$ [10]. When $\delta = 0$, the MGPE degenerates to the GPE. And the existence and uniqueness of the ground state has been thoroughly studied and we refer the readers to [7,8,36]. Therefore, throughout the paper, we will only consider the case $\delta \geq 0$ for the computation of the ground state of MGPE and assume the ground state is real-valued.

Numerous numerical methods have been proposed to compute the ground state of the classical GPE, such as a Runge–Kutta spectral method with spectral discretization in space and Runge–Kutta type integration in time by Adhikari et al. in [34], Gauss–Seidel-type methods in [21] by Lin et al., a finite element method by directly minimizing the energy functional in [16] by Bao and Tang, a regularized newton method by Wu, Wen and Bao in [43], a preconditioned nonlinear conjugate gradient method [5] by Antoine et al., an adaptive finite element method [24] and a Riemannian conjugate gradient method [25] for the rotating BEC. Among all the methods, the normalized gradient flow method, also named the imaginary time