Journal of Computational Physics 343 (2017) 92–109

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Efficient spectral computation of the stationary states of rotating Bose–Einstein condensates by preconditioned nonlinear conjugate gradient methods

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ARTICLE INFO

Article history:
Received 6 November 2016
Received in revised form 20 March 2017
Accepted 15 April 2017
Available online 21 April 2017

Keywords:
Bose–Einstein condensation
Rotating Gross–Pitaevskii equation
Stationary states
Fourier spectral method
Steepest descent
Conjugate gradient
Optimization algorithms on Riemannian manifolds
Preconditioner

ABSTRACT

We propose a preconditioned nonlinear conjugate gradient method coupled with a spectral spatial discretization scheme for computing the ground states (GS) of rotating Bose–Einstein condensates (BEC), modeled by the Gross–Pitaevskii Equation (GPE). We first start by reviewing the classical gradient flow (also known as *imaginary time* (IMT)) method which considers the problem from the PDE standpoint, leading to numerically solve a dissipative equation. Based on this IMT equation, we analyze the forward Euler (FE), Crank–Nicolson (CN) and the classical backward Euler (BE) schemes for linear problems and recognize classical power iterations, allowing us to derive convergence rates. By considering the alternative point of view of minimization problems, we propose the preconditioned steepest descent (PSD) and conjugate gradient (PCG) methods for the GS computation of the GPE. We investigate the choice of the preconditioner, which plays a key role in the acceleration of the convergence process. The performance of the new algorithms is tested in 1D, 2D and 3D. We conclude that the PCG method outperforms all the previous methods, most particularly for 2D and 3D fast rotating BECs, while being simple to implement.

1. Introduction

Bose–Einstein Condensates (BECs) were first predicted theoretically by S.N. Bose and A. Einstein, before being realized experimentally in 1995 [4,20,28,31]. This state of matter has the interesting feature that macroscopic quantum physics properties can emerge and be observed in laboratory experiments. The literature on BECs has grown extremely fast over the last 20 years in atomic, molecular, optics and condensed matter physics, and applications from this new physics are starting to appear in quantum computation for instance [22]. Among the most important directions, a particular attention has been paid towards the understanding of the nucleation of vortices [1,21,37–39,41,48] and the properties of dipolar gases [13,14] or multi-components BECs [11–13]. At temperatures T which are much smaller than the critical temperature T_c, the macroscopic behavior of a BEC can be well described by a condensate wave function ψ which is solution to a Gross–Pitaevskii

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http://dx.doi.org/10.1016/j.jcp.2017.04.040
0021-9991/

Equation (GPE). Being able to compute efficiently the numerical solution of such a class of equations is therefore extremely useful. Among the most crucial questions are the calculations of stationary states, i.e. ground/excited states, and of the real-time dynamics [5,9,13,34,35].

To fully analyze a representative and nontrivial example that can be extended to other more general cases, we consider in this paper a BEC that can be modeled by the rotating (dimensionless) GPE. In this setting, the computation of a ground state of a d-dimensional BEC takes the form of a constrained minimization problem:

$$\text{Find} \quad \phi \in L^2(\mathbb{R}^d) \qquad \text{s.t.} \qquad \phi \in \underset{\|\phi\|=1}{\arg\min} E(\phi), \tag{1.1}$$

here $\|\phi\| = \int_{\mathbb{R}^d} |\phi|^2$ is the standard L^2-norm and E is the associated energy functional. Several approaches can be developed for computing the stationary state solution to the rotating GPE. For example, some techniques are based on appropriate discretizations of the continuous normalized gradient flow/imaginary-time formulation [3,7,9,13,15,19,25,26,49], leading to various iterative algorithms. These approaches are general and can be applied to many situations (dipolar interactions, multi-components GPEs...). We refer for instance to the recent freely distributed Matlab solver GPELab that provides the stationary states computation [6] (and real-time dynamics [8]) for a wide variety of GPEs based on the so-called BESP (Backward Euler pseudo-Spectral) scheme [7,9,13,15] (see also Sections 4 and 6). Other methods are related to the numerical solution of the nonlinear eigenvalue problem [32,46] or on optimization techniques under constraints [17,23,29,30]. As we will see below in Section 4, some connections exist between these approaches. Finally, a regularized Newton-type method was proposed recently in [47].

Optimization problems with orthogonal or normalization constraints also occur in different branches of computational science. An elementary but fundamental example is the case of a quadratic energy, where solving the minimization problem is equivalent to finding an eigenvector associated with the lowest eigenvalue of the symmetric matrix representing the quadratic form. A natural generalization is a class of orthogonalized minimization problems, which for a quadratic energy reduce to finding the N first eigenvectors of a matrix. Many problems in electronic structure theory are of this form, including the celebrated Kohn–Sham and Hartree–Fock models [24,44]. Correspondingly, a large amount of effort has been devoted to finding efficient discretization and minimization schemes. A workhorse of these approaches is the nonlinear preconditioned conjugate gradient method, developed in the 80s [40], as well as several variants of this (the Davidson algorithm, or the LOBPCG method [36]).

Although similar, there are significant differences between the mathematical structure of the problem in electronic structure theory and the Gross–Pitaevskii equation. In some respects, solving the GPE is easier: there is only one wavefunction (or only a few for multi-species gases), and the nonlinearity is often local (at least when dipolar effects are not taken into account), with a simpler mathematical form than many electronic structure models. On the other hand, the Gross–Pitaevskii equation describes the formation of vortices: the discretization schemes must represent these very accurately, and the energy landscape presents shallower minima, leading to a more difficult optimization problem.

In the present paper, we consider the constrained nonlinear conjugate gradient method for solving the rotating GPE (Section 2) with a pseudo-Spectral discretization scheme (see Section 3). This approach provides an efficient and robust way to solve the minimization problem. Before introducing the algorithm, we review in Section 4 the discretization of the gradient flow/imaginary-time equation by standard schemes (explicit/implicit Euler and Crank–Nicolson schemes). This enables us to make some interesting and meaningful connections between these approaches and some techniques related to eigenvalue problems, such as the power method. In Sections 5.1 and 5.2, we introduce the projected preconditioned steepest descent (PSD) and preconditioned conjugate gradient (PCG) methods for solving the minimization problem on the Riemannian manifold defined by the spherical constraints. In particular, we provide some formulae to compute the stepsize arising in such iterative methods to get the energy decay assumption fulfilled. The stopping criteria and convergence analysis are discussed in Sections 5.3 and 5.4. We then investigate the design of preconditioners (Section 5.5). In particular, we propose a new simple symmetrical combined preconditioner, denoted by P_C. In Section 6, we consider the numerical study of the minimization algorithms for the 1D, 2D and 3D GPEs (without and with rotation). We first propose in Section 6.1 a thorough analysis in the one-dimensional case. This shows that the PCG approach with combined preconditioner P_C and pseudo-Spectral discretization, called PCG_C method, outperforms all the other approaches, most particularly for very large nonlinearities. In Sections 6.2 and 6.3, we confirm these properties in 2D and 3D, respectively, and show how the PCG_C algorithm behaves with respect to increasing the rotation speed. Finally, Section 7 provides a conclusion.

2. Definitions and notations

For the considered minimization problem (1.1), the energy functional E is defined by

$$E(\phi) = \int_{\mathbb{R}^d} \left[\frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \frac{\eta}{2}|\phi|^4 - \omega\phi^* L_z \phi \right],$$

where V is an external potential, η is the nonlinearity strength, ω is the rotation speed, and $L_z = i(y\partial_x - x\partial_y)$ is the angular momentum operator.