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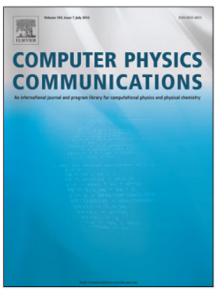

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Acceleration of the imaginary time method for spectrally computing the stationary states of Gross-Pitaevskii equations

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Abstract

The aim of this paper is to propose a simple accelerated spectral gradient flow formulation for solving the Gross-Pitaevskii Equation (GPE) when computing the stationary states of Bose-Einstein Condensates. The new algorithm, based on the recent iPiano minimization algorithm [36], converges three to four times faster than the standard implicit gradient scheme. To support the method, we provide a complete numerical study for 1d-2d-3d GPEs, including rotation and dipolar terms.

Keywords: Bose-Einstein condensation; rotating Gross-Pitaevskii equation; stationary states; imaginary time formulation; accelerated gradient; pseudospectral approximation.

1. Introduction

At temperatures T which are smaller than the critical temperature T_c, the Gross-Pitaevskii equation (GPE) can be used to model the behavior of Bose-Einstein Condensates (BECs). The first experimental realization of BECs was in 1995 [4, 8, 17, 24, 27] while they were theoretically predicted seventy years before by S.N. Bose and A. Einstein. This state of matter leads to the possibility of studying quantum physics at the macroscopic scale. Later, the nucleation of quantum vortices was observed [1, 18, 31, 32, 33, 37, 41] leading to the understanding of such BECs, modeled by the rotating GPE. More precisely, for a given initial data $\psi(t=0,\mathbf{x}) = \psi_0(\mathbf{x})$, a rotating BEC is represented by a wave function $\psi(t,\mathbf{x})$ solution to the dimensionless time-dependent GPE [8, 12]

$$i\partial_t \psi(t,\mathbf{x}) = -\frac{1}{2}\Delta\psi(t,\mathbf{x}) + V(\mathbf{x})\psi(t,\mathbf{x}) + \beta|\psi(t,\mathbf{x})|^2\psi(t,\mathbf{x}) - \mathbf{\Omega}\cdot\mathbf{L}\psi(t,\mathbf{x}), \tag{1}$$

for $\mathbf{x}\in\mathbb{R}^d$, $d=1,2,3$, $t>0$ and $\Delta := \sum_{j=1}^d \partial^2_{x_j}$. The function V is the confining potential. The parameter β is the nonlinearity strength that describes the (attractive or repulsive) interactions between atoms within the condensate. Essentially, we consider a cubic nonlinearity but the case of dipolar gases [8, 12] is also analyzed at the end of the paper to show that our contribution is general. In order to obtain the nucleation of vortices [1, 18, 31, 32, 33, 37, 41], the following rotating term is added

$$\mathbf{\Omega}\cdot\mathbf{L} = \Omega L_z = -i\Omega(x\partial_y - y\partial_x), \tag{2}$$

assuming $\mathbf{\Omega} = (0,0,\Omega)^t$, Ω being called the rotational velocity.

In this paper, we wish to compute the stationary states of the GPE, i.e. a solution of the form

$$\psi(t,\mathbf{x}) = e^{-i\mu t}\phi(\mathbf{x}), \tag{3}$$

where μ is the chemical potential and ϕ is a function that only depends on $\mathbf{x}$. By using equation (1), we deduce a nonlinear elliptic equation which reads as

$$\mu\phi(\mathbf{x}) = -\frac{1}{2}\Delta\phi(\mathbf{x}) + V(\mathbf{x})\phi(\mathbf{x}) + \beta|\phi(\mathbf{x})|^2\phi(\mathbf{x}) - \Omega L_z\phi(\mathbf{x}), \tag{4}$$

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