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A Multigrid Method for Ground State Solution of Bose-Einstein Condensates

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Abstract. A multigrid method is proposed to compute the ground state solution of Bose-Einstein condensations by the finite element method based on the multilevel correction for eigenvalue problems and the multigrid method for linear boundary value problems. In this scheme, obtaining the optimal approximation for the ground state solution of Bose-Einstein condensates includes a sequence of solutions of the linear boundary value problems by the multigrid method on the multilevel meshes and some solutions of nonlinear eigenvalue problems some very low dimensional finite element space. The total computational work of this scheme can reach almost the same optimal order as solving the corresponding linear boundary value problem. Therefore, this type of multigrid scheme can improve the overall efficiency for the simulation of Bose-Einstein condensations. Some numerical experiments are provided to validate the efficiency of the proposed method.

AMS subject classifications: 65N30, 65N25, 65L15, 65B99

Key words: BEC, GPE, eigenvalue problem, multigrid, multilevel correction, finite element method.

1 Introduction

Bose-Einstein condensation (BEC), which is a gas of bosons that are in the same quantum state, is an active field [6,23,29]. In 2001, the Nobel Prize in Physics was awarded Eric A. Cornell, Wolfgang Ketterle and Carl E. Wieman [4,19,29] for their research in BEC. The properties of the condensate at zero or very low temperature [20,31] can be described by the well-known Gross-Pitaevskii equation (GPE) [24,28] which is a time-independent

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nonlinear Schrödinger equation [30]. So far, it is found that the GPE fits well for most of experiments [5, 18, 20, 26].

As we know that the wave function ψ of a sufficiently dilute condensates satisfies the following GPE

$$\left(-\frac{\hbar^2}{2m}\Delta+\widetilde{W}+\frac{4\pi\hbar^2 aN}{m}|\psi|^2\right)\psi=\mu\psi, \tag{1.1}$$

where $\widetilde{W}$ is the external potential, μ is the chemical potential and N is the number of atoms in the condensate. The effective two-body interaction is $4\pi\hbar^2 a/m$, where $\hbar$ is the Plank constant, a is the scattering length (positive for repulsive interaction and negative for attractive interaction) and m is the particle mass. In this paper, we assume the external potential $\widetilde{W}(x)$ is measurable and locally bounded and tends to infinity as $|x|\rightarrow\infty$ in the sense that

$$\inf_{|x|\geq r}\widetilde{W}(x)\rightarrow\infty \quad \text{for } r\rightarrow\infty.$$

Then the wave function ψ must vanish exponentially fast as $|x|\rightarrow\infty$. Furthermore, Eq. (1.1) can be written as

$$\left(-\Delta+\frac{2m}{\hbar^2}\widetilde{W}+8\pi aN|\psi|^2\right)\psi=\frac{2m\mu}{\hbar^2}\psi. \tag{1.2}$$

Hence in this paper, we are concerned with the following non-dimensionalized GPE problem:

Find $(\lambda,u)\in\mathbb{R}\times H^1(\Omega)$ such that

$$\begin{cases} -\Delta u+Wu+\zeta|u|^2u=\lambda u, & \text{in } \Omega,\\ u=0, & \text{on } \partial\Omega,\\ \int_\Omega |u|^2 d\Omega=1, \end{cases} \tag{1.3}$$

where $\Omega\subset\mathbb{R}^d$ $(d=1,2,3)$ denotes the computing domain which has the cone property [1], ζ is some positive constant and $W(x)=\gamma_1x_1^2+\cdots+\gamma_dx_d^2\geq 0$ with $\gamma_1,\cdots,\gamma_d>0$ [8, 39].

So far, there exist many papers discussing the numerical methods for the time-dependent GPEs and time-independent GPEs. Please refer to the papers [2, 3, 5–8, 13, 16, 18–22, 29, 34] and the papers cited therein. Especially, in [39], the convergence of the finite element method for GPEs was proved and a prior error estimates presented in [12] which will be used in this paper. In [14, 15, 27], two-grid finite element methods for GPE have been proposed and analyzed.

Recently, a type of multigrid method for eigenvalue problems has been proposed in [32, 35–37]. The aim of this paper is to present a multigrid scheme for GPE (1.3) based on the multilevel correction method in [32]. With this method, solving GPE will has