INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 16, Number 5, Pages 789–803

AN EFFICIENT MULTIGRID METHOD FOR GROUND STATE SOLUTION OF BOSE-EINSTEIN CONDENSATES

NING ZHANG, FEI XU, AND HEHU XIE

Abstract. An efficient multigrid method is proposed to compute the ground state solution of Bose-Einstein condensations by the finite element method based on the combination of the multigrid method for nonlinear eigenvalue problem and an efficient implementation for the nonlinear iteration. The proposed numerical method not only has the optimal convergence rate, but also has the asymptotically optimal computational efficiency which is independent from the nonlinearity of the problem. The independence from the nonlinearity means that the asymptotic estimate of the computational work can reach almost the same as that of solving the corresponding linear boundary value problem by the multigrid method. Some numerical experiments are provided to validate the efficiency of the proposed method.

Key words. BEC, GPE, nonlinear eigenvalue problem, multigrid, tensor, finite element method, asymptotically optimal efficiency.

1. Introduction

It is well known that Bose-Einstein condensation (BEC), which is a gas of bosons that are in the same quantum state, is an important and active field [2, 3, 4, 12, 19] in physics. The properties of the condensate at zero or very low temperature [13, 21] can be described by the well-known Gross-Pitaevskii equation (GPE) [15] which is a time-independent nonlinear Schrödinger equation [20].

Since this paper considers the numerical method for the nonlinear eigenvalue problem, we are concerned with the following non-dimensionalized GPE problem: Find $\lambda \in \mathbb{R}$ and a function u such that

$$
(1) \qquad \left\{ \begin{array}{rcll} -\Delta u + Wu + \zeta |u|^2 u &=& \lambda u, & \text{in } \Omega, \\ u &=& 0, & \text{on } \partial\Omega, \\ \int_\Omega |u|^2 d\Omega &=& 1, & \end{array} \right.
$$

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 $W(x) = \gamma_1 x_1^2 + \ldots + \gamma_d x_d^2 \geq 0$ with $\gamma_1, \ldots, \gamma_d > 0$ [5, 29]. It is well known that the ground state solution for (1) is unique.

The convergence of the finite element method for GPEs is first proved in [29] and [8] gives prior error estimates which will be used in the analysis of our method. There also exist two-grid finite element methods for GPE in [9, 10, 17]. Recently, a type of multigrid method for eigenvalue problems has been proposed in [22, 24, 25, 26, 27]. Especially, [27] gives a multigrid method for GPE (1) and the corresponding error estimates. This type of multigrid method is designed based on the multilevel correction method in [22], and a sequence of nested finite element spaces with different levels of accuracy which can be built in the same way as the multilevel method for boundary value problems [28]. The corresponding error estimates have already been obtained in [27]. Furthermore, the estimate of computational work has also been given in [27]. The computational work of the multigrid in [27] is linear

Received by the editors May 8, 2018 and, in revised form, November 23, 2018.
2000 *Mathematics Subject Classification.* 65N30, 65N25, 65L15, 65B99.

scale but depends on the nonlinearity (i.e. the value of ζ) in some sense. The aim of this paper is to improve the efficiency further with a special implementing method for the multigrid iteration by using the tensor tool [14] for the GPE. With the tensor tool, the nonlinear iteration can be implemented only in the coarsest mesh and needs very small computational work. By using the proposed implementing technique, the multigrid method can really arrive the asymptotically optimal computational complexity which is almost independent of the nonlinearity of the GPE.

An outline of the paper goes as follows. In Section 2, we introduce finite element method for the ground state solution of BEC, i.e. non-dimensionalized GPE (1). A type of one correction step is given in Sections 3. In Section 4, we propose an efficient implementing technique for the nonlinear eigenvalue problem included in the one correction step. A type of multigrid algorithm for solving the non-dimensionalized GPE by the finite element method will be stated in Section 5. Three numerical examples are provided in Section 6 to validate the efficiency of the proposed numerical method in this paper. Some concluding remarks are given in the last section.

2. Finite element method for GPE problem

This section is devoted to introducing some notation and finite element method for the GPE (1). The letter C (with or without subscripts) denotes a generic positive constant which may be different at its different occurrences. For convenience, the symbols $\lesssim$, $\gtrsim$ and $\approx$ will be used in this paper. That $x_1 \lesssim y_1, x_2 \gtrsim y_2$ and $x_3 \approx y_3$, mean that $x_1 \leq C_1 y_1$, $x_2 \geq c_2 y_2$ and $c_3 x_3 \leq y_3 \leq C_3 x_3$ for some constants C_1, c_2, c_3 and C_3 that are independent of mesh sizes (see, e.g., [28]). The standard notation for the Sobolev spaces $W^{s,p}(\Omega)$ and their associated norms $\|\cdot\|_{s,p,\Omega}$ and seminorms $|\cdot|_{s,p,\Omega}$ (see, e.g., [1]) will be used. For $p = 2$, we denote $H^s(\Omega) = W^{s,2}(\Omega)$ and $H_0^1(\Omega) = \{v \in H^1(\Omega) : \ v|_{\partial\Omega} = 0\}$, where $v|_{\partial\Omega} = 0$ is in the sense of trace and $\|\cdot\|_{s,\Omega} = \|\cdot\|_{s,2,\Omega}$. In this paper, we set $V = H_0^1(\Omega)$ and use $\|\cdot\|_s$ to denote $\|\cdot\|_{s,\Omega}$ for simplicity.

For the aim of finite element discretization, we define the corresponding weak form for (1) as follows: Find $(\lambda, u) \in \mathbb{R} \times V$ such that $b(u, u) = 1$ and

$$a(u, v) = \lambda b(u, v), \quad \forall v \in V, \tag{2}$$

where

$$a(u, v) := \int_\Omega \big(\nabla u \nabla v + W uv + \zeta |u|^2 uv\big) d\Omega, \qquad b(u, v) := \int_\Omega uv d\Omega.$$

Now, let us define the finite element method [7, 11] for the problem (2). First we generate a shape-regular decomposition of the computing domain $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$ into triangles or rectangles for $d = 2$ (tetrahedrons or hexahedrons for $d = 3$). The diameter of a cell $K \in \mathcal{T}_h$ is denoted by h_K and define h as $h := \max_{K \in \mathcal{T}_h} h_K$. Then the corresponding linear finite element space $V_h \subset V$ can be built on the mesh $\mathcal{T}_h$. We assume that $V_h \subset V$ is a family of finite-dimensional spaces that satisfy the following assumption:

$$\lim_{h \to 0} \inf_{v_h \in V_h} \|w - v_h\|_1 = 0, \quad \forall w \in V. \tag{3}$$

The standard finite element method for (2) is to solve the following eigenvalue problem: Find $(\bar{\lambda}_h, \bar{u}_h) \in \mathbb{R} \times V_h$ such that $b(\bar{u}_h, \bar{u}_h) = 1$ and

$$a(\bar{u}_h, v_h) = \bar{\lambda}_h b(\bar{u}_h, v_h), \quad \forall v_h \in V_h. \tag{4}$$