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An Adaptive Finite Element Method with Hybrid Basis for Singularly Perturbed Nonlinear Eigenvalue Problems

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Abstract. In this paper, we propose an uniformly convergent adaptive finite element method with hybrid basis (AFEM-HB) for the discretization of singularly perturbed nonlinear eigenvalue problems under constraints with applications in Bose-Einstein condensation (BEC) and quantum chemistry. We begin with the time-independent Gross-Pitaevskii equation and show how to reformulate it into a singularly perturbed nonlinear eigenvalue problem under a constraint. Matched asymptotic approximations for the problem are reviewed to confirm the asymptotic behaviors of the solutions in the boundary/interior layer regions. By using the normalized gradient flow, we propose an adaptive finite element with hybrid basis to solve the singularly perturbed nonlinear eigenvalue problem. Our basis functions and the mesh are chosen adaptively to the small parameter ε. Extensive numerical results are reported to show the uniform convergence property of our method. We also apply the AFEM-HB to compute the ground and excited states of BEC with box/harmonic/optical lattice potential in the semiclassical regime ($0<\varepsilon\ll 1$). In addition, we give a detailed error analysis of our AFEM-HB to a simpler singularly perturbed two point boundary value problem, show that our method has a minimum uniform convergence order $\mathcal{O}(1/(N\ln N)^{\frac{2}{3}})$.

AMS subject classifications: 35P30, 35Q55, 65N25, 65N06, 65N30, 81Q05

Key words: Adaptive finite element, hybrid basis, nonlinear eigenvalue problem, singularly perturbed problem, Bose-Einstein condensation, uniform convergence.

1 Introduction

We consider the following nonlinear eigenvalue problem which is known as the time independent Gross-Pitaevskii equation (GPE) in Bose-Einstein condensation (BEC) [2, 4,

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9, 14]:

$$\mu\phi(\mathbf{x}) = -\frac{1}{2}\Delta\phi(\mathbf{x}) + V(\mathbf{x})\phi(\mathbf{x}) + \beta|\phi(\mathbf{x})|^2\phi(\mathbf{x}), \qquad \mathbf{x}\in\Omega, \tag{1.1}$$

$$\phi(\mathbf{x}) = 0, \qquad \mathbf{x}\in\partial\Omega, \tag{1.2}$$

where $\mathbf{x} = (x_1,\cdots,x_d)^T$ is the spatial coordinate, Ω is a subdomain of $\mathbb{R}^d$ ($d = 1,2,3$), $V(\mathbf{x})$ is a real-valued potential, and β is a constant. The wave function ϕ is required to satisfy the normalization condition

$$\|\phi\|^2 = \int_\Omega |\phi(\mathbf{x})|^2 d\mathbf{x} = 1. \tag{1.3}$$

The eigenvalue (chemical potential) μ is computed by

$$\mu(\phi) = \int_\Omega \left(\frac{1}{2}|\nabla\phi(\mathbf{x})|^2 + V(\mathbf{x})|\phi(\mathbf{x})|^2 + \beta|\phi(\mathbf{x})|^4\right) d\mathbf{x}. \tag{1.4}$$

The energy is computed by

$$E(\phi) = \int_\Omega \left(\frac{1}{2}|\nabla\phi(\mathbf{x})|^2 + V(\mathbf{x})|\phi(\mathbf{x})|^2 + \frac{\beta}{2}|\phi(\mathbf{x})|^4\right) d\mathbf{x}. \tag{1.5}$$

In fact, the nonlinear eigenvalue problem (1.1)-(1.2) can be viewed as the Euler-Lagrange equation of the energy functional $E(\phi)$ under the normalization constraint (1.3). In physical literatures [3, 11, 37], the ground state $\phi_g(\mathbf{x})$ and k-th excited state $\phi_k(\mathbf{x})$ are defined as the local minimizer of the energy functional over the unit sphere

$$S = \{\phi \,|\, \|\phi\| = 1,\ \ E(\phi) < \infty\}, \tag{1.6}$$

which are ranked according to their energies, i.e.,

$$E(\phi_g) < E(\phi_1) < E(\phi_2) < \cdots. \tag{1.7}$$

One of the fundamental problems in numerical simulation of BEC is to find its ground and excited states so as to compare the numerical results with experimental observations and to prepare initial data for studying the dynamics of BEC. Different numerical methods were proposed for computing the ground and excited states of BEC. For example, Bao and Du [9] presented a continuous normalized gradient flow with diminishing energy for computing the ground and first excited states in BEC. This idea was extended to multi-component BEC [4,10], rotating BEC [16], spin-1 BEC [7,12,15] and dipolar BEC [6]. Bao and Tang [14] proposed a method by directly minimizing the energy functional via finite element approximation to obtain the ground and excited states. Zhou [45, 46] and Shen and Zhou [42] provided error estimates for the finite element approximations for some nonlinear eigenvalue problems. In recent years, Zhou et al. [17, 24, 41] also used the adaptive finite element method to compute some eigenvalue problems arising in