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A Uniformly Convergent Numerical Method for Singularly Perturbed Nonlinear Eigenvalue Problems

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Abstract. In this paper we propose a uniformly convergent numerical method for discretizing singularly perturbed nonlinear eigenvalue problems under constraints with applications in Bose-Einstein condensation 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 presented to locate the positions and characterize the widths of boundary layers and/or interior layers in the solution. A uniformly convergent numerical method is proposed by using the normalized gradient flow and piecewise uniform mesh techniques based on the asymptotic approximations for the problem. Extensive numerical results are reported to demonstrate the effectiveness of our numerical method for the problems. Finally, the method is applied to compute ground and excited states of Bose-Einstein condensation in the semiclassical regime and some conclusive findings are reported.

AMS subject classifications: 35P30, 35Q55, 65N25, 65N06, 81Q05, 81V45

Key words: Nonlinear eigenvalue problem, Bose-Einstein condensation, ground state, excited state, energy, chemical potential, piecewise uniform mesh.

1 Introduction

We consider the following nonlinear eigenvalue problem [2, 5, 10]

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

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

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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 whose shape is determined by the type of system under investigation, and β is a constant. Eq. (1.1) is also known as the time-independent Gross-Pitaevskii equation (GPE) in Bose-Einstein condensation (BEC) [3, 7, 24], where ϕ is the macroscopic wave function of the condensate and β positive/negative corresponds to repulsive/attractive interaction between atoms. The wave function ϕ is required to satisfy the normalization condition

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

For the nonlinear eigenvalue problem (1.1)-(1.2) under the constraint (1.3), any eigenvalue μ which is also called as chemical potential in quantum physics can be computed from its corresponding eigenfunction ϕ by

$$\begin{aligned}\mu := \mu_\beta(\phi) &= \int_\Omega \left[\frac{1}{2}|\nabla\phi(\mathbf{x})|^2 + V(\mathbf{x})|\phi(\mathbf{x})|^2 + \beta|\phi(\mathbf{x})|^4\right] d\mathbf{x} \\ &= E_\beta(\phi) + \frac{\beta}{2}\int_\Omega |\phi(\mathbf{x})|^4 \, d\mathbf{x},\end{aligned} \tag{1.4}$$

where $E_\beta(\phi)$ is the energy per particle in BEC and is defined as

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

In fact, the nonlinear eigenvalue problem (1.1)-(1.2) can be viewed as the Euler-Lagrange equation of the energy functional $E_\beta(\phi)$ in (1.5) under the constraint (1.3). In physics literatures [3, 7, 24], the ground state is defined as the minimizer of the energy functional in (1.5) over the unit sphere

$$S = \{\phi \mid \|\phi\| = 1, \quad E_\beta(\phi) < \infty\}.$$

Any other eigenfunctions of the nonlinear eigenvalue problem (1.1)-(1.2) under the constraint (1.3), whose energy are greater than that of the ground state, are usually known as excited states.

Different numerical methods were proposed in the literatures for computing the eigenfunctions, i.e., ground and excited states, of the nonlinear eigenvalue problem (1.1)-(1.2) under the constraint (1.3). For example, Edwards and Burnett [21] presented a Runge-Kutta type method and used it to solve one dimensional (1D) and 3D ground states with spherical symmetry. Adhikari [1] used this approach to get the ground state solution of GPE in 2D with radial symmetry. Ruprecht et al. [26] used the Crank-Nicolson finite difference method for solving BEC ground state. Bao and Tang [10] proposed a method by directly minimizing the energy functional via finite element approximation to obtain the ground and excited states. Bao and Du [5] presented a continuous normalized gradient