Advances in Applied Mathematics and Mechanics
Adv. Appl. Math. Mech., Vol. **3**, No. 4, pp. 493-518

DOI: 10.4208/aamm.10-m1057
August 2011

Adaptive Finite Element Approximations for a Class of Nonlinear Eigenvalue Problems in Quantum Physics

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Received 24 September 2010; Accepted (in revised version) 21 December 2010

Available online 10 July 2011

Abstract. In this paper, we study an adaptive finite element method for a class of nonlinear eigenvalue problems resulting from quantum physics that may have a nonconvex energy functional. We prove the convergence of adaptive finite element approximations and present several numerical examples of micro-structure of matter calculations that support our theory.

AMS subject classifications: 35Q55, 65N15, 65N25, 65N30, 81Q05

Key words: Adaptive finite element, convergence, micro-structure, nonlinear eigenvalue.

1 Introduction

In this paper, we study adaptive finite element approximations for a class of nonlinear eigenvalue problems: find $(\lambda, u)\in\mathbb{R}\times H_0^1(\Omega)$ such that

$$\begin{cases} \big(-\alpha\Delta + V + \mathcal{N}(u^2)\big)u = \lambda u, & \text{in } \Omega, \\ \displaystyle\int_\Omega |u|^2 = Z, \end{cases} \tag{1.1}$$

where $\Omega\subset\mathbb{R}^3$, $Z\in\mathbb{N}$, $\alpha\in(0,\infty)$, $V:\Omega\to\mathbb{R}$ is a given function, $\mathcal{N}$ maps a nonnegative function over Ω to some function defined on Ω.

Many physical models for micro-structures of matter are nonlinear eigenvalue problems of type (1.1), for instance, the Thomas-Fermi-von Weizsäcker (TFW) type orbital-free model used for electronic structure calculations [15, 31, 41] and the Gross-Pitaevskii equation (GPE) describing the Bose-Einstein condensates (BEC) [4, 42]. In

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the context of simulations of electronic structure calculations, the basis functions used to discretize models like (1.1) are traditionally plane wave bases or typically Gaussian approximations of the eigenfunctions of a hydrogen-like operator. The former is very well adapted to solid state calculations and the latter is incredibly efficient for calculations of molecular systems. However, there are several disadvantages and limitations involved in such methods. For example, the boundary condition does not correspond to that of an actual system; extensive global communications in dealing with plane waves reduce the efficiency of a massive parallelization, which is necessary for complex systems; and the generation of a large supercell is needed for non-periodic systems, which certainly increases the computational cost. The finite element method uses local piecewise polynomial basis functions, which does not involve problems mentioned above and has several advantages. Although it uses more degrees of freedom than that of traditional methods, strictly local basis functions produce well structured sparse Hamiltonian matrices; arbitrary boundary conditions can be easily incorporated; more importantly, since ground state solutions oscillate obviously near the nuclei, it is relatively straightforward to implement adaptive refinement techniques for describing regions around nuclei or chemical bonds where the electron density varies rapidly, while treating the other zones with a coarser description, by which computational accuracy and efficiency can be well controlled. Thus it should be natural to apply adaptive finite element methods to solve nonlinear eigenvalue problems resulting from modeling electronic structures. Indeed the adaptive finite element method is a powerful approach to computing ground state energies and densities in quantum chemistry, materials science, molecular biology and nanosciences [5,30].

The basic idea of a standard adaptive finite element method is to repeat the following procedure until a certain accuracy is obtained:

$$\text{Solve} \rightarrow \text{Estimate} \rightarrow \text{Mark} \rightarrow \text{Refine}.$$

Adaptive finite element methods have been studied extensively since Babuška and Rheinboldt [3] and have been successful in the practice of engineering and scientific computing. In particular, Dörfler [21] presented the first multidimensional convergence result, which has been improved and generalized, see, e.g., [6,8,32–35,38] for linear boundary value problems, [11,16,20,27,28,39] for nonlinear boundary value problems, and [12,18,22–24] for linear eigenvalue problems. To our best knowledge, there has been no work on the convergence of adaptive finite element approximations for nonlinear eigenvalue problems, though some a priori error analyses of finite dimensional Galerkin discretizations for such nonlinear eigenvalue problems have been shown in [9,10,13,29,42,43].

In this paper, we shall present a posteriori error analysis of an adaptive finite element method for a class of nonlinear eigenvalue problems and prove that the adaptive finite element algorithm will produce a sequence of approximations that converge to exact ground state solutions. As an illustration, we shall also report several numerical experiments on electronic structure calculations based on the adaptive finite element discretization [5,15,30], which support our theory. Since the nonlinear term occurs,