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A LOCAL COMPUTATIONAL SCHEME FOR HIGHER ORDER FINITE ELEMENT EIGENVALUE APPROXIMATIONS

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Abstract. Based on some coupled discretizations, a local computational scheme is proposed and analyzed in this paper for a class of higher order finite element eigenvalue approximations. Its efficiency is proven by theoretical and numerical evidences. It is shown that the solution of an eigenvalue problem in a higher order finite element space may be reduced to the solution of an eigenvalue problem in a lower order finite element space, and the solutions of some linear algebraic systems in the higher order finite element space by some local and parallel procedure.

Key Words. Eigenvalue, finite element, higher order, local computation.

1. Introduction

Motivated by efficient eigenvalue computations in quantum chemistry, in this paper, a local computation scheme is proposed and analyzed for a class of higher order finite element eigenvalue approximations. With this new proposed scheme, solving an elliptic eigenvalue problem will not be much more difficult than the local solutions of some standard elliptic boundary value problem. Our scheme is an iterative approach, which is related to that in [18, 19]. The scheme in this paper, however, is based on global and local coupled discretizations.

It is well known that efficient electronic structure computations are usually desired in quantum chemistry and nano-materials computations. In modern electronic structure computations, the so-called density functional theory is fundamental, with which Kohn-Sham equations need to be solved [7, 15, 16, 17, 21]. Note that Kohn-Sham equations are nonlinear eigenvalue systems in three dimensions, the matrices resulting from both real space and reciprocal space techniques are large, and the number of eigenvalues and eigenvectors required is proportional to the number of atoms in the molecular system. Hence, an iteration procedure of solving a large number of eigenvalues of large scale linear systems must be involved. Moreover, in order to obtain the numerical solution with satisfactory accuracy, the number of iterations are usually very large, too. In a word, efficient electronic structure computations require large scale eigenvalue computing [7, 11, 16, 17, 22, 26, 29, 30]. Therefore, it is significant to improve the approximation accuracy or reduce the computational cost in solving such linear eigenvalue problems (in three dimensions) at each iteration step.

As the finite element method is one of most effective numerical methods, we shall consider to use the finite element scheme to discretize eigenvalue problems.

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Although the finite element method is capable of providing accurate solutions to both all-electron [27] and pseudopotential [6, 23] formulations of Kohn-Sham equations, its application to all-electron problems in molecules and solids has so far been limited by the large number of basis functions required to adequately describe all-electron solutions near nuclei, where the solutions can have cusps and oscillate rapidly [7, 22, 31, 34]. To make the finite element method to be competitive with conventional methods in the all-electron context, specialize basis functions, such as isolated atomic solutions or Gaussian functions, will likely need to be added to the standard finite element basis to increase the efficiency of the representation. In the context of pseudopotentional setting, however, the original Kohn-Sham equations become smooth and their solutions are much smoother and simpler [6, 7, 22, 23, 27]. Thus the finite element method with piecewise polynomial bases is immediately applicable. Since higher order finite elements are usually recommended when the data is smooth, it is very natural to apply a higher order finite element method to the pseudopotential formulation of Kohn-Sham equations. Indeed, the higher order finite element approach has been proved to be accurate and efficient in modern electronic structure computations (see, e.g., [1, 7, 14, 30, 31, 32, 34]).

The computational complexity of higher order finite element discretizations, however, is larger than that of lower order finite element discretizations. To reduce the complexity, in this paper, we will propose some new technique for fast higher order finite element eigenvalue approximations. This technique is based on our understanding of local behaviors of finite elements solutions to some elliptic problems. By using this technique, the computational complexity can be resolved through some coupled discretizations that can be carried out in local. The main idea of our new algorithm is to use a lower order finite element to approximate the low frequency of the solution and then to use some linear algebraic systems to correct the residual (which contains mostly high frequencies) in the higher order finite element space by some local and parallel procedure.

The central computation in solving Kohn-Sham equations is the repeated solution of the following model eigenvalue problem, which is also called as a Schrödinger equation, posed on a convex polygonal domain $\Omega \subset \mathbb{R}^3$:

$$\left\{ \begin{array}{rcl} -\Delta u + Vu & = & \lambda u \text{ in } \Omega, \\ u & = & 0 \text{ on } \partial\Omega, \end{array} \right. \tag{1.1}$$

where V is some potential function and is smooth in the pseudopotential setting.

Let us now use such a simple example to give a little more detailed but informal description of the main idea and the main result in this paper. Let $S_0^{h,1}(\Omega)$ and $S_0^{h,2}(\Omega)$, satisfying $S_0^{h,1}(\Omega) \subset S_0^{h,2}(\Omega) \subset H_0^1(\Omega)$, be the linear finite element space and the quadratic finite element space associated with a finite element grid $T^h(\Omega)$, respectively. We may employ the following algorithm to discretize (1.1) to obtain eigenvector approximations (on $\Omega_0 \subset \Omega$ locally) (see Section 3.1):

(1) Solve an eigenvalue problem in the linear finite element space: Find $\lambda_{h,1} \in \mathbb{R}^1, u_{h,1} \in S_0^{h,1}(\Omega)$ such that $\|u_{h,1}\|_{0,\Omega} = 1$ and

$$\int_\Omega (\nabla u_{h,1} \cdot \nabla v + V u_{h,1} v) = \lambda_{h,1} \int_\Omega u_{h,1} v \quad \forall v \in S_0^{h,1}(\Omega).$$