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A TWO-SCALE HIGHER-ORDER FINITE ELEMENT DISCRETIZATION FOR SCHRÖDINGER EQUATION*

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Abstract

In this paper, a two-scale higher-order finite element discretization scheme is proposed and analyzed for a Schrödinger equation on tensor product domains. With the scheme, the solution of the eigenvalue problem on a fine grid can be reduced to an eigenvalue problem on a much coarser grid together with some eigenvalue problems on partially fine grids. It is shown theoretically and numerically that the proposed two-scale higher-order scheme not only significantly reduces the number of degrees of freedom but also produces very accurate approximations.

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Key words: Higher-order, Finite element, Discretization, Eigenvalue, Schrödinger equation, Two-scale.

1. Introduction

Theoretical analysis of the electronic structure of matter is usually based on the energy-levels and wavefunctions of the many-body particle system. As a result, a number of eigenvalues and eigenfunctions of the Schrödinger type equations are required to be computed accurately and efficiently. However, it is a challenging task to solve multi-dimensional eigenvalue problems by conventional discretization methods, due to storage requirements and computational complexity.

In order to reduce the computational costs, such as the computational time and the storage requirement, we will introduce a two-scale higher-order finite element discretization scheme to solve the associated eigenvalue problem. With the scheme, the solution of the eigenvalue problem on a fine grid can be reduced to an eigenvalue problem on a much coarser grid and some eigenvalue problems on partially fine grids. It is shown by both theory and numerics that the scheme is efficient. The work of this paper may be viewed as a generalization of that in [14, 21, 22], in which some two-scale linear finite element discretizations for solving partial differential equations in multi-dimensions were developed.

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In the modern electronic structure computation of large scale, the pseudopotential formulations of the Kohn-Sham equations should be used. Note that in the pseudopotentional setting, the associated effective potentials of the Kohn-Sham equations are smooth [4, 5, 23, 24, 27], though the original effective potentials are singular. Hence we may start our investigation from the following Schrödinger equation:

$$\begin{cases} -\frac{1}{2}\Delta u + Vu = \lambda u & \text{in} \quad \Omega, \\ \qquad\qquad u = 0 & \text{on} \quad \partial\Omega, \end{cases} \tag{1.1}$$

where $\Omega = (0,1)^3$ and the effective potential V is smooth, say, $V \in W^{1,\infty}(\Omega)$.

We now give a somewhat more detailed description of the main ideas and results in this paper. Let $S_0^{h_1,h_2,h_3}(\Omega) \subset H_0^1(\Omega)$ be the standard triquadratic finite element space associated with the finite element mesh $T^{h_1,h_2,h_3}(\Omega)$ with mesh size h_1 in x-direction, h_2 in y-direction and h_3 in z-direction, respectively. One prototype scheme to discretize (1.1), say for the first eigenvalue λ with its corresponding eigenfunction u with $\int_\Omega |u|^2 = 1$, is as follows:

1. Solve (1.1) on a globally coarse grid: Find $(u_{H,H,H}, \lambda_{H,H,H}) \in S_0^{H,H,H}(\Omega) \times \mathbb{R}$ such that $\int_\Omega |u_{H,H,H}|^2 = 1$ and

$$\int_\Omega \frac{1}{2}\nabla u_{H,H,H} \cdot \nabla v + V u_{H,H,H} \cdot v = \lambda_{H,H,H} \int_\Omega u_{H,H,H} \cdot v, \quad \forall v \in S_0^{H,H,H}(\Omega).$$

2. Solve (1.1) on some partially fine grids in parallel:
   Find $(u_{h,H,H}, \lambda_{h,H,H}) \in S_0^{h,H,H}(\Omega) \times \mathbb{R}$ such that $\int_\Omega |u_{h,H,H}|^2 = 1$ and

$$\int_\Omega \frac{1}{2}\nabla u_{h,H,H} \cdot \nabla v + V u_{h,H,H} \cdot v = \lambda_{h,H,H} \int_\Omega u_{h,H,H} \cdot v, \quad \forall v \in S_0^{h,H,H}(\Omega);$$

   Find $(u_{H,h,H}, \lambda_{H,h,H}) \in S_0^{H,h,H}(\Omega) \times \mathbb{R}$ such that $\int_\Omega |u_{H,h,H}|^2 = 1$ and

$$\int_\Omega \frac{1}{2}\nabla u_{H,h,H} \cdot \nabla v + V u_{H,h,H} \cdot v = \lambda_{H,h,H} \int_\Omega u_{H,h,H} \cdot v, \quad \forall v \in S_0^{H,h,H}(\Omega);$$

   Find $(u_{H,H,h}, \lambda_{H,H,h}) \in S_0^{H,H,h}(\Omega) \times \mathbb{R}$ such that $\int_\Omega |u_{H,H,h}|^2 = 1$ and

$$\int_\Omega \frac{1}{2}\nabla u_{H,H,h} \cdot \nabla v + V u_{H,H,h} \cdot v = \lambda_{H,H,h} \int_\Omega u_{H,H,h} \cdot v, \quad \forall v \in S_0^{H,H,h}(\Omega).$$

3. Set

$$\begin{aligned} u_{H,H,H}^h &= u_{h,H,H} + u_{H,h,H} + u_{H,H,h} - 2u_{H,H,H}, \\ \lambda_{H,H,H}^h &= \lambda_{h,H,H} + \lambda_{H,h,H} + \lambda_{H,H,h} - 2\lambda_{H,H,H}. \end{aligned}$$

If, for example, $\lambda_{H,H,H}$, $\lambda_{h,H,H}$, $\lambda_{H,h,H}$, and $\lambda_{H,H,h}$ are the first eigenvalues of the corresponding problems, then we can establish the following results (see Theorem 4.1 in Section 4 below)

$$\left(\int_\Omega |u - u_{H,H,H}^h|^2\right)^{1/2} = \mathcal{O}(h^3 + H^5) \text{ and } |\lambda - \lambda_{H,H,H}^h| = \mathcal{O}(h^4 + H^6)$$