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A Nonnested Augmented Subspace Method for Kohn-Sham Equation

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Abstract. In this paper, a novel adaptive finite element method is proposed to solve the Kohn-Sham equation based on the moving mesh (nonnested mesh) adaptive technique and the augmented subspace method. Different from the classical self-consistent field iterative algorithm which requires solving the Kohn-Sham equation directly in each adaptive finite element space, our algorithm transforms the Kohn-Sham equation into some linear boundary value problems of the same scale in each adaptive finite element space, and then the wavefunctions derived from the linear boundary value problems are corrected by solving a small-scale Kohn-Sham equation defined in a low-dimensional augmented subspace. Since the new algorithm avoids solving large-scale Kohn-Sham equation directly, a significant improvement for the solving efficiency can be obtained. In addition, the adaptive moving mesh technique is used to generate the nonnested adaptive mesh for the nonnested augmented subspace method according to the singularity of the approximate wavefunctions. The modified Hessian matrix of the approximate wavefunctions is used as the metric matrix to redistribute the mesh. Through the moving mesh adaptive technique, the redistributed mesh is almost optimal. A number of numerical experiments are carried out to verify the efficiency and the accuracy of the proposed algorithm.

AMS subject classifications: 65N30, 65N25, 65L15, 65B99

Key words: Density functional theory, Kohn-Sham equation, nonnested mesh, augmented subspace method.

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1 Introduction

Density functional theory (DFT) is one of the major breakthroughs in quantum physics and quantum chemistry. In the framework of density functional theory, the many-body problem can be simplified as the motion of electrons without interaction in the effective potential field, which includes the Coulomb potential of the external potential field, the Hartree potential generated by the interaction between electrons, and the exchange-correlation potential for the nonclassical Coulomb interaction. For the exchange-correlation potential, it has always been a difficulty in density functional theory. At present, there is no exact analytical expression for the exchange-correlation potential. Generally, it is approximately described by the local density approximation (LDA), the local spin density approximation (LSDA) and the generalized gradient approximation (GGA), etc. The Kohn-Sham equation is one of the most important models in the calculation of electronic structure, which transforms the wavefunctions (in $\mathbb{R}^{3N}$ space) describing N particle states into density function (in $\mathbb{R}^3$ space), so as to reduce the degrees of freedom of equation and reduce the computational work of numerical simulation. The idea of Kohn-Sham equation can be traced back to Thomas-Fermi model in 1927. The model gave a primary description of the electronic structure of atoms. The strict theoretical analysis was described by Hohenberg and Kohn in [27], which proved the correctness and feasibility of using single electron orbit to replace the wavefunctions describing multiple electrons.

So far, lots of numerical methods for solving Kohn-Sham equation have been developed. For instance, plane-wave method [10,38] is the most popular method in the computational quantum chemistry community. Since the basis function is independent from the ionic position, plane-wave method has advantage in calculating intermolecular force. Combined with the pseudopotential method, plane-wave method plays an important role in the study of the ground and excited states calculations, and geometry optimization of the electronic structures. Although the plane-wave method is the most popular one in the computational quantum chemistry community, it is inefficient in solving non-periodic systems like molecules, nano-clusters, or materials systems with defects, etc. Furthermore, the plane-wave method uses the global basis which significantly affect the scalability on parallel computing platforms. The atomic-orbital-type basis sets [22,23] are also widely used for simulating materials systems such as molecules and clusters. However, they are well-suited only for isolated systems with special boundary conditions. It is difficult to develop a systematic basis-set for all materials systems. Thus over the past decades, more and more attentions are attracted to develop efficient and scalable grid-based methods such as the finite element method for electronic structure calculations. The advantages of grid-based methods include that it can use unstructured meshes and local basis sets, hence owing high scalability on parallel computing platforms. So far, the applications of the finite element method in solving Kohn-Sham equation have been studied systematically. We refer to [6, 8, 11, 36, 39, 42, 43, 45, 46, 50, 51, 53] and references therein for a comprehensive overview.