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Convergence and Complexity of an Adaptive Planewave Method for Eigenvalue Computations

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Abstract. In this paper, we study the adaptive planewave discretization for a cluster of eigenvalues of second-order elliptic partial differential equations. We first design an a posteriori error estimator and prove both the upper and lower bounds. Based on the a posteriori error estimator, we propose an adaptive planewave method. We then prove that the adaptive planewave approximations have the linear convergence rate and quasi-optimal complexity.

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Key words: Adaptive planewave method, convergence rate, complexity, eigenvalue.

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1 Introduction

The mathematical understanding of the adaptive computational methods has attracted much attention in mathematical community. An efficient and reliable a posteriori error estimator plays an essential role in adaptive methods. We particularly note that the a posteriori error estimates and the adaptive finite element methods have been extensively investigated (see, e.g., [4,5,10,11,13–17,19–21,23,26,29,30,32] and references cited therein). The spectral and the pseudospectral methods have been successfully applied in scientific and engineering computation, such as heat conduction, fluid dynamics, quantum physics and so on. For instance, the planewave discretization methods have been widely

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used in electronic structure calculations based on the Kohn-Sham equations [3,12,24,28]. However, for the planewave method, there is far less literature on the a posteriori error estimates and adaptive planewave approximations of the partial differential equations. We refer to [7, 18] for a posteriori error estimates, [22, 25] for the applications in electronic structure calculations, and [8,9] for the numerical analysis of linear elliptic source problems. There is no any reference on the numerical analysis for adaptive planewave approximations of eigenvalue problems up to now.

In this paper, we first design a residual-type a posteriori error estimator for the planewave approximations of a class of linear second-order elliptic eigenvalue problems. We prove that the error estimator can yield both the upper and lower bounds for the error of the approximations. Based on the a posteriori error estimator, we then propose an adaptive planewave method with the Dörfler marking strategy [17], which is a typical marking strategy used in adaptive finite element approximations and different from the adaptive planewave method by updating the energy cut-off for planewave discretizations in [25]. Following [15,16], by the perturbation arguments, we prove that the adaptive planewave approximations for a cluster of eigenvalues have the asymptotic linear convergence rate and asymptotic quasi-optimal complexity under some reasonable assumptions. More precisely, under the assumption that the initial planewave basis are sufficiently rich, we obtain that:

- the associated adaptive planewave approximate eigenspaces $\mathscr{M}_{\mathbb{G}_n}$ will converge to the exact eigenspaces $\mathscr{M}$ with some convergence rate (see Theorem 4.2):

  $$\delta_{H^1_p(\Omega)}(\mathscr{M},\mathscr{M}_{\mathbb{G}_n}) \lesssim \alpha^n,$$

  where $\alpha \in (0,1)$ is some constant.

- if $M(\lambda_{(i)}) \subset \mathcal{A}^s$ for $i=1,2,\ldots,m$ and the marked indexes are of minimal cardinality, the adaptive planewave approximations have a quasi-optimal complexity as follows (see Theorem 4.4):

  $$\delta_{H^1_p(\Omega)}(\mathscr{M},\mathscr{M}_{\mathbb{G}_n}) \lesssim (|\mathbb{G}_n| - |\mathbb{G}_0|)^{-s}.$$

We refer to Section 4 for more details.

The rest of this paper is organized as follows. In Section 2, we describe some basic notation and review the existing results of planewave approximations for a class of linear second-order elliptic source and eigenvalue problems that will be useful in our analysis. In Section 3, we present a posteriori error estimators from the relationship between the elliptic eigenvalue approximations with the associated source approximations. We then propose an adaptive planewave method and its feasible version for an elliptic eigenvalue problem. In Section 4, we analyze the asymptotic convergence and asymptotic quasi-optimal complexity of the adaptive planewave method. Finally, some conclusion remarks are given in Section 5.