

Adaptive Finite Element Eigenvalue Computations with Applications to Quantum Chemistry

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In this presentation, we will talk about some adaptive finite element approach to a class of singular eigenvalue problems and its applications to electronic structure study. We will report several numerical experiments in quantum chemistry, which show that our approach is efficient. This talk is based on some joint works with X. Dai, X. Gong, L. Shen, J. Xu, and D. Zhang.