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Split representation of adaptively compressed polarizability operator. (English) \[Zbl 07389178\]

Summary: The polarizability operator plays a central role in density functional perturbation theory and other perturbative treatment of first principle electronic structure theories. The cost of computing the polarizability operator generally scales as \(O(N_e^4)\) where \(N_e\) is the number of electrons in the system. The recently developed adaptively compressed polarizability operator (ACP) formulation [L. Lin, Z. Xu and L. Ying, Multiscale Model. Simul. 2017] reduces such complexity to \(O(N_e^3)\) in the context of phonon calculations with a large basis set for the first time, and demonstrates its effectiveness for model problems. In this paper, we improve the performance of the ACP formulation by splitting the polarizability into a near singular component that is statically compressed, and a smooth component that is adaptively compressed. The new split representation maintains the \(O(N_e^3)\) complexity, and accelerates nearly all components of the ACP formulation, including Chebyshev interpolation of energy levels, iterative solution of Sternheimer equations, and convergence of the Dyson equations. For simulation of real materials, we discuss how to incorporate nonlocal pseudopotentials and finite temperature effects. We demonstrate the effectiveness of our method using one-dimensional model problem in insulating and metallic regimes, as well as its accuracy for real molecules and solids.

MSC:

65F10 Iterative numerical methods for linear systems
65F30 Other matrix algorithms (MSC2010)
65Z05 Applications to the sciences

Keywords:
density functional perturbation theory; phonon calculations; vibration properties; adaptive compression; split representation; polarizability operator; sternheimer equation; Dyson equation

Software:
lobpcg.m; KSSOLV; AAA

Full Text: DOI

References:


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