Zhou, Yunkai; **Saad, Yousef**; **Tiago, Murilo L.**; **Chelikowsky, James R.**
Self-consistent-field calculations using Chebyshev-filtered subspace iteration. (English)
Zbl 1105.65111
J. Comput. Phys. 219, No. 1, 172-184 (2006).

Summary: The power of density functional theory is often limited by the high computational demand in solving an eigenvalue problem at each self-consistent-field (SCF) iteration. The method presented in this paper replaces the explicit eigenvalue calculations by an approximation of the wanted invariant subspace, obtained with the help of well-selected Chebyshev polynomial filters. In this approach, only the initial SCF iteration requires solving an eigenvalue problem, in order to provide a good initial subspace. In the remaining SCF iterations, no iterative eigensolvers are involved. Instead, Chebyshev polynomials are used to refine the subspace. The subspace iteration at each step is easily five to ten times faster than solving a corresponding eigenproblem by the most efficient eigen-algorithms. Moreover, the subspace iteration reaches self-consistency within roughly the same number of steps as an eigensolver-based approach. This results in a significantly faster SCF iteration.

MSC:

65N25	Numerical methods for eigenvalue problems for boundary value problems involving PDEs	Cited in **32** Documents
35P15	Estimates of eigenvalues in context of PDEs	
35P30	Nonlinear eigenvalue problems and nonlinear spectral theory for PDEs	

Keywords:

density functional theory; Chebyshev polynomial filter; subspace iteration; eigenproblem; real-space pseudopotential; numerical examples; Kohn-Sham equations; self-consistent-field iteration; eigenvalue; invariant subspace

Software:

ARPACK; eigs

Full Text: DOI