Diagonalization-free real space DFT calculations using Chebyshev filtered subspace iteration

Yunkai Zhou

Department of mathematics, Southern Methodist University
Dallas, Texas 75275, USA

The Chebyshev-filtered subspace iteration (CheFSI) method [1–5] has resulted in significant speedup over iterative diagonalization-based methods in DFT calculations. An order of magnitude speedup can be routinely obtained for material systems with thousands of atoms. However, the previous CheFSI method is not diagonalization-free. It resorts to iterative diagonalization at the first step of a self-consistent loop to provide initial vectors for the latter more efficient subspace filtering.

We propose a novel approach to completely avoid the expensive first-step diagonalization. This is achieved by suitably chosen polynomial filters. The new approach costs about half of the memory requirement of diagonalization-based methods. In addition, this filtering can provide better initial vectors than diagonalization-based methods, which reduces the overall self-consistency iteration steps.

[1] Y. Zhou, Y. Saad, M. L. Tiago, and J. R. Chelikowsky. Self-consistent-field calculation using Chebyshev-filtered subspace iteration. *J. Comput. Phys.*, 219(1):172–184, 2006.

[2] M. L. Tiago, Y. Zhou, M. Alemany, Y. Saad, and J. R. Chelikowsky. Evolution of magnetism in iron from the atom to the bulk. *Phys. Rev. Lett.*, 97:147201, 2006. *J. Comput. Phys.*, 219(1):172–184, 2006.

[3] Y. Zhou, Y. Saad, M. L. Tiago, and J. R. Chelikowsky. Parallel self-consistent-field calculations using Chebyshev-filtered subspace acceleration. *Phys. Rev. E*, 74(6):066704, 2006.

[4] M. Alemany, M. Jain, M. L. Tiago, Y. Zhou, Y. Saad, and J. R. Chelikowsky. Efficient first-principles calculations of the electronic structure of periodic systems. *Comp. Phys. Comm.*, 177(4):339–347, 2007.

[5] J. R. Chelikowsky, Y. Saad, T.-L. Chan, M. L. Tiago, A. T. Zayak, and Y. Zhou. Pseudopotentials on grids: Application to the electronic, optical, and vibrational properties of silicon nanocrystals. *J. Comput. Theoret. Nanoscience*, 6(6):1247–1261, 2009.