

Computation of Maximally Localized Wannier Functions and Compact Representations of Kohn-Sham Invariant Subspaces

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Maximally Localized Wannier Functions (MLWFs) are useful for computations of physical properties such as the polarization in insulators. They can be computed using iterative algorithms to minimize the wavefunction spread, but also by approximate simultaneous diagonalization of non-commuting matrices [1]. In large-scale electronic structure calculations, the cost of a simultaneous diagonalization scales as $O(N^3)$ for N electrons. This unfavorable scaling makes it necessary to develop efficient scalable algorithms for massively parallel computers. We present a new parallel algorithm for simultaneous diagonalization and demonstrate its scalability on up to 1024 processors for applications to the calculations of MLWFs.

Simultaneous diagonalization can also be used to compute reduced numerical representations of the solutions of the Kohn-Sham equations. We present a data compression method that allows for *a priori* control of the error caused by the reduction process. When applied to Kohn-Sham wavefunctions expanded on a plane-wave basis, this approach leads to a substantial reduction of the size of the datasets used to restart first-principles simulations, with controlled loss of accuracy. Examples of applications to liquid water and carbon nanotubes will be presented.

[1]F. Gygi, J.-L. Fattebert and E. Schwegler, Comput. Phys. Comm. 155, 1 (2003).