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Sub-linear scaling methods for electronic structure computations in materials.

Carlos J. García-Cervera.[1]

We introduce a class of sub-linear scaling algorithms for analyzing the electronic structure of crystalline solids with isolated defects based on a quantum-mechanical description of the system, in the context of Density Functional Theory (DFT).

Kohn-Sham DFT [1, 2, 3] is a very popular tool for electronic structure analysis, with applications in materials science, chemistry, and other areas. Compared with the quantum many-body problem, which describes a system with N electrons by a $3N$-dimensional antisymmetric wave function (ignoring spin degeneracy), the Kohn-Sham density functional theory describes such a system by N one-particle wave functions. By suitably approximating the functionals, Kohn-Sham DFT can become a very effective alternative to the quantum many-body problem, with satisfactory accuracy and much improved efficiency [4].

The Kohn-Sham equations are a system of nonlinear eigenvalue problems. The traditional self-consistent approach [2] for the solution of this eigenvalue problem consists of two nested iterations: in the inner iteration, the orbitals $\{\psi_j\}_{j=1}^N$ are obtained by a process of diagonalization and orthogonalization; in the outer iteration, the electron density is updated until self-consistency is reached. The diagonalization and/or orthogonalization procedure scales typically as $O(N^3)$, which is prohibitively expensive for relatively small problems.

I will describe in detail the linear scaling algorithm introduced in [5, 6]. The algorithm is based on a subspace iteration procedure with localized non-orthogonal wave functions.

Our fundamental assumption in our study of crystalline materials is that the positions of the atoms are distributed smoothly except for small isolated regions that contain defects. We use this smoothness assumption to perform asymptotic analysis of the DFT models, with arbitrarily high order accuracy. In the smooth region, we can then solve the DFT models to any specified accuracy requirement, by solving the asymptotic equations that we have derived. These asymptotic equations can be solved on coarse grids whose grid size depends only on the smoothness of the atomic positions and the error tolerance, not on the atomic spacing. The results can then be used to solve the problem for the non-smooth region – the solution in the smooth region provides the environment for solving for the electronic structure in the non-smooth region.

References

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[1]Mathematics Department
University of California, Santa Barbara, USA