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A Tensor-product approach for large scale electronic structure calculations using Kohn–Sham density functional theory

Motamarri, Phani, phanim@umich.edu, Gavini, Vikram, University of Michigan, United States; Blesgen, Thomas, Max-Planck-Institute for Mathematics in the Sciences, Germany

ABSTRACT

Quantum-mechanical calculations based on Kohn–Sham density functional theory (DFT) played a significant role in accurately predicting various aspects of materials behavior over the past decade. The Kohn–Sham approach to DFT reduces the many-body Schrodinger (eigen value) problem of interacting electrons into an equivalent problem of noninteracting electrons in an effective mean field that is governed by electron-density. Despite the reduced computational complexity of Kohn–Sham DFT, large-scale DFT calculations are still computationally very demanding with the resulting computational complexity scaling cubically with number of atoms in a given materials system. Numerical algorithms with reduced scaling behavior which are robust, computationally efficient and scalable on parallel computing architectures are always desirable to enable simulations at larger scales and on more complex systems. Following this line of thought, this study explores the use of tensor structured methods for ab-initio numerical solution of Kohn–Sham equations arising in DFT calculations. Earlier studies on tensor-structured methods have been quite successful in the accurate calculation of Hartree and the nonlocal exchange operators arising in the Hartree–Fock equations. A recent investigation of low-rank Tucker-type decomposition of the electron-density of large aluminum clusters (obtained from the finite-element discretization of orbital free DFT) shows the exponential decay of approximation error with respect to Tucker rank (number of tensor-basis functions in Tucker type representation). The results also indicate a smaller Tucker rank for the accurate representation of the electron density and is only weakly dependent on the system sizes studied. The promising success of tensor-structured techniques in resolving the electronic structure of material systems has enabled us to take a step further. In this study, we propose a systematic way of computing a globally adapted Tucker-type basis for solving the Kohn–Sham DFT problem by using a separable approximation of the Kohn–Sham Hamiltonian. Further, the resulting Kohn–Sham eigenvalue problem is projected into the aforementioned Tucker basis and is solved for ground-state energy using a self-consistent field iteration. The rank of the resulting Tucker representation and the computational complexity of the calculation are examined on representative benchmark examples involving metallic and insulating systems.