Self-Consistent Solution of Kohn-Sham Equation by Real-Space Finite-Difference Method

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Electronic-structure calculations play a fundamental role in predicting important physical (optical, electrical, etc) properties of condensed matter. Based on density functional theory (DFT), Kohn-Sham (KS) equation replaces the interacting many-body (electrons) problem by an equivalent set of self-consistent single-particle equations. Different from well-adopted basis set approach, we present a real-space finite-difference method to discretize the KS equation where the Laplacian operator is represented by high-order differences. After spatial discretization, a derived nonlinear eigenvalue problem is solved by a self-consistent field (SCF) iteration scheme with the update of electron density and potentials. In spite of the simplicity and versatility of the finite-difference method, one has to perform large-scale calculations of both eigenvalue and electrostatic problems at each iteration step. For eigenvalue problems, we minimize the Rayleigh quotients by the conjugate gradient method; and find minimum eigenvalues of interest through subspace diagonalization without Gram-Schmidt procedure. For obtaining electrostatic potentials, we use Dirichlet boundary condition to truncate the computational domain after inserting electron density and Gaussian compensating charge density together into Poisson's equation. Then a preconditioned Krylov subspace solver is employed to solve the Poisson's equation. A three-dimensional quantum dot with few spin-polarized electrons (each electron has spin up) is simulated by the real-space DFT incorporating local spin density (LSD) approximation. Wave function, electron density, eigen-energy, and total energy are calculated and compared to published results. The real-space finite-difference method produces reliable simulation results with a high computational efficiency. This work is fundamentally important to quantum-mechanical ab-initio calculation.

Numerical results of spin-polarized 6-electron quantum dot are presented with atomic units. Computational domain occupies $[-8, 8]^3$ with a grid size of 0.2; eigen-energies: {2.74, 3.07, 3.07, 3.07, 3.43, 3.43}; total energy: 13.01. The electron density and squared wave functions (1^{th}, 3^{th}, 6^{th} eigenstates) are shown.