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Heuristics for Accelerating Electronic Structure Calculations

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Under the Kohn-Sham density functional theory framework, the electron density (rho) associated with a ground state atomistic system can be obtained by solving the nonlinear equation rho=diag(f(H(rho))) where f is the Fermi-Dirac distribution function and H is the Kohn-Sham Hamiltonian. One way to solve this nonlinear equation is to apply a Broyden type of method. I will discuss a number of heuristics for constructing an effective Jacobian approximation and efficient ways to evaluate diag(f(H(rho))).