An Approximate Eigensolver for Self-Consistent Field Calculations

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We discuss an approximate solution method for the generalized eigenvalue problems arising for instance in the context of electronic structure computations based on density functional theory. The solution method is demonstrated to excel as compared to established solvers in both computational effort and scaling for parallelization. Furthermore, we estimate the error resulting from our proposed subspace method starting from the initial approximations for instance provided in the course of the self-consistent field iteration, showing that in general the approximation quality is improved by our method to yield sufficiently accurate eigenvalues.