Preconditioners for Electronic Structure Calculation

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Electronic structure calculations often require solving nonlinear equations by iterative methods. The convergence of these methods can be improved by using appropriate preconditioners. The construction of these preconditioners requires a good understanding of the Jacobian associated with the underlying nonlinear operator. For electronic structure calculations, properties of these Jacobians can often be revealed by performing perturbation analysis of a related eigenvalue problem. We will demonstrate this type of approach using two examples. One originates from a Kohn-Sham density functional theory based calculation, and the other originates from the coupled cluster approximation to the ground states of a many-electron system. We will show the benefit of using preconditioners constructed from perturbative analysis by numerical examples.

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