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"Solving Nonlinear Eigenvalue Problems in Electronic Structure Calculation"

Abstract:
One of the fundamental problems in electronic structure calculation is to determine electron orbitals associated with the minimum total energy of a large atomistic system. The total energy minimization problem is often formulated as a nonlinear eigenvalue problem and solved by an iterative procedure called the self-consistent field (SCF) iteration. In this talk, I will examine the convergence properties of the SCF iteration and present an alternative algorithm that minimizes the total energy directly. The key ingredients of the direct minimization algorithm involve projecting the total energy into a sequences of low dimensional subspaces and seeking the minimizer of the total energy within each subspace. The solution to each projected problem not only enables us to construct a good search direction along which the total energy decreases rapidly but also tells us how far we should move along the search direction. Numerical examples will be presented to demonstrate that this new direct minimization algorithm is more efficient and robust than the SCF iteration.

Friday, April 13, 2007
3:00 PM in 372 Jabara Hall

Please come join us for refreshments before the lecture
at 2:30 p.m. in room 353 Jabara Hall.