1057-65-316 **Chao Yang*** (cyang@lbl.gov), Lawrence Berkeley National Laboratory, MS-50F, 1 Cyclotron Rd, Berkeley, CA 94720. *Solving Nonlinear Eigenvalue Problems in Electronic Structure Calculations.*

One of the fundamental problems in electronic structure calculations is to determine the electron density associated with the minimum total energy of molecules, solids or other types of nanoscale materials. This can, in theory, be done by computing the smallest eigenvalue and the corresponding eigenfunction of a many-body Schrodinger's operator. However, such an approach is computationally infeasible except for systems with only a few electrons. Through the density functional theory formalism, the many-body eigenvalue problem can be reduced to a single particle eigenvalue problem with far fewer degrees of freedom. However, the eigenvalue problem is nonlinear in the sense that the matrix Hamiltonian to be diagonalized is a function of the eigenfunctions to be computed. In this talk, I will discuss a number of approaches for solving this type of problem and examine their convergence properties. (Received January 25, 2010)