Direct Minimzation and A Posteriori Error Estimators in Density Functional Theory

Reinhold Schneider
Institut für Mathematik, Technische Universität Berlin, Berlin
schneidr@math.tu-berlin.de

Density functional theory provides a simplified quantum mechanical model for the ground state an N-electron system inside the electro-static field given by fixed nuclei. It requires the minimization of the Kohn Sahm energy with respect to orthogonality between N unknown orbital functions. Usually this problem is treated by solving the canonical Kohn Sham equations which form a coupled nonlinear eigenvalue type problem. Alternatively, such kind of minimization problem could be solved by a projected preconditioned steepest decent iteration. We investigate the convergence of this direct minimization procedure. The present algorithm applies also for a simultanous computation of the first N eigenpairs. We present also an a posteriori analysis of the discretization of error in the energies.