

General correlated rotations and orbital correlation – some new concepts in electronic structure theory

Henrik Koch

Department of Chemistry
Norwegian University of Science and Technology
N-7014 Trondheim
Norway

Based on an alternative parameterization of state vectors we develop a novel approach to the approximate treatment of electron correlation. The main properties of this general correlated rotations (GCR) hierarchy are the uniform treatment of correlated orbitals, size extensivity, gauge invariance and the variational method to determine optimal parameters is computationally feasible. We argue that this hierarchy represents the natural generalization of the Hartree-Fock model to include electron correlation, as opposed to the standard linear or non-linear superposition of Slater determinants.