

Quasiparticle Pair Coupled Cluster and the Pairing Hamiltonian

Thomas M. Henderson

Department of Chemistry and Department of Physics and Astronomy, Rice University

While a conventional excitation-based truncation in coupled cluster theory yields an efficient description of dynamic correlations, it is much less effective for the description of strong static correlations where the mean-field picture breaks down. However, a seniority-based truncation in which spinorbitals are treated as pairs shows interesting potential as an alternative. Recently, Ayers and coworkers have shown that a simple pair coupled cluster doubles with optimized orbitals and pairing schemes gives results very similar to a pair full configuration interaction for a wide variety of systems. This connection breaks down when the effective two-body interaction is attractive rather than repulsive and the lowest energy mean-field breaks particle number symmetry. In this talk, I discuss the extension of pair coupled cluster theory to the case of a number broken reference and show results for the pairing Hamiltonian, which provides a useful model for the description of superconductivity.