Post-AGP Correlated Methods

Thomas M. Henderson

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

While the antisymmetrized geminal power (AGP) wave function has a long history in manybody physics, it is generally insufficiently accurate for chemical applications. What is needed, it would seem, is some way to incorporate correlations beyond those included in the simple AGP form. In this talk I will discuss several initial attempts to correlate AGP, designed in analogy with post-Hartree–Fock techniques. I will show applications to the pairing or reduced BCS Hamiltonian, which provides a useful model for the description of superconductivity and which greatly simplifies post-AGP calculations.