Correlated N-Particle States Totally Determined by One Particle Generalized Spin Orbitals

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The independent particle picture has been successfully utilized by chemists for more than half a century fundamentally because it allows the modeling of molecular structure and chemical reactions in an accessible pictorial manner. However it suffers from the drawback that it is based on an uncorrelated N-electron state, which often does not provide an accurate enough description of physical processes. A one electron theory of many electron systems that does explicitly describes electron-electron correlation may, however, be based on the observation that Antisymmetrized Geminal Power (AGP) states are *completely* characterized by a set of *unnormalized but orthogonal* Canonical General Spin Orbitals (CGSO's). This coupled with the observation that one can form a generalization of the independent particle Fock operator to express the total state energy in terms of ionization energies, kinetic energies and potential energies of these CGSOs leads to a one electron picture of chemical bonding that maintains the conceptual and pictorial advantages enjoyed by the independent particle model, while at the same time describing correlation. In this talk I will present some details of this correlated one particle theory.

Further, I will briefly review that AGP states have had a long history in quantum chemistry and physics ranging from their use in the analysis of the N-representability problem to their utilization in the description of many physical phenomena such as the determination of excitation energies and transition probabilities based on the Polarization Propagator, Superconductivity and the Fractional Quantum Hall Effect.