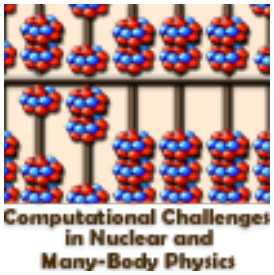

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Unconventional Coupled Cluster Theories for Strong and Weak Correlations

Coupled cluster (CC) theory with single and double excitations accurately describes weak electron correlation but is known to fail in cases of strong static correlation. Fascinatingly, however, pair coupled cluster doubles (p-CCD), a simplified version of the theory limited to pair excitations that preserve the seniority of the reference determinant (i.e., the number of unpaired electrons) has mean field computational cost and is an excellent approximation to the full configuration interaction (FCI) of the paired space provided that the orbital basis is optimized to adequately define a pairing scheme. In previous work [1], we have shown that optimization of the pairing scheme in the seniority zero FCI leads to a very accurate description of static correlation. The same conclusion extends to p-CCD [2] if the orbitals are optimized to make the p-CCD energy stationary [3]. The extension of this pair model to quasiparticles will be addressed [4]. We additionally discuss renormalized Hamiltonians via similarity transformation based on Gutzwiller projectors and other exponential forms to describe residual weak correlations [5].

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