

Coupled Cluster theory as a Local and Non-local method in Self-Energy Embedding Theory(SEET)

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We investigate the performance of Green's function coupled cluster singles and doubles (CCSD) method as a solver for Green's function embedding methods. To develop an efficient CC solver, we construct the one-particle Green's function from the coupled cluster (CC) wave function based on a non-hermitian Lanczos algorithm. We have tested the applicability of the CC Green's function solver in the weakly to strongly correlated regimes by employing it for a half-filled 1D Hubbard model projected onto a single site impurity problem and a half-filled 2D Hubbard model projected onto a 4-site impurity problem. For the 1D Hubbard model, for all interaction strengths, we observe an excellent agreement with the Exact Diagonalization (ED) technique, both for the self-energy and spectral function. For the 2D Hubbard, we have employed an open-shell version of the current implementation and observed some discrepancies from ED in the strongly correlated regime. Finally, on an example of a small ammonia cluster, we analyze the performance of the Green's function CCSD solver within the self-energy embedding theory (SEET) with Hartee-Fock (HF) and Green's function second order (GF2) for the treatment of the environment.

We have explored another situation where we seek to improve the non-local part of a problem by employing CC self-energy, instead of often used low-order perturbation theories, like GW or GF2. Here our target applications are for strongly correlated systems involving d- and f-elements.