Self-consistent second-order Green's function theory embedded into mean-field theory

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Abstract

Many-body Greens functions methods provide a direct way of calculating experimentally measurable electronic properties of the system. Self-consistent Green's function perturbation theory (GF2) provide a systematic way to study weakly correlated and many moderately strongly correlated systems. Unfortunately, the computational complexity of this technique makes calculations of large realistic systems unfeasible. Embedding methods in which the high-level description of the small subsystem is embedded into the environment described at low-level of theory have lower computational cost and in many cases can provide an accurate description of the electronic properties of both the embedded fragment and the total system. We have developed the simplest Green's function embedding theory in which GF2 is embedded into the mean-field theory (MF) such as Hartree–Fock (HF) or density functional theory (DFT). We call this embedding scheme GF2-in-MF. We will demonstrate the application of GF2-in-MF for covalently bounded and weakly interacting fragments. Additionally, we will show that the locality of electron-electron correlation allows for a reduction of the computational cost of calculations and thus provide a way to obtain correlated Green's functions for large realistic systems.