Correlation Energy Densities from Coupled Cluster Theory

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(Semi-)local density functional approximations (DFAs) are the workhorse electronic structure methods in condensed matter theory and surface science. Central to defining such DFAs is the exchange-correlation energy density e_{xc}, a spatial function that yields the exchange-correlation energy E_{xc} upon integration.

Unlike E_{xc}, e_{xc} is not uniquely defined. Indeed, there are infinitely many functions that integrate to the correct E_{xc} for a given electron density ρ. The challenge for constructing a useful DFA is to find a systematic connection between ρ and ε_{xc}. While several empirical and rigorous approaches to this problem are known, there has been little innovation with respect to the fundamental functional forms of DFAs in recent years.

Herein, we discuss a less explored route to constructing DFAs. Specifically, a recipe for deriving e_{xc} directly from many-body wavefunctions is presented. The corresponding energy densities are analyzed and (semi-)local approximations are presented. The extension to non-local DFAs will be discussed.