Modern Coupled Cluster Theory for the Uniform Electron Gas

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Condensed matter applications for quantum chemical techniques represent an important forefront for our field. The variation of the 'chemical environments' present in these systems present a substantial challenge to even sophisticated methods. Model systems, such as the uniform electron gas, allow us to test methods to gauge their suitability for development for use in the solid state and their simplicity allows for a more straightforward interpretation of the physics involved. This poster aims to examine the applicability of coupled cluster to studying these problems by applying them to the uniform (or homogeneous) electron gas model.

We examine:

(a) how to test for divergences arising in the correlation energy from approximate theories,

(b) a screened CCSD(T) model for highly accurate correlation energies,

(c) diagrammatic channels in the electron gas, and

(d) a new range-separation scheme for coupled cluster.

This builds on the wealth of known physics concerning the uniform electron gas, and particularly new exact ground-state energy benchmarks available from full configuration interaction quantum Monte Carlo.

This will draw on material from:

(1) Phys. Rev. Lett., 110, 226401 (2013);

(2) arXiv: 1310.6425;

(3) arXiv:1310.6806.