Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Developments in Coupled Cluster Theory for the Homogenous Electron Gas[1] JAMES J. SHEPHERD, TOM M. HENDERSON, Rice University, ANDREAS GRÜNEIS, University of Vienna, GUSTAVO E. SCUSERIA, Rice University — In a series of recent communications the correlation energy for the ground-state homogeneous electron gas has been precisely determined by full configuration interaction quantum Monte Carlo. The power of this new approach is that energies going beyond fixed-node approxmation and at finite basis set sizes are now available. This has opened up the possibility of benchmarking and further developing quantum chemical methods which involve finite basis sets for periodic systems, in particular coupled cluster theory. We will discuss: A) extensivity and divergences in approximate correlation energies, B) diagrammatic channels in the gas, and C) screening and range-separation in modern coupled cluster theory. This talk will draw on material from: 1) Phys. Rev. B 85, 081103 (2012); 2) Phys. Rev. B 86, 035111 (2012); 3) Phys. Rev. Lett., 110, 226401 (2013); 4) arXiv: 1310.6425; 5) arXiv:1310.6806.

[1]JJS thanks the Royal Commission for the Exhibition of 1851 for a Research Fellowship

James Shepherd
Rice University

Date submitted: 07 Nov 2013 Electronic form version 1.4