Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Full Configuration Interaction Quantum Monte Carlo and Diffusion Monte Carlo: A Comparative Study of the 3D Homogeneous Electron Gas JAMES J. SHEPHERD, PABLO LÓPEZ RÍOS, RICHARD J. NEEDS, University of Cambridge, UK, NEIL D. DRUMMOND, University of Lancaster, UK, JENNIFER A.-F. MOHR, University of Cambridge, UK, GEORGE H. BOOTH, Princeton University, USA, ANDREAS GRÜNEIS, GEORG KRESSE, University of Vienna, Austria, ALI ALAVI, University of Cambridge, UK — Full configuration interaction quantum Monte Carlo[1] (FCIQMC) and its initiator adaptation[2] allow for exact solutions to the Schrödinger equation to be obtained within a finite-basis wavefunction *ansatz*. In this talk, we explore an application of FCIQMC to the homogeneous electron gas (HEG). In particular we use these exact finite-basis energies to compare with approximate quantum chemical calculations from the VASP code[3]. After removing the basis set incompleteness error by extrapolation[4,5], we compare our energies with state-of-the-art diffusion Monte Carlo calculations from the CASINO package[6]. Using a combined approach of the two quantum Monte Carlo methods, we present the highest-accuracy thermodynamic (infinite-particle) limit energies for the HEG achieved to date. [1] G. H. Booth, A. Thom, and A. Alavi, J. Chem. Phys. 131, 054106 (2009). [2] D. Cleland, G. H. Booth, and A. Alavi, J. Chem. Phys. 132, 041103 (2010). [3] www.vasp.at (2012). [4] J. J. Shepherd, A. Grüneis, G. H. Booth, G. Kresse, and A. Alavi, Phys. Rev. B. 86, 035111 (2012). [5] J. J. Shepherd, G. H. Booth, and A. Alavi, J. Chem. Phys. 136, 244101 (2012). [6] R. Needs, M. Towler, N. Drummond, and P. L. Ríos, J. Phys.: Condensed Matter 22, 023201 (2010).

James J. Shepherd
University of Cambridge, UK

Date submitted: 03 Jan 2013 Electronic form version 1.4