



A Full Configuration Interaction (Quantum Monte Carlo) Perspective on the 3D Homogeneous Electron Gas

A TALK BY JAMES J. SHEPHERD

University of Cambridge, United Kingdom | http://www.alavi.ch.cam.ac.uk/members/james_shepherd/

DATE / TIME	Monday, 1 st of October 2012, 04:00 p.m. (CET)
LOCATION	Seminar Room 138C, Vienna University of Technology, "Freihaus"- building, 9th floor, "yellow" – Wiedner Hauptstraße 8-10, A-1040 Vienna, AUSTRIA)

James J. Sheperd | js615@cam.ac.uk

Computer modelling of electronic correlations is becoming an increasingly important tool in our understanding of materials, and there is a need for increasingly powerful and accurate numerical electronic-structure theories to sit alongside experiment and theoretical analysis. As computers approach the petascale era, this need is naturally best-filled by quantum Monte Carlo techniques, which can immediately take advantage of highly-parallel architectures.

Full configuration interaction quantum Monte Carlo (FCIQMC) is one such technique that efficiently finds the exact ground-state solution to the many-fermion Schrödinger equation by simulating a 'Game of Life, Death and Annihilation' in Slater determinant space. Here, this method is applied to the 3D homogeneous electron gas (HEG), a system for which other quantum Monte Carlo techniques have been developed over the past three decades yielding increasingly accurate ground-state energies and properties. In spite of such intense investigation -- is there a new perspective to be found? This question will be discussed in terms of new ground-state energies and analysis of the (FCI) wavefunction of the HEG.