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The Homogeneous Electron Gas: Beyond Fixed Nodes

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— The ground state energy of the homogeneous electron gas (HEG) still presents a significant challenge to Quantum Chemical methods, in spite of being a model Hamiltonian that has been studied for many decades and is often regarded as the archetypal system in solid state physics and in Fermi liquid theory. To date the only truly successful methods to yield accurate ground state energies at a range of densities have been quantum Monte Carlo techniques, in particular Diffusion Monte Carlo (DMC). Attempts to go beyond the fixed-node approximation have been met with some success, however elimination of this error all-together has not been achieved. Full Configuration Interaction (FCI) would provide an exact solution to this problem in the limit of an infinite basis set, which can be approached in a systematically improvable way. However, this is prohibitively expensive, scaling exponentially in the electron number and the size of the underlying one-electron basis with very large pre-factors. We present the application of a new method, FCI Quantum Monte Carlo, which stochastically samples the exact wavefunction producing FCI accuracy at a greatly improved computational cost, to the high-density HEG.

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