Accurate exchange-correlation energies for the warm dense electron gas from density matrix quantum Monte Carlo

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The exchange correlation energy of the uniform electron gas at finite temperature is required for a high quality temperature-dependent local density approximation functional [1,2].

Path integral quantum Monte Carlo methods can be used to obtain high accuracy energies at non-zero temperatures. Two different path integral methods, one based in real space (Brown et. al [3]) and the other in reciprocal/configuration space (Schoff et. al [4]), have recently been used to study warm dense gas. These studies have found significantly different energies (~10% E_{xc}) at high density (r_s = 1.0) for temperatures below the Fermi temperature.

Here, we attempt to resolve this disagreement by using an exact-on-average technique known as density matrix quantum Monte Carlo (DMQMC). This method, developed by Foulkes and coworkers [5], expands the density matrix in a complete basis of Slater determinant outer products. These are extremely numerous and are then sampled by a Monte Carlo scheme inspired by full configuration interaction quantum Monte Carlo [6].

This talk discusses first how specialized modifications were made to the DMQMC algorithm to study the warm dense electron gas [7], before moving on to examining the magnitude of numerical error in exchange correlation energies from current path integral calculations.

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