MONTE CARLO SIMULATION OF UNIFORM ELECTRON GAS: PAIR CORRELATION FUNCTIONS AND MOMENTUM DISTRIBUTIONS IN STRONGLY NON-IDEAL REGIME

Larkin A.S.,* Filinov V.S., Levashov P.R.

JIHT RAS, Moscow, Russia

**alexanderlarkin@rambler.ru*

The uniform electron gas (UEG) is a model system consisting of electrons and the homogeneous positive-charged neutralizing background. Being the quantum analogue of the one-component plasma, it reproduces many physical phenomena such as Wigner crystallization and screening. Also UEG is a simple model of alkali metals, a cornerstone in Fermi liquid theory and a workbench for the development of quantum Monte Carlo (QMC) methods. Also UEG properties are essential for density functional theory (DFT) being the source of the data for the exchangeâ€“correlation energy. A theoretical studies of the thermodynamical states of UEG with strong coupling and significant degeneracy are quite challenging due to inapplicability of the perturbative analytical approaches or classical molecular dynamics. Quantum Monte Carlo methods, based on path integral formalism, are much more suitable for this issue.

In this work we are using our numerical method SMPIMC (Single Momentum Path Integral Monte Carlo) to study some thermodynamical properties of the UEG in the regime of strong non-ideality ($\Gamma \lesssim 36$) with degeneracy varying from weak to significant ($kT = 0.5E_F$). We calculated the pair correlation functions, momentum distribution functions and average kinetic and potential energies. It was discovered that the momentum distribution function becomes wider than the Fermi distribution for the ideal system due to quantum effects, when coupling is high enough.