THERMODYNAMIC PROPERTIES OF UNIFORM ELECTRON GAS IN WARM DENSE MATTER REGIME: MONTE CARLO SIMULATIONS

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Uniform electron gas (UEG) is a model Coulomb system consisting of electrons and neutralizing positive-charged rigid background. Being one of the simplest quantum many-body Coulomb systems, it has important and various applications in modern physics, including general theory of Coulomb systems, physics of metals and density functional theory. Thermodynamic state of unpolarized UEG is usually characterized by two parameters — the Brueckner parameter and the reduced temperature:

$$r_s = \left(\frac{3}{4\pi n a_0^3}\right)^{1/3}, \quad \theta = \frac{kT}{E_F},$$

In the warm dense matter (WDM) regime, when the UEG is significantly non-ideal and degenerate, perturbative analytical approaches are not applicable, so the numerical simulation is required.

In this work we have been studied the UEG in WDM regime using the new single-momentum path integral Monte Carlo (SMPIMC) method. There are presented the results for the following thermodynamical properties and values: average energy (kinetic and potential), momentum distribution functions and pair correlation functions. The range of states corresponding to the values of r_s from 0.2 to several tens and θ from 4.0 to 0.5 is considered in detail. The influence of non-ideality on the momentum distribution functions has been discovered. When r_s increases from a certain value (at fixed θ), the momentum distribution functions deviate from the Fermi distribution towards larger momenta. It has been shown that the appearance of such high-momenta ¡¡tails¿¿ is associated with the appearance of maxima in the pair correlation functions, indicating the liquid-like behavior of the UEG. The work is supported by the Russian Science Foundation, grant No. 20-42-04421.