Thermodynamics of uniform electron gas at finite temperature by path integral Monte Carlo simulations with improved sign problem treatment

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In this work we study thermodynamic properties of uniform electron gas (UEG) over wide density and temperature range, using the improved fermionic-path-integral Monte Carlo (FPIMC) method. This method demonstrates a significant reduction of the "fermionic sign problem", which takes place in standard path-integral Monte Carlo simulations of degenerate fermionic systems. We introduce three basic improvements. The first one is the improved treatment of exchange interaction, achieved by the proper change of variables in the path-integral measure. The second improvement is the inclusion of long-range Coulomb effects into an angle-averaged effective potential, as proposed by E. Yakub and C. Ronchi. The third improvement is the angle-averaging of an exchange determinant, describing the fermionic exchange interaction not only between particles in the main Monte Carlo cell, but also with electrons in the nearest periodic images. The FPIMC shows very good agreement with analytical data for ideal Fermi gas. For strongly coupled UEG under warm dense matter conditions we obtain lower absolute values of the total and exchange-correlation energy in comparison with other Monte Carlo approaches. Pressure and entropy of non-ideal quantum UEG will be also presented.
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