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Ab Initio Quantum Monte Carlo Simulation of Warm Dense Electrons

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The accurate thermodynamic description of electrons using Quantum Monte Carlo (QMC) methods is of paramount importance for the theoretical description of warm dense matter – an exotic state that is of relevance for the description of astrophysical objects and inertial confinement fusion. Until recently, the most accurate QMC data were obtained using the fixed node approximation (RPIMC) [1]. Here we show how to perform ab initio QMC simulations of the uniform electron gas (UEG) without the fixed node approximation [2] and address the extrapolation to the thermodynamic limit [3].

These new results are subsequently used as input for the construction of a complete parametrization of the exchange-correlation free energy of the UEG with respect to density, temperature and spin-polarization covering the entire relevant parameter regime [4], thereby providing a complete thermodynamic description of the UEG [5]. We expect this new exchange-correlation functional to be of high importance as input for many applications, including thermal density functional theory simulations of warm dense matter and astrophysical models.

In addition, we investigate the effect of a harmonic perturbation, which allow us to obtain highly accurate data for the static density response (and, thus, the local field correction) of the warm dense electron gas [5,6] and compare our new results to dielectric approximations such as RPA and STLS.

References

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