Ab initio thermodynamic quantities of the strongly degenerate electron gas from Configuration Path Integral Monte-Carlo simulations

MICHAEL BONITZ, TIM SCHOOF, SIMON GROTH, Institute for Theoretical Physics and Astrophysics, CAU Kiel — Thermodynamic properties of the homogeneous electron gas (HEG) at finite temperatures are of high importance for many systems, including dense quantum plasmas, warm dense matter or plasmas in the interior of compact stars. Recently, Restricted Path Integral Monte-Carlo data for low to moderate densities ($r_s = \bar{r}/a_B \geq 1$) have been presented [1], while the high-density regime was not accessible due to the Fermion sign problem. Here we apply the recently developed Configuration PIMC (CPIMC) method [2,3] to the HEG at high densities ($r_s \leq 0.5$) and low to moderate temperatures ($\Theta = k_B T/E_F \leq 1$).

We demonstrate that CPIMC allows for efficient ab-initio equilibrium calculations of thermodynamic properties of highly degenerate, moderately coupled electrons. It is based on the representation of the N-particle density operator in a basis of antisymmetrized N-particle states [2]) and does not suffer from the Fermion sign problem in the non-interacting limit.


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