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Ab initio thermodynamic results for warm dense matter[1]

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Warm dense matter (WDM) – an exotic state where electrons are quantum degenerate and ions may be strongly correlated – is ubiquitous in dense astrophysical plasmas and highly compressed laboratory systems including inertial fusion. Accurate theoretical predictions require precision thermodynamic data for the electron gas at high density and finite temperature around the Fermi temperature. First such data have been obtained by restricted path integral Monte Carlo (restricted PIMC) simulations [1] and transformed into analytical fits for the free energy [2]. Such results are also key input for novel finite temperature density functional theory.

However, the RPIMC data of Ref. 1 are limited to moderate densities, and even there turned out to be surprisingly inaccurate, which is a consequence of the fermion sign problem. These problems were recently overcome by the development of alternative QMC approaches in Kiel (configuration PIMC [3, 4] and permutation blocking PIMC [5]) and Imperial College (Density matrix QMC [5]). The three methods have their strengths and limitations in complementary parameter regions and provide highly accurate thermodynamic data for the electronic contributions in WDM. While the original results [4-7] were obtained for small particle numbers, recently accurate finite size corrections were derived allowing to compute ab initio thermodynamic data with an unprecedented accuracy of better than 0.3 percent. This provides the final step for the use as benchmark data for experiments and models of Warm dense matter.

[1] E.W. Brown et al., Phys. Rev. Lett. **110**, 146405 (2013). [2] V.V. Karasiev et al., Phys. Rev. Lett. **112**, 076403 (2014). [3] T. Schoof et al., Contrib. Plasma Phys. **51**, 687 (2011). [4] T. Schoof et al. Phys. Rev. Lett. **115**, 130402 (2015) [5] T. Dornheim et al., J. Chem. Phys. **143**, 204101 (2015). [6] F.D. Malone et al., J. Chem. Phys. **143**, 044116 (2015). [7] S. Groth, T. Dornheim, et al., Phys. Rev. B **93**, 085102 and 205134 (2016).

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