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Restricted Configuration Path integral Monte Carlo for warm dense matter[1] ARIF OKTAY YILMAZ, KAI HUNGER, MICHAEL BONITZ, SIMON GROTH, Kiel University, TOBIAS DORNHEIM, CASUS — Quantum Monte Carlo is the most accurate method for simulating the homogeneous electron gas under warm dense matter conditions [T. Dornheim et al., Phys. Reports 744, 1-86 (2018)] However, due to the notorious fermion sign problem, previous ab initio approaches were restricted to temperatures above half the Fermi temperature, i.e. $\Theta = k_B T/E_F \geq 0.5$. Also, the method of choice for the degenerate Fermi gas – configuration path integral Monte Carlo (CPIMC) [T. Schoof et al., Contrib. Plasma Phys. 51, 687 (2011)] – is restricted to high density, i.e. $r_s = \bar{r}/a_B \leq 1$. Here, we construct two new approximations – RCPIMC and RCPIMC+ – that neglect some classes of Monte Carlo updates. While RCPIMC+ reduces the sign problem, RPCIMC completely eliminates it, at the price of a systematic error. We investigate the magnitude of the errors by comparing new finite size corrected [T. Dornheim et al., Phys. Rev. Lett. 117, 156403 (2016)] simulations to the parametrization [S. Groth et al., Phys. Rev. Lett. 115, 135001(2017)]. As a result we conclude that RCPIMC+ allows for accurate simulations of thermodynamic properties (deviations of less than 1%) at least up to $r_s = 3$ and $0.05 \leq \Theta \leq 0.3$, significantly extending the range of CPIMC.

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