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Fermionic Quantum Monte Carlo simulations without fixed nodes

TOBIAS DORNHEIM, TIM SCHOOF, SIMON GROTH, MICHAEL BONITZ,
Kiel university — Recent restricted PIMC (RPIMC) simulations [PRL **110**, 146405 (2013)] of the uniform electron gas (UEG) at finite temperature have turned out to be surprisingly inaccurate [PRL **115**, 130402 (2015)]. Therefore, there exists a high need for alternative approaches which circumvent the fermion sign problem (FSP). In this work, we present two independent approaches which exhibit a complementary behavior. The configuration PIMC (CPIMC) method [Contrib. Plasma Phys. **51**, 687-697 (2011)], which operates in Fock space, excels at high density and allows for cutting edge results at strong degeneracy. In contrast, the permutation blocking PIMC (PB-PIMC) approach [New J. Phys. **17**, 073017 (2015)] is formulated in coordinate space and combines antisymmetric imaginary time propagators (determinants) with a higher order factorization of the density matrix. This leads to a significant reduction of the sign problem and extends the range of applicability of standard PIMC towards higher density and lower temperature [arXiv:1508.03221 (2015)]. Joining these two complementary methods allows us to present accurate thermodynamic results for the uniform electron gas over a broad parameter range and, therefore, to partly avoid the FSP.

Tobias Dornheim
Kiel university

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