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Simulations of Dense Hydrogen and Helium Plasmas Without the Fixed-Node Approximation¹ ALEXEY FILINOV, MICHAEL BONITZ, Kiel University, PAVEL LEVASHOV, JIHT RAS Russia — Quantum Monte Carlo belongs to the most accurate simulation techniques. For Fermi systems, however, its applicability at strong degeneracy is limited by the fermion sign problem. Recently, a significant progress has been achieved for uniform electron gas with configuration path integral Monte Carlo (CPIMC) and permutation blocking (PB-PIMC) [1]. Both methods are free from uncontrolled errors introduced by the fixed nodes approximations. Here we develop a generalization of the PB-PIMC [1] suitable for the grandcanonical ensemble and, in combination with the improved Kelbg potential [2], perform simulations for hydrogen and helium plasmas down to temperatures $3 \cdot 10^4$ K. The obtained isotherms of pressure and internal energy are compared with the restricted PIMC [3] allowing us to conclude on the accuracy of the fixed-node approximation at weak and strong degeneracy, and how the bound state formation affects the results. Some thermodynamic properties are compared with finite temperature DFT simulations [4]. [1] T. Dornheim et al., Phys.Rep. 744, 1-86(2018); A. Filinov et al., Phys.Rev.E 70, 046411 (2004); [3] B. Milizer et al., Phys.Rev.B 84, 224109 (2011); [4] D. Knyazev and, P. Levashov, Phys. Plasmas 23, 102708 (2016).

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