Verification of the "Identical Permutation" path integral Monte Carlo Method for the Uniform Electron Gas

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The calculation of thermodynamic properties of strongly nonideal quantum Fermi systems remains a great challenge. Direct solution of quantum equations of motion for many-particle system, in contrast to classical molecular dynamics, is infeasible both theoretically and practically. Consequently, Path Integral Monte Carlo (PIMC) methods are of significant interest. However, the most straightforward and formally exact Direct PIMC (DPIMC) explicitly accounting for fermion permutations, is practically inapplicable for systems with more than 10 particles due to the factorial growth of the number of terms, while more sophisticated fermionic Monte Carlo approaches suffer from serious limitations or lack sufficient verification.
This work aims to verify the PIMC method based on the exchange determinant within the "Identical Permutation" approximation in case of the uniform electron gas (UEG). A series of calculations was performed for a small number of particles, with direct comparison to the exact DPIMC method. The results demonstrate that the error in the exchange-correlation corrections to internal energy and pressure is about 10% in the worst case, in the regime where the nonideality and degeneracy parameters are about 1, and rapidly decreases with increasing nonideality. In the strongly nonideal regime ($\Gamma \gtrsim$) and for wide range of degeneracy, the error remains less than 1%. Thus, the considered Identical Permutation approximation can be expected to provide good accuracy in the most physically relevant region of high nonideality and strong degeneracy, confirming its potential for further applications in quantum statistical physics.