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Path Integral Monte Carlo Methods for Fermions[1] ETHAN ETHAN, University of Illinois at Urbana-Champaign and Lawrence Livermore National Laboratory, JONATHAN DUBOIS, Lawrence Livermore National Laboratory, DAVID CEPERLEY, University of Illinois at Urbana-Champaign — In general, Quantum Monte Carlo methods suffer from a sign problem when simulating fermionic systems. This causes the efficiency of a simulation to decrease exponentially with the number of particles and inverse temperature. To circumvent this issue, a nodal constraint is often implemented, restricting the Monte Carlo procedure from sampling paths that cause the many-body density matrix to change sign. Unfortunately, this high-dimensional nodal surface is not a priori known unless the system is exactly solvable, resulting in uncontrolled errors. We will discuss two possible routes to extend the applicability of finite-temperatue path integral Monte Carlo. First we extend the regime where signful simulations are possible through a novel permutation sampling scheme. Afterwards, we discuss a method to variationally improve the nodal surface by minimizing a free energy during simulation. Applications of these methods will include both free and interacting electron gases, concluding with discussion concerning extension to inhomogeneous systems.

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