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Overcoming the fermion sign problem in homogeneous systems
ETHAN BROWN, ETH Zürich, JONATHAN DUBOIS, BERNI ALDER, Lawrence Livermore National Laboratory — Explicit treatment of many-body Fermi statistics in path integral Monte Carlo results in exponentially scaling computational cost due to the near cancellation of contributions to observables from even and odd permutations. Through direct analysis of exchange statistics we find that individual exchange probabilities in homogeneous systems are, barring known combinatorial factors, independent of the configuration of other permutations present. For two representative systems, 3-He and the homogeneous electron gas, we find that this allows the entire antisymmetrized density matrix to be generated from a simple model depending on only a few parameters obtainable directly from a standard PIMC simulation. Finally, we show this model may be extended to arbitrary order, resulting in a polynomial scaling algorithm for measuring fermionic observables.

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