

Abstract Submitted
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By-passing the sign-problem in Fermion Path Integral Monte Carlo simulations by use of high-order propagators¹ SIU A. CHIN, Texas A and M University — The sign-problem in PIMC simulations of non-relativistic fermions increases in severity with the number of fermions and the number of beads (or time-slices) of the simulation. A large number of beads is usually needed, because the conventional primitive propagator is only second-order and the usual thermodynamic energy-estimator converges very slowly from below with the total imaginary time. The Hamiltonian energy-estimator, while more complicated to evaluate, is a variational upper-bound and converges much faster with the total imaginary time, thereby requiring fewer beads. This work shows that when the Hamiltonian estimator is used in conjunction with fourth-order propagators with optimizable parameters, the ground state energies of 2D parabolic quantum-dots with approximately 10 completely polarized electrons can be obtained with ONLY 3-5 beads, before the onset of severe sign problems.

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