Approaching Strongly Correlated Systems Using Partial Node FCIQMC

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Finding the ground state of a fermionic Hamiltonian is a difficult problem, due to the Fermion sign problem. While still scaling exponentially, full configuration-interaction Monte Carlo (FCI-QMC) [1] mitigates some of the exponential variance by allowing annihilation of noise – whenever two walkers arrive at the same configuration with opposite signs, they are removed from the simulation. While FCI-QMC has been quite successful for quantum chemistry problems, it has had less success with strongly correlated systems; for example, it is unstable for even small systems sizes when applied to the one of the simplest many-body systems: the Fermi-Polaron. In this talk, we explore a series of algorithmic improvements which significantly increase its effectiveness. These improvements include modifying fixed node to work in this method, developing a partial node approach which allows for an extrapolation to the exact answer and developing a variant of release node. Additionally, we find a way to work directly in the thermodynamic limit for some subset of important systems. We apply these new approaches to the Fermi-Polaron finding that it accurately reproduces known analytic and numerical results going beyond them in certain cases [2].

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[1] G.H. Booth, A. J. W. Thom, and A. Alavi, J. Chem. Phys **131**, 5 (2009).

[2] M. Kolodrubetz and B.K. Clark, arxiv:1204.1490

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