Abstract Submitted
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Approximations beyond the initiator approach for ameliorating the sign problem[1] ADAM HOLMES, CYRUS UMRIGAR, Laboratory of Atomic and Solid State Physics, Cornell University, BRYAN CLARK, Kavli Institute of Theoretical Physics, University of California at Santa Barbara; Physics Department, University of Illinois at Urbana Champaign — Full CI Quantum Monte Carlo [1-2] is a computationally expensive method that projects out the ground state in a given basis without resorting to the fixed-node approximation. Instead, it has an initiator bias, which disappears as one approaches the infinite walker limit. While the semistochastic improvement on the method increases the efficiency by about three orders of magnitude [3], converging the ground state energy with respect to the walker population can still require prohibitively many walkers, not only as the number of electrons is increased, but even as the size of the basis is increased for a fixed number of electrons. We therefore investigate other approaches to ameliorating the sign problem, e.g., fixed-node and partial-node approximations [4], and compare the tradeoffs between accuracy and efficiency. [1] George H. Booth, Alex JW Thom and Ali Alavi, J. Chem. Phys. **131**, 054106 (2009). [2] Cleland, Deidre, George H. Booth and Ali Alavi, J. Chem. Phys. **132**, 041103 (2010). [3] F. R. Petruzielo, A. A. Holmes, Hitesh J. Changlani, M. P. Nightingale and C. J. Umrigar, Phys. Rev. Lett. **109**, 30201 (2012). [4] M. Kolodrubetz and B. K. Clark. Phys. Rev. B **86**, 075109 (2012).

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Adam Holmes
Laboratory of Atomic and Solid State Physics, Cornell University

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