Abstract Submitted
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Symmetry in Auxiliary-Field Quatnum Monte Carlo Calculations[1] HAO SHI, SHIWEI ZHANG, physics department, College of William and Mary — We discuss how symmetry properties can be preserved rigorously to improve the accuracy and efficiency in auxiliary-field quantum Monte Carlo (AFQMC) calculations. Using the Hubbard model as an example, we study the effect of symmetry in two aspects of ground-state AFQMC calculations, the Hubbard-Straonovich transformation and the form of the trial wave function. In unconstrained calculations, the implementation of symmetry often leads to shorter convergence time and much smaller statistical errors, thereby resulting in a substantial reduction of the sign problem and allowing exact calculations for larger and more strongly correlated systems. Moreover, certain excited states become possible to calculate which are otherwise beyond reach. In calculations with constraints,[2,3] it is shown that the use of symmetry can often reduce the systematic error significantly. Results are presented for the two-dimensional repulsive Hubbard model.

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[2]S. Zhang, J. Carlson, and J. Gubernatis, Phys. Rev. B **55**, 7464 (1997)
[3]C. Change, S. Zhang, Phys. Rev. B **78**, 165101 (2008)

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