Recent developments in auxiliary-field quantum Monte Carlo: symmetry and constraint release

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We discuss the use of symmetry properties to increase the accuracy and efficiency in auxiliary-field quantum Monte Carlo (AFQMC) calculations of electronic systems. With the Hubbard model as an example, we study the effect of preserving symmetry in two aspects of ground-state AFQMC calculations, the Hubbard-Straonovich transformation and the form of the initial trial wave function. It is shown that significant improvement over state-of-the-art calculations can be achieved. In calculations with constraints, the use of symmetry can greatly reduce the systematic error. In calculations in which the constraint is released, the implementation of symmetry often leads to shorter convergence time and much smaller statistical errors, thereby alleviating the sign problem. Moreover, certain excited states become possible to calculate which are otherwise beyond reach. We also discuss the use of the energy variance to help monitor and accelerate convergence in ground-state projections. Detailed comparisons are made with exact results from direct diagonalization in smaller systems. Near-exact ground-state energies can be obtained with our method for systems with 100 lattice sites (basis functions).

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