

## Semistochastic Quantum Monte Carlo with the use of spatial and time reversal symmetries

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Exact Diagonalization of a Hamiltonian relies on the ability to perform sparse matrix vector multiplications, and Quantum Monte Carlo performs the same operations stochastically at the cost of the infamous sign problem. To mitigate deficiencies with either method, we have recently proposed a hybrid method, namely semistochastic Quantum Monte Carlo [Petruzielo et al., Phys. Rev. Lett. 109, 230201]. The method is semistochastic in that the matrix multiplication is partially implemented numerically exactly and partially stochastically with respect to expectation values only. Though the idea is quite general, we use elements from the recently proposed Full Configuration Interaction Quantum Monte Carlo (FCIQMC) method [Booth et al. J. Chem. Phys., 131, 054106, (2009)] to demonstrate that its semistochastic version significantly reduces the computational time required to obtain the eigenvalue to a specified statistical uncertainty. This is demonstrated by the application of the semistochastic quantum Monte Carlo method to systems with a sign problem: the fermion Hubbard model and the carbon dimer. In addition, we show how we can make these calculations more efficient with the use of symmetries of the Hamiltonian. We use spatial (and time reversal) symmetries for the square lattice Hubbard model and time reversal symmetry for singlet ground states of quantum chemical Hamiltonians.