

Abstract Submitted  
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**Evaluation of expectation values in full configuration interaction quantum Monte Carlo** J.S. SPENCER, W.M.C. FOULKES, Imperial College London — The full configuration interaction quantum Monte Carlo (FCIQMC) method[1-3] provides access to the exact ground state energy. However, like diffusion Monte Carlo, it is hard to precisely calculate expectation values of operators which do not commute with the Hamiltonian due to the stochastic representation of the wavefunction. Following related work on diffusion Monte Carlo[4], we have formulated an approach to stochastically sample additional operators in FCIQMC by using the Hellmann-Feynman theorem and sampling pumped equations of motion coupled to the standard equation of motion used to evolve the wavefunction. Our approach requires only minor modifications to existing FCIQMC programs and can be used to evaluate expectation values of arbitrary operators. We will present example calculations on the Hubbard model and molecular systems.

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