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Equilibration of walkers and correlation of samples in QMC simulations D. NISSENBAUM, B. BARBIELLINI, A. BANSIL, Northeastern U. — When using the Metropolis algorithm from an unequilibrated starting point to obtain properly distributed samples for a Quantum Monte Carlo (QMC) calculation, and when analyzing the accuracy of the results after equilibration, one needs to properly handle two factors: the time taken for the walkers to equilibrate, and the presence of correlations in the sample points after the walkers have equilibrated. Inclusion of unequilibrated data gives a bias to the computed averages, while dealing appropriately with correlated data is essential in order to obtain accurate error bars. In this connection, we are developing reliable techniques to determine equilibration time and compute observable error bars. We present a careful study of several Li clusters, ranging from the Li dimer to a cluster containing 64 Li atoms, and focus particularly on scaling properties of the equilibration time with the size of the system. Work supported in part by the USDOE.

Daniel Nissenbaum
Northeastern University

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