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Decorrelation of samples in Quantum Monte Carlo calculations and applications to metallic nanoclusters[1] DANIEL NISSENBAUM, BERNARDO BARBIELLINI, ARUN BANSIL, Northeastern University — We discuss decorrelation of samples in Quantum Monte Carlo (QMC) ground-state energy calculations for large lithium and water nanoclusters and show how accurate results can be obtained without the need for decorrelating samples. The scaling of the integrated autocorrelation time τ is analyzed as a function of nanocluster size. τ is found to scale quadratically in Li nanoclusters, which adds a quadratic factor to the scaling of the total computation time in this metallic case, a factor which does not appear in computations of non-metallic H_2O nanoclusters. We choose nanoclusters which are relatively large in the context of QMC to demonstrate the application of these techniques - lithium nanoclusters with up to 64 atoms and water nanoclusters with up to 20 molecules.

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