Decorrelation of samples in Quantum Monte Carlo calculations and applications to metallic nanoclusters\textsuperscript{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 \( \tau \) is analyzed as a function of nanocluster size. \( \tau \) 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 \( \text{H}_2\text{O} \) 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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