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Transient quantum Monte Carlo investigations of few-electron systems NORM TUBMAN, Northwestern University, JONATHAN DUBOIS, RANDOLPH HOOD, BERNI ALDER, Lawrence Livermore National Lab — Diffusion Monte Carlo (DMC) is one of the most accurate methods for calculating electronic structure and can be applied to systems containing thousands of electrons. Typical applications of DMC utilize the fixed-node approximation, in which the nodes are specified using an input trial wave function. Errors in the locations of the nodes lead to systematic errors in DMC energy estimators. Removing this nodal bias can be done using transient quantum Monte Carlo methods, which have previously been applied to the free-electron gas and a handful of other few-electron systems. The drawback in using transient methods is the significant increase in computational cost. We have studied several quantum systems of varying sizes in order to better understand the scaling properties of various transient methods. We have explored techniques for reducing the computational cost such as cancellation and correlated walkers. We have analyzed our data using Bayesian inference. Prepared by LLNL under Contract DE-AC52-07NA27344

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