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Addressing Autocorrelation in the Determinant Quantum Monte Carlo Method[1] ISAAC OWNBY, PHILLIP DEE, STEVEN JOHNSTON, The University of Tennessee, Knoxville — Autocorrelation is a prominent issue among all Monte Carlo methods. Autocorrelation times are especially bad when the simulation is close to a phase transition. This issue of "critical slowing" can often be reduced, even eliminated, using cluster algorithms. The algorithms update the degrees of freedom in large clusters or blocks to efficiently kick configurations out of local energy minima. Albeit, the updates often increase the computational cost of the simulation; thus, there is a balance in the minimization of autocorrelation times and runtime. One system with a severe autocorrelation problem is the half-filled 2D Holstein model, which exhibits a metal-to-insulator transition at sufficiently low temperatures. Using determinant quantum Monte Carlo to simulate this model, we study the dependence of the autocorrelation time on the type and frequency of MC updates as well as other simulation parameters. Our results suggest some useful ways to tune MC updates to yield shorter autocorrelation times without resorting to the overly expensive simulations.

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