Abstract Submitted
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Geometrically Constructed Markov Chain Monte Carlo Study of Quantum Spin-phonon Complex Systems[1] HIDEMARO SUWA, Department of Physics, Boston University — We have developed novel Monte Carlo methods for precisely calculating quantum spin-boson models and investigated the critical phenomena of the spin-Peierls systems. Three significant methods are presented. The first is a new optimization algorithm of the Markov chain transition kernel based on the geometric weight allocation. This algorithm, for the first time, satisfies the total balance generally without imposing the detailed balance and always minimizes the average rejection rate, being better than the Metropolis algorithm. The second is the extension of the worm (directed-loop) algorithm to non-conserved particles, which cannot be treated efficiently by the conventional methods. The third is the combination with the level spectroscopy. Proposing a new gap estimator, we are successful in eliminating the systematic error of the conventional moment method. Then we have elucidated the phase diagram and the universality class of the one-dimensional XXZ spin-Peierls system. The criticality is totally consistent with the $J_1 - J_2$ model, an effective model in the antiadiabatic limit. Through this research, we have succeeded in investigating the critical phenomena of the effectively frustrated quantum spin system by the quantum Monte Carlo method without the negative sign.

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