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Extending Monte Carlo Samples

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We discuss a proposal to improve the efficiency of numerical simulations of spin and quantum link systems via analytical extension of the Monte Carlo sample.

1. INTRODUCTION

Quantum Monte Carlo (QMC) simulations which use the loop cluster algorithm and its variants are successful because they can make large jumps in configuration space while maintaining ergodicity and satisfying detailed balance [1,2]. An important subclass of these algorithms is implemented in continuous euclidean time, as opposed to discretized time, and thereby derives significant savings in storage and execution time [3]. Because the paths in the path integrals sampled by the continuous time cluster algorithms (CTCAs) have only sporadic changes of state, with constant states between such transitions, the CTCAs lend themselves to an interesting extension of Monte Carlo sampling. The algorithm explored here extends the QMC sample by summing the contribution of all path configurations with the same ordering of states, but with different values of the time intervals between changes of state.

2. DISCUSSION

As an example, we study here the quantum antiferromagnetic Heisenberg model (AFHM), although CTCAs are of more general applicability, including quantum link models for gauge theories [4]. The AFHM Hamiltonian in d dimensions is

$$H = J \sum_{i,\mu} \vec{S}_i \cdot \vec{S}_{i+\hat{\mu}} \ , \quad \vec{S}_i^{\,2} = S(S+1) \ , \qquad (1)$$

where $J > 0$ is the antiferromagnetic exchange coupling, $\hat{\mu}$ denotes the d primitive translation vectors of the unit cell, and $\vec{S}_i$ is the quantum spin operator at position i (in this paper we discuss only spin $S = 1/2$.) This model has been extensively analyzed with the recent generation of cluster QMC algorithms [3,5–8].

Standard Trotter-Suzuki techniques transform this d-dimensional quantum model into a $(d+1)$-dimensional classical model by creating an additional "euclidean time" dimension of extent β. The partition function is thus mapped to a "worldline" path integral in the $(d+1)$-dimensional space. Until recently, numerical simulations implemented configuration sampling on such systems using discretized euclidean time, with a consequent systematic error and a necessary extrapolation to continuous euclidean time. However, it was realized that the path configurations in the worldline integral can be dealt with in continuous time [9], leading to the development of the CTCAs that efficiently sample these path integrals.

2.1. Typical configuration

In Fig. 1 we display a typical worldline configuration for the $(1+1)$-dimensional AFHM spin chain. Here the euclidean time dimension is vertical. This picture is for the discrete time cluster algorithm (DTCA) with periodic boundary conditions. Each column of circles represents a spin site at different times, and light and dark markings represent "spin up" and "spin down" states. The interactions are laid out in the familiar checkerboard pattern of plaquettes. There are 3 different types of plaquettes in this model. As discussed elsewhere [10], associated with each type i of plaquette is a different Boltzmann weight w_i. The relative weights are (in terms of $\epsilon \equiv 1/N$ for small

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ϵ): $w_1 = 1$, $w_2 = (1 + \exp(\epsilon\beta J))/2 \to 1 + \epsilon\beta J/2$, and $w_3 = (\exp(\epsilon\beta J) - 1)/2 \to \epsilon\beta J/2$.

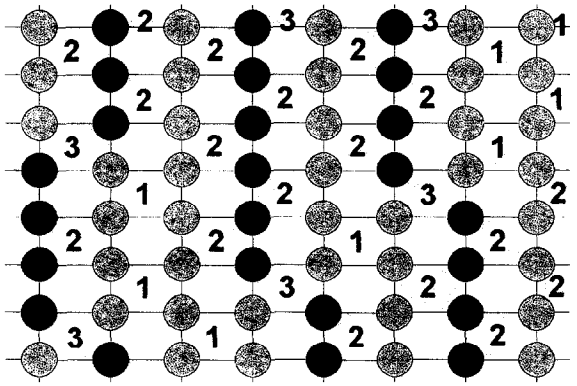

Figure 1. Quantum AFHM 8-spin chain in 1 + 1 dimensions, discrete time, Trotter $N = 4$.

In Fig. 2 we show the spin chain implemented in continuous time. The 8 vertical bands represent the 8 spin sites; light and dark markings represent "spin up" and "spin down" states. Note the spin states are constant in euclidean time, except for sporadic transitions from one state to another. Note also there are two different kinds of interfaces between spins: like and unlike, corresponding to plaquette types 1 and 2 in the DTCA. Also there are sporadic transitions which correspond to the type 3 plaquettes in the DTCA.

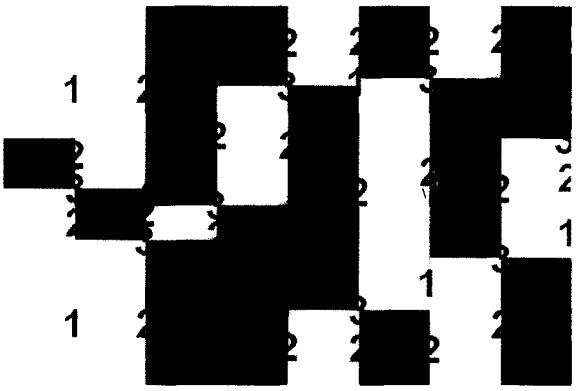

Figure 2. Quantum AFHM 8-spin chain in 1 + 1 dimensions, continuous time.

2.2. Boltzmann weight of configuration

The statistical weight W of a DTCA configuration is simply the product of the plaquette weights. In Fig. 1 this works out to $W = w_1^8 w_2^{18} w_3^6$. We can use the statistical weights $w_i(\epsilon \to 0)$ to compute the Boltzmann weight for CTCA configurations, with a minor wrinkle. The wrinkle is that any configuration with M transitions (state changes) picks up a factor of $w_3^M \propto \epsilon^M$, which vanishes as $\epsilon \to 0$. In the path integral, this is exactly compensated as $N \to \infty$ by the combinatorial factor $\binom{N}{M}$. In the technique we propose here, we will be averaging over configurations which all have the same number of transitions, so this factor can be ignored.

The rest of the calculation is straightforward: $w_1 = 1$ is trivial, and w_2^n for some $n \leq N$ gives an exponential. It is convenient to use $\tau \leq \beta$ for euclidean time intervals. For each single nearest-neighbor interaction with unlike spins and duration τ, we get a factor $\exp(\tau J/2)$. In Fig. 2, with $M = 8$ transitions, the weight is $W = (\epsilon\beta J/2)^M \exp(JT/2)$ where T is the sum of all the durations of unlike-spin nearest-neighbor interactions.

3. SUPERSAMPLING

We propose an extension to the Monte Carlo sample. We shall appropriate the term "supersampling" for this technique. The basic idea is that each configuration generated by the QMC algorithm is related to a subspace of configurations, each with the same euclidean-time-ordering of states but which have different time intervals between transitions. Taking account of all these additional states in the Monte Carlo sum should in principle result in a better simulation, i.e. a reduction of variance.

The strategy here is to integrate over all possible transition time locations, subject to the constraints that the ordering of states is fixed and of course that the total duration is β. At any given euclidean time, we need to count up the number of unlike-spin nearest neighbors; the contribution of that state to the Boltzmann weight will be multiplicative. In the following it will help to absorb the factor $1/2$ in $\exp(J\tau/2)$ into a multiplier n_i associated with a state i, that is, n_i for a given state of the system is half the number of unlike-spin interfaces. For a more general Hamiltonian, n_i will simply be the multiplier for a given state,

such that the contribution to the weight of an interval of duration τ_i is $\exp(n_i\tau_i)$.

The denominator of the estimator will be the integral

$$I = \int_0^\beta d\tau_0 \int_0^{\beta-\tau_0} d\tau_1 \int_0^{\beta-\tau_0-\tau_1} d\tau_2 \ldots \times \exp(n_0\tau_0 + n_1\tau_1 \ldots + n_M(\beta - \sum_{i=0}^{M-1} \tau_i)) \; .$$

This can be shown to equal

$$I = \sum_{i=0}^{M} C_i \exp(n_i\beta) \tag{2}$$

where

$$C_i \equiv \frac{1}{\prod_{j\neq i}(n_i - n_j)} \; , \tag{3}$$

provided that the factors n_i are not degenerate.

Consider the numerator of our estimator. Let us focus attention on observables like the staggered susceptibility which are evaluated as some weight per unit of euclidean time v_i – in other words, for which the numerator is

$$J = \int_0^\beta d\tau_0 \int_0^{\beta-\tau_0} d\tau_1 \int_0^{\beta-\tau_0-\tau_1} d\tau_2 \ldots \times (v_0\tau_0 + v_1\tau_1 \ldots) \times \exp(n_0\tau_0 + n_1\tau_1 \ldots + n_M(\beta - \sum_{i=0}^{M-1} \tau_i)) \; .$$

It can be shown that this evaluates to

$$J = \sum_{k=0}^{M} D_k \exp(n_k\beta) \tag{4}$$

where

$$D_k \equiv \frac{v_k\beta - \sum_{i\neq k} \frac{v_k - v_i}{n_k - n_i}}{\prod_{j\neq k}(n_k - n_j)} \; . \tag{5}$$

Implementing this estimator requires keeping track of the order of states in our configuration as it is updated by the Monte Carlo algorithm. In addition, we keep track of the Boltzmann weights n_i and the observable weights v_i. Our approach for handling degeneracies is to observe that varying the boundary between two intervals with the same weight factor n_i does not change the Boltzmann weight; hence we lump together all the intervals with the same weight and only supersample a restricted set of intervals, with non-degenerate weights.

Note this method does not improve topological observables like the helicity modulus. Also note some Hamiltonians, such as the XY model, have the same Boltzmann weight for like-spin and unlike-spin interactions; in such cases supersampling will be trivially ineffective.

4. PROSPECTS

Supersampling cluster algorithms for the AFHM are being coded, with the intention of verifying and quantifying the variance reduction associated with this technique. Also, attempts to merge this technique with the technique of cluster-based improved estimators are also underway.

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