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Bond-updating mechanism in cluster Monte Carlo calculations

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We study a cluster Monte Carlo method with an adjustable parameter: the number of energy levels of a demon mediating the exchange of bond energy with the heat bath. The efficiency of the algorithm in the case of the three-dimensional Ising model is studied as a function of the number of such levels. The optimum is found in the limit of an infinite number of levels, where the method reproduces the Wolff or the Swendsen-Wang algorithm. In this limit the size distribution of flipped clusters approximates a power law more closely than that for a finite number of energy levels.

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I. INTRODUCTION

One way to calculate thermodynamical quantities of model systems is by averaging over a sample of states selected by a Monte Carlo procedure [1]. This approach is especially useful for models that have not been solved by rigorous methods. In the course of time a number of different techniques have been developed. For example, in the so-called simple sampling method the states are chosen independently with equal probability. Especially when this method is applied at low temperatures, one tends to choose states with small Boltzmann factors, that do not contribute significantly to the thermal averages. Thus, at low temperatures the simple-sampling method becomes inefficient. A more efficient sampling procedure is "importance sampling:" one generates a Markov chain of states, with transition probabilities chosen such that each state occurs with the ensemble probability. The canonical ensemble is used most often, but alternative ensembles like the microcanonical ensemble have been used. In most applications of the Monte Carlo method, consecutive microstates in the Markov chain differ by only one or two particles. Therefore, in critical systems, where correlations over large distances exist, the effectivity of such importance sampling methods decreases because of the mechanism of critical slowing down.

In some special cases such as the Potts model, effective methods have been found for simulation in the neighborhood of the critical point. The equivalence of the Potts model [2] with the random-cluster model can be used to effect the change of large clusters of spins instead of single spins. This canonical importance sampling method with clusters was introduced by Swendsen and Wang [3].

A different approach to suppress critical slowing down in the case of the Potts model was made by Hu [4]. He introduced a method that may be characterized as simple sampling with respect to the number of states of the Potts model. Therefore critical slowing down is absent but the sampling method has been argued to become less effective for large system sizes when the number of states differs appreciably from 1 [5].

Recently Creutz [6] proposed a microcanonical importance sampling method with clusters. In this method, the system includes "demons," which can absorb or supply the energy change of a bond, when one of the spins connected by that bond is inverted. Equilibration is established by rearranging the demons over the bonds. Creutz also noted that the Swendsen-Wang cluster method can be formulated using demons. Then, the demons have an infinite number of states and are brought in equilibrium with a heat bath after each interaction with the spin system.

The microcanonical method by Creutz differs in two respects from the Swendsen-Wang method. On the one hand, he updates the spins according to a deterministic rule, and on the other hand, he uses demons with a finite number of energy levels. An attractive aspect of the deterministic updating method is that it should enable a fast algorithm. However, both aforementioned differences may affect the efficiency of the method: it remains to be investigated how the critical slowing down is affected. For an assessment of the method, separation of the two effects is desirable.

In this work we study the effects of a variation of the number of energy levels of the demons on the efficiency of a canonical cluster method. In principle such a study could yield Monte Carlo methods that are more effective than the presently known cluster algorithms. In Sec. II we formulate canonical sampling methods using intermediary demons, and review some possibilities for the bond-updating mechanism. In Sec. III we present the results of Monte Carlo calculations and in Sec. IV we draw some conclusions.

II. THE ACCESS TO THE ENERGY RESERVOIR

In importance-sampling methods energy is transferred to and from a heat bath. In our description of this energy-exchange mechanism we will make use of a system of Ising spins ($S = \pm 1$). In the Metropolis method the reservoir couples to the spins (in the case of Kawasaki [7] spin exchange dynamics it couples to pairs of spins). When a transition is made, the associated energy is transferred to or from the reservoir. In a microcanonical sampling method [8] the reservoir consists of a so-called demon

traveling along the sites. The spin at a site visited by the demon is flipped if the demon can change its energy by an amount that compensates for the change of energy of the spin system. Thus, given the energy and the energy spectrum of the demon, the microscopic dynamics of the spin system is deterministic.

Also in the case of other ensembles the transition probabilities can be formulated using a demon. A finite but large reservoir is used in the Gaussian [9] and dynamical ensemble [10]. An intermediary demon equilibrates with this reservoir. The amount of energy stored in the reservoir determines the probability that energy levels of the demon are occupied. The probability of a transition in the spin system depends on the amount of energy stored in the reservoir. In the Metropolis spin updating method according to the canonical ensemble, the demon equilibrates with an infinite heat bath at temperature T prior to every site visit. The transition probabilities are thus determined by the temperature and the energy spectrum of the demon. We choose demons with equidistant nondegenerate energy levels. The level spacings are multiples of the Ising energy quantum $2J$ where $-JS_iS_j$ is the interaction energy of a pair of neighboring spins S_i and S_j. If the demon has an infinite number of energy levels, it can always accept energy from the spin system. Thus a transition that lowers the energy of the spin system is always made. There is, however, a finite probability that the demon is in a low-energy level and cannot provide the energy to make the reverse transition. That transition is therefore made with the probability $\exp(-\beta\Delta E)$, where ΔE is the energy of the spin system after the transition minus that before the transition. The transition probabilities thus equal those of Fosdick [11].

In another extreme case the demon has only two energy levels. The level spacing is chosen to be $|\Delta E|$, which depends on the local configuration. The demon is able to accommodate the energy change with probability $1/(e^{\beta\Delta E}+1)$. In this case the transition probabilities are those of Yang [12].

The energy spectrum of the demon determines the microscopic dynamics. However, it is plausible that in this case the choice of the demon does not influence those critical dynamic properties contained in the Ising universality class with spin-flip dynamics. Results for critical exponents of systems with spin-flip dynamics are given in [13].

For cluster methods the heat bath couples to the bonds in the lattice. The bonds between interacting spins can be active or inactive. The state of a spin can only be changed if all spins connected to it by active bonds are changed at the same time in a compatible way. This defines the process of cluster construction used by Creutz [6]. For simplicity we consider pairwise interactions. More general constructions were treated by Kandel *et al.* [14]. An extension using dual spins was given by Andreichenko [15].

The relation between the canonical and microcanonical cluster methods is analogous to that described above in the case of single spin dynamics. Whereas in the microcanonical process demons interact only with the bonds, in the canonical cluster formation process the demon is brought in equilibrium with an infinite heat bath at temperature T before every bond visit. We denote the number of levels of the intermediate demon by n . The level spacing is chosen equal to the bond energy quantum $2J$. We consider the dependence of the dynamics on n. There is a probability

$$P_a = \frac{\exp(-2nJ/kT)}{\sum_{j=1}^{n}\exp(-2jJ/kT)} \tag{1}$$

that the demon is in its highest energy level. Then it cannot absorb a change of energy associated with a bond between a pair of antiparallel spins: this pair of spins has to be flipped simultaneously and the bond connecting this pair is active in the cluster formation process.

The probability that the demon is in its lowest energy level equals

$$P_p = \frac{\exp(-2J/kT)}{\sum_{j=1}^{n}\exp(-2jJ/kT)}. \tag{2}$$

A bond between parallel spins will therefore be active in the cluster formation process with a probability P_p. The spin updating operation comprises the simultaneous inversion of all the spins in a cluster connected by active bonds.

In the limit $n \to \infty$, the bond probabilities are such that the critical Ising model maps on the random-cluster model at its percolation threshold [2]. They satisfy $1-P_a = 1$ and $1-P_p = \exp(-2J/kT)$: these are the probabilities according to Swendsen and Wang. For finite n both probabilities acquire the same factor $1-P_a$, so that the percolation threshold will be exceeded. Therefore, in the limit of large L, we expect the best efficiency of a cluster algorithm for $n \to \infty$. For finite n the percolation and the Ising transition decouple and the clusters become too large when $L \to \infty$: their average size will approach a nonzero fraction of the system. However, for finite L the optimum may be at $n < \infty$. An interesting question is how the dynamics of the cluster process, in particular the efficiency of model simulations, will depend on the choice of n for finite systems.

III. MONTE CARLO SIMULATION

Given a method for the partition of the lattice in clusters of spins, one is free to choose the rule to update one or more clusters of spins. For the Ising model with nearest-neighbor interaction and Swendsen-Wang bond probabilities, Kerler [16] has compared the merits of several updating methods. In the method of Wolff [17] one site is chosen randomly. Only the spins in the cluster connected to that spin are changed. In this work we restrict ourselves to this updating method, which has the computational advantage that only one cluster need be constructed. Thus we investigate a generalization of the Wolff algorithm: the generalization is that we use demons with a finite number of energy levels as explained in Sec. II.

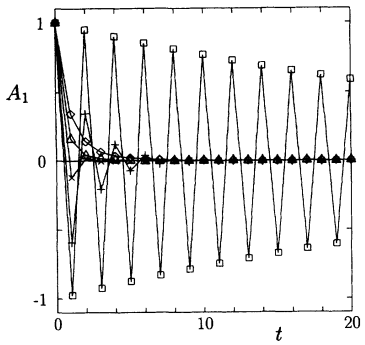

FIG. 1. Correlation function of the magnetization versus the number of cluster updates t for the three-dimensional Ising model at $K = 0.221\,653$ with system size 16^3. The results for n-level demons are denoted by $\square$ for $n = 2$, $+$ for $n = 4$, $\times$ for $n = 6$, Δ for $n = 8$, and $\diamond$ for $n = \infty$. The error bars do not exceed the symbol size. The lines are a guide to the eye.

The simulations used a three-dimensional Ising lattice with periodic boundaries and a linear size of $L = 16$ lattice units, at the estimated critical point: $J/kT = 0.221\,653$ (see [18] and references cited therein). In Fig. 1 we plot the time dependence of the autocorrelation function of the magnetization $A_1(t) = \langle m(0)m(t)\rangle/\langle m^2\rangle$, where the time t is counted as the number of cluster updates. The correlation function oscillates with t for small n. It decreases by an order of magnitude after a few cluster updates for $n > 2$. This is not the case for the square of the magnetization. In Fig. 2 we observe that the autocorrelation function of the square of the magnetization $A_2(t) = [\langle m^2(0)m^2(t)\rangle - \langle m^2\rangle^2]/[\langle m^4\rangle - \langle m^2\rangle^2]$ decays faster for large n. The probability that the cluster contains the majority of the spins is appreciable for small n. To provide more data with respect to this phenomenon we show the size distribution of flipped clusters in Fig. 3. It turns out that the larger the number of levels the closer the distribution approximates the power law distribution [19] expected for Wolff dynamics in an infinite lattice

$$q(x) \sim x^{-d/y_T}, \tag{3}$$

where q is the number of flipped clusters of size x, d is the

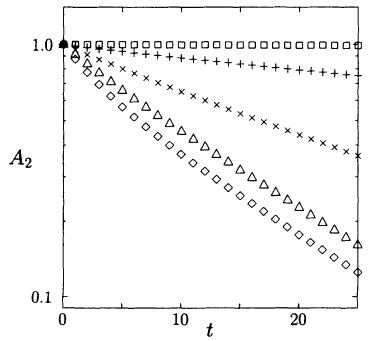

FIG. 2. Correlation function of the squared magnetization versus the number of cluster updates t for the three-dimensional Ising model at $K = 0.221\,653$ with system size 16^3. The results for n-level demons are denoted by $\square$ for $n = 2$, $+$ for $n = 4$, $\times$ for $n = 6$, Δ for $n = 8$ and $\diamond$ for $n = \infty$. The error bars do not exceed the symbol size.

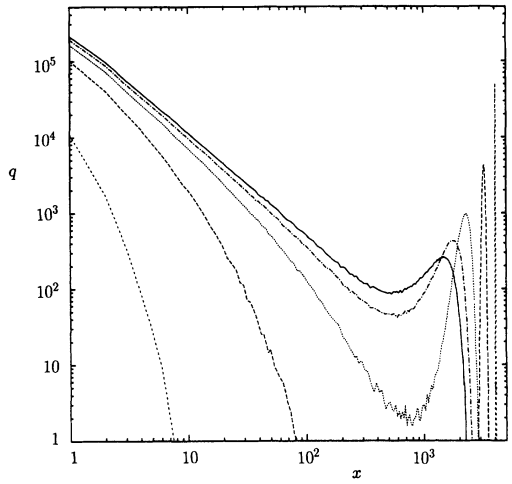

FIG. 3. Number of flipped clusters of size x versus cluster size for the three-dimensional Ising model at $K = 0.221\,653$ with system size 16^3. The distributions are shown after 10^6 cluster updates with a dashed line for $n = 2$, long dashes for $n = 4$, a dotted line for $n = 6$, a dash-dotted line for $n = 8$, and a full line for $n = \infty$. Bin widths increase from 1 to 20 on the x scale for larger clusters.

dimension of the lattice, and y_T is the leading temperaturelike exponent. For the smaller values of n there is a pronounced second maximum in the size distribution. For $n \leq 4$ the clusters contributing to this maximum contain the majority of the spins.

IV. CONCLUSION

For the critical three-dimensional Ising model we find that the dynamics using a demon with an infinite number of levels is most effective from the point of view of correlation times of the square of the magnetization. The size distribution of flipped clusters shows a maximum for the smallest clusters and a second maximum for large clusters. Decreasing n enhances the second peak and therefore increases the average cluster size. In principle such an increase might improve the efficiency of the simulation process. However, we observed that, although more spins are changed on average, this does not decrease the correlation time. For small n the clusters tend to become so large that they contain most of the spins. The effect of flipping such a cluster is equivalent to flipping the complement, which is small. This is a distinct disadvantage from the computational point of view. Not only is the effect of flipping a cluster small, it also takes many operations to generate such a cluster. Thus demons with a limited number of levels decrease the efficiency of the cluster algorithm in the case of the three-dimensional Ising system. We expect this to apply to the Creutz microcanonical method as well.

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