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Comment on the Calculation of Thermal Averages by Long-Time Monte Carlo Simulations

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It is shown that the effect of turnovers of the whole spin lattice for temperatures below the ordering temperature during a long-time computer simulation is not always satisfactorily reduced by considering the absolute value of the order parameter. A simple method to overcome this problem is suggested.

KEY WORDS: Monte Carlo simulations; "ergodic" time; multi-spin coding technique.

The ultimate goal of a Monte Carlo simulation is to compute expectation values for infinite systems. Because this is not possible in practice, one has to calculate finite-volume expectation values and then try to extrapolate. The Monte Carlo algorithm in principle is able to determine the exact finite-volume Gibbs distribution when performing an infinite number of spin-flip trial processes, and it is generally accepted that under certain circumstances the exact finite-volume Gibbs distribution is reasonably well represented by the configurations generated from a large but finite number of spin-flip trial processes.

When extrapolating from the finite-volume results to the infinite system one has to take into account the different physical behavior of finite and infinite systems concerning the following two effects.[1,2] First, when the thermal correlation length approaches the linear extension of the system the thermodynamic behavior becomes different from that of an infinite system. This effect is taken into account by the finite-size scaling

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theory.[1,2] Furthermore, it is well known[1-3] that in a Monte Carlo simulation for the phase transition of a finite spin system the whole spin lattice will turn over after a characteristic "ergodic" time, so that, for instance, the order parameter of an Ising ferromagnet, the magnetization M, will change from $+M$ to $-M$ or vice versa, even below the ordering temperature T_c. As a result, the thermal average of the order parameter will tend to zero for a long-time Monte Carlo simulation (simulation time much longer than the "ergodic" time) even in the ferromagnetic regime. Two methods have been suggested to avoid problems related to these turnovers:

1. Only simulation times smaller than the "ergodic" time are considered for averaging of the observables; see, for instance, ref. 3. To achieve a reasonable statistical accuracy, averages over many independent such short-time simulations must be performed, i.e., over simulations starting from different initial spin configurations. Thereby for each run the first few configurations generated must be discarded to allow for equilibrization of the spin system.

2. Simulation times longer than the "ergodic" time are considered, but the absolute value $|M|$ of the order parameter is used instead of the order parameter M itself to make the direction of the order parameter unimportant.[1] If the thermal averages are calculated after each Monte Carlo step per spin, and if the turnovers occurred abruptly, i.e., during one Monte Carlo step per spin, this procedure would be justified. Then—as was supposed in the paper of Landau[1]—lattice turnovers would be "immaterial" for the determination of $\langle |M| \rangle$. However, if the turnovers need several or many Monte Carlo steps per spin, it will affect not only the thermal average of the order parameter M, but also that of $|M|$. Exactly the same problem has been addressed by Mouritsen (ref. 4, pp. 17, 18), albeit not considered quantitatively.

It is the main point of the present paper to demonstrate that the latter case holds in general, i.e., that the effect of lattice turnovers may not be simply eliminated by considering $\langle |M| \rangle$ instead of $\langle M \rangle$, and that the reversals are not "immaterial" to the calculation of $\langle |M| \rangle$. This means that the turnover configurations (which are real thermal fluctuations of the finite-spin system) contribute significantly to the statistical average $\langle |M| \rangle$. However, the statistical weight of turnover configurations becomes smaller with increasing size of the system and is negligibly small for very large systems. Therefore, when extrapolating from the finite-volume results to the behavior of the infinite system, we must get rid of them in some way. It is the second point of the present paper to suggest a simple method which tries to cope with the lattice turnovers during a long-time simulation. This

method is not free of some arbitrariness, but it constitutes a reasonable approach which turns out to be successful at least for the Monte Carlo study of the simple cubic Ising model with random quenched nonmagnetic impurities (see below).

The use of such a modified long-time simulation may be motivated by the following two points:

(a) It is simpler than method 1, especially for temperatures close to T_c, where the "ergodic" time becomes shorter and shorter whereas the equilibrization time increases.[3]

(b) It saves computer time, because it requires discarding only once spin configurations for spin equilibrization, whereas in method 1, spin configurations must be discarded for each individual run. In the latter case, the arbitrary initial spin configurations (for instance, ferromagnetic or random configurations) are very much different from "typical" equilibrium configurations. They therefore appear only with very small statistical weight in the equilibrium ensemble and must be discarded when calculating thermal averages. In contrast, the turnover configurations of a long-time simulation represent large but real thermal fluctuations of a finite system contributing with some nonnegligible weight to the thermal average for the finite system because they occur typically after a time comparable to the "ergodic" time. They are rather similar in nature to other typical equilibrium configurations at least concerning the short-range spin order. As a result, the following configurations are very soon representative for the thermal average of a system with stable magnetization in one direction. This leads to the basic idea of the suggested method: Instead of performing many independent short-time simulations and discarding for each simulation a rather large number of spin configurations for equilibrization, we consider one long-time simulation and neglect the turnover configurations as well as only few of the following configurations when calculating $\langle |M| \rangle$, in a way discussed below.

To demonstrate the main point of the present paper and the suggested method, we have performed Monte Carlo simulations for the simple cubic Ising model with 32^3 spins and with random quenched nonmagnetic impurities of concentration $x = 0.2$ on the basis of the fully vectorized multi-spin coding algorithm with helical boundary conditions described in ref. 5, with 5×10^5 Monte Carlo steps per spin (MCS). Figure 1 exhibits the time evolution of the magnetization, averaged over subsets of 500 MCS (symbol $\langle \cdot \rangle_{500}$), respectively, for a temperature of $T = 3.450$ (in units of J/k_B) below the ordering temperature $T_c = 3.505$. For this temperature there are two lattice turnovers (for $n \approx 290$ and $n \approx 750$ in Fig. 1) which remain stable for a longer time. Furthermore there are several "spikes" for

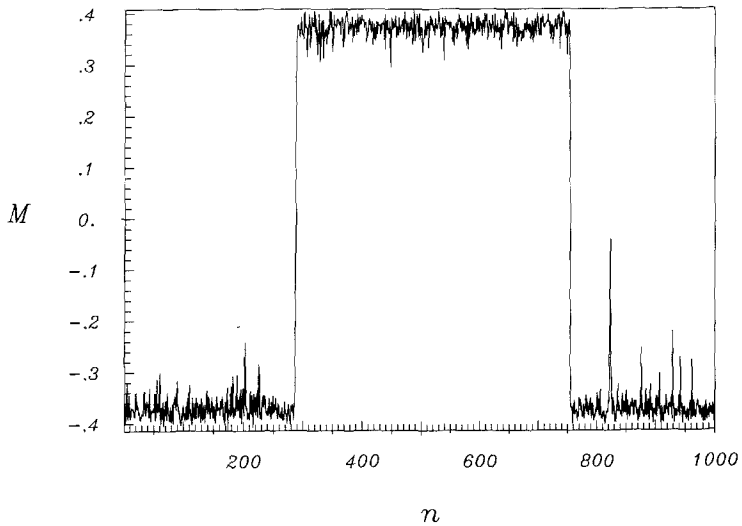

Fig. 1. Time evolution of the magnetization M (see text) averaged over 500 MCS. The number n labels the succeeding subsets of 500 MCS.

$n \approx 200$, 225, 820, etc., for which the magnetization fluctuates strongly. For each of the subsets of 500 MCS we have calculated $|\langle M \rangle_{500}|$ and $\langle |M| \rangle_{500}$. If these two quantities are not identical, there must be a change in the sign of M during the considered 500 MCS. In Fig. 1 this was the case for $n = 287$, $n = 288$ (which constitutes the first stable turnover), and $n = 754$ (second turnover) as well as for the "spike" at $n = 822$–824 and the one at $n = 962$. For all the other "spikes" $|\langle M \rangle_{500}|$ was exactly identical to $\langle |M| \rangle_{500}$, indicating that no change in sign occurred for the corresponding subsets.

Figure 2 represents some of the data (see below) close to T_c for the thermal average $\langle |M| \rangle$ (squares) calculated from the spin configurations after each of the 5×10^5 MCS (after having discarded the first 10%), together with the respective numbers of subsets in which turnovers occurred. In addition, we have determined $\langle |M| \rangle$ (triangles) by omitting the above specified subsets from the calculation for which a change in sign of M occurred. Obviously, there is a difference between the two sets of results which becomes relevant already for $T = 3.450$, for which only seven subsets of this type exist.

It should be noted that all the spikes with $|\langle M \rangle_{500}| = \langle |M| \rangle_{500}$, i.e., those for which no change in sign of M occurs, are kept for the thermal averages. Although this seems to be a self-suggesting procedure for projecting out the turnover configurations, it is not free of some arbitrariness: For

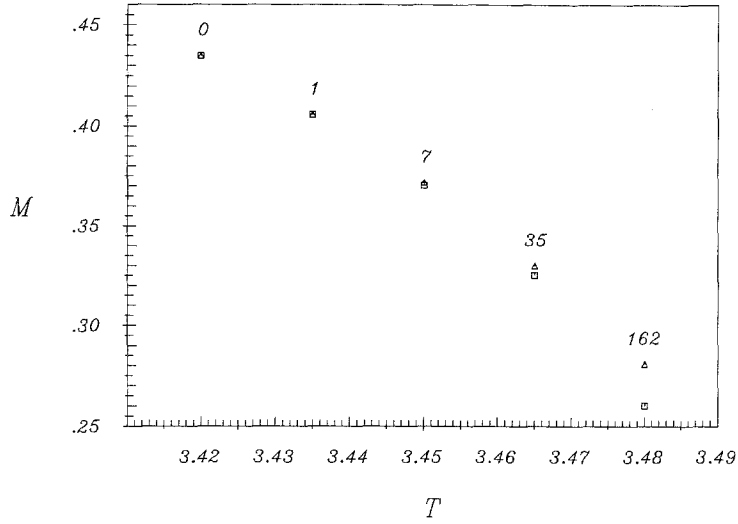

Fig. 2. Temperature dependence of the magnetization M averaged over 5×10^5 MCS with (□) and without (△) the undesired turnover states. The figures denote the number of subsets for the respective temperatures, for which $|\langle M \rangle_{500}| \neq \langle |M| \rangle_{500}$.

instance, for $T = 3.450$ (Fig. 1) some of those spikes are even larger in amplitude than the one for $n = 962$ (which is discarded because of $|\langle M \rangle_{500}| \neq \langle |M| \rangle_{500}$). Some of the spin configurations in the corresponding subsets may be close to a change in sign of M and therefore also may represent large fluctuations which occur only in a finite system.

In spite of this arbitrariness, the above-discussed procedure of projecting out the turnover configurations appears to be reasonable: For the displayed temperature range the so corrected data (triangles) are nearly identical to those from a conventional Monte Carlo simulation for 40^3 spins with only 1.5×10^4 MCS, for which no turnover occurred.[5,6] Accordingly, the Kouvel–Fisher analysis[5,6] of the corrected data yields similar values for the critical exponent β and the ordering temperature T_c, whereas a Kouvel–Fisher analysis of the uncorrected data is nearly impossible due to the irregularities introduced by the turnovers.

Altogether, our calculations clearly demonstrate that the effect of turnovers may not be satisfactorily reduced just by considering the absolute value of M, i.e., the turnovers are not immaterial, in contrast to the statement in ref. 1. Furthermore, we have shown that our procedure of projecting out the turnover configurations works reasonably well at least for the diluted three-dimensional Ising model: It yields results which are almost identical to those from short-time simulations, for which no turnovers occur (method 1). It should be noted, however, that the suggested proce-

dure becomes more and more arbitrary when approaching T_c. Then the thermal fluctuations are very large, so that the turnover may occur for $T \lesssim T_c$ also for an equivalent-sized subsystem of an infinitely extended system. Although it is expected that the number of turnovers in the finite system is still larger than that in the equivalent-sized subsystem, there is no way to distinguish between "regular" turnovers and those initiated by the finite size of the system.

To avoid confusion, we remark that the suggested procedure is only able to reduce the effect of turnovers, but does not eliminate the finite-size effects described by the finite-size analysis, which of course also occur if there is no turnover at all during the simulation. In Fig. 2 we display only those data which—according to the Kouvel–Fisher analysis of all the data—are not spoiled by those finite-size effects and which are in the critical regime.

Finally, it should be noted that the tendency for turnovers is triggered by the dilution of the system with nonmagnetic impurities. For the pure Ising model we observed for the 32^3 lattice no turnover in the ferromagnetic regime, neither for a conventional Monte Carlo simulation with periodic boundary conditions and 1.25×10^5 MCS, nor for the fully vectorized multispin program with helical boundary conditions and 5×10^5 MCS. In contrast, in the case of the diluted Ising model a comparable number of turnovers appeared for both types of programs when performing the calculations exactly for the same configuration and, for instance, for $T = 3.48$.

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