Monte Carlo mean-field method for spin systems

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We use a Monte Carlo mean-field method proposed by Netz and Berker to analyze the critical behavior of an Ising square lattice. We show that this method demands longer sampling times as compared with the conventional Monte Carlo simulations. Also, similar mean-field results can be obtained from self-consistent analytic calculations for small clusters of spins.

In some recent publications, Netz and Berker[1] proposed a Monte Carlo mean-field theory to account for the thermodynamic behavior of spin systems. The method incorporates the hard-spin conditions of local degrees of freedom and should be especially useful in the case of frustrated systems, for which the standard mean-field approximation may lead to completely wrong results. Furthermore, Netz and Berker claim that this method converges faster, and works with much less sampling, than the conventional Monte Carlo simulations. So far, this Monte Carlo mean-field method (which we call MCMFM) has been applied to just a few special spin systems (as a stacking of frustrated triangular Ising lattices). We then decided to perform some calculations to gauge the real capabilities of the method. In this publication, we report simulations for a ferromagnetic Ising square lattice in zero field. We point out the limitations of this scheme, which still produces essentially mean-field results, and does demand a considerable amount of sampling time (Monte Carlo steps).

Let us describe the method for an Ising Hamiltonian,

$$\mathbf{H}=-J\sum_{(ij)}\sigma_i\sigma_j-H\sum_{i=1}^{N}\sigma_i\ , \tag{1}$$

where $\sigma_i=\pm1$, for all sites of a crystal lattice, and the first sum is over nearest-neighbor pairs of sites. In zero external field, we can write the standard mean-field equations,

$$\langle\sigma_i\rangle=\tanh(\beta JH_i),\ \text{and}\ H_i=\sum_{j(i)}\langle\sigma_j\rangle\ , \tag{2}$$

where $\beta=(k_BT)^{-1}$, and the sum is over the nearest neighbors of site i. The idea of Netz and Berker consists in writing the effective field H_i in the form

$$H_i=\sum_{j(i)}\sigma_j\ , \tag{3}$$

and choosing the signs of σ_j according to the formula

$$\sigma_j=\mathrm{sgn}(m_j-r)\ , \tag{4}$$

where r is a random number in the interval $[-1,+1]$, and $m_j=\langle\sigma_j\rangle$. In a sequential version, we update m_j for each site of the lattice and store the quantity to be measured.

According to Banavar, Cieplak, and Maritan,[2] the method of Netz and Berker could be interpreted as an approximation based on Callen's identity,

$$\langle\sigma_i\rangle=\left\langle\tanh\left[\beta J\sum_{j(i)}\sigma_j\right]\right\rangle\ , \tag{5}$$

where the averages are taken with respect to the canonical ensemble. Using a factorized stationary probability distribution,

$$P(\{\sigma\})=\prod_i\frac{1}{2}(1+\sigma_i\langle\sigma_i\rangle)\ , \tag{6}$$

we can write a system of self-consistent equations for the set $\{\langle\sigma_i\rangle\}$. Netz and Berker[3] agree with this interpretation and claim that the simultaneous implementation of the hard-spin condition and of mean-field theory can indeed be carried out even without using Monte Carlo samplings. We have reasons, however, to disagree with this interpretation. The closed-form scheme of Banavar, Cieplak, and Maritan[2] is identical to a self-consistent method proposed by Mamada and Takano[4] some time ago. However, there is no obvious deduction of a stationary probability distribution in the Monte Carlo mean-field method. Choosing a random number in the interval $[-1,+1]$, at the Monte Carlo time step τ, and setting $\sigma_j(\tau+1)=\mathrm{sgn}[m_j(\tau)-r]$, at the next time step $\tau+1$, is entirely equivalent to using a single-site transition probability

$$W[\sigma_j(\tau+1)]=\frac{1+\sigma_j(\tau+1)m_j(\tau)}{2}\ , \tag{7}$$

but it is not equivalent to using an equilibrium distribution as in Eq. (6). Although displaying similar analytical expressions, these quantities are known to have quite different meanings. In a standard Monte Carlo simulation[7] we choose a transition probability such that the process of simulation generates an equilibrium or stationary distribution (for example, we may write a condition of detailed balance to establish a connection between transition and equilibrium probabilities). It is interesting to remark that the dynamics of Netz and Berker's algorithm may be written in terms of a transition probability, $W(m_i\rightarrow m_i')$, from an old to a new value of the magnetization per spin. For an Ising chain, for example, we have

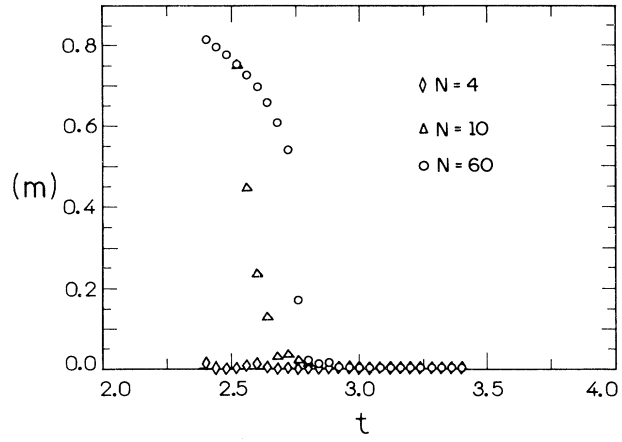

FIG. 1. Absolute value of the magnetization per spin $|m|$ versus temperature, $t=k_BT/J$, for $N=4$, 10, and 60.

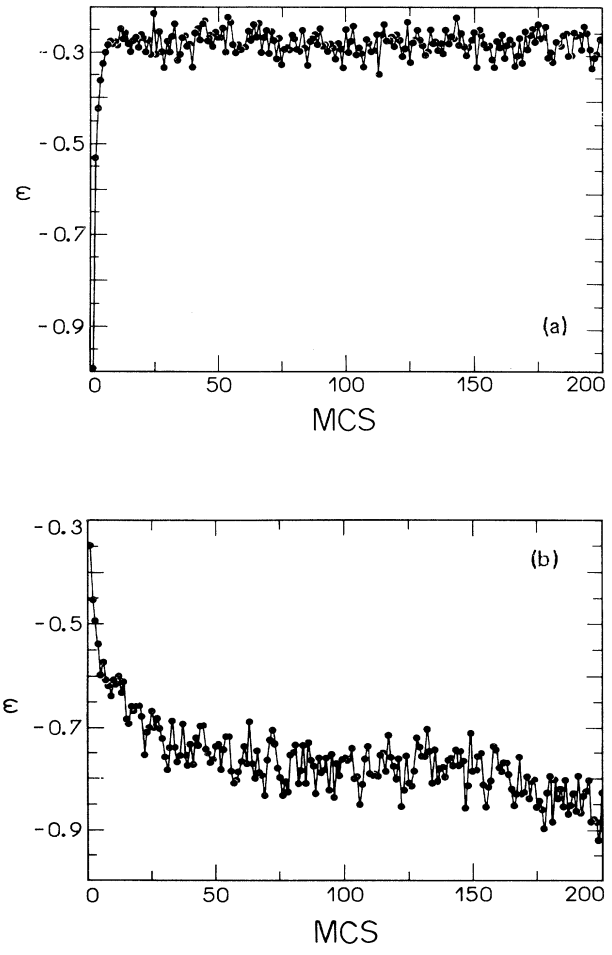

FIG. 2. Plots of the internal energy per spin ϵ versus the number of Monte Carlo steps (MCS): (a) $N=60$, and $t=4.00$; (b) $N=60$, and $t=2.72$. The solid lines are a guide for the eyes.

TABLE I. Some typical values to compare the performance of the MCMFM and a standard Monte Carlo simulation in the vicinity of the critical temperature (at $t\approx 2.72$ for the MCMFM, and $t\approx 2.269$ for a Metropolis simulation). The standard simulations require a smaller number of MCS's to yield similar estimates for u (with errors of about 1%).

N	u	σ_u^2	S_i	MCS (MCMFM)	MCS [Landau (Ref. 5)]
10	−0.901	7.6×10^{-2}	14±3	10 000–15 000	4000–10 000
60	−0.895	2.4×10^{-3}	~400	~12 000	1000–2500

$$W(m_i\rightarrow m_i'=0)=\tfrac{1}{2}(1-m_{i+1}m_{i-1})\ , \tag{8}$$

if σ_{i+1} and σ_{i-1} have opposite signs, and

$$W[m_i\rightarrow m_i'=\pm\tanh(2\beta J)]=\tfrac{1}{4}(1\pm m_{i+1})(1\pm m_{i-1})\ , \tag{9}$$

if $\sigma_{i+1}=\sigma_{i-1}=\pm1$. We thus can find the probability of transition from the set $\{m_i\}$ to the new set $\{m_i'\}$. There is no obvious deduction of the stationary equilibrium distribution $P(\{m_i\})$. It is even less obvious how to deduce the more relevant quantity $P(\{\sigma_i\})$.

We now report an application of the sequential form of the MCMFM to the analysis of the ferromagnetic Ising model on a square lattice of $N\times N$ sites, with periodic boundary conditions. In Fig. 1, we show plots of the absolute value of the magnetization per spin,

$$|m|=\left\langle\left|\frac{1}{N^2}\sum_{i=1}^{N^2}m_i\right|\right\rangle\ , \tag{10}$$

where $\langle\cdots\rangle$ is a Monte Carlo average, versus the temperature $t=k_BT/J$, for $N=4$, 10, and 60. We have used 10^6 Monte Carlo steps (MCS) for $N=4$, 6.5×10^4 MCS for $N=10$, and 1.25×10^4 MCS for $N=60$. The quantity m is not particularly adequate for numerical purposes,[5] but it seem to have been used by Netz and Berker. For estimating the critical temperature, we have calculated the internal energy per spin,

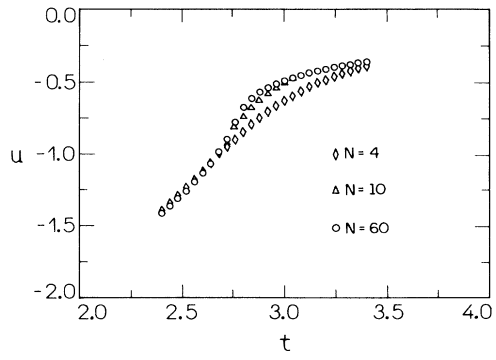

FIG. 3. Plots of the mean internal energy per spin as a function of temperature, for $N=4$, 10, and 60.

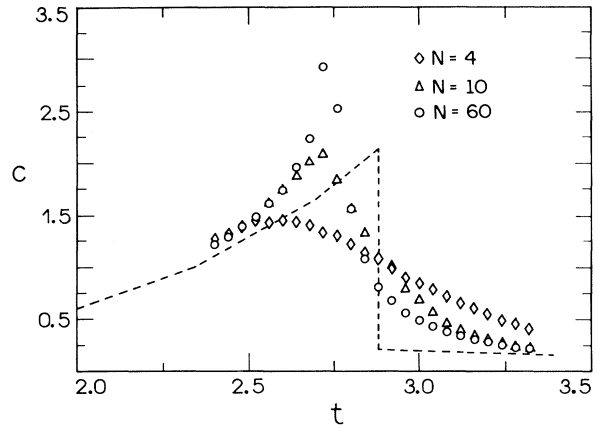

FIG. 4. Plots of the specific heat per spin versus temperature, for $N=4$, 10, and 60. The dashed line corresponds to the Bethe-Peierls approximation.

$$\epsilon=\frac{1}{N^2}\sum_{(ij)}\sigma_i\sigma_j\ , \tag{11}$$

for each Monte Carlo step. In Fig. 2, we show graphs of ϵ as a function of the number of Monte Carlo steps, for $N=60$, at temperatures $t=4.0$, and $t=2.72$. Near the critical temperature, the convergence is quite slow for the bigger lattices. In Table I, we compare the performance of the MCMFM with a conventional application of the Metropolis algorithm (as used by Landau[5] to study finite-size effects in the Ising square lattice). The values of the mean internal energy per spin u in the neighborhood of the critical temperature, were calculated according to the algorithm of Netz and Berker (σ_u^2 is the variance of the values of the energy, and S_i is the statistical inefficiency). We also give the number of Monte Carlo steps to obtain convergence, with errors on the order of 1% in u, both in the present calculations and in the work of Landau. An inspection of this table already indicates the limitations of Netz and Berker's method. In fact, for the same values of u, the conventional Monte Carlo method may demand a shorter sampling time. Also, to evaluate the critical temperature, $T_c(N)$, from the maxima of the specific heat per spin, $c(N)$, we were forced to use substantially larger samples. As the method does not generate Boltzmann states, we cannot make $c(N)=N^2\sigma_u^2/t^2$, although this formula has been used by Netz and Berker.[1] In Figs. 3 and 4, we show the internal energy and the specific heat for $N=4$, 10, and 60, using the same number of MCS's as before (the dashed line in Fig. 4 represents the specific heat in the Bethe-Peierls approximation). From the location of the maxima of the specific heat, we draw the graph of $T_c(N)$ versus $1/N$ shown in Fig. 5. An extrapolation for $N\to\infty$ (which does not seem to be justified by finite-size arguments in this case), yields the estimate $T_c(N\to\infty)=2.72\pm0.04$, which should be compared with $T_c=4$, for the mean-field approximation, $T_c=3.089\ldots$, according to Mamada and Takano,[4] in agreement with Banavar, Cieplak, and Maritan,[2] $T_c=2.885\ldots$, in the well known Bethe-Peierls approximation, and $T_c=2.269\ldots$, from Onsager's exact result.

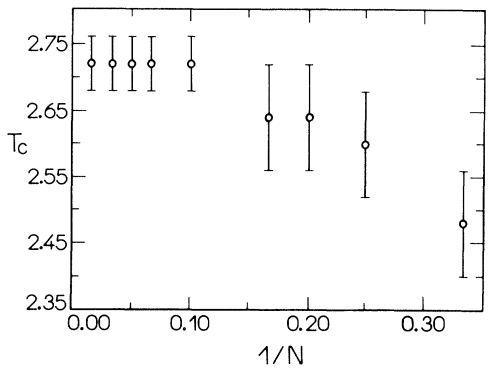

FIG. 5. Plots of the estimated critical temperature, from the maxima of the specific heat versus $1/N$.

In conclusion, we have used the ferromagnetic Ising model on a square lattice to test a recently proposed Monte Carlo mean-field method (MCMFM). We show that this procedure demands longer sampling times than conventional Monte Carlo simulations to achieve a comparable degree of convergence. Also, we still obtain essentially mean-field results, which could as well have been obtained by a variety of self-consistent cluster approximations. It is not immediate to associate an equilibrium distribution with the transition probabilities of the MCMFM. In fact, we show that a self-consistent closed-form approximation based on a single-site distribution, as proposed by Banavar, Cieplak, and Maritan,[2] gives different results from the Monte Carlo implementation of the mean-field method. As shown in a recent paper by Kabakçioglu, Berker, and Yalabik,[6] different implementations of the hard-spin conditions may indeed lead to different results for the field-temperature phase diagram of the antiferromagnetic Ising model on a triangular lattice. In spite of all these limitations, mean-field calculations taking into account the hard-spin conditions may be useful to obtain qualitatively correct results for spin systems with a high degree of frustration.

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