Entropy of the two-dimensional Ising model

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A numerical calculation of the entropy of the two-dimensional Ising model is described, for nonzero external field. The calculation makes use of the Monte Carlo method to simulate a kind of microcanonical ensemble.

I. METHOD OF CALCULATION

The purpose of this paper is to describe a numerical calculation of the entropy of the two-dimensional Ising model, for nonzero external field. For zero external field the model can be solved analytically, the Onsager solution. The calculation for nonzero field involves the use of the Monte Carlo method. What is novel about this calculation is that the probability distribution sampled by the Monte Carlo method is not the Boltzmann distribution.

The two-dimensional Ising model consists of a spin $s(x)$, which can take the values $+1$ or -1, at each point x of a two-dimensional lattice. In the computer simulation the lattice size is finite with periodic boundary conditions. The energy of the Ising spins is

$$E(s)=-\sum_{x,i} s(x)s(x+e_i) , \tag{1}$$

where e_1 and e_2 are the unit lattice vectors; the magnetization is

$$M(s)=\sum_{x} s(x) . \tag{2}$$

The problem is to compute the entropy $S(E,M)$, defined by

$$S(E,M)=\ln\rho(E,M) , \tag{3}$$

where $\rho(E,M)$ is the density of states in the (E,M) plane. The entropy is an intrinsic property of the Ising spins, independent of temperature or external field. It is an important quantity because it relates the microscopic interaction to thermodynamics. In particular, the form of $S(E,M)$ determines the phase structure of the system; for the Ising model it must create the low-temperature phase transition between spin-up and spin-down ordered states.

The basic idea of my calculation of $S(E,M)$ is to integrate the thermodynamic relations[1]

$$\beta=(\partial S/\partial E)_{\text{eq}} \quad \text{and} \quad h=-(\partial S/\partial M)_{\text{eq}} ; \tag{4}$$

here β is the inverse temperature, h/β is the external field, and the subscript eq indicates that the derivatives are evaluated at the equilibrium values of E and M, denoted $\bar{E}$ and $\bar{M}$. To obtain $S(E,M)$ by integrating Eq. (4), β and h must be computed for a sufficiently dense set of points in the (E,M) plane. Then Eq. (4) can be used to estimate $S(E,M)$, up to an additive constant, by numerical integration.

In a conventional Monte Carlo simulation of the Ising model, the Boltzmann distribution is sampled, i.e., the distribution

$$e^{-\beta E(s)}e^{hM(s)}/Z , \tag{5}$$

where Z is the partition function. This is the distribution of states in the canonical ensemble, i.e., for thermal equilibrium with an infinite heat bath in the presence of an external field $H=h/\beta$. For input (β,h) a set of configurations is generated with this distribution, and $\bar{E}$ and $\bar{M}$ are estimated by their averages in this set. However, this simulation cannot be used to compute $S(E,M)$ from Eq. (4), because of effects of the first-order phase transition. As (β,h) varies through the transition, $\bar{E}$ and $\bar{M}$ change discontinuously when the system changes phase. Intermediate points between the two phases are inaccessible, because they are not stable for any (β,h). Therefore the derivatives $\partial S/\partial E$ and $\partial S/\partial M$ cannot be determined in the intermediate region. Furthermore, a phenomenon resembling hysteresis occurs:[2] the point (β,h) at which the phase change occurs depends on the starting configuration, because the two phases are both metastable in a neighborhood of the transition. The hysteresis adds another element of ambiguity to the calculation of the derivatives. Since I must know the derivatives throughout the (E,M) plane to compute $S(E,M)$, a conventional Monte Carlo simulation does not provide the necessary information.

It has been found in recent studies of other models that the information can be obtained by sampling a distribution other than the Boltzmann distribution.[3–8] Consider for example a system Q with a first-order transition as a function of β, with no external field. Then the entropy is a function $S(E)$, and the inverse temperature is $\beta=(dS/dE)_{\text{eq}}$. If the Boltzmann distribution $\exp(-\beta E)$ is sampled then $\bar{E}$ changes discontinuously, with hysteresis, for β near the transition temperature. However, if a Gaussian distribution $P(E)=\exp[-a(E_c-E)^2]$ is sampled, then as E_c varies the system changes continuously from one phase to the other, without hysteresis. The Gaussian distribution can be interpreted[5,6] as the distribution of states in the microcanonical ensemble of an analog system that consists of the system of interest Q in thermal equilibrium with an auxiliary system, called the demon system. If the demon variables interact with the variables of Q by an ergodic dynamics that conserves the combined energy, then the distribution of Q states is $P_d(E_c-E)$, where $P_d(E_d)$ is the density of states of the demon system

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at demon energy E_d. The Gaussian distribution corresponds to a hypothetical demon system with Gaussian density of states. The inverse temperature in the microcanonical ensemble is[5,6,9]

$$\beta=[d\ln P(E)/dE]_{eq}=2a(\bar{E}-E_c) . \qquad (6)$$

Thus this microcanonical ensemble is simulated by sampling $P(E)$, measuring $\bar{E}$ and β as E_c varies. The experience of the use of this approach in an example with classical spins[5] and examples of lattice gauge theories,[6–8] examples with first-order phase transitions, is that the system changes continuously as E_c varies, without hysteresis. Interestingly, near the phase transition $\bar{E}$ is not a single-valued function of β.

The idea of using a microcanonical ensemble can be generalized to the case of an external field, for the Ising model calculation considered here. The difference is that here the demon system interacts with the Ising spins such that the total *magnetization* is conserved, rather than the total energy.[10] The precise definition of the analog system is as follows. Let the internal interactions of the Ising variables be in thermal equilibrium with an infinite heat bath at temperature β; in addition let the Ising spins be in equilibrium with a set of demon Ising spins s_d. The demon spins have no interaction among themselves, nor with the heat bath. Then the probability distribution of the Ising spin states is of the form

$$P(s)=Ke^{-\beta E(s)}P_M(M(s)) , \qquad (7)$$

where K is a normalization constant. The magnetization distribution $P_M(M)$ is derived from the assumption that the Ising spins interact with the demon spins by an ergodic dynamics with constant combined magnetization. In the computer simulation the number of demon spins is equal to the number of lattice sites N, although this is not necessary. The combined magnetization is

$$M_c=M(s)+M(s_d) , \qquad (8)$$

and the statement that the dynamics is ergodic means that all states with magnetization M_c are equally likely. The distribution of Ising spins $P_M(M)$ is obtained by summing over the possible demon spin states. The number of such states is the binomial coefficient (N,n_+), where n_+ is the number of demon spins with $s_d=+1$. Thus $P_M(M)$ is the binomial distribution

$$P_M(M(s))=\frac{N!}{[(N-M_d)/2]![(N+M_d)/2]!} , \qquad (9)$$

where $M_d=M_c-M(s)$. As M_c varies between $-2N$ and $2N$, the peak position of $P_M(M)$ varies between $-N$ and N; thus M_c acts like an external field. However, the form of the distribution is different than the Boltzmann distribution. Therefore, for reasons that will be explained in Sec. III, the Ising system changes continuously as M_c varies, without hysteresis, even across the phase boundary separating spin-up and spin-down ordered states.

I call $P(s)$ a microcanonical distribution, but it should be remembered that the internal Ising interactions are in equilibrium with an infinite heat bath.[10] The term "microcanonical" refers to the fact that the total magnetization is constant in the analog system.

To summarize, the calculation is to sample the distribution of states $P(s)$ by the Monte Carlo method, computing the mean values $\bar{E}$ and $\bar{M}$. These results yield measurements of the partial derivatives of $S(E,M)$ at $(\bar{E},\bar{M})$, by Eq. (4). The derivative $(\partial S/\partial E)_{eq}$ is equal to β, the input value in $P(s)$. A formula for the other derivative $(\partial S/\partial M)_{eq}$, which is denoted $-h$, can be derived from the theory of the microcanonical ensemble:[9] The partition function is[1]

$$Z=\sum_{\text{states}} e^{-\beta E(s)}P_M(M(s)) = \int\int e^{S(E,M)}e^{-\beta E}P_M(M)dE\,dM . \qquad (10)$$

For the canonical ensemble the magnetization distribution $P_M(M)$ is e^{hM}. Because S, E, and M are extensive quantities, the integrand is sharply peaked at the maximum of the function

$$F_{\beta h}(E,M)=S(E,M)-\beta E+hM , \qquad (11)$$

i.e., at the minimum of the free energy; thus $(\bar{E},\bar{M})$ is at the maximum of this function. For the canonical ensemble this constitutes a proof of Eq. (4). For the microcanonical ensemble the relevant function is instead

$$F_{\beta M_c}(E,M)=S(E,M)-\beta E+\ln P_M(M) , \qquad (12)$$

i.e., $(\bar{E},\bar{M})$ is at the maximum of this function. Therefore the definition of the external field in the microcanonical ensemble is

$$h=-(\partial S/\partial M)_{eq}=(\partial \ln P_M/\partial M)_{eq} , \qquad (13)$$

in a notation in which M takes a continuum of values.[1] For the Ising model, in which the possible values of M are even integers, a suitable definition of h is

$$h=-[S(\bar{E},\bar{M}+2)-S(\bar{E},\bar{M}-2)]/4 = \tfrac{1}{4}\ln[P_M(\bar{M}+2)/P_M(\bar{M}-2)] . \qquad (14)$$

The thermodynamic relations in Eqs. (4) and (14) are exact in the limit of an infinite lattice. For a finite lattice there are corrections of order $1/N$ compared to the lowest-order terms. That is, the mean values $(\bar{E},\bar{M})$ do differ slightly from the values (E',M') that maximize $F_{\beta M_c}(E,M)$; the difference is of order 1, compared to E and M which are of order N. In the computer simulation the lattice size is 20×20, giving $N=400$ spins. This appears to be sufficiently large that the calculation of $S(E,M)$ is not very sensitive to the finite-size correction. Evidence for this statement will be described in Sec. IV.

Finally, it should be noted that a Monte Carlo calculation of the entropy of the Ising model has also been described by Binder.[11] However, in Binder's calculation the Boltzmann distribution is sampled, and the entropy calculation is quite different than that described here.

II. RESULTS

The results are based on Monte Carlo calculations in which the distribution $P(s)$ defined in Eqs. (7) and (9) is sampled by the Metropolis method. The calculations are for a 20×20 lattice, with periodic boundary conditions; the number of Ising spins is $N=400$. There are two parameters in $P(s)$, namely β and M_c. For each (β,M_c) a Monte Carlo calculation was done, consisting of 5000 sweeps of the lattice, measuring the average energy $\bar{E}$ and magnetization $\bar{M}$, and computing the external field h from Eq. (14). The parameter values were first for M_c fixed at $M_c=0$, with β varying by

$$\beta/\beta_c=0.0 \text{ to } 1.5 \text{ step } 0.1 \ , \tag{15a}$$

then for β/β_c fixed at 0.6, 0.8, 0.9, 1.0, 1.1, 1.2, and 1.4, with M_c varying by

$$M_c=-1.2N \text{ to } 1.2N \text{ step } 0.1N \ . \tag{15b}$$

Figure 1 shows the resulting averages $(\bar{E},\bar{M})$. At these points in the (E,M) plane the two partial derivatives of $S(E,M)$ are known. These points are sufficiently dense to yield an accurate estimate of $S(E,M)$ by numerical integration.

The numerical integration was done in two steps. The entropy can only be determined up to an additive constant, so $S(E,M)$ was arbitrarily set equal to 0 at $(E,M)=(0,0)$. In the first step, the string of results in Eq. (15a) was used. For these calculations with $M_c=0$ the mean magnetization is $\bar{M}=0$; note that unlike the canonical ensemble, states with $\bar{M}=0$ are stable in the microcanonical ensemble even at temperatures below the critical point. Thus these results were used to determine $S(E,0)$ by integrating the first relation in Eq. (4). In the second step, the strings of results with fixed β in Eq. (15b) were used. For each string the entropy at $M=0$ is the starting point for integrating along the string away from $M=0$. There is a consistency check on the accuracy, from the fact that all these strings end in the corner $E\rightarrow-2N$ and $|M|\rightarrow N$; the different strings gave consistent results for $S(E,M)$ in the corner. By this process $S(E,M)$ was estimated throughout the space covered by the points in Fig. 1.

The entropy $S(E,M)$ is maximum at $(E,M)=(0,0)$, which corresponds to a random spin state; it decreases monotonically as (E,M) varies away from this point. Rather than display the entropy itself, it is more interesting to display the function $F_{\beta h}(E,M)$ defined in Eq. (11), with $h=0$ and β near β_c, the critical point. The critical point is known from the Onsager solution for an infinite lattice,

$$\beta_c=\tfrac{1}{2}\ln(\sqrt{2}+1) \ . \tag{16}$$

The function $F_{\beta 0}(E,M)$ is a more sensitive function of E and M than the entropy. As explained at Eq. (11), the states in the canonical ensemble fluctuate about the maximum of $F_{\beta h}(E,M)$. For $\beta>\beta_c$ the equilibrium states for $h=0+$ and $h=0-$ are spin-up or spin-down ordered states. Thus the position of the maximum of $F_{\beta h}(E,M)$ jumps from nonzero $M>0$ to nonzero $M<0$ as h moves from $0+$ to $0-$. However, for $\beta<\beta_c$ the equilibrium states have $M=0$ at $h=0$, and the position of the maximum of $F_{\beta h}(E,M)$ varies continuously with h. Therefore the function $F_{\beta h}(E,M)$ depends sensitively on (E,M) for β near β_c and $h=0$.

Figure 2 shows a contour plot of $F_{\beta 0}(E,M)$ for $\beta=\beta_c$. This function has two equal local maxima, at $E/2N=-0.75$ and $M/N=\pm0.8$. The existence of the two maxima implies that the system remains aware of the two symmetry-breaking states even at the critical temperature. In the canonical ensemble with $\beta=\beta_c$ and $h=0$,

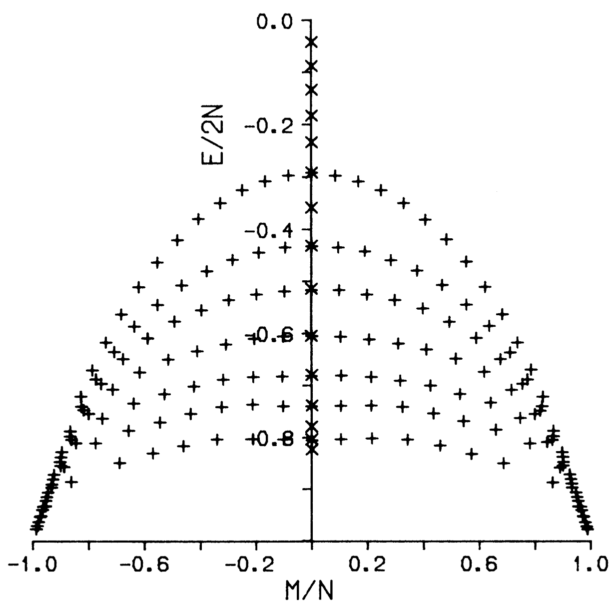

FIG. 1. Mean magnetization per spin $\bar{M}/N$ and mean Ising interaction energy per lattice link $\bar{E}/2N$ from the Monte Carlo calculations with parameters in Eqs. (15a) and (15b).

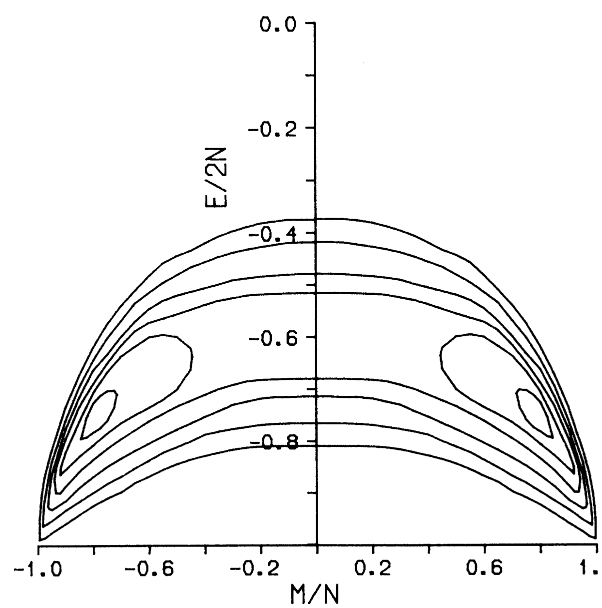

FIG. 2. Contour plot of $F_{\beta h}(E,M)$ for $\beta=\beta_c$ and $h=0$. The contour levels are 0.20, 0.21, 0.22, 0.225, 0.23, and 0.2345.

the system should fluctuate most of the time about these two maxima. Figure 3 demonstrates that this is indeed the case; Fig. 3 is a scatter plot of states produced by a Monte Carlo simulation using the Boltzmann distribution with $\beta=\beta_c$ and $h=0$. Here 2000 sweeps were done, and after each sweep the value of (E,M) was plotted on the graph. For the 20×20 lattice the system changes from one symmetry-breaking phase to the other several times in the course of 2000 sweeps. However, the transitions occur quickly, in a few sweeps. During most of the simulation the system fluctuates in one phase or the other. The point (E,M) about which the system fluctuates in either of these metastable states is at the maximum of $F_{\beta_c 0}(E,M)$ seen on the contour plot in Fig. 2.

It is easy to see how the equilibrium state changes as β and h vary away from the values β_c and 0. The equilibrium state is at the maximum of $F_{\beta h}(E,M)$. If β increases above β_c, the two maxima in Fig. 2 grow, and move to lower E and higher $|M|$. If h is then turned on, one maximum rises relative to the other. On the other hand, if β decreases below β_c, the maxima move toward $M=0$ and toward higher E. At some point the two maxima coalesce on the $M=0$ axis. If h is turned on in this symmetric phase, the maximum just moves continuously away from $M=0$.

Figure 4 shows a contour plot of $F_{\beta 0}(E,M)$ for $\beta=0.9\beta_c$. Here there is a single maximum at $E/2N=-0.52$ and $M/N=0$, as expected above the critical temperature, in the symmetric phase. Figure 5 shows a scatter plot for 2000 sweeps of the Boltzmann distribution with $\beta=0.9\beta_c$ and $h=0$. Again the configurations are centered at the maximum of $F_{\beta 0}(E,M)$, but they undergo large fluctuations because the maximum is very flat.

Finally a brief discussion of the uncertainty of the contours in Figs. 2 and 4 is needed. The uncertainty due to statistical error in the Monte Carlo calculations is small compared to that due to the numerical integration, which is simply the trapezoidal rule interpolating between points on Fig. 1. I estimate that the uncertainty in the value of $S(E,M)$ at any point (E,M) is at most ± 0.001, and relative uncertainties of nearby points are even smaller. Then the uncertainty in the contour position is at most ± 0.002 in either $E/2N$ or M/N for any small segment of a contour.

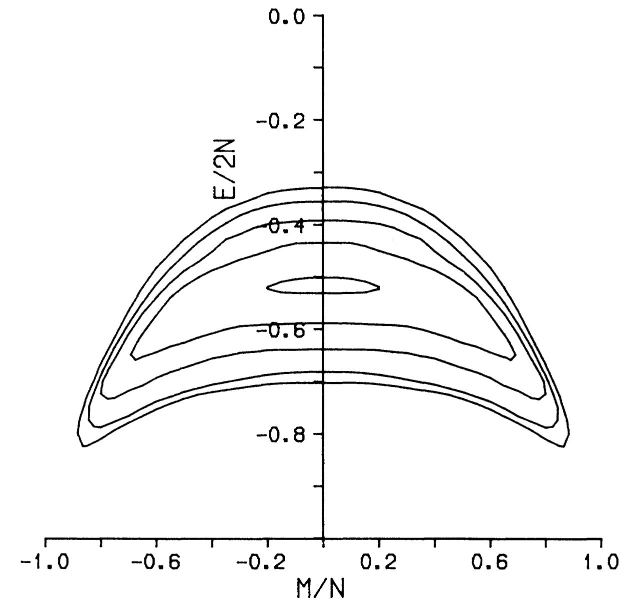

FIG. 4. Contour plot of $F_{\beta h}(E,M)$ for $\beta=0.9\beta_c$ and $h=0$. The contour levels are 0.16, 0.165, 0.17, 0.175, and 0.1795.

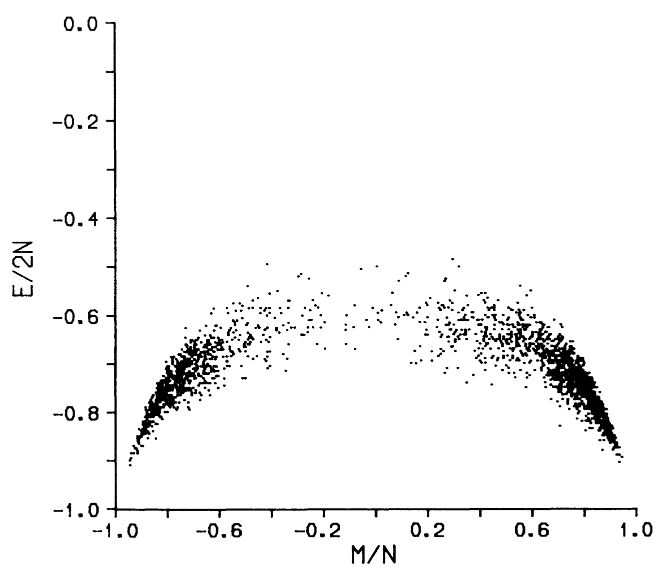

FIG. 3. Scatter plot of M/N and $E/2N$ from a Monte Carlo simulation with $\beta=\beta_c$ and $h=0$.

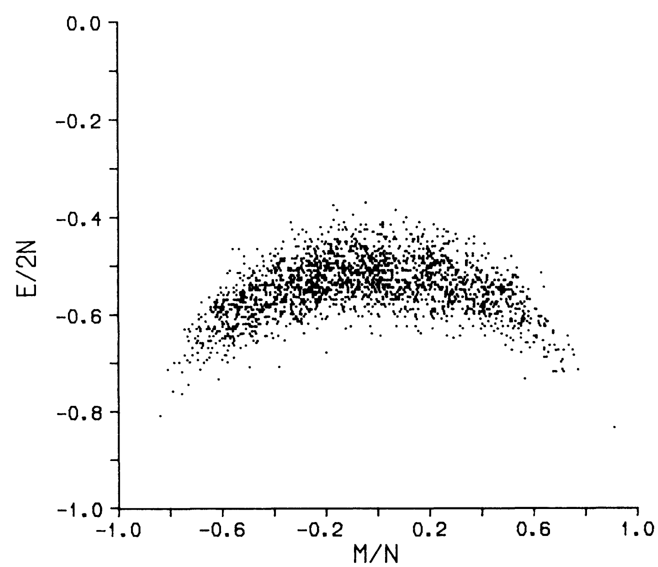

FIG. 5. Scatter plot of M/N and $E/2N$ from a Monte Carlo simulation with $\beta=0.9\beta_c$ and $h=0$.

III. DISCUSSION

The equilibrium state for inverse temperature β and external field $H = h/\beta$ occurs at the maximum of the free-energy function $F_{\beta h}(E,M)$. As β and h vary, the position of the maximum varies; if $\beta > \beta_c$ and h crosses the phase boundary at $h = 0$, then the position of the absolute maximum jumps from one symmetry-breaking phase to the other.

Figure 2 demonstrates that the function $F_{\beta 0}(E,M)$ has two local maxima for $\beta > \beta_c$, for the 20×20 lattice. This result explains why the equilibrium state changes discontinuously, with hysteresis, when the Boltzmann distribution is sampled: for $|h|$ sufficiently small there are two local maxima of $F_{\beta h}(E,M)$, both creating metastable states. Thus if the system is initially in the spin-down ordered phase, and then h increases to a value slightly greater than 0, the system remains in the spin-down phase for many Monte Carlo sweeps, even though $h > 0$. If h increases further the local maximum of the spin-down phase diminishes; when h is sufficiently large this ceases to be a local maximum, and the system jumps to the spin-up phase. In contrast, the microcanonical equilibrium state is at the maximum of $F_{\beta M_c}(E,M)$, which has only a single local maximum for any (β, M_c); therefore the system changes continuously, without hysteresis, as (β, M_c) varies.

The fact that $F_{\beta 0}(E,M)$ has two local maxima for $\beta > \beta_c$ implies that for a 20×20 lattice the entropy violates a convexity condition. To describe the violation of this convexity condition, let $\rho(M)$ be the density of states as a function of magnetization for fixed $\beta > \beta_c$; i.e., the distribution[1]

$$\rho(M) = \int e^{S(E,M)} e^{-\beta E} dE/Z = e^{S_r(M)} , \qquad (17)$$

where $S_r(M)$ will be called the reduced entropy. The average magnetization for external field $H = h/\beta$ is[1]

$$\overline{M} = \int e^{S_r(M)} e^{hM} M\, dM \Big/ \int e^{S_r(M)} e^{hM} dM . \qquad (18)$$

Since $S_r(M)$ and M are extensive quantities, the magnetization is sharply peaked at the maximum of the function

$$F_h(M) = S_r(M) + hM . \qquad (19)$$

If $S_r(M)$ has two equal local maxima at $\pm M_0$, then the position of the absolute maximum of $F_h(M)$ jumps from $-M_0$ to $+M_0$ discontinuously as h varies from $0-$ to $0+$. This is precisely what happens for $\beta > \beta_c$. The fact that $S_r(M)$ has two local maxima for $\beta > \beta_c$ follows from the existence of two local maxima of $F_{\beta_c 0}(E,M)$ in Fig. 2. But to see the two peaks directly, $S_r(M)$ itself can be computed: Since the equilibrium state is at the maximum of $F_h(M)$,

$$(dS_r/dM)_{\rm eq} = -h ; \qquad (20)$$

the microcanonical measurements of h and $\overline{M}$ for fixed β yield this derivative, which can be integrated to compute $S_r(M)$, up to an additive constant.

Figure 6 shows $\overline{M}$ versus h computed by sampling the Boltzmann distribution (plotted as points joined by line segments), and the microcanonical distribution $P(s)$ (plotted as crosses), for $\beta = 1.4\beta_c$, i.e., at a temperature far below the critical point. In the canonical ensemble the system jumps from spin up to spin down or vice versa, with hysteresis, as h varies. In the microcanonical ensemble the system changes continuously from one phase to the other, but $\overline{M}$ is not a single-valued function of h. It is significant that the limit of metastability in the canonical ensemble is the same as the range of the multivalued crossover region in the microcanonical ensemble. Now, integrating $-h$ as a function of $\overline{M}$ yields the reduced entropy $S_r(M)$, up to an additive constant. Arbitrarily normalizing $S_r(0) = 0$, I obtain the result shown in Fig. 7; the two maxima of $S_r(M)$ are at $\pm M_0$, where $M_0/N = 0.98$.

The double maximum of $S_r(M)$ violates the usual convexity condition. The susceptibility χ is defined by

$$\chi = d\overline{M}/dH = -\beta[(d^2S_r/dM^2)_{\rm eq}]^{-1} . \qquad (21)$$

To have $\chi > 0$, the function $S_r(M)$ must be convex, with $d^2S_r/dM^2 < 0$. But the double maximum of $S_r(M)$ means that $d^2S_r/dM^2 > 0$ over some range of M between the peaks. This region cannot be measured in the canonical ensemble, since M jumps from one peak to the other as h varies. But $S_r(M)$ is an intrinsic property of the system, independent of the external field; and its dependence on M between the peaks is particularly interesting.

In an infinite system $S_r(M)$ does not have two peaks. Rather, $S_r(M)$ is constant at the value $S_r(\pm M_0)$ for M in the range $(-M_0, M_0)$, because of domain formation. The

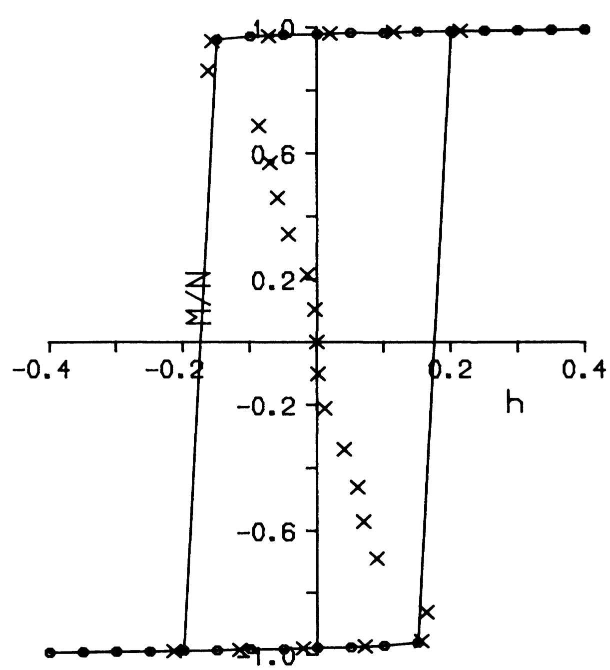

FIG. 6. Mean magnetization per spin $\overline{M}/N$ vs external field h from simulation of the canonical ensemble (points connected by line segments) and microcanonical ensemble (crosses), for $\beta = 1.4\beta_c$.

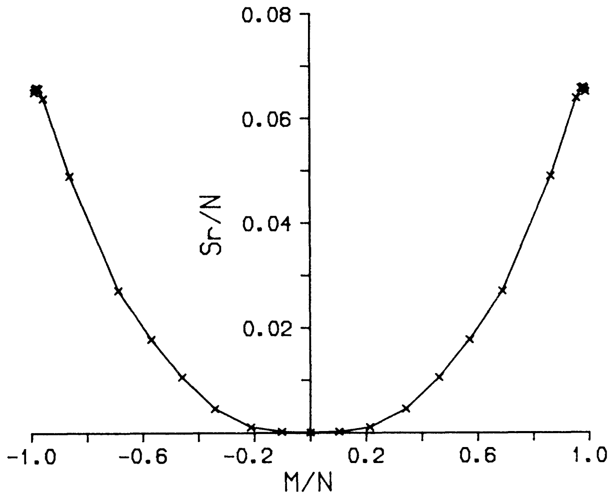

FIG. 7. Reduced entropy per spin S_r/N vs magnetization per spin M/N for $\beta=1.4\beta_c$. The entropy $S_r(M)$ is normalized to be 0 at $M=0$.

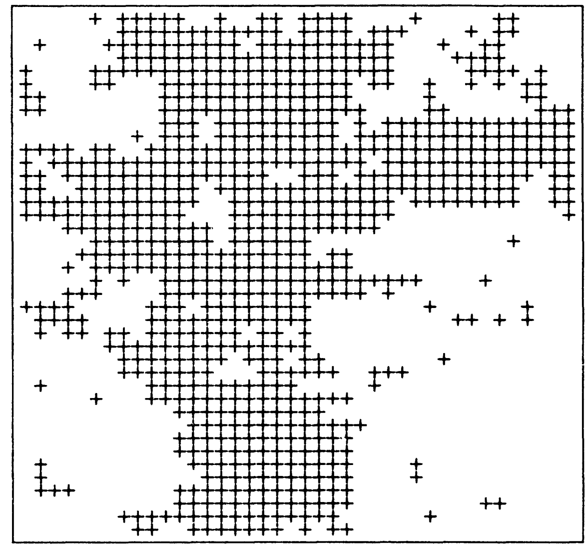

FIG. 8. Typical configuration generated in the simulation of the microcanonical ensemble for $\beta=\beta_c$ and $M_c=0$. The crosses $(+)$ are plotted at lattice sites where the Ising spin is $s=+1$.

energy of a configuration consisting of spin-up phase in a fraction f of the lattice and spin-down phase in the other fraction $1-f$, is the sum of the volume energies of the two domains, plus the surface energy of the boundary between the domains. But in an infinite lattice the surface energy is negligible. Therefore states with different domain fractions f are equally likely. Since any magnetization between $-M_0$ and M_0 can be achieved by the correct choice of f, $S_r(M)$ is constant.

In the 20×20 lattice the surface energy of the boundary between spin-up and spin-down domains is not negligible compared to the volume energy. Therefore these states of intermediate M are pushed to higher energy relative to the pure phases, leaving behind an *entropy deficiency* in the intermediate range of M. The region of entropy deficiency creates the double maximum of $S_r(M)$, and is ultimately the cause of the first-order phase transition. An interesting question is whether this statement applies to every system with a first-order phase transition: that a small, i.e., not macroscopically large, sample has an entropy deficiency in the region of configuration space intermediate between the pure phases.

The striking difference between the microcanonical and canonical ensembles is that for $\beta>\beta_c$ there are stable equilibrium states intermediate between pure spin-up or spin-down states in the microcanonical case. The reason is that the equilibrium state of the microcanonical ensemble is at the maximum of

$$F_{M_c}(M)=S_r(M)+\ln P_M(M)\ , \tag{22}$$

which moves throughout the domain $(-M_0,M_0)$ as M_c varies. In particular, for $M_c=0$ the mean magnetization is $\overline{M}=0$. Figure 8 shows a typical configuration for $M_c=0$ at $\beta=\beta_c$, for a 40×40 lattice. The spins are fairly well separated into spin-up and spin-down domains, but with an irregular domain boundary. If β decreases the domain boundary lengthens, until eventually the domains break up. If β increases the domain boundary shortens, and the spins separate into two compact ordered domains.

IV. COMMENT ON FINITE LATTICE SIZE

The thermodynamic relations in Eqs. (4) and (14) are the basis of the calculation of $S(E,M)$. These relations are only exact in the infinite volume limit. For a finite lattice, the mean value $(\overline{E},\overline{M})$ does differ slightly from the value (E',M') that maximizes the function $F_{\beta M_c}(E,M)$. The difference is only of order 1 where E and M are of order N, so for a 20×20 lattice it is small. But the question arises whether the calculation of $S(E,M)$ is sensitive to this small error.

There are three pieces of qualitative evidence that indicate that $S(E,M)$ is not very sensitive to the finite-size error. First, the free-energy function $F_{\beta 0}(E,M)$ computed from the microcanonical data, shown in Figs. 2 and 4, predicts correctly the result of the canonical ensemble simulation, shown in Figs. 3 and 5. Second, the curves of $\overline{M}$ versus h obtained from microcanonical and canonical ensembles with the same β are virtually identical for $\beta<\beta_c$. For $\beta>\beta_c$ they differ only in the hysteresis region; and even in the hysteresis there is similarity in that the limit of metastability in the canonical ensemble is the same as the range of the microcanonical crossover, as shown in Fig. 6. Third, there is a self-consistency check on the calculation of the derivatives of $S(E,M)$: Equation (4) implies that

$$\partial\beta/\partial\overline{M}=-\partial h/\partial\overline{E}\ ;$$

the numerical results obey this relation, to within the accuracy of the calculation.

It is not obvious how to determine the finite-size error precisely. It is not sufficient to compare results for different lattice sizes, because the entropy itself changes with lattice size.

However, a further, more quantitative test of the accuracy of the microcanonical method may be obtained by calculating the magnetization distribution

$$\rho(M)=\sum_{\{s\}} e^{-\beta E(s)}\delta(M,M(s)) \quad (23)$$

in two different ways. On the one hand, $\rho(M)$ can be calculated directly, by sampling the Boltzmann distribution $\exp[-\beta E(s)]$ by the Monte Carlo method and plotting a histogram of the magnetizations of the states in the sample. Figures 9 and 10 show histograms[12] for $\beta=\beta_c$ and $\beta=0.9\beta_c$, where β_c is the critical temperature of the infinite two-dimensional Ising model, Eq. (16). The number of Monte Carlo sweeps, which is the number of points in each histogram, is 6000.

On the other hand, $\rho(M)$ can also be calculated by the microcanonical method. The distribution of states sampled in the microcanonical calculation is

$$e^{-\beta E(s)}e^{S_d[M_c-M(s)]}, \quad (24)$$

where $S_d(M_d)$ is the entropy of the system of demon spins and M_c is the combined magnetization of the Ising spins and the demon spins. Thus the distribution of M in the microcanonical sample is

$$\rho(M)e^{S_d(M_c-M)}=e^{S_r(M)+S_d(M_c-M)}, \quad (25)$$

where $S_r(M)=\ln\rho(M)$. This distribution is sharply peaked at the maximum of the function $S_r(M)+S_d(M_c-M)$; therefore, the mean magnetization $\overline{M}$ obeys approximately the relation

$$S_r'(\overline{M})=S_d'(M_c-\overline{M})=-h(\overline{M}), \quad (26)$$

where the second equation defines the external field h. This formula is the basis of the microcanonical calculation: For each M_c a Monte Carlo calculation yields a measurement of $\overline{M}$ and $h(\overline{M})$; as M_c varies, $S_r'(M)$ is determined for all M. Then $\rho(M)$ can be estimated by integrating $h(M)$,

$$\rho(M)=K\exp\left[-\int_0^M h(M')dM'\right], \quad (27)$$

where K is a suitable normalization constant. However, the relation (26) is only exact in the limit of an infinite lattice; this is the origin of the finite-size error in the microcanonical method. For a 20×20 lattice, with $N=400$ spins, the error is expected to be small; the purpose of this calculation is to verify that it is small.

Figure 11 shows the external field h as a function of the mean magnetization per spin M/N, measured in microcanonical Monte Carlo calculations, for $\beta=\beta_c$ and $0.9\beta_c$.[12] The curves in Figs. 9 and 10 show the resulting $\rho(M)$ obtained from Eq. (27), normalized such that the integral is 6000, the same as that of the histograms. For $\beta=0.9\beta_c$ there is no significant difference between the

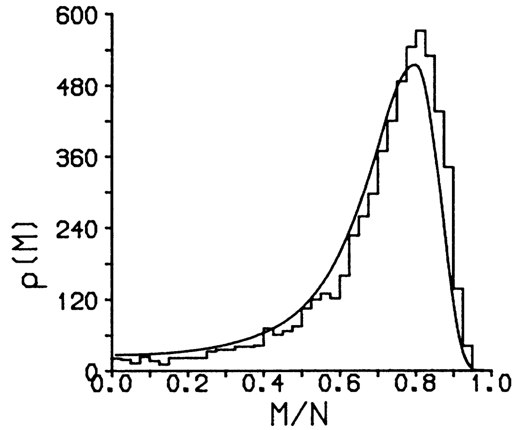

FIG. 9. The magnetization distribution $\rho(M)$ for $\beta=\beta_c$ on a 20×20 lattice with periodic boundary conditions; M/N is the magnetization per spin. The histogram consists of 6000 samples from the Boltzmann distribution. The curve was derived by integrating the external field vs M measured in microcanonical calculations.

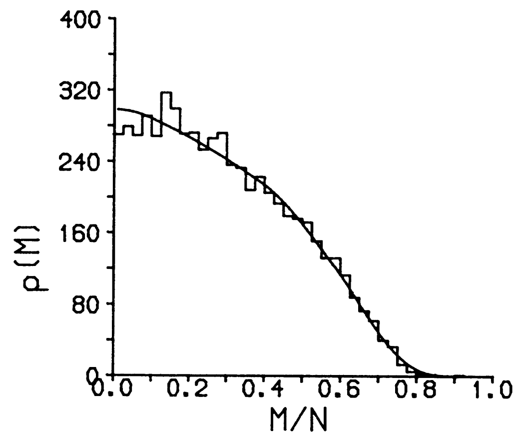

FIG. 10. The magnetization distribution $\rho(M)$ for $\beta=0.9\beta_c$; the curves have the same meaning as in Fig. 9.

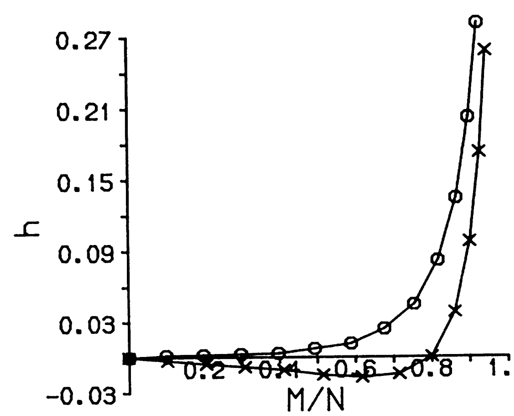

FIG. 11. External field h vs mean magnetization per spin M/N measured in microcanonical calculations, for $\beta=\beta_c$ (points plotted as crosses $\times$) and $0.9\beta_c$ (points plotted as circles $\circ$). Values between the measurements are estimated by linear interpolation.

results of the two calculations of $\rho(M)$. For $\beta=\beta_c$ there is a discernible difference between the two distributions, with the most probable value of M slightly larger in the canonical ensemble than predicted by the microcanonical result. However, the error is quite small, and the large change in $\rho(M)$ from $\beta=0.9\beta_c$ to β_c is correctly predicted by the microcanonical calculations. For β far from β_c the finite-size error is even smaller than in Figs. 9 or 10, because the error is largest at the critical point where there is long-range correlation between fluctuations of the spins.

Section II describes a calculation of the entropy function $S(E,M)$. The distribution $\rho(M)$ is related to $S(E,M)$ by Eq. (17). The finite-size errors in the estimates of $S(E,M)$ and $S_r(M)$ should be of the same order of magnitude. Figures 9 and 10 indicate that the error is small for a lattice size as small as 20×20. This does not imply that $S(E,M)$ is the same for a 20×20 lattice as for an infinite lattice, but only that the microcanonical method of estimating $S(E,M)$ is accurate for a lattice as small as 20×20.

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[1]For simplicity I have used a notation in which the energy E and magnetization M can take a continuum of values. For the Ising model, for which E and M are integer valued, the interpretation of this notation is as follows: derivatives with respect to E or M mean finite differences, and integrals over E or M mean sums.

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