Canonical-ensemble results for the Ising model with random bonds in two dimensions

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The purpose of this paper is to show how some interesting numerically exact thermal averages can be computed for finite two-dimensional Ising models by a transfer-matrix method, and to apply these methods to the Ising version of the Edwards-Anderson (EA) model of a spin-glass to ascertain whether there is a phase transition. We do not study the spatial dependence of $\langle \sigma_0 \sigma_l \rangle$ for, as we show with an example, its behavior for finite systems can be misleading. It is first shown how to obtain χ'_{EA} , defined by $\chi'_{EA} = N^{-1} \sum \langle \langle \sigma_i \sigma_j \rangle_T^2 \rangle_J$. We compute χ'_{EA} and study the quantity $\Lambda = -\partial \ln(\chi'_{EA})/\partial T$, both as a function of temperature (T) and of the number of spins (N) in the system. The results obtained for square systems of up to 100 spins in the case where $J = \pm 1$ with equal probability and for square systems of up to 121 spins in the case where each J is normally distributed about J=0 are in accord with the existence of a critical point at $T_0 \simeq 1.0$ and at $T_0 \simeq 0.6$, respectively. In addition the value $\nu \approx 1$ is obtained. The value q = 0 for T > 0 is consistent with the results obtained. The low-temperature entropy per spin (S) is computed for long strips of different widths. Extrapolation to an infinite width yields $S/k \simeq 0.07$. It is also shown how to calculate the probability, $P(\eta)$, that the quantity, $\eta = N^{-1} \sum \tau_i \sigma_i$, where each $\tau_i = 0, \pm 1$ take any value in the range $1 \le \eta \le 1$. The probability, $P(\eta)$, obtained for the EA model at low temperatures often has several maxima separated by regions of improbable values of η , as is to be expected of a system with metastable states.

I. INTRODUCTION

Spin-glasses¹ have been the subject of interest in the past few years. The so-called canonical² spinglasses are metallic alloys of a magnetic-transitionmetal solute in a noble metal, such as CuMn or AuFe at low solute concentrations. The magnetic atoms are quenched in supposedly random positions and interact amongst themselves through the Ruderman, Kittel, Kasuya, Yosida³ (RKKY) exchange. The random location of the local moments plus the longrange oscillatory nature of the RKKY interaction produce a random mesh of ferromagnetic and antiferromagnetic bonds, some of which must necessarily be broken even in the ground state. This property, known as frustration,⁴ and strong frozen disorder have come to be recognized as the essential features of, not just the canonical spin-glasses, but of all spinglasses.⁵ A different example of a spin-glass is the insulating system⁶ Eu_xSr_{1-x}S, where two magnetic atoms (Eu) interact ferromagnetically if they are nearest neighbors, but they interact antiferromagnetically if they are second nearest neighbors. At suitable values of x (concentration of magnetic atoms), there is again both: (a) strong disorder in the position of the moments; (b) consequently, not all ferromagnetic and antiferromagnetic bonds can be satisifed, i.e., the system is *frustrated*.

Due to the combined effects of disorder and frustration, the low-temperature properties of spin-glasses are not fully understood. Whether a sharp phase transition exists separating the paramagnetic and spin-glass phases has not yet been established either. Early Mössbauer studies⁷ showed that, at least for the observation times of this type of experiment (10^{-7} sec) , the spins in the system freeze, that is, the quantity

$$q(t) = N^{-1} \sum_{i} \left\langle \vec{\mathbf{S}}_{i}(0) \cdot \vec{\mathbf{S}}_{i}(t) \right\rangle \quad , \tag{1}$$

where $\overline{S}_{i}(t)$ is the *i*th spin at time *t*, the sum is over the *N* spins in the system, and $\langle \rangle$ denote thermal averages, does not vanish at low temperatures for $t \leq 10^{-7}$ sec. Furthermore, it followed from the Mössbauer work, and was confirmed by neutron scattering experiments,⁸ that different spins freeze in different random directions, that is,

$$\mathbf{V}^{-2} \sum_{ij} \langle \vec{\mathbf{S}}_i \cdot \vec{\mathbf{S}}_j \rangle \exp(i \vec{\mathbf{Q}} \cdot \vec{\mathbf{R}}_{ij}) = 0$$
 (2)

for any \vec{Q} , where \vec{R}_{ij} is the position of the *i*th spin with respect to the *j*th one.

Initial results obtained by Edwards and Anderson⁹ (EA) for their model agreed with Eq. (2) and they obtained a nonvanishing order parameter,

$$q = N^{-1} \sum_{i} \langle \vec{\mathbf{S}}_i \rangle^2 \quad , \tag{3}$$

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below the freezing temperature, T_f . The Ising version of the EA model, with a Hamiltonian given by,

$$\mathfrak{K} = -\sum_{ij} J_{ij} \sigma_i \sigma_j - H \sum_{i} \sigma_i : \sigma_i = \pm 1 \quad , \tag{4}$$

where each J_{ij} is an independent random variable with a probability density $p(J_{ij}) \propto \exp(-J^2_{ij}/2)$ if i and j are nearest neighbors of $J = \pm 1$ with equal probability, has been the most widely studied spin-glass model. It is a strongly disordered system with frustration.⁴ In the following, we shall be referring to this model unless stated otherwise. Monte Carlo (MC) work¹⁰ seemed to confirm at first that $q \neq 0$ at low temperatures in two and three dimensions. Instead, Bray et al.¹¹ argued that the MC results showed that q(t) vanishes, albeit very slowly, as $t \rightarrow \infty$ at low temperatures. More recently, Morgenstern and Binder¹² have used a transfer-matrix method (see Sec. II of this paper) to obtain results indicating that q vanishes for $T \neq 0$ in two dimensions. As is well known, the behavior of q(t) as $t \rightarrow \infty$ bears directly on the behavior of the susceptibility in the Ising version of the EA model, since¹³

$$\chi(t) = (1/kT)[1 - q(t)] , \qquad (5)$$

where $\chi(t)$ is the magnetization of the system at time t divided by a vanishingly small external field which is switched on at t = 0. Thus, if q(t) does not vanish as $t \rightarrow \infty$, then the equilibrium susceptibility, $\chi(t \rightarrow \infty)$, is purely paramagnetic, as follows from Eq. (5), and any observed departure from such a behavior would be a time dependent effect, as stressed by Bray *et al.*¹¹

The previous remarks pertain to the lowtemperature nature of spin-glasses; however, whether a sharp phase transition exists separating the paramagnetic and spin-glass phase, a question of considerable recent interest, cannot be settled by showing that q vanishes for all $T \neq 0$; q = 0 does not rule out a phase transition as in the XY model.¹⁴

The existence of (or lack of) a sharp phase transition has not been established unambiguously by experimental work.¹⁵ Different interpretations of neutron scattering results have led to different views on this question.¹⁶ On the other hand, the magnetic susceptibility as a function of frequency, $\chi(\omega)$, can be obtained by magnetic resonance work. A sharp cusp in $\chi(\omega)$ vs T at some temperature $T_f(\omega)$ implies a sharp phase transition if $T_f(\omega)$ lends to some nonzero value as $\omega \rightarrow 0$; otherwise, the susceptibility cusp would be a transient effect, albeit, a very long lived one. Again, there seems to be no general agreement on this point.¹⁷

Most theoretical work and computer simulations have been done on the Ising version of the EA model. Different renormalization-group calculations¹⁸ have produced different answers regarding the existence of a true phase transition in 2 or 3 space dimensions. A critical review of renormalizationgroup results and their reliability has been given by Kirkpatrick.¹⁹

More recently, Morgenstern and Binder (MB)¹² have applied the transfer matrix method (see Sec. II of this paper) to the Ising EA model in two dimensions. We have also developed and applied this method independently.²⁰ This method provides numerically exact results for any one system with a given set of exchange constants. Since it is a numerically exact method, it avoids some of the pitfalls of MC and of the renormalization-group work. There are two main limitations in the application of this method however: (a) practical considerations do not allow the applicability of this method to large systems; (b) averages over an *infinite* set of systems with different exchange constants cannot, of course, be carried out.

By an approximate method, MB first obtain the spin directions in a ground state of the system. Let $\tau_i = 1(-1)$ if the *i*th spin points up (down) in such a ground state. They then compute, for that particular ground state, the quantity ψ , given by,

$$\psi^2 = N^{-2} \sum_{i,j} \tau_i \tau_j \langle \sigma_i \sigma_j \rangle_T \quad , \tag{6}$$

where the sum is over all $1 \le i \le N$ and all $1 \le j \le N$ and $\langle \rangle_T$ denotes a thermal average. The results of MB obtained for finite N point towards $\psi \to 0$ as $N \to \infty$ if T > 0. For the EA model with each $J = \pm 1$, ψ seems to vanish as $N \to \infty$ even at T = 0. The vanishing of ψ suggests that q vanishes also, although as MB remark, it is not necessarily so if T > 0.

In this paper, we study the quantity,

$$\chi'_{\rm EA} = N^{-1} \sum \left\langle \left\langle \sigma_i \sigma_j \right\rangle_T^2 \right\rangle_J \quad , \tag{7}$$

where $\langle \rangle_j$ denotes an average over systems with different sets exchange constants, and the double sum extends over all values of *i* and *j*. This quantity has the virtue of not being tied to any ground state as ψ is, furthermore, the relation

$$N^{-1}\chi'_{\mathrm{EA}} \underset{N \to \infty}{\longrightarrow} q^2 \tag{8}$$

is valid at any temperature. In addition, as has been pointed out by Chalupa,²¹ the quantity χ_2 , defined by, $\chi = \chi_0 + \chi_2 h^2 + \cdots$, where *h* is the applied magnetic field, and χ'_{EA} are related; the relation simplifies if χ_2 diverges, then, as $T \rightarrow T_f$ from above,

$$\chi_2 \rightarrow -3\chi'_{\rm EA}/kT \quad , \tag{9}$$

where k is Boltzmann's constant. On the other hand, as is well known, $-\chi_2$ must be very large in the vicinity of T_f , for quite small applied fields are enough to round the cusp in χ vs T. Indeed, the experimental results of Miyako *et al.*²² indicate a diverging χ_2 at T_f . We therefore explore (in Sec. II) the distinct

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possibility that, in the EA model, $\chi_{EA} \rightarrow \infty$ at T_0 , whether q = 0 for $T < T_0$ (in analogy with the XY model in two dimensions) or not.

The nature of the spin-glass phase (quite independently of whether a sharp phase transition separates it from the paramagnetic phase) has not been fully established yet. Experimental^{1,2} work shows that there are many states available at low temperature, since the entropy (S) is linear in T. Monte Carlo¹⁰ work has also produced $S \propto T$ at low T for the EA model with J normally distributed and²³ $S \rightarrow 0.10$ as $T \rightarrow 0$ for the two-dimensional EA model with $J = \pm 1$, which is significantly larger than the value S = 0.07found by MB by the transfer matrix method. The likely origin of the discrepancy in these two values is easily understood. First note that in MC work, as the temperature is gradually lowered the relaxation times becomes longer and the energy (E) of the system fails to reach its equilibrium values by ever larger amounts, thus, from

$$C = \frac{\partial E}{\partial T} \quad , \tag{10}$$

one gets a value of C (specific heat) which is lower than its equilibrium value. Now, S is obtained¹¹ calorimetrically⁴ in MC work, that is by means of,

$$S(T) = S(T \to \infty) - \int_0^\infty [C(T)/T] dT \quad , \qquad (11)$$

whence an overestimate of S(T=0) follows. Such an effect has been anticipated¹³ by theoretical work on Ising chains with random bonds and has been observed experimentally.²⁴ This discrepancy in the $T \rightarrow 0$ limiting values of S illustrates the importance of long-time effects spin-glasses.

It is thought^{13,25} that many of the states available to spin-glasses at low temperatures are metastable states, which are responsible for their slow relaxation. The transfer matrix method is also useful in this regard to check this idea. Consider any spin configuration $\{\tau_1, \tau_2, \ldots, \tau_N\}$, and let

$$\eta = N^{-1} \sum \tau_i \sigma_i \quad . \tag{12}$$

The probability that η take any value in the range $-1 \le \eta \le 1$ can be obtained (see Sec. II D) at any temperature. If $\tau_i = 1$ for every *i*, for instance, then η is the magnetization per spin; on the other hand, if the value of each τ_i is chosen according to ground-state spin configuration, then $P(\eta = 1) \rightarrow 1$ and $P(\eta \neq 1) \rightarrow 0$ if there is no ground-state degeneracy. If the picture of multiple metastable states at low temperatures is right, the $P(\eta)$ should have some humps associated with metastable states separated by regions where P is small. The quantity $P(\eta)$ contains additional information as well, such as the value of ψ studied by MB, since

$$\psi^2 = \sum_{\eta} \eta^2 P(\eta) \quad , \tag{13}$$

as follows from Eqs. (5) and (9). The magnetic susceptibility at any field H can, of course, be calculated from $P(\eta)$ if $\tau_i = 1$.

The paper is organized as follows: Our methods and results are presented in Sec. II, while the conclusions appear in Sec. III. Section II comprises several parts. In Sec. II A an explanation is given of the application of the transfer matrix method to the computation of the equilibrium values of the twodimensional Ising model with any given set of exchange constants. In Sec. II B it is shown how to obtain χ'_{EA} , defined in Eq. (7), and its critical behavior is studied. Our results for the EA model in two dimensions are consistent with $\xi \sim (T - T_0)^{-\nu}$, with $\nu = 1 \pm 0.5$, $T_0 \simeq 1.0$ for the case in which $J = \pm 1$, but $T_0 \simeq 0.6$ for the case in which J is in the form of a Gaussian distribution. In Sec. IIC, the entropy of very long strips of EA systems with $J = \pm 1$ is obtained at a very low temperature (T = 0.1) for different widths; the value of the entropy, extrapolated to an infinite width, is in agreement with the result of MB. In Sec. II D, we show how to calculate the probability $P(\eta)$ that η , defined in Eq. (9), take a given value. It is obtained for some temperatures for a couple of choices of the set $\{\tau_i\}$.

In Sec. III we conclude that there is a phase transition in the two-dimensional Ising version of the EA model. To support this conclusion, we contrast our results with: (i) χ'_{EA} for an Ising model with random bonds in one dimension (where one knows that no phase transition exists); (ii) the quantity $\chi' = \sum_{ij} \langle \sigma_i \sigma_j \rangle$ for an ordinary Ising ferromagnet in two dimensions, where a phase transition is known to exist. It is also shown that $\langle \sigma_i \sigma_j \rangle \approx A \exp(-r_{ii}/\xi)$, for a finite Ising ferromagnet of 10×25 spins at T = 2.2 (note that $T_c \simeq 2.27$). This result is to be contrasted with $\langle \sigma_i \sigma_j \rangle \sim r^{-1/4}$ which is the known²⁶ behavior for an *infinite* system at $T = T_c$ ($T_c \simeq 2.27$). This result undermines the conclusion of MB that there is no phase transition in the EA model in two dimensions, since their conclusion is based on their result that $\langle \langle \sigma_i \sigma_j \rangle_T^2 \rangle_J \sim \exp(-r_{ij}/\xi)$ for a finite system at low temperatures with the points i and jwithin a distance smaller than ξ to the boundary of the system. Thus, the possibility that $\langle \langle \sigma_i \sigma_j \rangle_T^2 \rangle_J$ $\sim r_{ij}^{-x}$ below some temperature for an *infinite* EA model cannot be excluded.

II. METHODS AND RESULTS

A. Transfer matrix

Consider a square lattice of spins with columns and rows with semiperiodic boundary conditions: the lattice is on a cylindrical surface with its columns parallel to the cylinder's axis. We could just as easily deal with a system with free boundary conditions, but it will not do so here. On the other hand, to use fully periodic boundary conditions is impractical, as may be appreciated below. Let all the spins $(\sigma'_1, \sigma'_2, \ldots, \sigma'_M)$ on the uppermost row (let it be the *n*th one) be fixed while a sum all over the other spins in the system is performed, and let $Z(\sigma'_1, \sigma'_2, \ldots, \sigma'_M)$ be such a partial sum over states. Clearly, the partition function Z_n fulfills

$$Z_n = \sum Z(\sigma'_1, \sigma'_2, \dots, \sigma'_M)$$
(14)

and

$$Z_{n+1}(\sigma_1, \sigma_2, \ldots, \sigma_M) = \exp\left(\beta \sum_i \sigma_i (J_i' \sigma_{i+1} + H)\right) \prod_i \sum_{\sigma_i'} \exp(\beta J_i \sigma_i \sigma_i') Z(\sigma_1', \sigma_2', \ldots, \sigma_M') \quad , \tag{15}$$

where $\{J_i'\}$ is the set of horizontal bonds in the (n+1)th row, and $\{J_i\}$ is the set of bonds connecting the *n*th and (n+1)th rows. Equations (14) and (15) suggest immediately the iterative procedure to be followed to obtain Z_n . Note that performing the operations in the order indicated in Eq. (15) leads to a computing time which goes as $MN2^M$, not as 2^{MN} , where M(N) is the number of columns (rows).

B. Edwards-Anderson susceptibility

To obtain χ'_{EA} , defined by Eq. (7), first let

$$\chi_0 = N^{-1} \lim_{N \to \infty} \lim_{H \to 0} (\beta)^{-2} \partial^2 \ln Z / \partial H^2 , \qquad (16)$$

which yields

$$\chi_0 = N^{-1} \sum \langle \sigma_i \sigma_j \rangle_T \quad , \tag{17}$$

since $\langle \sigma_i \rangle_T = 0$, due to the unusual order in which the limits are taken in Eq. (16). Clearly, χ_0 only equals the physical susceptibility if no symmetry is broken, i.e., if $\langle \sigma_i \rangle_T = 0$. To perform Eq. (16) numerically, we use $\Delta H = 10^{-2} N^{-1}$ kT. Now note that

$$\langle \chi_0^2 \rangle_J - \langle \chi_0 \rangle_J^2 = 2N^{-2} \sum_{ij}' \langle \langle \sigma_i \sigma_j \rangle_T^2 \rangle_J \quad , \tag{18}$$

where the prime indicates that the term i = j is excluded, since

$$\langle \langle \sigma_i \sigma_j \rangle_T \langle \sigma_l \sigma_m \rangle_T \rangle_J$$

$$= \langle \langle \sigma_i \sigma_j \rangle_T^2 \rangle_J (\delta_{il} \delta_{jm} + \delta_{im} \delta_{jl}) + \delta_{ij} \delta_{lm} \quad . \quad (19)$$

It follows from the definition of χ'_{EA} , Eq. (7), that

$$\chi'_{\rm EA} = (N/2) \left(\langle \chi_0^2 \rangle_J - \langle \chi_0 \rangle_J^2 \right) + 1 \quad . \tag{20}$$

Thus, averaging χ_0 and χ_0^2 over systems with different sets of $\{J_{ij}\}$ yields χ_{EA} . Note that $\langle \chi_0 \rangle_J = 1$. It would be more convenient to study the quantity,

$$\chi_{\rm EA} = \chi'_{\rm EA} - N^{-1} \sum_{i,j} \langle \langle \sigma_i \rangle_T^2 \langle \sigma_j \rangle_T^2 \rangle_J \quad , \tag{21}$$

than to study χ'_{EA} , for if there were a phase transition at some T_0 , and if in addition $\langle \langle \sigma \rangle_T^2 \rangle_J \neq 0$ for $T < T_0$, then χ_{EA} would conveniently peak (diverge if $N \to \infty$) there, whereas χ'_{EA} would just increase monotonically as T decreases. Unfortunately $\langle \langle \sigma_i \rangle_T^2 \langle \sigma_j \rangle_T^2 \rangle_J$ can only be obtained for a very large system $(N \to \infty)$, to have a broken symmetry), and we consequently only obtain χ'_{EA} and not χ_{EA} ; if, on the other hand, there is either no phase transition or there is a phase transition as in the XY model, in which χ_{EA} would diverge at some T_0 but q = 0 for any $T \neq 0$, then, of course, $\chi'_{EA} = \chi_{EA}$ for all $T \neq 0$. Anyway, it is most convenient to study the quantity

$$\Lambda = -\frac{\partial \ln(\chi_{\rm EA})}{\partial T} \quad , \tag{22}$$

for reasons that will become immediately clear. Let us first assume that, at least for $T > T_0$,

$$\chi'_{\rm EA} \sim \xi^x$$
 , (23)

where ξ is a correlation length, as follows if

$$\langle \langle \sigma_i \sigma_j \rangle_T^2 \rangle_J = f(r_{ij}/\xi)/r_{ij}^y \quad . \tag{24}$$

Now, if in addition $\xi \sim |1 - T/T_0|^{-\nu}$, then,

$$\Lambda \sim |1 - T/T_0|^{-1} , \qquad (25)$$

whence,

$$\Lambda \sim \xi^{1/\nu} , \qquad (26)$$

for an infinite system. However, for a finite system, Λ saturates when ξ becomes comparable to L. Therefore,

$$\Lambda \sim L^{1/\nu} \quad , \tag{27}$$

at $\xi(T) \approx L$, where L is the side of the square system. On the other hand, since

$$\chi'_{\rm EA} \leq N$$
 , (28)

it follows from the definition of Λ , Eq. (22), that

$$\int_0^\infty \Lambda(T) dT \le \ln(N) \quad . \tag{29}$$

From Eqs. (27) and (29), it follows that if ξ diverges at some nonvanishing temperature T_0 with a finite ν then plots of Λ vs T, for systems of different sizes, will show maxima in Λ at T_0 , and these maxima, $\Lambda(T_0)$, will obey Eq. (27). We now summarize our procedure to obtain Λ . Following a given rule (for instance, each $J = \pm 1$ with equal probability) all the exchange constants of the system are assigned. Next, χ_0 is computed by means of Eq. (16) for this one system. Assigning a new set of \mathcal{F} s we compute a second χ_0 , and so on up to \tilde{n} times. Equation (20) yields χ'_{EA} only in the limit $\tilde{n} \rightarrow \infty$. Let the value of χ'_{EA} , obtained by applying Eq. (20) to a set of \tilde{n} systems, be $\chi'_{EA}(\tilde{n})$, and let the corresponding value of Λ , obtained from Eq. (21), be $\Lambda(\tilde{n})$. Since,

$$\Lambda = \lim_{\tilde{n} \to \infty} \Lambda(\tilde{n}) \quad , \tag{30}$$

we have examined $\Lambda(\tilde{n})$ vs \tilde{n} . It is shown for some particular cases in Fig. 1 for the case $J = \pm 1$, and in Fig. 2 for the case in which J is distributed normally. From curves such as the ones shown in Figs. 1 and 2 follow the estimated statistical errors of the values of Λ we quote.

We have calculated Λ for systems for $L \times L$ spins both for $J = \pm 1$ with equal probability and for J distributed normally about J = 0. In the first case $(J = \pm 1)$ values of Λ were obtained for: L = 4, 6, 8and 10, by averaging over 600 systems for L = 4, 6,



FIG. 1. The values of Λ [defined in Eq. (22)] obtained are shown for a system of 8×8 spins at T = 0.5 vs the number (\tilde{n}) of systems averaged over. Each system contains a particular set of J values assigned by means of a *Gaussian* random number generator. The two dotted lines show 2.3 ± 0.2 (1200/ \tilde{n})^{1/2} where 2.3 is the best value of Λ [i.e., $\Lambda(\tilde{n} = 1200)$], 0.2 is the estimated statistical error in this value of Λ . The statistical error (0.2 in this case) is estimated with the criterion that most of the values $\Lambda(\tilde{n})$ obtained must lie within the dotted lines.



FIG. 2. As in Fig. 1, the values of Λ , defined in Eq. (22), obtained are shown for a system of 8×8 spins at T = 0.9 vs the number (\tilde{n}) of systems averaged over. Each system contains a particular set of J values assigned by means of an unbiased random number generator which yields +1 or -1. The dotted lines show $1.87 \pm 0.20 \ (600/\tilde{n})^{1/2}$ where 1.87 is the best value of Λ [i.e., $\Lambda(\tilde{n} = 600)$], 0.2 is the estimated statistical error in this value of Λ . The statistical error (0.2 in this case) is estimated with the criterion that most of the values $\Lambda(\tilde{n})$ obtained must lie within the dotted lines.



FIG. 3. The quantity Λ is shown for systems of various sizes vs the temperature (*T*). The values of *J* are ± 1 with equal probability.



FIG. 4. As in Fig. 3, the quantity Λ is shown for systems of various sizes vs the temperature (*T*). The values of *J* are normally distributed.

and 8, and over 420 systems for L = 10; the results obtained are shown in Fig. 3. In the second case (J in the form of a Gaussian distribution), values of Λ have been obtained for L = 4, 6, 8, and 11, by averaging over 1200 systems for L = 4, 6 and 8, and over 300 systems for L = 11, the results are shown in Fig. 4.

Both Figs. 3 and 4 exhibit maxima, $\Lambda(T_0)$, at temperatures which appear to be independent of the size of the system. In addition, $\Lambda(T_0)$ increases as L increases, as is exhibited explicitly in Fig. 5.

For comparison, we have also computed

$$\Lambda_F = -\frac{\partial \ln X'}{\partial T} \quad , \tag{31}$$

where $\chi' = N^{-1} \sum \langle \sigma_i \sigma_j \rangle_T$, for the Ising ferromagnet. Furthermore, we have computed Λ , as defined by Eq. (31), with $\chi' = N^{-1} \sum |\langle \sigma_i \sigma_j \rangle|$, for the modified Mattis model. These results are also shown in Fig. 5. They are analyzed in Sec. III.

C. Entropy

The low-temperature entropy of systems of *n* spins wide by *l* spins long has been computed for the case of $J = \pm 1$ with equal probability. The entropy is computed by means of

$$S = \Delta (kT \ln Z) / \Delta T \quad . \tag{32}$$

We have carried out this calculation, using



FIG. 5. The maximum value attained by $(\partial \ln \chi' / \partial T)$ as a function of temperature is shown for square systems of side L as a function of L for (i) an Ising ferromagnet (open squares) $(\chi' \equiv N^{-1} \sum \langle \sigma_i \sigma_j \rangle)$; (ii) the modified Mattis model (crosses) $(\chi' \equiv N^{-1} \sum \langle |\langle \sigma_i \sigma_j \rangle|)$; (iii) the Edwards-Anderson model (open triangles for $J = \pm 1$ and open circles for J normally distributed) $\chi' = \chi'_{EA}$. In all cases, the boundary conditions are semiperiodic. Note that the modified Mattis model and the ferromagnet yield the same results. The statistical errors for the EA model increase from 0.1 for L = 4 to 0.5 for L = 11.

 $\Delta T = 0.1$, for systems 300 spins long with a width in the range $4 \le n \le 10$. For any given *n*, the results were averaged over 10 systems with different sets of exchange constants.

The entropy per spin in units of k is shown in Fig. 6 as a function of n for T = 0.1. Two distinct branches can be seen in the figure: a high one for n even and a lower one for n odd. Both branches seem to converge as $n \rightarrow \infty$.

To understand why there are two branches in Fig. 6, one for n even and one for n odd, consider a close path around the cylinder on which the system is placed and the number (p) of broken vertical bonds cut by such a path. Note that due to frustration some bonds will usually be broken in the ground state. Now, if all spins above the closed path are flipped with all spins below fixed, the energy will change by,

$$\Delta E = 2J(n-2p) \quad , \tag{33}$$

which can only vanish for n even. Thus, there is an extra ground-state degeneracy for systems with an



FIG. 6. The entropy of strips of 300n spins is shown vs 1/n for (i) (+) for n = 4, 6, 8, 10; (ii) (0) for n = 5, 7, 9. Each point shown represents an average over 10 strips.

even number of spins across. To estimate the resulting excess entropy per spin, ΔS , note that each closed path with 2p = n around the cylinder contributes with a factor of 2 to the degeneracy. It follows that if these special paths are a distance λ_n apart on the average, then

$$(\Delta S/k) \simeq (1/n\lambda_n) \ln(2) \tag{34}$$

in the ground state. This expression fits the points in Fig. 6 with $\lambda_n \approx 5$. We estimate a value of $S/k \approx 0.07$ as the extrapolated value as $n \to \infty$.

The above discussion leads us to the following observation: the value of the correlation function, $\langle \sigma_i \sigma_{i+k} \rangle$ will differ significantly from the value it takes for an infinite system if $J = \pm 1$, if the number of spins across the system is even and if k is comparable with the width of the system, since $\lambda_n \approx n$. It is reasonable to expect that $\langle \langle \sigma_i \sigma_{i+k} \rangle_T^2 \rangle_J$ would be too small by the factor $\exp(-k/\lambda_n)$.

D. Probability $P(\eta)$

We next explain how to calculate the probability $P(\eta)$ that the quantity

$$\eta = N^{-1} \sum_{i} \tau_i \sigma_i \quad , \tag{35}$$

where each $\tau_i = \pm 1$, take a given value. Clearly, η can take N + 1 equally spaced values in the range $-1 \le \eta \le 1$. Let

$$Z(\eta) = \sum_{i}^{\prime} e^{-\beta E_{i}} , \qquad (36)$$

where the sum is over all the states of the system with a given value of η . Obviously,

$$Z = \sum Z(\eta) \quad , \tag{37}$$

and

$$P(\eta) = Z(\eta)/Z \quad . \tag{38}$$

To obtain $Z(\eta)$, let

$$Z(Q) = \sum_{\eta} Z(\eta) \exp(-iQ\eta) \quad , \tag{39}$$

and note that this quantity can be obtained by the procedure used in Sec. II A for obtaining Z, by just letting

$$\mathfrak{K} \to \mathfrak{K} + i Q \eta / \beta \quad . \tag{40}$$

If we now let

$$Q = (1 + N^{-1})\pi S \quad , \tag{41}$$

where $S = 0, 1, 2, \ldots, N$, then Fourier inversion yields

$$Z(\eta) = (N+1)^{-1} \sum_{Q} Z(Q) e^{iQ\eta} .$$
 (42)

Thus, to obtain $P(\eta)$, one must first obtain Z(Q) for N+1 values of Q.

We exhibit in Fig. 7 the results obtained for one system of 10×10 with J distributed normally and $\tau_i = 1$ for every *i* (i.e., $\eta = N^{-1} \sum \sigma_i$ in this case). Note that at low temperatures $(T = 0.2) P(\eta)$ has



FIG. 7. The probability that the magnetization $(N^{-1}\sum_{i} \sigma_{i})$ take a given value η is shown vs η for a system of 10×10 spins with each J given by a Gaussian random number generator. The lines are drawn as a visual aid.



FIG. 8. The probability that η take a given value is shown for various temperatures vs η for a system of 10×10 spins with the value of each J assigned by a Gaussian random number generator. Each τ_i in the definition of $\eta(\eta = N^{-1} \sum_{i} \tau_i \sigma_i)$ in this figure) is chosen to agree with the spin configuration obtained for this system after cooling it gradually by means of a Monte Carlo simulation. The lines are drawn as a visual aid.

one maximum at $\eta = 0.06$ and another one at $\eta = 0.10$ and that they are separated by a small value of $P(\eta)$ at $\eta = 0.08$. Such a behavior is to be expected of a system with multiple metastable states. In the $T \rightarrow 0$ limit, $P(\eta)$ must become 1 for one value of η and vanish otherwise in this case. It is noteworthy, that at a temperature as low as T = 0.2the most probable value of n is only realized 14% of the times, as Fig. 7 shows. Figure 8 exhibits $P(\eta)$ for the same system but the values of τ_i in Eq. (35) are chosen to agree with a configuration of spins which was obtained²⁷ by Monte Carlo simulation, cooling to T = 0.5 (at this temperature the system becomes extremely slow in relaxing to equilibrium). Such set of τ_i corresponds to a low-energy configuration. Figure 8 shows how far it is from the groundstate configuration. For comparison, $P(\eta)$ is shown in Fig. 9 for the ordinary Ising model (J = +1) for temperatures not far from $T_c(T_c \simeq 2.27)$.

Figure 10 shows $P(\eta)$ for one system of 10×10 spins with each J chosen to be +1 or -1 with equal probability and $\tau_i = 1$ for each *i*. It is not sharply different from Fig. 7.



FIG. 9. The probability that the magnetization $(N^{-1}\sum_{i} \sigma_{i})$ take a value η is shown vs η for an Ising ferromagnet of 10×10 spins for T = 1.7 and for T = 2.6 spins. Note that Onsager's solution yields $T_{c} = 2.27$.



FIG. 10. The probability that the magnetization $(N^{-1}\sum_{i} \sigma_i)$ take a value η is shown for various temperatures vs η for a system of 10 × 10 spins with the value of each J assigned at random to be ±1 without bias.

III. COMMENTS AND CONCLUSIONS

We shall first comment on the main argument of MB against a phase transition in the Ising model in two dimensions. They obtain $\langle \sigma_i \sigma_j \rangle_T^2$ as a function of the distance, r_{ij} , at low temperatures, both for the case in which $J = \pm 1$ as for the case in which J is normally distributed. They find that $\langle \langle \sigma_i \sigma_j \rangle_T^2 \rangle_J$ $\sim \exp(-r_{ij}/\xi)$ instead of $\langle \langle \sigma_i \sigma_j \rangle_T^2 \rangle_J \rightarrow c$ as $r_{ij} \rightarrow \infty$ as one would for $T < T_c$ for an ordinary Ising model. An algebraic decay, that is $\langle \langle \sigma_i \sigma_j \rangle_T^2 \rangle_J \sim r_{ij}^{-x}$, as in the XY model below its critical temperature, was ruled out by MB. However, the result of MB was obtained for a finite system, and the points i and jwere allowed to be within a distance smaller than ξ from the boundary of the system, and such a procedure will in general affect the qualitative form of $\langle \langle \sigma_i \sigma_j \rangle_T^2 \rangle_J$. To illustrate this point, we exhibit in Figs. 11 and 12 $\langle \sigma_i \sigma_j \rangle$ vs r_{ii} , for an ordinary Ising model (J = 1) of 10×25 at $T = 2.2(T_c \simeq 2.27)$. Figures 11 and 12 clearly favor the form $\langle \sigma_i \sigma_j \rangle$ $\simeq A \exp(-r_{ij}/\xi)$ for $r_{ij} \ge 3$. The analytic result for an *infinite* system is,²⁶ of course, $\langle \sigma_i \sigma_j \rangle \sim r^{-1/4}$ at $T = T_c$. Clearly, the possibility that $\langle \langle \sigma_i \sigma_j \rangle_T^2 \rangle_J \sim r^{-x}$ for the EA model below some critical temperature cannot therefore be ruled out.

For comparison, we next show the behavior of Λ vs T for (i) an Ising chain with random bonds (where one knows that $\chi'_{EA} \rightarrow \infty$ as $T \rightarrow 0$), and (ii) for an Ising ferromagnet (J = +1) in two dimensions (where one knows that $N^{-1} \sum \langle \sigma_i \sigma_j \rangle \rightarrow \infty$ as



FIG. 11. The correlation function $\langle \sigma_i \sigma_{i+l} \rangle$ is shown on a log-log scale vs *l* for an ordinary Ising system of 10×25 spins in two dimensions. The system is on a cylinder, 10 spins along the circumference and 25 spins parallel to the cylinder's axis. The *i*th spin is 5 lattice spacings from the rim of the cylinder and the (i + l)th one is *l* lattice spacings away along a line parallel to the cylinder's axis. Notice the deviation from the power-law $l^{-1/2}$ behavior predicted for large *l* for an *infinite* system.



FIG. 12. As in Fig. 11, the correlation function $\langle \sigma_i \sigma_{i+l} \rangle$ is shown on a semilog scale vs *l* for an ordinary Ising system of 10 × 25 spins in two dimensions. The system is on a cylinder, 10 spins along the circumference and 25 spins parallel to the cylinder's axis. The *i*th spin is 5 lattice spacings from the rim of the cylinder and the (i + l)th one is *l* lattice spacings away along a line parallel to the cylinder's axis.

 $T \rightarrow T_c$). The Ising chain can be treated analytically. A high-temperature series expansion²⁸ yields

$$\langle \sigma_i \sigma_j \rangle = v_i v_{i+1} \dots v_{j-1}$$
, (43)

where $v_i = \tanh(\beta J_i)$ and J_i couples σ_i with σ_{i+1} . Defining

$$\langle v^2 \rangle = (2\pi)^{-1/2} \int [\tanh(\beta J)]^2 \exp(-J^2/2) dJ$$
, (44)

it follows easily that

$$\chi_{\rm EA} = (1 + \langle v^2 \rangle) / (1 - \langle v^2 \rangle) \quad . \tag{45}$$

Therefore, $T\chi'_{EA} \rightarrow (2\pi)^{-1/2}$ as $T \rightarrow 0$, and $\chi'_{EA} \rightarrow 1$ as $T \rightarrow \infty$. These results hold for an *infinite* chain. Figure 13 shows Λ [defined in Eq. (22)] versus T for some finite chains as well. By the transfer matrix method, we have also computed the quantity,

$$\chi' = N^{-1} \sum_{ij} \langle \sigma_i \sigma_j \rangle \quad , \tag{46}$$

for the Ising ferromagnet (J = 1) in two dimensions for systems of various sizes. The quantity Λ_F , defined in Eq. (31), is exhibited in Fig. 14 as a function of temperature. Note that it peaks at T_c as expected $(T_c = 2.27)$, and that the maximum value of Λ_F vs T grows linearly with L, which, according to Eq. (27), agrees with the known²⁶ exact value of $\nu = 1$. For $T \ll T_c$, Λ_F seems fairly independent of L which contrasts somewhat with the low-temperature



FIG. 13. The quantity Λ , defined by Eq. (22), is shown vs temperature for Ising *chains* of different lengths. The values of each J was assigned by a Gaussian random number generator. The curve for the infinite chain was obtained using Eq. (45).



FIG. 14. $\Lambda_F = \partial \ln(N^{-1} \sum_{ij} \langle \sigma_i \sigma_j \rangle) / \partial T$ is shown vs temperature for ordinary Ising ferromagnets of various sizes in two dimensions. Note that Onsager's solution yields $T_c \simeq 2.27$.

behavior of Λ shown in Figs. 3 and 4 for the EA model. We look into this point below.

The results of Sec. II B exhibited in Figs. 3-5 are consistent with a correlation length obeying

$$\xi \sim (T - T_0)^{-\nu}$$
 (47)

for the EA model in two dimensions, where $\nu = 1.0 \pm 0.5$ in both cases, $T_0 \simeq 0.6$ for the case in which J is distributed normally and $T \simeq 1.0$ for the case in which J = 1. We now wish to argue that this expression is more than just a sufficient possibility to fit the results shown in Figs. 3 and 4. The following argument shows that Eq. (47) *follows*, at least in the range

$$4 \leq \xi \leq 10 \tag{48}$$

from the data shown in Figs. 3 and 4. Note first that $\langle \langle \sigma_i \sigma_j \rangle_T^2 \rangle_J = f(r_{ij}/\xi) r^{-y}$ implies that $\chi'_{EA} \sim \xi^x$, whence

$$\Lambda = -x \frac{\partial \ln \xi}{\partial T} \quad , \tag{49}$$

as follows from the definition of Λ , Eq. (22). Now, Λ must saturate when ξ becomes as large as *l* (the linear dimension of the system). Therefore

$$-x\left(\frac{\partial \ln\xi}{\partial T}\right)_{\xi=l} \approx \Lambda_{\max} \quad . \tag{50}$$

On the other hand, $\Lambda_{\max} = cL^{1/\nu}$ in the range of values of L studied ($4 \le L \le 10$ for $J = \pm 1$ and $4 \le L \le 11$ for J distributed normally); consequently, Eq. (50) becomes

$$-x\left(\frac{\partial \ln\xi}{\partial T}\right) \approx c\,\xi^{1/\nu} \quad . \tag{51}$$

Integration yields

$$\xi^{-1} = \left(\frac{c}{vx}(T - T_0)\right)^{\nu} , \qquad (52)$$

where T_0 is an undetermined constant of integration up to this point. To determine T_0 from our results, consider now two systems one of $L_1 \times L_1$ spins and another one of $L_2 \times L_2$ spins, and let T_1 and T_2 be such that $\xi(T_1) = l_1$ and $\xi(T_2) = L_2$. It follows from Eq. (52) that

$$(T_1 - T_0)^{\nu} / (T_2 - T_0)^{\nu} = L_2 / L_1$$
, (53)

which yields

$$T_0 - T_2 = \epsilon / [(L_2/L_1)^{1/\nu} - 1] , \qquad (54)$$

where $\epsilon = T_1 - T_2$. Now, since the maximum in Λ occurs at a temperature which is fairly independent of the size of the system, as can be gathered from Figs. 3 and 4, it follows that $\epsilon << 1$ and consequently that

 $T_0 \approx T_2$, since $\nu \approx 1$. Thus, Eq. (47) follows, at least for the range of ξ studied, i.e., for $4 \leq \xi \leq 10$ for the case in which $J = \pm 1$ and for $4 \leq \xi \leq 11$ for the case in which J is normally distributed. It is worthwhile noticing where the above derivation would proceed differently in the case of the Ising *chain*. It is only the non-negligible value of ϵ that allows a vanishing T_0 to obtain for the chain.

We next discuss whether q = 0 or not for $T = T_0$ on the basis of our results. This question cannot be answered solely on the behavior of Λ at T_0 as a function of L, since as was shown in Sec. II, $\Lambda(T_0) \sim L^{1/\nu}$ follows if $\xi \sim (T - T_0)^{-\nu}$ for $T > T_0$, quite independently of whether below T_0 there is strong long-range order $(q \neq 0)$ as in the Ising ferromagnet or whether there is weak long-range order (in which case q = 0) as in the XY model. Clearly if there were strong long-range order, then Eq. (8) would imply that $\Lambda \rightarrow 2\partial \ln(q)/\partial T$ as $N \rightarrow \infty$ for

- ¹For reviews of the theory of spin-glasses, see A. Blandin, J. Phys. (Paris) 39, C6-1499 (1978).
- ²K. H. Fisher, Physica <u>86-88B</u>, 813 (1977).
- ³M. A. Ruderman and C. Kittel, Phys. Rev. <u>96</u>, 99 (1954);
 J. Kasuya, Prog. Theor. Phys. <u>16</u>, 45 (1956); K. Yosida, Phys. Rev. <u>106</u>, 893 (1957); P. F. de Chatel, J. Appl. Phys. 52, 1727 (1981).
- ⁴G. Toulouse, Commun. Phys. 2, 115 (1977).
- ⁵P. W. Anderson, in *Ill-Condensed Matter*, edited by R. Balian, R. Maynard, and G. Toulouse (North-Holland, New York, 1979), p. 159; K. Binder, in *Fundamental Problems in Statistical Mechanics*, edited by E. G. D. Cohen (North-Holland, Amsterdam, in press).
- ⁶H. Maletta, J. Phys. (Paris) <u>41</u>, C-115 (1980); H. Maletta and W. Felsch, Phys. Rev. B <u>20</u>, 1245 (1979); K. Binder, W. Kinzel, H. Maletta, and D. Stauffer, J. Magn. Magn. Mater. <u>15-18</u>, 189 (1980).
- ⁷C. E. Violet and R. J. Borg, Phys. Rev. <u>149</u>, 540 (1966); B. Window, Phys. Rev. B <u>6</u>, 2013 (1972).
- ⁸A. Arrot, J. Appl. Phys. <u>36</u>, 1093 (1965).
- ⁹S. F. Edwards and P. W. Anderson, J. Phys. F <u>5</u>, 965 (1975).
- ¹⁰K. Binder and K. Schröder, Phys. Rev. B <u>14</u>, 2142 (1976); D. Stauffer and K. Binder, Z. Phys. B <u>30</u>, <u>313</u> (1978).
- ¹¹A. J. Bray, M. A. Moore, and P. Reed, J. Phys. C <u>11</u>, 1187 (1978).
- ¹²I. Morgenstern and K. Binder, Phys. Rev. Lett. <u>43</u>, 1615 (1979); Phys. Rev. B 22, 288 (1980).
- ¹³J. F. Fernández and R. Medina, Phys. Rev. B <u>19</u>, 356 (1979).
- ¹⁴J. M. Kosterlitz and D. J. Thouless, J. Phys. C <u>6</u>, 1181 (1973).
- ¹⁵For reviews of experimental work and further references, see B. Coles, J. Magn. Magn. Mater. <u>15-18</u>, 103 (1980);

 $T < T_0$, that is, Λ would become independent of N for N sufficiently large. Now, as Figs. 3 and 4 show, that is not the case for the EA finite systems studied here. Note that for the Ising ferromagnet, Fig. 14, Λ is indeed approximately independent of L for $L \ge 4$ if $T \le 0.7T_c$. On the other hand, if $\langle \langle \sigma_0 \sigma_1 \rangle^2 \rangle \sim r^{-y}$ for $T < T_0$, then $\Lambda \sim \ln(N)$, which is in fair agreement with our results, within our accuracy. Thus, our results favor weak long-range order below T_0 and consequently q = 0. It follows then, from Eq. (9), that χ is not linear in h for $T < T_0$ no matter how small h may be.

ACKNOWLEDGMENTS

I am indebted to Dr. R. Medina for interesting discussions and to T. Streit and Z. Andérico for reading the manuscript with care.

A. P. Murani, J. Phys. (Paris) 39, C6-1517 (1978).

- ¹⁶For a recent version of disagreeing views and further references, see A. P. Murani, Phys. Rev. B <u>22</u>, 3495 (1980); K. Levin, C. M. Soukoulis, and G. S. Grest, *ibid*. <u>22</u>, 3500 (1980).
- ¹⁷For a view in favor of a transition, see, E. D. Dahlberg, M. Hardiman, R. Orbach, and J. Souletie, Phys. Rev. Lett. <u>42</u>, 401 (1979); E. M. Gray, J. Magn. Magn. Mater. <u>15-18</u>, 177 (1980); for a different view, see J. L. Tholence, Solid State Commun. <u>35</u>, 113 (1980).
- ¹⁸C. Jayaprakash, J. Chalupa, and M. Wortis, Phys. Rev. B <u>15</u>, 1495 (1977); B. W. Southern and A. P. Young, J. Phys. C <u>10</u>, 2170 (1977); P. W. Anderson and C. M. Pond, Phys. Rev. Lett. <u>40</u>, 903 (1978); S. Kirkpatrick, Phys. Rev. B <u>15</u>, 1533 (1977); A. P. Young and R. Stinchcombe, J. Phys. C <u>8</u>, L535 (1975); W. Kinzel and K. H. Fisher, *ibid.* <u>6</u>, 118 (1978).
- ¹⁹S. Kirkpatrick, in *III Condensed Matter*, edited by R. Balian, R. Maynard, and G. Toulouse (North-Holland, New York, 1979), p. 321.
- ²⁰J. F. Fernández, Bull. Am. Phys. Soc. <u>25</u>, 12 (1980); J. Phys. C <u>13</u>, L555 (1980).
- ²¹J. Chalupa, Solid State Commun. <u>22</u>, 315 (1977).
- ²²Y. Miyako, S. Chikazawa, T. Sato, and T. Saita, J. Magn. Magn. Mater. <u>15-18</u>, 139 (1980).
- ²³S. Kirkpatrick, Phys. Rev. B <u>16</u>, 4630 (1977).
- ²⁴G. J. Neiuwenhuys and J. A. Mydosh, Physica (Utrecht) <u>86B</u>, 880 (1977).
- ²⁵C. Dasgupta, S. Ma, and C. K. Hu, Phys. Rev. B <u>20</u>, 3837 (1979).
- ²⁶H. E. Stanley, Introduction to Phase Transitions and Critical Phenomena (Clarendon, Oxford, 1971), p. 47.
- ²⁷R. Medina (private communication).
- ²⁸Stanley, Ref. 26, p. 147.