Exact results for the site-dilute antiferromagnetic Ising model on finite triangular lattices

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(Received 8 September 1987)

Exact analytical and numerical results for the site-diluted antiferromagnetic Ising model on the triangular lattice (AFIT) are presented. For infinitesimal dilution the change in the free energy of the system is related to the distribution of local fields, and it is shown that for a frustrated system such as the AFIT, dilution lowers the entropy per spin. For lattices of finite size and dilution the transfer matrix for the partition function is evaluated numerically. The entropy per spin shows a marked minimum near a concentration of spins $x=0.70$, in some disagreement with earlier transfer-matrix results.

I. INTRODUCTION

The antiferromagnetic Ising model on the triangular lattice (AFIT) is a fully frustrated system which fails to order even at zero temperature. Wannier[1] has solved this problem exactly by Onsager's method and calculates the ground-state entropy per spin to $S(0)=0.324$ (Ref. 2) (in this paper we take $k_B=1$). It is now generally accepted that frustration is a necessary ingredient, along with randomness, for a system to exhibit spin-glass behavior. Therefore, when random quenched vacancies are introduced into the AFIT, it is reasonable to consider the possibility that this system might freeze at sufficiently low temperatures.

While the general wisdom seems to be that the lower critical dimension for spin-glass behavior is $d_c=3$ (Refs. 3–6), Monte Carlo calculations of the distribution of local fields[7] for the AFIT show a pronounced "zero-field hole" characteristic of the spin-glass state. In addition it has been shown[8] that for small dilution the entropy of the AFIT decreases with dilution. This argument is reproduced in Sec. II.

One of the serious drawbacks of Monte Carlo calculations in a system such as this is the possibility that it will be trapped for long times in metastable states, and for this reason, it is useful to consider exact calculations of the free energy. In Sec. III we outline an algorithm for evaluating the partition function of the dilute AFIT, and in Sec. IV we present the results of our numerical calculations. In Sec. V we discuss these results within the context of spin-glass behavior.

II. FREE ENERGY OF WEAKLY DILUTED ISING MODELS

The ordered phase of systems with random, quenched impurities is a subject of recent and current interest in several fields. In this paper we consider the effect of random, quenched vacancies on the free energy of a nearest-neighbor Ising model.

The Hamiltonian for the dilute nearest-neighbor Ising model is

$$H=-J\sum_{\langle i,j\rangle}^{N(1-y)}{}' S_{i'}S_{j'}\ , \tag{1}$$

where the prime on the summation index indicates that the sum is over occupied sites only. N is the number of lattice sites, and y is the fraction of those sites which are vacant. Each site has an independent probability y to be vacant (or occupied by a nonmagnetic impurity). The Hamiltonian (1) is defined for a particular configuration of the diluted lattice. If the summation is extended over all the sites of the lattice, the Hamiltonian can be expressed as the sum of two terms $H=H_0+H_1$, where H_0 is the Ising Hamiltonian for the perfect lattice,

$$H_0=-J\sum_{\langle i,j\rangle}^{N} S_iS_j \tag{2}$$

and H_1 contains all the "missing terms" due to dilution, which, if $y\ll 1$, can be written as

$$H_1=\sum_{i''}^{Ny}{}'' h_{i''}S_{i''}\ . \tag{3}$$

The double prime on the summation index in (3) indicates that the sum is over vacant sites only, and h_i is the local exchange field at site i

$$h_i=J\sum_{j'(i)} S_{j'}\ . \tag{4}$$

The partition function Z for the diluted lattice is

$$Z=\operatorname*{Tr}_{\{S_{i'}\}} e^{-\beta H}\ . \tag{5}$$

One can think of a vacancy as an occupied site to which the exchange couplings are zero. These "ghost" spins are completely free and contribute an entropy $Ny\ln 2$. Therefore the trace over the spins on occupied sites can be extended for the entire lattice by multiplying the partition function by the normalization factor 2^{-Ny}

$$Z=Z_0 2^{-Ny}\left\langle\prod_{i''}^{Ny}{}'' e^{-\beta h_{i''}S_{i''}}\right\rangle_0\ . \tag{6}$$

The ensemble average in (6) is taken with respect to the

Hamiltonian H_0, and Z_0 is the partition function for the perfect lattice.

For sufficiently small dilution the vacancies will be well isolated. So long as the separation between vacancies is much larger than the correlation length we can invoke the cluster property and replace the average of the product in (6) by the product of the averages for single vacancies. We will in fact be interested in the limit $y \to 0$, in which case the above argument becomes exact.

At this point we introduce into the trace (6) a resolution of the identity, $1 = \sum_h \delta(h - h_i)$, where $\delta(h - h_i)$ is the Kronecker symbol. In the nearest-neighbor Ising model the local field takes on values which are integer multiples of the exchange coupling J from $-qJ$ to qJ, where q is the coordination number of the lattice. The partition function for a single isolated vacancy is then

$$Z_1 = \tfrac{1}{2} Z_0 \sum_h \langle \delta(h - h_0)(\cosh\beta h - S_0 \sinh\beta h) \rangle_0 , \tag{7}$$

where we have assigned the vacancy to site $i = 0$.

The distribution function for the local field $P(h)$ is defined as

$$P(h) = \langle \delta(h - h_i) \rangle_0 . \tag{8}$$

In terms of $P(h)$, (7) becomes

$$Z_1 = \tfrac{1}{2} Z_0 \sum_h P(h) \operatorname{sech}\beta h . \tag{9}$$

As we have argued above, the contributions to the free energy from a small fraction of vacancies Ny will be additive in the limit $y \ll 1$, and the free energy of the weakly diluted lattice is

$$F = F_0 + NyT \ln 2 - NyT \ln \left[\sum_h P(h) \operatorname{sech}\beta h \right] . \tag{10}$$

In the case of a frustrated system, such as the AFIT, the distribution of local fields at low temperatures shows a maximum at $h = 0$ (Ref. 9), and this term will dominate the sum in (10). Therefore we have

$$F = F_0 + NyT[\ln 2 - \ln P(0)] . \tag{11}$$

The entropy is given by

$$S = -\frac{\partial F}{\partial T} = S_0 - Ny[\ln 2 - \ln P(0)] + NyT \frac{\partial \ln P(0)}{\partial T} . \tag{12}$$

Assuming that $P(h = 0)$ does not vanish as $T \to 0$, we see from (12) that the entropy of the AFIT is lowered on dilution, and a similar conclusion holds for any Ising model with local interactions and nonvanishing $P(h = 0)$. Exact results for the AFIT at $T = 0$ are known for the entropy[4] and $P(h)$ (Ref. 9), which allow us to predict from (12) that

$$\frac{\partial}{\partial x} \left[\frac{S}{N} \right] \Bigg|_{\substack{T=0 \\ x=1}} = 1.593 . \tag{13}$$

This result disagrees with early numerical transfer matrix calculations,[10] but agrees well with the numerical results presented in Sec. IV.

III. THE TRANSFER MATRIX FOR THE PARTITION FUNCTION

The Hamiltonian for the dilute AFIT can also be written as

$$H = -J \sum_{\langle i,j \rangle} x_i x_j S_i S_k , \quad J < 0 \tag{14}$$

where we now introduce new random variables x_i governed by the binomial probability distribution

$$P(x_i) = x\delta(1 - x_i) + (1 - x)\delta(x_i) , \tag{15}$$

where x is the mean concentration of spins on the lattice.

The partition function is given by

$$Z(\{x_i\}) = \operatorname*{Tr}'_{\{S_i\}} e^{-\beta H(\{x_i\})} , \tag{16}$$

where the prime again indicates that the trace is over occupied sites only. The trace can be extended over the entire lattice if the partition function is normalized by a factor 2^{-N_v}, where N_v is the number of vacant sites. Thus for a particular configuration of vacancies,

$$Z(\{x_i\}) = 2^{-N_v} \operatorname*{Tr}_{\{S_i\}} e^{\beta J \sum_{\langle i,j \rangle} x_i x_j S_i S_j} . \tag{17}$$

Since

$$e^{\beta J x_i x_j S_i S_j} = \cosh\beta J x_i x_j + S_i S_j \sinh\beta J x_i x_j ,$$

the partition function can be written as

$$Z(\{x_i\}) = 2^{-N_v} \prod_{\langle i,j \rangle} \cosh(\beta J x_i x_j) \operatorname{Tr} \prod_{\langle i,j \rangle} [1 + t x_i x_j S_i S_j] , \tag{18}$$

where $\tanh\beta J x_i x_j = x_i x_j \tanh\beta J = x_i x_j t$.

We now consider a finite lattice of width N and length M. The product and trace operations are carried out in a sequence of steps. We begin by collecting all terms in (18) which arise from couplings between spins in a single row and label each spin by its row and column (n,m) and then define for the kth row

$$Z_k(S_{k,1}, \ldots, S_{k,N}) = \prod_j^N (1 + t x_{k,j} x_{k,j+1} S_{k,j} S_{k,j+1}) , \tag{19}$$

where N is the number of sites in a row. Each spin $S_{k,j}$ is coupled to two spins in the next row $S_{k+1,j}$ and $S_{k+1,j-1}$, by the factor

$$W_{k,j}(S_{k+1,j-1} S_{k+1,j}; S_{k,j}) = (1 + t x_{k+1,j-1} x_{k,j} S_{k+1,j-1} S_{k,j})(1 + t x_{k+1,j} x_{k,j} S_{k+1,j} S_{k,j}) . \tag{20}$$

Suppressing for a moment the dependence of each function on $\{S_{i,j}\}$, the trace in (18) takes the form

$$T=\operatorname*{Tr}_{\{S\}} Z_M W_{M-1,1}\cdots W_{M-1,N}\cdots Z_2 W_{1,1}\cdots W_{1,N-1}W_{1,N}Z_1 \ . \tag{21}$$

The trace can now be carried out one spin at a time starting with spin $S_{1,N}$. Let us define

$$Y_N(S_{2,N-1},S_{2,N}S_{1,1},\ldots,S_{1,N-1})=\operatorname*{Tr}_{S_{1,N}} W_{1,N}(S_{2,N-1},S_{2,N};S_{1,N})Z_1(S_{1,1}\cdots S_{1,N}) \ . \tag{22}$$

Then

$$T=\operatorname*{Tr}_{\{S\}} Z_M W_{M-1,1}\cdots W_{M-1,N}\cdots Z_2 W_{1,1}\cdots W_{1,N-1}Y_N \ . \tag{23}$$

As each spin in row 1 is traced over, the variables from the first row are replaced by those from the second. Note that while the Z's depend on N variables, the Y's depend on $N+1$.

Finally in the last step the trace over $S_{1,1}$ gives

$$U_2(S_{2,1},\ldots,S_{2,N})=\operatorname*{Tr}_{S_{1,1}} W_{1,1}(S_{2,N},S_{2,1};S_{1,1})Y_1(S_{2,1},\ldots,S_{2,N},S_{1,1}) \ . \tag{24}$$

The product $\tilde{Z}_2=U_2Z_2$ is again a function of the N spin variables $S_{2,1},\ldots,S_{2,N}$, and the trace over the spins in the second row can now be carried out. When the penultimate row $M-1$ has been traced over, the partition function is given by

$$Z=2^{-N}v\prod_{\langle i,j\rangle}\cosh(x_ix_j\beta J)\operatorname*{Tr}_{\{S_{M,1}\cdots S_{M,N}\}} \times\tilde{Z}_M(S_{M,1},\ldots,S_{M,N}) \ . \tag{25}$$

Once the partition function for a particular fixed set of vacancies has been computed, the free energy is calculated for several such distributions, and averaged, which we denote by $(\cdots)_x$. Thus

$$-\beta(F)_x=-(N_v)_x\ln 2+\left[\sum_{\langle i,j\rangle}\ln\cosh(x_ix_j\beta J)\right]_x +[\ln(T\{x_i\})]_x \ . \tag{26}$$

IV. EVALUATION OF THE FREE ENERGY

When the algorithm described in Sec. II is implemented on an IBM 3081 computer, the evaluation of the partition function for a single choice of vacancies on a 10×20 triangular lattice takes roughly 9 s. Of course the width of the lattice which can be studied by this method is limited by the length of the array Y_k which contains 2^{N+1} components. The length of the lattice M is limited only by the largest and smallest numbers which can be handled by the computer.

In Fig. 1 we show the entropy per spin as a function of concentration for $T/J=0.3$. The straight line passing through $x=1$ is the theoretical result (13) and clearly agrees quite well with the numerical results. The upper curve is taken from Anderico, Fernandez, and Streit. Numerically the derivative of S at $x=1$ is

$$\left.\frac{\partial S}{\partial x}\right|_{\substack{T=0.3J\\x=1}}=1.61 \ . \tag{27}$$

The slight discrepancy with (13) can be attributed to the finite site of the system and to the fact that we are not evaluating the entropy at $T=0$. For example, the bulk entropy per spin at $T=0$ is $S(0)=0.324$, while for the 10×20 lattice at $T/J=0.3$, $S=0.310$.

The entropy continues to decrease with x until approximately $x=0.70$ where a minimum is obtained. One expects that as the percolation threshold $x=0.5$ is approached, the contribution of finite clusters to the entropy will be large and the entropy will turn up again. Since we are more interested in the properties of the largest (percolating) cluster, we have "cleaned" the lattice by re-

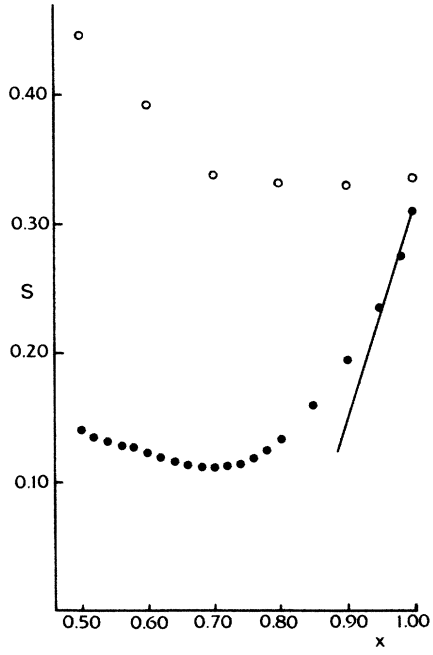

FIG. 1. Dependence of the entropy per spin (s) on concentration for $T/J=0.3$ for a 10×20 triangular lattice. Straight line through $x=1$ is the theoretical prediction (13). The upper curve (○) is taken from Anderico, Fernandez, and Streit (Ref. 10).

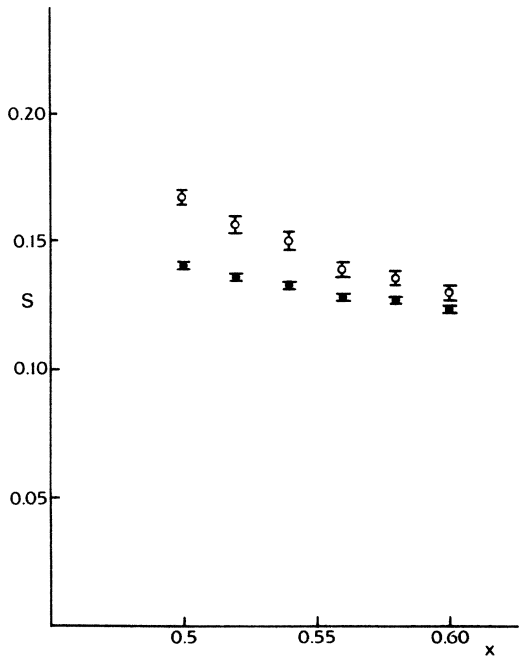

FIG. 2. Comparison of the entropy per spin (s) near percolation. Upper curve ($\overline{\Sigma}$) is lattice containing isolated clusters, lower curve (●) is the entropy per spin of the largest connected cluster only.

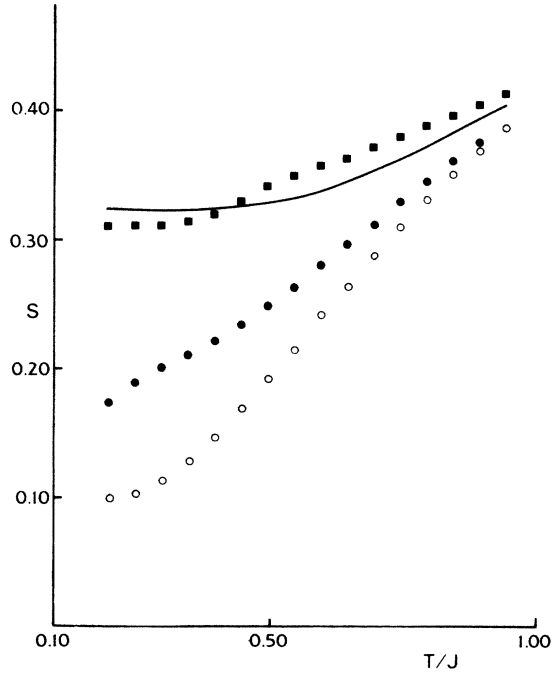

FIG. 3. Entropy per spin (s) as a function of temperature for $x=1.0$ (■), $x=0.90$ (●), and $x=0.75$ (○). The solid curve is the exact result for the infinite lattice (Ref. 1).

moving all but the largest cluster. In Fig. 2 we show the entropy per spin near percolation before and after cleaning. Figure 3 shows the entropy per spin as a function of temperature for several values of the concentration. The continuing decrease in the entropy with temperature for the diluted lattices indicates a tendency toward order.

V. DISCUSSION

The transfer-matrix calculations presented here demonstrate the strong tendency of the AFIT model to order when diluted. These results support earlier Monte Carlo studies[7] of the distribution of local fields and the Edwards-Anderson order parameter $q(t)$. There is a growing body of evidence from high-temperature expansions,[3,4] numerical simulations,[5] and scaling arguments[6] that the lower critical dimension for spin-glass behavior is $d_c=3$. However, a proof of this conjecture does not yet exist. On the other hand, the site-diluted AFIT model does seem to exhibit some of the properties one would expect of a spin glass. If indeed $2<d_c$, then a careful study of systems which are in some sense close to being spin glasses ought to help in clarifying the nature of the spin-glass state.

ACKNOWLEDGMENTS

The authors are indebted to M. Farach for developing the cluster-cleaning algorithm and to J. F. Fernandez for introducing us to the transfer matrix method. This work was partially supported by National Science Foundation Grant No. DMR-8506690.

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