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Abstract

Calculations of the specific heat and magnetization of quenched, site-diluted, N×N square and triangular Ising lattices have been carried out by a Monte Carlo method. For spin concentrations x of 0.8 and 0.9, lattices of size N=64 did not give sharp transitions. For a triangular lattice with N=128 and x=0.904, we found a well-defined peak in the specific heat and an abrupt change in the magnetization at $T=0.865\ T_c(1)$. Linear interpolation gives $s \equiv d/dx[T_c(x)/T_c(1)]_{x=1} = 1.40 \pm 0.05$, in excellent agreement with the high temperature series calculations of Rushbrooke et al. For the square lattice we calculate $s=1.5\pm0.1$. We also determined site magnetization as a function of the number of "live" nearest neighbors.

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ABSTRACT

Calculations of the specific heat and magnetization of quenched, site-diluted, N x N square and triangular Ising lattices have been carried out by a Monte Carlo method. For spin concentrations x of 0.8 and 0.9, lattices of size N = 64 did not give sharp transitions. For a triangular lattice with N = 128 and x = 0.904, we found a well-defined peak in the specific heat and an abrupt change in the magnetization at $T = 0.865\ T_c(1)$. Linear interpolation gives

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I. INTRODUCTION

For many years there has been great interest in the properties of randomly diluted magnetic systems. A simple theoretical model for such systems, which has been widely studied, is the randomly diluted Ising model, which we write as

$$\mathcal{H} = -J \sum_{\langle ij \rangle} p_i p_j \sigma_i \sigma_j, \qquad (1)$$

where $\langle ij \rangle$ indicates that the sum is over pairs of nearest neighbors, $\sigma_i = \pm 1$ is an Ising variable, and p_i is a random variable equal to unity if the site i is occupied and is zero otherwise. In the "quenched" model which we consider the free energy is taken to be the configurational average, denoted by $\langle\langle \ \rangle\rangle$, of the free energy over the occupation variables. We assume the p_i's to be uncorrelated with $\langle\langle p_i \rangle\rangle = x$.

In early work,[1] the thermodynamic functions of this model were studied via series expansions in powers of either (J/kT), where T is the temperature, or x. More recently, renormalization group treatments have been given[2,3] which indicate that for 2 < d < 4, where d is the spatial dimensionality, one expects cross-over behavior such that for $\epsilon \equiv [T - T_c(x)]/T_c(1)$ sufficiently small one enters a randomness dominated regime where the critical exponents assume values characteristic of local disorder. Here $T_c(x)$ is the transition temperature (defined by the onset of long range order) for concentration x. In this paper we present a Monte-Carlo study of this model in the hope of elucidating the noncritical behavior. Heretofore, such information has only been obtained by series methods or via approximations[4] wherein fluctuations in local environment are treated in an average way. By using a simulation method we are able to study the importance of these fluctuations and also to give a qualitative picture of the thermodynamic properties over the entire range of temperature.

This paper is organized as follows. In Sec. II we describe briefly the numerical approach used, and we discuss our results in Sec. III.

II. MONTE-CARLO TECHNIQUE

The calculations were made by a method similar to that used by Ogita et al[5] and by Stoll et al.[6] Toroidal periodic boundary conditions were used. Pseudo-random numbers were obtained using two well-tested generators.[7] One sequence was used to choose the jth spin. The other determined the new value, σ_j, of the jth spin according to the Boltzmann distribution:

$$P(\sigma_j) = \{1 - \tanh[E_j/kT]\}/2, \qquad (2)$$

where E_j is the energy of the jth spin in the field of its neighbors. The program was checked by performing calculations on an undiluted system and comparing the results with the exact results for a finite lattice given by Ferdinand and Fisher.[8] There were no statistically significant errors in the Monte-Carlo results for x = 1 at any temperature.

For each lattice a distribution of impurities was chosen by using the random number generator. The same impurity distribution was used at all temperatures for a given concentration. On each run, the lattice was allowed to reach thermal equilibrium and then its behavior was averaged over 1000 times steps in order to simulate the thermal average. (On the average, each spin is examined once per time step.) Temperatures of interest were run two or three times.

III. DISCUSSION

In Fig. 1 we show results for the specific heat obtained by graphically differentiating our Monte Carlo results for the internal energy for two sizes of triangular lattices. The apparent divergences seen in Fig. 1 occur at the same temperature, $T_c(x)$, determined by the onset of long range order. The smaller peak in the specific heat for x = 0.904 at a temperature below the main transition is attributed to the effects of metastable states. It is clear that our data does not permit us to discuss the possible modification of the critical exponents due to random dilution. For the transition temperature we obtained the value $T_c(0.904) = (0.865 \pm 0.005)\ T_c(1)$. Judging from the value of the transition temperature for x = 0.8 as indicated by our results shown in Fig. 1, we conclude that $T_c(x)$ is a nearly linear function of x for $0.9 \lesssim x \leq 1$. Thus, we deduce the limiting slope $s \equiv T_c(1)^{-1}\ dT_c/dx|_{x=1} = 1.40 \pm 0.05$, in excellent agreement with the high temperature series calculations of Rushbrooke et al.[1] We have performed similar calculations for the square lattice which give $s = 1.5 \pm 0.1$.

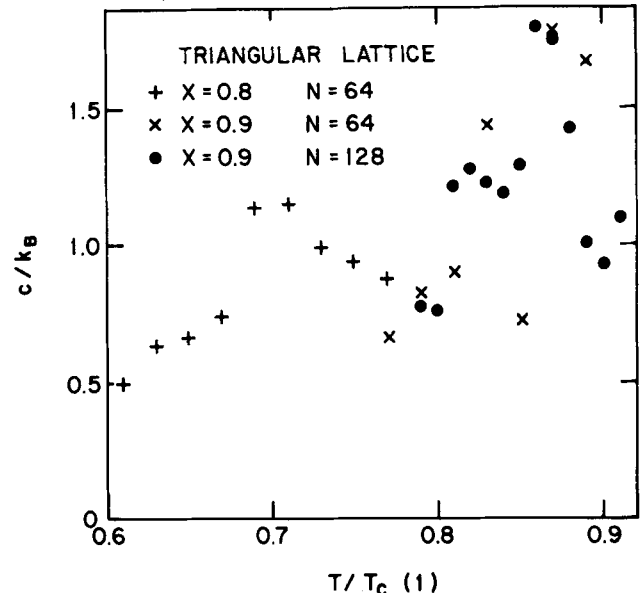In Fig. 2 we show $\sigma_z(T)$, the magnetization of sites classified according to the number, z, of "live"

TRIANGULAR LATTICE
+ X = 0.8   N = 64
x X = 0.9   N = 64
● X = 0.9   N = 128

c/k_B

T/ T_c (1)

Figure 1

Specific heat per spin, c, of N x N randomly diluted triangular lattices with spin concentration x subject to periodic boundary conditions. The points were obtained by a finite difference method from a direct calculation of the energy.

nearest neighbors. Thus, if z_i is the number of live nearest neighbors of the site i, we define

$$\sigma_z(T) = \sum_{z_i = z} \langle \sigma_i \rangle_T / \sum_{z_i = z} P_i, \qquad (3)$$

where $\langle \; \rangle_T$ indicates a thermal average. In the simplest theories[4] one assumes that $\langle \sigma_i \rangle_T$ is independent of i. However, as our data shows, this is not even approximately true. In fact, we see that the effective field acting on a site with z neighbors is approximately proportional to z. A difficulty in making this idea quantitative is caused by the inaccuracy inherent in the use of mean field theory for a two dimensional model. One can define an effective field via the relation

$$\sigma_z(T) = \tanh[H_{eff}(z)/k_B T]. \qquad (4)$$

For x = 0.904 and T = 0.80 T_c(1) the data of Fig. 2 inserted in Eq. (4) gives $H_{eff}/k_B T$ = 0.38, 0.56, 0.84, 1.13, and 1.45 for z = 2, 3, 4, 5, and 6, respectively. Qualitatively, one has a linear relation between H_{eff}(z) and z. As one would expect, deviations from linearity are such as to cause H_{eff}(z)/z to increase slightly as z increases. Physically, we expect that $\langle \sigma_i \rangle_T$ is almost completely characterized by the value of z_i.

· In Fig. 2 we see a regime for $0 \le \epsilon \le 0.05$ where magnetization occurs in our finite sample using a limited time average, but probably would not occur for an infinite sample. The size of this interval is the same as that below T_c(x) where the specific heat results (for x = 0.904) are seen to display anomalous behavior.

Domain wall excitations are known[9] to play a role in the dynamics of pure systems. These effects become even stronger in the presence of dilution, since the energy of formation of a domain wall is proportional to the number of live bonds in the wall. In fact, it is clear that in the dilute system, in contrast to the pure case, domain walls in such low energy configurations are metastable and give rise to thermally activated relaxation mechanisms. This domain
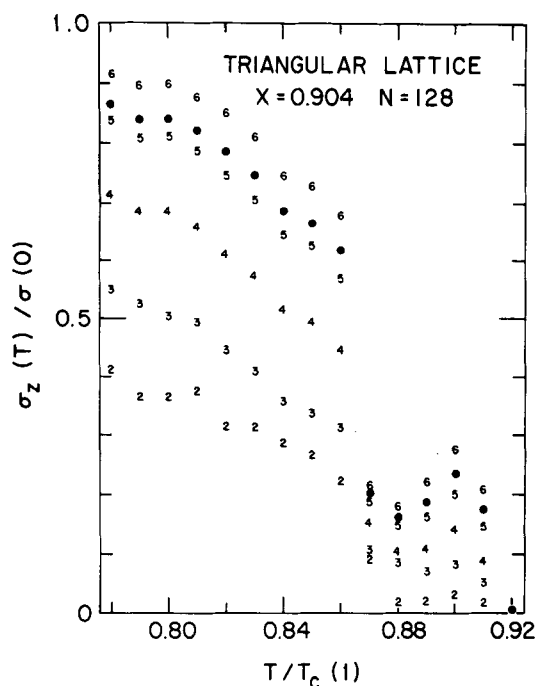

Figure 2

Thermal average magnetization per spin, σ_z(T), as a function of temperature, T, for various values of z, the number of "live" nearest neighbors. The dots · show the average magnetization per spin of the entire lattice.
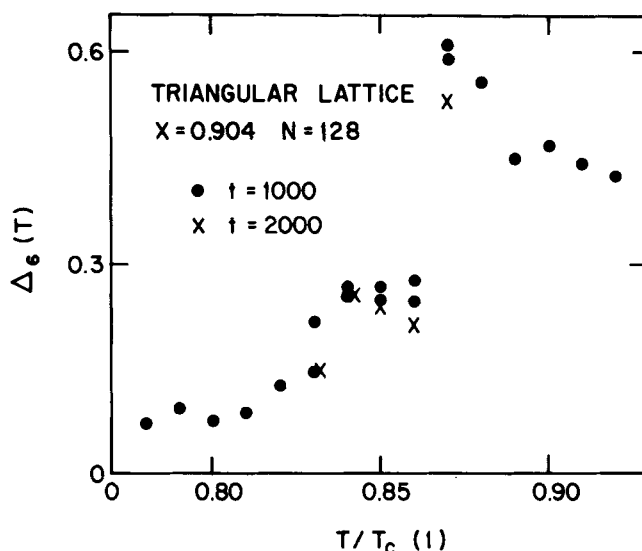

Figure 3

Standard deviation, Δ_6(T), of the average magnetization of sites with 6 "live" nearest neighbors as defined by Eq. (5) versus temperature.

wall pinning below the transition causes the shape of the fluctuation regions of reversed spin to be more irregular in the dilute system than in the pure case. As a consequence of their irregular shape, large scale fluctuations tend to be unstable with respect to breaking up. Above the transition temperature the energy of the fluctuations is less important than their entropy, and irregularly shaped domains are rarer than regularly shaped ones. For these more circular domains piecewise decay is less likely and a longer relaxation time results. These domains with "giant moments" may explain the occurrence of apparent magnetization in our finite samples for $0 \le \epsilon \le 0.05$ for x = 0.904.

Numerically, we may study these fluctuations by studying the way they influence the finite time averages we calculate. As in Eq. (3) we may define the dispersion, Δ_z(T), as

$$\Delta_z^2(T) = \left\{ \sum_{z_i = z} \langle \sigma_i \rangle_T^2 / \sum_{z_i = z} P_i \right\} - \sigma_z(T)^2. \qquad (5)$$

By the central limit theorem, we expect

$$\Delta_z^2(T,t) = \Delta_z^2(T,\infty) + \tau_k/t, \qquad (6)$$

where τ_k is a kinetic relaxation time. Large values of Δ_z(T,∞) indicate that our system is trapped in a metastable configuration. Data for t = 1000 and 2000 time steps in shown in Fig. 3.

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