RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 31, NUMBER 5 1 MARCH 1985

Instability under dilution of an antiferromagnetic Ising model on an fcc lattice: A Monte Carlo study

H. A. Farach, R. J. Creswick, J. M. Knight, and C. P. Poole, Jr.
University of South Carolina, Columbia, South Carolina 29208

J. F. Fernandez
Centro de Fisica, Instituto Venezolano de Investigaciones Cientificas (IVIC), Apartado 1827, Caracas 1010A, Venezuela

(Received 3 December 1984)

We study an Ising antiferromagnet with nearest-neighbor interactions only on an fcc (frustrated) lattice with *no* external field. We show that if a fraction $(1-x)$ of the lattice sites is *randomly* unoccupied by spins then the system becomes unstable against the formation of domains. The mechanism producing the instability works somewhat like the one which destroys ferromagnetism in the *random-field* Ising model. Monte Carlo results are obtained for low temperatures as a function of x for fcc lattices of $(12\times12\times12)\times4$ sites. A transition from an antiferromagnetic state at $x=1$ to a disordered state for a small amount of dilution is clearly observed.

I. INTRODUCTION

The nature of the low-temperature magnetic state of diluted antiferromagnets in frustrated lattices is not well known. The possibility that such a state is a spin-glass[1] has been pursued recently both by experiment[2] and Monte Carlo simulation.[3] The results obtained have been far from conclusive.

We first say a word about the fully occupied lattice. It has not been trivial to establish the nature of the low-temperature phase of an antiferromagnetic Ising model in a *fully* occupied fcc lattice, for this is a fully frustrated system. For type-I ordering there is no binding energy between adjacent antiferromagnetically ordered planes in the ground state since half of the exchange bonds are broken. If all the spins within one plane are inverted, then all broken (fulfilled) bonds become fulfilled (broken). Nevertheless, Young[4] has shown that this degeneracy is lifted for $T>0$, and that the lowest free-energy state is perfectly antiferromagnetically ordered.

We study here an Ising antiferromagnet with nearest-neighbor (nn) interactions only on an fcc lattice with a fraction (x) of all lattice points occupied randomly by spins and *no* external field.

We give, in Sec. II, a simple argument to show that for any amount of dilution, however small, antiferromagnetic order is unstable against the formation of domains. The argument given here follows the one given by Imry and Ma[5] to show that any weak random field destroys ferromagnetism in an Ising model for $d\leq 2$ (where d is the spatial dimensionality of the system). We then report the results of Monte Carlo calculations that we have performed on an Ising antiferromagnet with nn interactions only on an fcc lattice. The results obtained indicate that there is indeed a transition from an ordered state at $x=1$ to a disordered state for a small amount of dilution.

II. INSTABILITY OF ANTIFERROMAGNETIC ORDER

Consider antiferromagnetic order of type I on a fcc lattice. If all sites are occupied $(x=1)$, then there is no binding energy between any two adjacent parallel antiferromagnetically ordered planes since half of the exchange bonds joining the planes are broken. If all the spins within one plane are inverted, then all broken (fulfilled) bonds become fulfilled (broken), and the energy is therefore unchanged. Doman[6] has argued that any amount of dilution, however small, will lift this degeneracy in an infinite system. Briefly, if two vacancies in two adjacent antiferromagnetic planes are nearest neighbors, then flipping all of the spins in one plane will raise (lower) the energy if the missing spins were parallel (antiparallel). We now argue that, in addition, these antiferromagnetically ordered planes break up into domains. To see this, consider a region of linear size l in one of these planes. The number of nn vacancy pairs is $N_p\sim(1-x)^2l^2$, and the excess number of broken bonds over fulfilled bonds joining them is $\sqrt{N_p}$, which leads to the binding energy,

$$\epsilon_r\sim J(1-x)l \ . \tag{1}$$

The number of bonds broken within the plane on which the domain lies is equal to twice the number of bonds cutting the domain interface. Consequently, for smooth interfaces, the domain surface energy is

$$\epsilon_s\sim Jxl \ . \tag{2}$$

Now, if $\epsilon_r<\epsilon_s$, then a domain will be formed. The situation here is analogous to the random-field[7] Ising model (RFIM) in two dimensions. For any spatial dimension d,

$$\epsilon_s\sim Jl^{d-1} \tag{3}$$

is the interface energy necessary to form a domain in that case, and

$$\epsilon_r\sim hl^{d/2} \tag{4}$$

is the field energy gained (or lost), for smooth interfaces. Clearly, for $d=2$, these expressions become like Eqs. (1) and (2). For $d<2$, it follows that $\epsilon r<\epsilon_s$ for any h if l is sufficiently large for the RFIM. For $d=2$, a more careful analysis is necessary. Renormalization-group work[8] indicates that the RFIM is unstable to domain formation for $d=2$ as well. These results have been corroborated numeri-

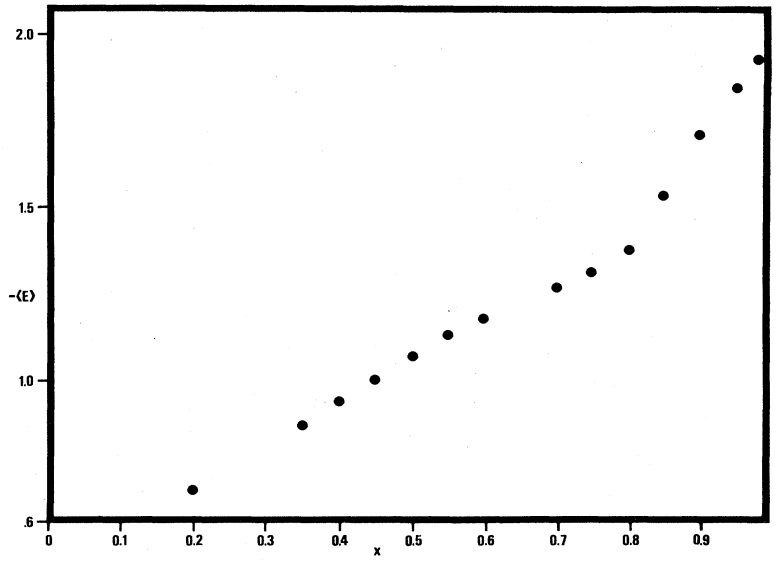

FIG. 1. Average energy $\langle E \rangle$ as a function of concentration at $T = 1.2$.

cally.[9] On this groud, we expect a diluted antiferromagnetic Ising model on a fcc lattice to be disordered.

III. MONTE CARLO RESULTS

We study the Ising antiferromagnet in an fcc lattice using the well-known Monte Carlo procedure with Glauber spin dynamics. The face-centered cubic lattice contains $N = 4 \times 12^3 = 6912$ sites, and the equilibrium is established by quenching the system from an infinite temperature and then running for 10^3 Monte Carlo steps per spin.

Figure 1 shows the computed energy per spin as a function of x for $T = 0.8$ J. The change in slope at $x \sim 0.8$ is suggestive of a phase transition. To gain more information we compute the quantities $\langle S_{\mathbf{q}} \rangle$ and $\langle |S_{\mathbf{q}}|^2 \rangle$, where

$$S_{\mathbf{q}} = \sum_{\mathbf{r}} S_{\mathbf{r}} e^{i\mathbf{q}\cdot\mathbf{r}} \quad . \tag{5}$$

In a perfectly ordered antiferromagnetic state $S_{\mathbf{q}} = N\delta_{q,q_0}$, where $q_0 = (0, 0, 1)$, for example, for a type-I antiferromagnet. In a completely disordered state, $\langle |S_{\mathbf{q}}|^2 \rangle \sim N$. Our Monte Carlo results are shown in Fig. 2 for $T = 0.8$ J and $T = 1.5$ J as a function of x. As a reference point for the values of T given here, recall that there is a first-order transition for the pure system[10] ($x = 1$) at[11] $T \approx 1.8$ J. For $T = 1.5$ J, there is a sharp jump in $\langle |S_{\mathbf{q}}|^2 \rangle$ at $x \approx 0.93$ which suggests a first-order transition. For $T = 0.8$ J, $\langle |S_{\mathbf{q}}|^2 \rangle$ drops less abruptly as x decreases to $x \approx 0.75$. We discuss the significance of these results in the next section.

IV. DISCUSSION

We have argued in Sec. II that a nn Ising antiferromagnet with *no* external field, in a diluted ($x < 1$) fcc (frustrated) lattice is unstable to the formation of domains. The mechanism which produces domains is akin to the one which destroys ferromagnetic order in the random-field Ising model.[5]

Our Monte Carlo results support our argument, even though antiferromagnetic order would seem to disappear only for $x \lesssim 0.8$ for $T = 0.8$ J. Allowance must be made for the fact that these results are for a *finite* ($12^3 \times 4$ sites) system. One expects that domains cannot be too small if the system is weakly ($1 - x << 1$) diluted.

Proceeding by analogy with the random-field Ising model where it has been shown by Fernandez and Pytte[9] that the

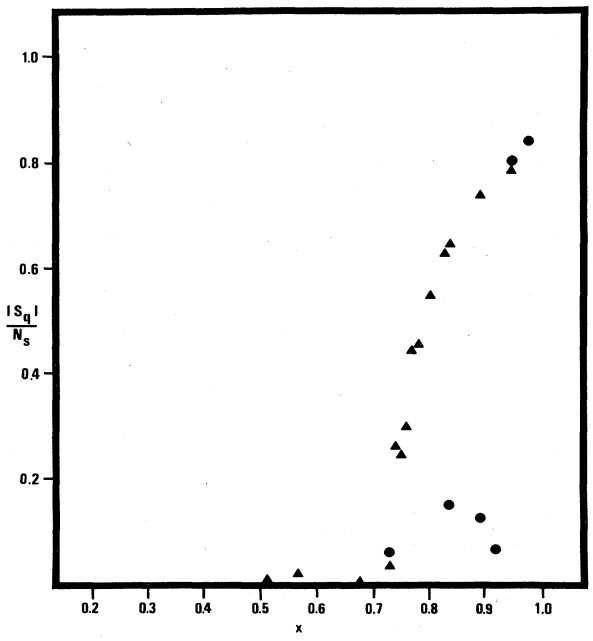

FIG. 2. Dependence of $|S_q|/N_s$ on the concentration x for the temperatures $T = 0.8$ (▲) and $T = 1.5$ (●), where $N_s = xN$.

correlation length (ξ) diverges with h as

$$\xi \sim \exp(a/h^2) \tag{6}$$

in two dimensions, we expect that the typical linear size (l) of our domains here will fulfill

$$l \sim \exp[a/(1-x)^2] \tag{7}$$

for the diluted Ising antiferromagnet on a fcc lattice with *no* applied field. It follows therefore that for small enough values of $1-x$ the length l is larger than the linear dimension of the system, and consequently the system is ordered.

It seems worthwhile to extend the Monte Carlo work reported here to cover systems of different sizes to check that the transition to a disordered state does indeed occur at a value of x which approaches unity as the size of the system becomes infinite. It would be interesting to check, perhaps using finite-size scaling, whether Eq. (7) holds.

ACKNOWLEDGMENT

This work was partially supported by the National Science Foundation (NSF) under Grant No. ISP-80-11451.

[1]For a review of spin-glasses, see, for instance, A. P. Young, J. Stat. Phys. **34**, 871 (1984).

[2]T. Giebultowicz, H. Kepa, B. Buras, K. Clausen, and R. R. Galazka, Solid State Commun. **40**, 499 (1980); G. Dolling, T. M. Holden, V. F. Sears, J. K. Furdyna, and W. Giriat, J. Appl. Phys. **53**, 7644 (1982); R. R. Galazka, S. Nagata, and P. H. Keeson, Phys. Rev. B **22**, 3344 (1981); S. Oseroff, *ibid.* **25**, 6584 (1982).

[3]G. S. Grest and E. G. Gabl, Phys. Rev. Lett. **16**, 1182 (1979); J. F. Fernandez, H. Farach, C. P. Poole, and M. Puma, Phys. Rev. B **27**, 4274 (1983).

[4]N. D. Mackenzie and A. P. Young, J. Phys. C **14**, 3927 (1981).

[5]Y. Imry and S. K. Ma, Phys. Rev. Lett. **35**, 1399 (1975).

[6]B. G. S. Doman, J. Phys. C **14**, 1765 (1981).

[7]For a recent review of the random-field Ising model problem see, for instance, Y. Imry, J. Stat. Phys. **34**, 849 (1984); G. Grinstein, J. Appl. Phys. **55**, 2371 (1984).

[8]G. Grinstein and S. K. Ma, Phys. Rev. Lett. **49**, 6685 (1982); Phys. Rev. B **28**, 2588 (1983); J. Villain, J. Phys. (Paris) Lett. **43**, L551 (1982).

[9]J. F. Fernandez and E. Pytte (unpublished).

[10]D. Mukamel and S. Krinsky, Phys. Rev. B **13**, 5078 (1976).

[11]M. K. Phani, J. L. Lebowitz, and M. H. Kalos, Phys. Rev. B **21**, 4027 (1980).