Weakly diluted $n \geq 2$ Ising antiferromagnets: Loss of long-range order and crossover effects

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The effect of small amounts of bond or site dilution on $n \geq 2$ Ising antiferromagnets (AF) in zero external field is studied. It is shown (a) that such impurities generate spatially random symmetry breaking, much like a random anisotropy along a few axes; (b) that any small amount of these impurities obliterates long-range order in $d < 2$ (and very likely in $d = 2$) dimensions in these systems; and (c) that the corresponding crossover exponent for these systems is, for any spatial dimensionality, $\phi = \gamma - 2\beta$ (instead of $\phi = \alpha$, as prescribed by the Harris criterion for random ferromagnets). Both transfer-matrix (TM) and Monte Carlo (MC) results are obtained for an Ising AF with nearest- *and* next-nearest-neighbor interactions. The TM data, obtained for long narrow strips at low temperature, and the MC results, for two-dimensional systems in the critical region, support the above conclusions.

I. INTRODUCTION

Effects produced by small amounts of impurities on magnetic systems have been the subject of great interest for well over a decade now. Random impurities which couple linearly to the order parameter, such as spatially random magnetic fields acting on a ferromagnet, easily disrupt long-range order for systems of low dimensionality, as was originally suggested by Imry and Ma.[1,2] Even for higher dimensionalities, random fields affect critical behavior.[3] On the other hand, according to the Harris criterion,[4] small amounts of nonmagnetic impurities (such as nonmagnetic atoms substituting magnetic atoms at random in zero applied field) affect critical behavior of ferromagnets as follows: critical indices are unaffected if the specific-heat exponent (α) fulfills $\alpha < 0$; for $\alpha > 0$, there is a crossover from a regime free of impurity effects, for $t \gg t_c$ (where $t = |T/T_c - 1|$ and t_c is, by definition, the crossover value for t), into an impurity dominated regime, for $t \ll t_c$; furthermore $t_c \sim (\delta J)^{1/\alpha}$, where δJ stands for random variation in the exchange constant. Neither random fields nor random anisotropies are covered by the Harris criterion.

The purpose of this paper is to show that random *site* dilution (substitution of magnetic atoms, chosen at random, by nonmagnetic ones) as well as random *bond* dilution (removal of some exchange bonds chosen at random) in *zero external field* plays a role akin to random anisotropy for *antiferromagnets* (AF's) with n-fold degenerate ground states if $n \geq 2$. Such AF's turn out *not* to be covered by the Harris criterion. These AF's will be referred to here as *frustrated*[5] *random-exchange* AF's (FREAF). Arguments and numerical results are presented to show that any small amount of bond or site dilution obliterates long-range order in a concrete example of an $n = 2$ AF in $d < 2$. It is also argued that the reduced crossover temperature (t_c) into the impurity dominated regime is (for any dimensionality) given by

$$t_c \sim (\delta J)^{1/\phi} , \tag{1}$$

and

$$\phi = \gamma - 2\beta , \tag{2}$$

where γ and β are the exponents for the magnetic susceptibility and for the staggered magnetization, respectively. Numerical results supporting this conclusion are presented for two dimensions.

Briefly (see Sec. II for a more detailed explanation) the effect discussed here comes about in FREAF which have some special symmetry (with a corresponding degenerate ground state) and in which removal of bonds or spins breaks this symmetry. Which ground state will end up with the lowest energy will be seen to depend on which particular bond is removed. Since bond (or site) dilution is random, it generates local *random symmetry breaking* (RSB), which therefore produces a spatially random ground-state bias. This RSB turns out to mimic a random anisotropy (with n axes for an n-fold degenerate ground state).

The plan of the paper is as follows. Section II describes in detail how RSB is generated by either bond or site dilution in the nearest-neighbor + next-nearest-neighbor (NN + NNN) Ising model[6] (a two-dimensional FREAF) and how long-range order is destroyed therein by any small amount of dilution. It is also argued in Sec. II that RSB is generated by bond or site dilution in all (types[7] I, II, and III) of three-dimensional Ising AF on fcc lattices as well as in Ising AF's of type II on bcc lattices (type I AF on bcc lattices are *un*frustrated and act, upon dilution, in zero field as a ferromagnet does, obeying the Harris criterion). Crossover effects are looked into in Sec. III. Equations (1) and (2) are obtained in Sec. III, following in part Aharony's[8] treatment of the random-field problem. Numerical results are presented in Sec. IV: transfer-matrix results for bond diluted long strips (effectively $d = 1$ systems) exhibiting destruction of

long-range order (as well as the predicted crossover behavior) by bond dilution; and Monte Carlo (MC) results for bond diluted NN+NNN Ising model (in $d=2$) exhibiting crossover behavior in agreement with Eqs. (1) and (2). Finally, a summary of results and some remarks make up Sec. V.

II. MODELS AND RSB

Some frustrated random-exchange antiferromagnetic models in two and three dimensions are described in this section. (Some of the subject matter in this section has already been presented in brief form elsewhere,[9] but is included here for completeness.) It is also shown how bond or site dilution in zero applied field generates random symmetry breaking for each of these models as well as some of the disruptive effects it produces. The ordered AF states of these systems, which are very well known,[7] are, nevertheless, described here in some detail to help the reader picture how RSB occurs and what it does to these systems.

A. The NN+NNN Ising model and its symmetries

Consider a set of spins on a square lattice (see Fig. 1) with nearest-neighbor (NN) and next-nearest-neighbor (NNN) interactions J_1 and J_2, respectively, with Hamiltonian

$$H=-\sum_{i,j} J_{ij}S_iS_j \ , \tag{3}$$

where $S_i=\pm 1$ is the spin on the ith site, $\sum_{i,j}$ stands for a sum over all i and j, and $J_{ij}=J_1$ if i and j are NN and $J_{ij}=J_2$ if i and j are NNN. This model has been called the NN+NNN model by Barber.[6]

Consider first the pure case: each lattice site occupied by a spin and all J_1 and J_2 bonds in place and let $J_2<0$. For $J_1=0$, the system clearly breaks up into two uncoupled antiferromagnetic sublattices (see Fig. 1). Even for $J_1\neq 0$, the ground state corresponds to two interpenetrating antiferromagnets if J_1 is sufficiently small. In order to see just how small J_1 must be, as well as to be able to look into the symmetries of H, define

$$J(\mathbf{k})=\sum_j J_{ij}\exp(-i\mathbf{k}\cdot\mathbf{r}_{ij})$$

and

$$S(\mathbf{k})=N^{-1/2}\sum_i S_i\exp(-i\mathbf{k}\cdot\mathbf{r}_i) \ .$$

It follows from Eq. (3) that

$$H=-\tfrac{1}{2}\sum_{\mathbf{k}} J(\mathbf{k})S(\mathbf{k})(-\mathbf{k}) \ . \tag{4}$$

It is straightforward to check that, for

$$J_2<0 \text{ and } |J_1|<2|J_2| \ , \tag{5}$$

$J(\mathbf{k})$ has its maxima at $\mathbf{k}=\mathbf{k}_1=(\pi/a)(0,1)$ and $\mathbf{k}=\mathbf{k}_2=(\pi/a)(1,0)$. Thus $S(\mathbf{k}_1)$ and $S(\mathbf{k}_2)$ correspond to the two ground-state spin configurations. One can easily verify that given an $S(\mathbf{k}_1)$ configuration, reversal of all spins on only one sublattice (call it the R_S transformation) produces an $S(\mathbf{k}_2)$ configuration. Unless otherwise stated, Eq. (5) will be emplicitely assumed to hold throughout this paper for the NN+NNN model.

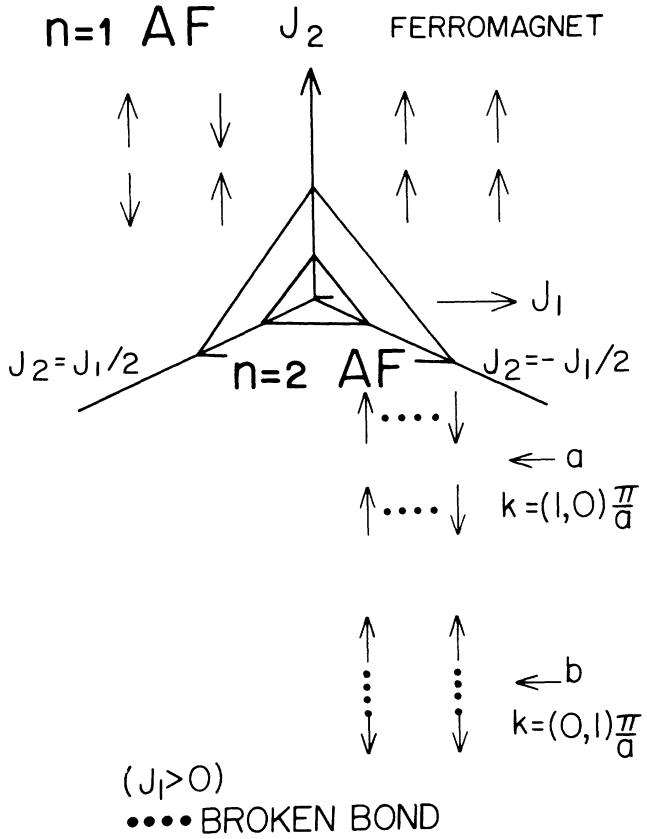

FIG. 1. Phase diagram for the two-dimensional NN+NNN Ising model (for the ground state, or in mean-field theory for any $T<T_c$). The two degenerate ground-state spin configurations for the lower third part of the phase diagram are shown. Broken (NN) J_1 bonds are shown, assuming $J_1>0$.

This model shares the property of *ground-state* energy invariance under an R_S transformation with the Baxter model and with the Ashkin-Teller model. This point has been stressed by Barber.[6] All three models exhibit nonuniversal behavior. Critical exponents for them have been computed by Swendsen and Krinsky[10] as a function of J_1/J_2. However, whereas R_S is an exact symmetry for the Baxter and Ashkin-Teller models, it is *not* an exact symmetry of the NN+NNN model—although the ground-state energy remains invariant under an R_S transformation, energies of other states do *not*, as consideration of almost any particular state will show. There is, however, an exact symmetry for the NN+NNN model: in k space, the exchange of each $S(\mathbf{k}_x,\mathbf{k}_y)$ with $\mathbf{S}(\mathbf{k}_y,\mathbf{k}_x)$. (Note that this transformation is equivalent to the R_S transformation of the *ground state* but *not* of any state.) The sum over the first Brillouin zone in Eq. (4) can consequently be reduced to a sum over half the zone—over $\mathbf{k}_y>\mathbf{k}_x$—defining $S^{(1)}(\mathbf{k}_x,\mathbf{k}_y)=S(\mathbf{k}_x,\mathbf{k}_y)$ and $S^{(2)}(\mathbf{k}_x,\mathbf{k}_y)=S(\mathbf{k}_y,\mathbf{k}_x)$, but summing now also over the two newly defined S components. The NN+NNN Ising model is therefore, in effect, a two-component ($n=2$) model; for one ground state, $S^{(1)}(0,\pi/a)=N^{1/2}$, $S^{(1)}(\mathbf{k})=0$ for

$\mathbf{k} \neq 0, \pi$, and $S^{(2)}(\mathbf{k})=0$ for all $\mathbf{k}$; while for the other ground state, $S^{(2)}(0,\pi/a)=N^{1/2}$, $S^{(2)}(\mathbf{k})=0$ for $\mathbf{k} \neq (0,\pi/a)$, and $S^{(1)}(\mathbf{k})=0$ for all $\mathbf{k}$.

B. Local RSB generated by dilution in the NN+NNN model

The two ground-state spin configurations are shown in Fig. 1. Assume, for the sake of definiteness, that $J_1 > 0$. Then, all horizontal J_1 bonds are broken in the spin configuration depicted as a in Fig. 1, while all J_1 vertical bonds are broken in the spin configuration depicted as b in Fig. 1. It follows that removal of a horizontal (vertical) J_1 bond leads to a lower energy for configuration a (b) in Fig. 1. (Removal of a J_2 bond does not lift the degeneracy.) Note that reversal of *all* spins is still a symmetry of the system, and that the state denoted as a (b) in Fig. 1 corresponds to $S^{(1)}(\mathbf{k}_1)=N^{1/2}$ [$S^{(2)}(\mathbf{k}_1)=N^{1/2}$]. Clearly, random removal of J_1 bonds generates RSB of a particular type: random anisotropy (with only two easy axes possible).

Removal of a fraction x of J_1 bonds in any region R of linear size b leads to an unbalanced number, $\delta n \sim b^{d/2}[x(1-x)]^{1/2}$ of vertical and horizontal bonds, and a corresponding energy bias $\varepsilon_b \sim J_1\,\delta n$. Following Imry and Ma,[11] consider reversing all spins within R in *only one* sublattice. It costs a wall energy, $\varepsilon_w \sim J_2 b^{(d-1)}$. Clearly, a domain will be formed if $\varepsilon_b > \varepsilon_w$, which is possible if $b > \xi$, where

$$\xi \sim (J_2/J_1)^{2/(2-d)}[x(1-x)]^{-\nu}, \quad \text{for } d<2\ , \tag{6}$$

and $\nu = 1/(2-d)$. Just as for the random-field Ising problem,[1] $d=2$ appears to be the lower critical dimension, and one, therefore, expects[12]

$$\xi \sim \exp\{J_2^2/[J_1^2 x(1-x)]\}$$

for $d=2$.

Numerical transfer-matrix[13] (TM) results for strips[9] support these predictions. The TM method, which yields numerically exact equilibrium averages, is a particularly suitable technique for this problem, for one expects, by analogy with the random-field Ising model, that there must be exceedingly long relaxation times[14] to equilibrium at low temperatures, a very undesirable feature for MC simulations. Let

$$S = 2N^{-1}\left[\sum_1 \langle S_i S_j\rangle + \sum_2 \langle S_i S_j\rangle\right], \tag{7}$$

where $\sum_1$ ($\sum_2$) stands for sums over all i and j on the first (second) sublattice, N is the number of sites in the whole lattice, and $\langle\ \rangle$ stands for thermal average. S can easily[13] be computed for strips of ω spins across and L spins along the long dimension. All the results shown in Ref. 9 are for $J_2 = j_1 < 0$, $k_B T = 0.2 J_2$, and values of x and L such that $\xi \gg \omega$ and $\xi \ll L$; then, $\xi = S/2\omega$, which allows ξ versus x to be obtained. By the same arguments that lead to Eq. (6)—but note that $\varepsilon_b \sim J_1[x(1-x)\omega L]^{1/2}$ and $\varepsilon_\omega \sim J_2\omega$ for strips—one is led to expect that

$$\xi \sim (J_2/J_1)2\omega/[x(1-x)] \tag{8}$$

for strips, in agreement with numerical TM results.[9] (See also Sec. IV.)

For *site* dilution, removal of just one spin removes the corresponding four J_1 bonds, but does *not* remove the ground-state degeneracy. On the other hand, a missing *pair* on NN spins does lift the degeneracy, since an unequal number (four against three) of vertical and horizontal J_1 bonds are then missing, which produces a bias for one of the ground states, just as one missing bond does. The fact that missing *pairs* of NN spins are necessary to lift the degeneracy implies that $x(1-x)$ comes in squared in the derivation of Eq. (6) for *site* dilution, and consequently Eq. (7) still holds, but with $\nu = 2/(2-d)$.

C. Local RSB generated by dilution in three-dimensional (3D) antiferromagnets

As in Sec. II B, consider an Ising model with NN and NNN exchange interactions J_1 and J_2. Consider the bcc lattice first, with all bonds and spins in place. The values of $\mathbf{k}$ which maximize $J(\mathbf{k})$ define the ground state. There are three solutions[15] depending on the values of J_1 and J_2: (a) ferromagnetic order for $J_1 > 0$ and $J_2 > -(\frac{1}{2})J_1$; (b) type-I AF order (see Fig. 2) for $J_1 < 0$ and $J_2 > (\frac{2}{3})J_1$;

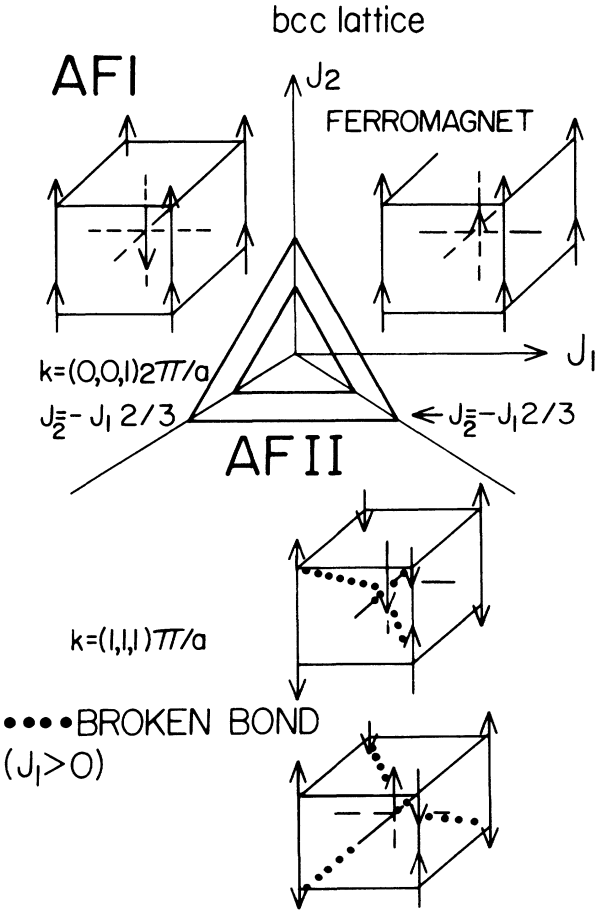

FIG. 2. Phase diagram for Ising model with NN (J_1) bonds and NNN (J_2) bonds on a bcc lattice. There are no broken bonds and no degeneracy in any of the two phases at the top. For the lower $n=2$ phase, there are broken bonds, shown as the dotted line, assuming $J_1 > 0$, for the two degenerate ground states. Note that J_1 bonds which are broken (fulfilled) in one phase become fulfilled (broken) in the other phase.

and (c) type-II AF order for $J_2 < -(\frac{2}{3})|J_1|$. Since neither the ferromagnetic case nor type-I AF (which can be transformed to a ferromagnet by reversing and redefining all spins in the body-centered sites) have any ground-state degeneracy, they are free of the effects of interest here. Consider however an AF of type II. Inspection of Fig. 2 shows that half of the J_1 bonds are broken and the other half are fulfilled in the ground state. One can think of the bcc lattice as two interpenetrating simple-cubic sublattices, and just as for the NN+NNN model, reversal of all spins on one sublattice leaves the ground-state energy invariant. Such a transformation is not an *exact* symmetry; however, in close analogy with the NN+NNN model, there is an exact mirror symmetry with respect to any of the faces of the nonprimitive unit cell.

In complete analogy with the NN+NNN model, removal of a J_1 bond lifts the ground-state degeneracy and produces a random anisotropy (along two axes). In contrast with the two-dimensional case, the surface energy prevents the formation of domains for $d=3$ [see expressions above Eq. (6) for ε_b, δn, and ε_w]. Crossover effects are discussed in Sec. III.

Consider now an Ising model in an fcc lattice. There are four types[15] of maxima for $J(k)$ depending on the values of J_1 and J_2, which define the corresponding ground states (see Fig. 3), mainly: (a) a ferromagnetic ground state for $J_1>0$ and $J_2>-J_1$; (b) an AF of type I for $J_1<0$ and $J_2>0$; (c) an AF type III for $J_2<0$ and $J_2>J_1/2$; and (d) an AF of type II for $J_2<J_1/2$ and $J_2<-J_1$. All three types of AF are degenerate in the fcc lattice.

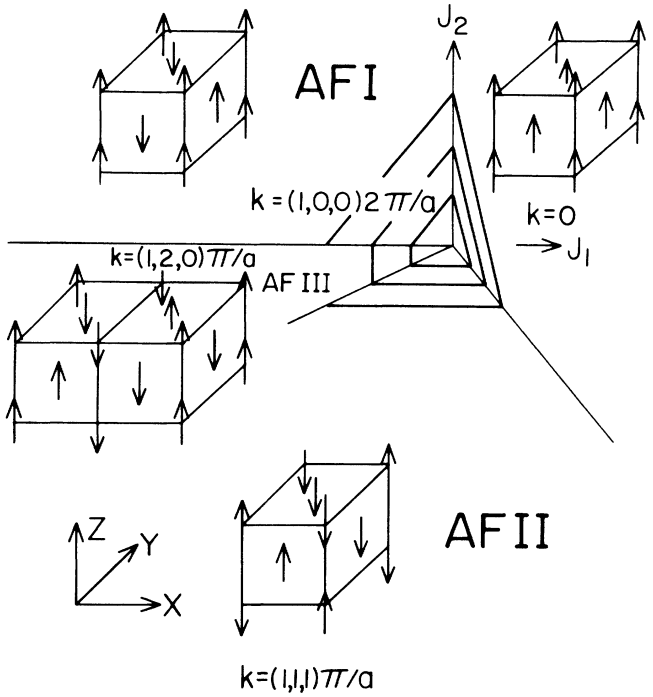

FIG. 3. Phase diagram for Ising model with NN (J_1) bonds and NNN (J_2) bonds on an fcc lattice. There are broken bonds and degeneracy in all AF I, AF II, and AF III phases. There are three degenerate spin configurations ($n=3$) in the AF I phase. The configuration $\mathbf{k}=(2\pi/a)(1,0,0)$ is shown; permutations of 1,0,0 produce the other two configurations. All permutations (6) of the three components of $\mathbf{k}=(\pi/a)(1,2,0)$ in the AF III phase give the six degenerate ground-state configurations. In addition to the spin configuration shown, for $\mathbf{k}=(\pi/a)(1,1,1)$, for AF II, there are three more: $\mathbf{k}=(\pi/a)(-1,1,1)$ and its other two permutations.

There are three degenerate ground states for AF of type I. Ferromagnetic planes are either perpendicular to the x, y, or z axis, and spins on adjacent ferromagnetic planes point in opposite directions (see Fig. 3). All J_1 bonds which lie on ferromagnetic planes are broken, but all other bonds are fulfilled. Therefore, random removal of bonds selects for the ground state one of *three* orientations: the one for which the ferromagnetic planes contain the largest possible number of missing J_1 bonds.

A maximum of $J(\mathbf{k})$ occurs for $\mathbf{k}=(1,2,0)\pi/a$ for AF type III—see Fig. 3. All six permutations of (1,2,0) give all the maxima of $J(\mathbf{k})$. Note, by inspection of Fig. 3, that for $\mathbf{k}=(1,2,0)\pi/a$, all J_2 bonds along the x axis are fulfilled but the rest are broken. On the other hand, all J_1 bonds in planes perpendicular to the x axis are fulfilled while half of the other J_1 bonds are fulfilled and half are broken (the broken and fulfilled bonds exchange roles if the two $\mathbf{k}$ components 2 and 0 are interchanged). Clearly, random removal of bonds generates, once more, RSB, and a concomitant spatially varying bias for the different ground states. Obviously, removal of J_2 bonds does contribute to RSB in the case of AF of type III.

There are *four* spin configurations (maxima of $J_{\mathbf{k}}$) with the same ground-state energy for J_2 and J_1 in the region corresponding to AF II in Fig. 3; they correspond to $\mathbf{k}_1(\pi/a)(1,1,1)$, $\mathbf{k}_2=(\pi/a)(-1,1,1)$, $\mathbf{k}_3=(\pi/a)(1,-1,1)$, and $\mathbf{k}_4=(\pi/a)(1,1-1)$, where a is the nonprimitive unit cell lattice constant. These four $\mathbf{k}$ vectors define ferromagnetic planes; spins in adjacent planes point in opposite directions.[7,16] All J_2 bonds are fulfilled, and all six J_1 bonds which lie on ferromagnetic planes are broken while the rest are fulfilled. It follows as for AF's of type I that random removal of bonds will select the orientation for which ferromagnetic planes contain the largest number of missing bonds.

In every one of the above cases in 3D lattices, the surface energy prevents domain formation. The effect of dilution on crossover behavior to the impurity dominated critical regime is discussed in Sec. III.

III. PREDICTIONS FOR CROSSOVER EFFECTS

Whereas $t_c \sim [J_1^2 x(1-x)]^{1/\alpha}$ for random-exchange ferromagnets (REF), according to the Harris criterion,[14] we expect Eqs. (1) and (2) to hold for the $n \geq 2$ Ising systems studied here. Intuitively, as has been argued in Ref. 9, a thermal fluctuation of linear size x costs a free energy $k_B T_c$ in the pure system. Random behavior sets in if the random energy ε_R of such a fluctuation in the diluted system fulfills $\varepsilon_R > k_B T_c$; now, $\varepsilon_R \sim J_1[nx(1-x)]^{1/2}$, where n is the effective number of spins contributing, that is, $n \sim \sum_i \langle S_0 S_i \rangle$. Thus, n diverges like the susceptibility, that is, $n \sim t^{-\gamma}$. This crude argument yiels $\phi=\gamma$, which differs a bit from Eq. (2). A more careful treatment of the problem follows.

Following Aharony's[8] treatment of the random-field Ising problem, a small perturbation is introduced; let

$$H \rightarrow H + \sum_{i,j} \delta J_{ij} S_i S_j \ , \tag{9}$$

where H is the Hamiltonian for the pure system, the sum is over all ij pairs, and δJ_{ij} is an independent random variable. (For NN bond dilution, if i and j are NN, $\delta J_{ij}=0$ if the ij bond is in place, and $\delta J_{ij}=-J_1$ if the ij bond is missing; the following argument is not restricted to bond dilution, however.) Now, $(\delta J_{ij}\,\delta J_{kn})_{\rm av}=0$ if ij kn are not the same pair, where $(\cdots)_{\rm av}$ stands for an average over different realizations of random bonds. For simplicity's sake, the following derivations, and numerical work, are restricted to randomness in NN bonds only. Generalization to randomness in other bonds is straightforward. Let $\delta J^2=(\delta J_{ij})^2_{\rm av}$; then, a cumulant expansion[17] of F (the free energy) in powers of δJ^2 yields

$$-\beta F = -\beta F_0 + \beta^2(\delta J^2/2) \sum [\langle (S_i S_j)^2 \rangle - \langle S_i S_j \rangle^2] \ , \tag{10}$$

to order δJ^2, where the sum is over NN pairs only. Note that $(S_i S_j)^2=1$, therefore $\langle S_i S_j \rangle^2$ is the term which can provide the singular contribution of F to order $(\delta J)^2$.

On the other hand, assume scaling,[18]

$$F \sim t^{2-\alpha} f((\delta J)^2/t^{\phi}) \ , \tag{11}$$

where f is some function (every subscripted f, as well as unsubscripted, stands for some function everywhere below). Now,

$$F \sim t^{2-\alpha}[f(0)+f'(0)(\delta J)^2/t^{\phi}] \ ,$$

to order $(\delta J)^2$, whence, by comparison with Eq. (10), it follows that

$$t^{2-\alpha-\phi} \sim \langle S_i S_{i+\delta} \rangle^2 \ , \tag{12}$$

where i and $i+\delta$ are nearest neighbors. If (as in the case of a *ferro*magnet, and see below) $\langle S_i S_{i+\delta} \rangle \sim$ energy, then $\langle S_i S_{i+\delta} \rangle \sim t^{1-\alpha}$, and the Harris criterion follows (see also below). It is next shown that $\langle S_i S_{i+\delta} \rangle \sim t^{2\beta}$ for the AF studied here ($n \geq 2$), which, in conjunction with Eq. (12) and the scaling relation[18] $\alpha+2\beta+\gamma=2$, yields Eq. (2).

Consider first the NN+NNN model, and let

$$\langle S_i S_{i+\delta} \rangle = (\psi+\varepsilon_1)/2 \ , \tag{13}$$

where, $\psi=\langle S_i(S_{i+\delta}-S_{i+\delta'})\rangle$, $\varepsilon_1=\langle S_i(S_{i+\delta}+S_{i+\delta'})\rangle$, and sites $i+\delta$ and $i+\delta'$ are NN to site i and are themselves *NN* sites. The term ε_1 is the NN interaction contribution to the energy from each spin. Thus $\varepsilon_1 \sim t^{1-\alpha}$ is expected. ψ is a different type of term; it vanishes for $T>T_c$, by the $x \leftrightarrow y$ symmetry discussed in Sec. II A, since sites $i+\delta$ and $i+\delta'$ are exchanged by that transformation if the i site is taken for the origin. To see how ψ behaves below T_c, where the $x \leftrightarrow y$ symmetry is broken, assume, say, that $S(\mathbf{k}_1)\neq 0$ and $S(\mathbf{k}_2)=0$, where $k_1=(\mathbf{k}_x=\pi/a, \mathbf{k}_y=0)$, and $\mathbf{k}_2=(\mathbf{k}_x=0,\pi/a)$. Then,

$$\psi = -2N^{-1} |\langle S(\mathbf{k}_1) \rangle|^2 + N^{-1} \sum{}' |S(\mathbf{k})|^2 [\exp(ik_x)-\exp(ik_y)] \ , \tag{14}$$

where $\sum'$ stands for sum over all k within the first Brillouin zone, except $\mathbf{k}=\mathbf{k}_1$ and $\mathbf{k}=\mathbf{k}_2$, and the -2 factor arises out of a term

$$[\exp(ik_{1x})-\exp(ik_{1y})]$$

[the δ and δ' sites have been identified with the sites to the right and up of site i, respectively). Now, even below T_c, $|\langle S(\mathbf{k}_x,\mathbf{k}_y)\rangle|^2 = |\langle S(\mathbf{k}_y,\mathbf{k}_x)\rangle|^2$ for all $\mathbf{k}$ except $\mathbf{k}_1$ and $\mathbf{k}_2$. Straightforward considerations of the Ginzburg-Landau-Wilson Hamiltonian[19] of this model show that it is so. Therefore, the second term in Eq. (13) vanishes, whence

$$\psi = 2\langle S_i \rangle \langle S_j \rangle \ , \tag{15}$$

or equivalently, $\psi=\langle S_i \rangle \langle S_{i+\delta}-S_{i+\delta'} \rangle$. Thus, $\psi \sim t^{2\beta}$, and this is the most singular term in Eq. (13) (except, of course, if $1-\alpha<2\beta$). As stated below Eq. (12), Eq. (2) follows. A numerical check of these results is given in Sec. IV A. Note that $\psi=0$ for ferromagnets and for $n=1$ Af, where—see Eq. (13) and above—the Harris criterion follows for those systems.

Everything works much the same for AF of type II in the bcc lattice as for the NN+NNN model above. For the fcc lattice a few details are slightly different. Consider first AF of type I (see Fig. 3). Everything up to Eq. (13) is applicable again, but now, $\psi=\langle S_i(2S_j-S_n-S_m)\rangle_{\frac{2}{3}}$ and $\varepsilon_1=\langle S_i(S_j+S_n+S_n+S_m)\rangle_{\frac{2}{3}}$, where site i is at the origin and sites j, n, and m serve as the primitive basis of the fcc lattice. Instead of the $x \leftrightarrow y$ symmetry of the NN+NNN model, there is, in this case, a threefold rotational symmetry (corresponding to the three equivalent orientations of the ferromagnetic planes). Just as for the NN+NNN model above: (a) ε_1 is proportional to the NN bond contribution to the energy, consequently one expects $\varepsilon_1 \sim t^{1-\alpha}$; and (b) $\psi=\langle S_i \rangle \langle S_j - S_m \rangle$, whence $\psi \sim t^{2\beta}$, and Eq. (2) follows once more. The arguments for AF of types II and III proceed along similar lines.

IV. NUMERICAL RESULTS

All numerical results to be shown in this section are for $J_2=J_1<0$.

A. Transfer-matrix results for strips

Results for long (length $\gg\xi$) narrow ($\omega \ll \xi$) strips obtained by the numerical TM method[13] are shown. There are periodic boundary conditions along the width of the strips and free boundaries at the distant ends. First note that for a pure quasi-one-dimensional Ising model,[20] $\langle S_i S_{i+\delta} \rangle^2$ does not go like a power of t near $T=0$. Therefore, neither Eq. (12) nor Eq. (11), from which Eq. (12) follows, can hold. Since $S \sim (\delta J)^{-2}$ in the $T \rightarrow 0$ limit—see Eq. (8) and above—and $S \rightarrow g^{-1}$ as $\delta J \rightarrow 0$, where $g=\exp(-2\omega J_2/k_B T)$ instead of $S \sim t^{-\gamma}$) for $k_B T \ll J_2$, scaling must be of the form,

$$S \sim g^{-1} f((\delta J)^2/g) \ . \tag{16}$$

Figure 4 shows, for strips with a fraction x of NN bonds missing, $\ln(Sg)$ versus $\ln\{g/[x(1-x)]\}$ (recall that $[x(1-x)]=(\delta J/J_1)^2$ for $\omega=2$ and $k_B T=0.2\,|J_2|$. The agreement with the predicted form of f is rather good. For $(\delta J)^2/g \ll 1$, which corresponds to the pure system limit, Sg becomes constant as expected. On the other hand, from arguments in Sec. III—see Eq. (8) and above—one expects $S \to \sim 1/[x(1-x)]$ as $T \to 0$, or, equivalently, $Sg \to \sim g/(\delta J)^2$ as $(\delta J)^2/g \to \infty$, which is indeed the behavior shown in Fig. 4. This behavior is not at all what one expects from the Harris criterion. These results for narrow strips provide a clear case of a system not covered by the Harris criterion, according to which, impurities should be irrelevant if $\xi > t^{-2/d}$ as $T \to T_c$ (a condition clearly fulfilled in this case), contrary to the results obtained.

B. Monte Carlo results for the pure NN+NNN Ising model

All the Monte Carlo results shown in this paper were obtained applying the Metropolis[21] algorithm to systems with periodic boundary conditions. At least 10^3 MC sweeps to equilibrate and 10^4 MC sweeps in equilibrium were made in each run.

The values of T_c, γ/ν, α/ν, and ν are first established for the *pure* system according to the following scheme. From finite-size scaling,[18]

$$\chi \sim t^{-\gamma} f_1(\xi/L) \ . \tag{17}$$

Letting $t^{-\gamma}=L^{\gamma/\nu}(\xi/L)^{\gamma/\nu}$, and since $S \sim \chi$ or $T \geq T_c$, it follows that

$$S \sim L^{\gamma/\nu} \text{ at } T=T_c \ . \tag{18}$$

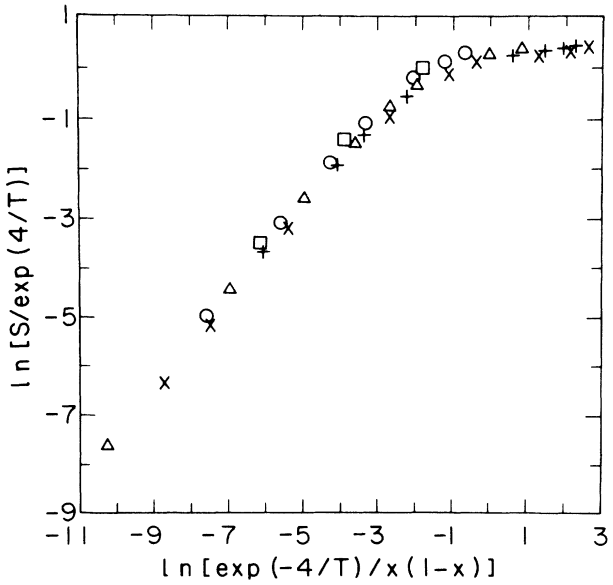

FIG. 4. Transfer-matrix results for long (length $\gg\xi$) narrow (two spins across, $\xi \gg 2$) NN+NNN Ising strips with x fraction of NN bonds missing, at temperature T, in units of $|J_2|/k_B$, for $J_2=J_1<0$. ×, +, △, ○, and □ stand for data for $x=0.01$, 0.02, 0.05, 0.1, and 0.2, respectively.

Similarly,

$$C \sim L^{\alpha/\nu}, \text{ at } T=T_c \ . \tag{19}$$

$\log(S)$ versus $\log(L)$ is shown in Fig. 5, for several values of T. For $T<T_c$, $S \to L^d$ (d is the dimensionality of the system) as $L \to \infty$, as follows directly from the definition of S in Eq. (7), whereas $S \to$ constant as $L \to \infty$, for $T>T_c$. Equation (18) is fulfilled only for $T=T_c$. Figure 5 yields $k_B T_c=(2.08\pm0.01)\,|J_2|$ and $\gamma/\nu=1.79\pm0.05$; The error values follow from statistical errors in the MC results. These, and other numerical results presented below, are recorded in Table I.

$\log[C(T_c)]$ as well as $\log(C_m)$ [the maximum value of $C(T)$ for each value of L] are shown in Fig. 6 versus $\log(L)$. Note that finite-size scaling gives $C \sim t^{-\alpha} f_c(\xi/L)$, where f_c is some function, or, equivalently [setting $t^{-\alpha} \sim L^{\alpha/\nu}(\xi/L)^{\alpha/\nu}$], $C \sim L^{\alpha/\nu} f_d(\xi/L)$; it follows that C has its maximum value, as a function of T, at $\xi/L=$constant. Therefore, $C_m \sim L^{\alpha/\nu}$. The two sets of data points for $C(T_c)$ and for C_m in Fig. 5 yield two values for α/ν: 0.46 and 0.47, respectively. Statistical error analysis of the MC results yield the value of α/ν shown in Table I.

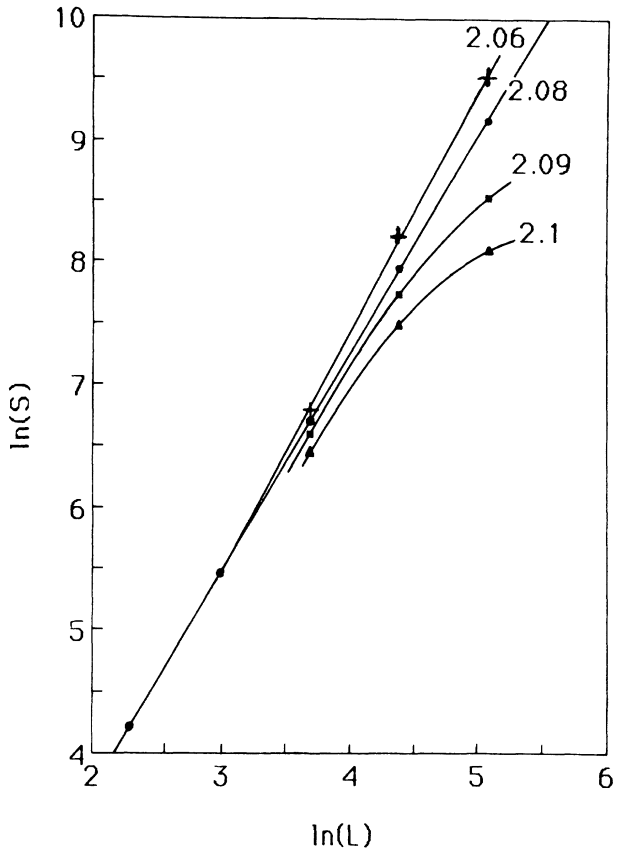

FIG. 5. $\mathrm{Ln}(S)$ is shown, at different temperatures, for NN+NNN Ising systems (with $J_1=J_2<0$) of $L \times L$ spins, vs $\ln(L)$. The numbers shown are the corresponding temperatures, in units of $|J_2|/k_B$, to each of the shown curves. Two curves are straight (for 2.06 and 2.08) lines and two (for 2.09 and 2.1) are parabolas. The slope of the $T=2.06$ curve is 1.97 (it must be 2 for $T<T_c$). The $T=2.08$ curve is shown in Fig. 6 also.

TABLE I. Values obtained for exponents and for T_c for the NN+NNN Ising model with $J_2 = J_1 < 0$.

Exponents	Source
$\gamma/\nu = 1.79 \pm 0.05$	See Figs. 5 and 6 and Eq. (18)
$\alpha/\nu = 0.46 \pm 0.02$	See Fig. 6 and Eq. (19)
$\nu = 0.79 \pm 0.05$	See Fig. 6 and above Eq. (20)
$\phi/\nu = 1.63 \pm 0.05$	See Fig. 6 and Eq. (26)
$\phi/\nu = 1.6 \pm 0.1$	Eq.(2) and see below Eq. (26)
$\gamma/\phi = 1.2 \pm 0.2$	See Fig. (8) and Eq. (28)
$k_B T_c = (2.08 \pm 0.01) \lvert J_2 \rvert$	

To obtain the value of ν, quantity $\Lambda = -\delta \ln(\chi)/\delta T$ is also plotted versus $\ln(L)$ in Fig. 6. (For a discussion on Λ, see Ref. 22.) Note that Eq. (17) implies that $\Lambda \sim t^{-1} f_\Lambda(\xi/L)$. It follows, by the same argument as for C_m above, that $\Lambda_m \sim L^{1/\nu}$. Fro the data shown in Fig. 6 and the associated errors, it follows that $\nu = 0.79 \pm 0.05$. (This value is a bit lower than the value $\nu = 0.87$ obtained by Swendsen and Krinsky[10] for $J_2 = J_1 < 0$. The values obtained here for γ/ν and ν yield $\gamma = 1.4$, which lies between Swendsen and Krinsky's[10] 1.5 and Oitmaa's[23] high-temperature series value of 1.3.) Note that the hyperscaling relation,

$$d\nu = 2 - \alpha \ , \tag{20}$$

is *not* violated—within the allowed errors.

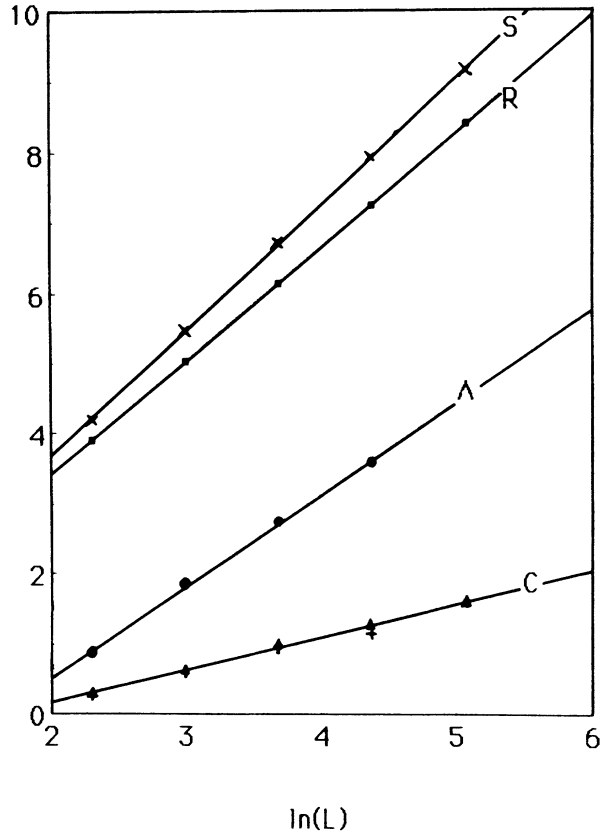

FIG. 6. Curves for $\ln(S)$, $\ln(R)$, $\ln(\Lambda)$, $\ln(C)$, and $\ln(C_m)$. All except C_m are for $T = T_c$ ($= 2.08$), are shown vs $\ln(L)$, for NN+NNN Ising systems (with $J_1 = J_2 < 0$) of $L \times L$ spins. S and R are defined in Eqs. (7) and (23), respectively, Λ is defined above Eq. (20), C is the specific heat and C_m is the maximum value of C as a function of T for each L. The lines shown are straight line fits. $\times$, $\square$, $\circ$, $\triangle$, and $+$ stand for data for $\ln(S)$, $\ln(R)$, $\ln(\Lambda)$, $\ln(C)$, and $\ln(C_m)$, and the slopes of the corresponding curves give the values of γ/ν, ϕ/ν, $1/\nu$, and α/ν [for $\ln(C)$ and for $\ln(C_m)$], respectively.

It is shown next how the value of ϕ is obtained. Consider a system without impurities. Let

$$H \to H - g \sum_i S_i S_{i+\delta} \ , \tag{21}$$

where $\sum_i$ stands for a sum over all i sites in the lattice and $i + \delta$ is a NN to site i. (*No* sum over δ is performed.) Then, using translational invariance,

$$N^{-1}(\delta F/\delta g)_0 = -\langle S_i S_{i+\delta} \rangle \ , \tag{22}$$

where the 0 subscript stands for the $g \to 0$ limit. Let $R = N^{-1}(\delta^2 F/\delta g^2)_0$, then,

$$R = N^{-1} \sum_i \sum_j (\langle S_i S_{i+\delta} S_j S_{j+\delta} \rangle - \langle S_i S_{i+\delta} \rangle \langle S_j S_{j+\delta} \rangle) \ . \tag{23}$$

Assuming scaling,

$$F \sim t^{2-\alpha} f_g(g/t^{\bar{\omega}}, \xi/L) \ . \tag{24}$$

It follows from Eq. (22) that $\langle S_i S_{i+\delta} \rangle \sim t^{2-\alpha-\bar{\omega}} f_s(\xi/L)$ and from Eq. (23) that $R \sim t^{2-\alpha-2\bar{\omega}} f_R(\xi/L)$, which, together with Eq. (12) yields

$$\phi = -2 + \alpha + 2\bar{\omega} \ . \tag{25}$$

Thus, $R \sim t^{-\phi} f_R(\xi/L)$, and, letting $t^{-\phi} = L^{\phi/\nu}(\xi/L)^{\phi/\nu}$, it follows that

$$R(T_c) \sim L^{\phi/\nu} \ . \tag{26}$$

The procedure used here to compute ϕ is the following: Equation (23) is the prescription used to compute $R(T)$, for each value of L, by MC simulation, then $\ln[R(k_B T = 2.08 \lvert J_2 \rvert)]$ is plotted versus $\ln(L)$. Such a plot is shown in Fig. 6. The slope yields $\phi/\nu = 1.63$. Statistical errors in MC results lead to an error of ≈ 0.05.

How does the value of ϕ/ν obtained compare with the value $(\gamma - 2\beta)/\nu$ predicted for it in Sec. III? The scaling relation $\alpha + 2\beta + \gamma = 2$ and Eq. (20) give $(\gamma - 2\beta)/\nu = 2\gamma/\nu - d$, which, from the result obtained for γ/ν, gives 1.58 ± 0.1 for ϕ/ν. There is, therefore, good agreement.

C. Impure NN+NNN model

The numerical value for ϕ/ν obtained above was extracted from the properties of the *pure* NN+NNN Ising model, making use of Eq. (12), which, in turn, follows from expanding F in powers of $(\delta J)^2$. In this subsection, the value of ϕ/γ is obtained fro the actual behavior of *impure* NN+NNN Ising systems.

Crossover behavior is illustrated in Fig. 7, which shows MC results for Λ defined above Eq. (20)—as a function of T for a pure system and for a system with 10% of its NN

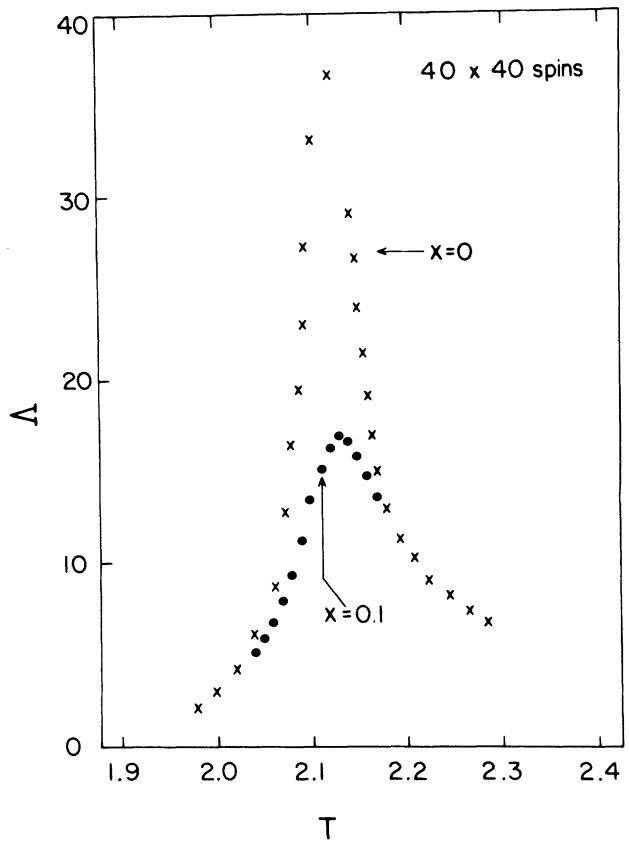

FIG. 7. Λ is shown for NN+NNN Ising systems (with $J_1=J_2<0$) of 40×40 spins vs T. The upper curve is for a pure system and the lower one is for an impure system (a particular case) with 10% of its NN bonds missing. The only purpose of this figure is to illustrate qualitatively crossover behavior. The data points shown were obtained by fitting $\ln(S)$ vs T with a cubic spline curve and taking its derivative.

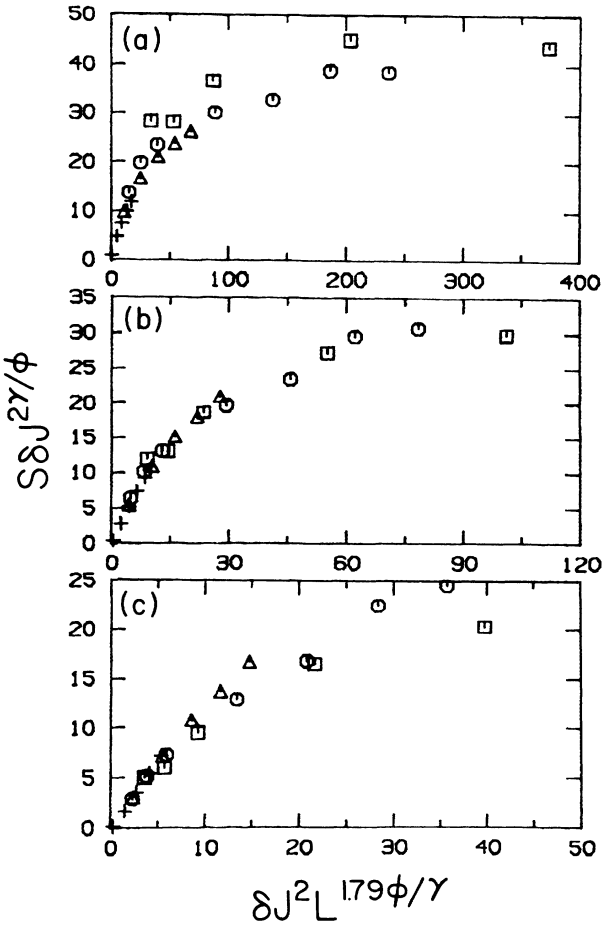

FIG. 8. Plot of $S(\delta J)^{2\gamma/\phi}$ vs $(\delta J)^2 L^{1.79\phi/\gamma}$, for *impure* NN+NNN Ising systems of $L\times L$ spins, with each NN given a value $J_1+(\delta J)_1$, where $(\delta J)_1$ is a random number with a flat distribution and a variance of $(\delta J)^2$. +, △, ○, and □ stand for $L=10$, 20, 40, and 80, respectively. The values $\phi/\gamma=1.0$, 1.2, and 1.4 were used in parts (a), (b), and (c), respectively.

bonds missing, on lattices of 40×40 sites in both cases. The critical point singularity of Λ is clearly suppressed by finite-size effects for the pure system; the Λ peak is further suppressed by impurities, as expected from the conclusions in Sec. III—that there is no ordered phase in two-dimensions (2D).

To obtain ϕ/ν, first note that S, defined in Eq. (7), fulfills $S\sim\chi$ (χ is the susceptibility) for $T\geq T_c$, since $\langle S_i\rangle=0$ then, for impurities of the type under consideration here do not break the up down symmetry of the system. Scaling is assumed once more, in particular,

$$S\sim t^{-\gamma}f((\delta J)^2/t^{\phi},\xi/L)\ . \tag{27}$$

First note, that given $f(x,y)$, one can define $f_1(x,xy^{-\phi/\nu})=f(x,y)$, which, substituting $\xi\sim t^{-\nu}$ and $t^{-\gamma}=(\delta J)^{-2\gamma/\phi}[(\delta J)^2/t^{\phi}]^{\gamma/\phi}$ above, leads to

$$S(T_c)\sim(\delta J)^{-(2\gamma/\phi)}f_1(\infty,(\delta J)^2L^{\phi/\nu})\ . \tag{28}$$

Substitution of the value $\gamma/\nu=1.79$—found in Sec. IV B—for ν above, leaves γ/ϕ as the only fitting parameter. Figures 8(a)–8(c) show MC results for $S(T_c)(\delta J)^{2\gamma/\phi}$ versus $(\delta J)^2L^{1.79\phi/\gamma}$ for various values of L, for $\gamma/\phi=1.0$, 1.2, and 1.4, respectively. Each data point represents an average over six realizations of random J_1 bonds. Each NN bond was assigned a value $J_1+(\delta J)_1$, where $(\delta J)_1$ is a random number with a flat distribution and a variance of δJ^2. Significant deviations from scaling behavior occur in Figs. 8(a) and 8(c), but reasonably good scaling is shown in Fig. 8(b). The value $\gamma/\phi=1.2\pm0.2$ follows therefore from Fig. 8, in reasonable agreement with what follows from the values determined above for γ/ν (1.79) and for ϕ/ν (1.58 and 1.63).

V. SUMMARY AND COMMENTS

The effect of small amounts of random impurities, such as bond or site dilution, on the critical behavior of $n\geq2$ Ising antiferromagnets, in *zero* external field, has been studied. More precisely, it has been shown that any small amount of bond or site dilution generates spatially random symmetry breaking, which acts as a random anisotropy (along a number of axes equal to the multiplicity of the ground state), and which (a) destroys long-range or-

der in $d \leq 2$ in the NN+NNN Ising antiferromagnet if $J_2 < 0$ and $|J_2| > |J_1|/2$, and (b) produces a crossover exponent with the value $\phi = \gamma - 2\beta$ (instead of $\phi = \alpha$, prescribed by the Harris criterion for random ferromagnets) for all Ising antiferromagnets on fcc lattices and all Ising antiferromagnets of type II on bcc lattices. These results are predicted in Secs. II and III, and are supported by transfer-matrix results for strips and by Monte Carlo simulations for two-dimensional NN+NNN Ising systems, presented in Sec. IV.

The result $\phi = \gamma - 2\beta$ differs markedly from the Harris criterion ($\phi = \alpha$ if $\alpha > 0$). The reason is that the mechanism, RSB, responsible for the crossover behavior predicted here for $n \geq 2$ AF is radically different from the mechanism associated with the Harris criterion, at work in ferromagnets (or $n = 1$ AF, such as type-I AF on a bcc lattice) with impurities. It may be worth remarking that the inapplicability of the Harris criterion to $n \geq 2$ AF has nothing to do with any possible violation of hyperscaling ($d\nu = 2 - \alpha$), which is only used towards the end in the derivation[4] of the Harris criterion to arrive at its final (usual) form ($\phi = \alpha$). The exponents of the NN+NNN Ising model (see Table I) do, in fact, fulfill hyperscaling within the allowed errors.

Most discussions and calculations in this paper deal with *bond* dilution, but the extension to the case of site dilution is simple. A *single* missing spin does not generate any bias for any ground state. A little thought shows that it takes a *pair* of NN missing spins to generate RSB. It follows that (for $x \ll 1$) x must be replaced by x^2 in Eqs. (6) and (8) for site dilution [or equivalently, for Eq. (6), $\nu \to 2/(d-2)$] and $\delta J = J_1 x$, instead of $\delta J = J_1 \sqrt{x}$, everywhere else in the paper.

It is unfortunate that most Ising AF in fcc lattices are unsuitable for experimental tests of the results predicted here, for they do *not* have a critical point, but undergo a first-order phase transition instead. According to renormalization-group work and numerical results,[24] the transition from the paramagnetic state to the AF state is a first-order one if $-0.25 < J_2/J_1 < 1$. More recent MC work[25] shows that this range is even larger, -0.25 should be replaced by some number smaller than -1. The situation is not drastically different for AF in bcc lattices. AF of type II undergo a *first*-order transition[26] unless perhaps if $J_2 \ll -2/3\,|J_1|$, that is, unless it is an AF deep into the type-II region. There is, however, an interesting possibility for experiments: AF with $J_2 \approx -2/3\,|J_1|$ and $J_1 < 0$, on bcc lattices, will, upon cooling, go through the multicritical point where the paramagnetic Af II and AF I phases meet. Such a system behaves as an $n = 3$ AF (2 from the AF II phase plus 1 from the AF I phase) and should exhibit the crossover behavior predicted by Eq. (2).

Whether long-range order in NN+NNN vector spin systems (Heisenberg and the like) is or is not destroyed for d small enough by any small amount of bond or site dilution is not immediately obvious; it turns out *not* to be destroyed.[27,28] For a hint for why this might be so, note that, in the NN+NNN XY model, the random anisotropy-like effect produced by dilution acts only along *two* axes—*not* isotropically at random.

On the other hand, the crossover effects, namely Eq. (2), predicted here for *Ising* systems should also hold for vector spin systems. There is nothing in the derivation (Sec. III) of Eq. (2) restricting it to Ising systems, and should therefore apply to Heisenberg AF in fcc and bcc lattices (except AF of type I on bcc lattices).

Diluted semimagnetic semiconductors,[29] such as $Cd_{1-x}Mn_xTe$, are realizations of the models studied in this paper, and may be viewed as AF with random anisotropy (produced by dilution) along a number of axes equal to the multiplicity of the ground state. These ideas have already been put to use by Geschwind *et al.*[30]

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