PHYSICAL REVIEW B VOLUME 39, NUMBER 7 1 MARCH 1989

Ground-state morphology of random frustrated XY systems

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(Received 2 May 1988)

Analytical and numerical results are presented on the ground-state properties of the frustrated XY spin model. One isolated antiferromagnetic (AF) bond in a periodic lattice of ferromagnetic bonds of strength J gives rise to a canted Villain ground state only if its strength exceeds a critical value K_c ($|K_c|=J$ for the square lattice). When two AF bonds are present, their interaction is short range below the threshold and long range (power law) above, and we give a Ginzburg-Landau energy functional that incorporates analytical results for that situation. For a finite density of randomly distributed AF bonds, numerical simulations on the square lattice show that the nature of the ground states differs markedly for small and large values of $|K|/J$, and a simple coherent-potential-approximation calculation is presented for the location of the line separating the two regimes. The simulations also indicate the existence of locally ordered domains, limited by grain boundaries pinned to strongly frustrated regions. A similar model has recently been invoked to interpret spin-glass-type features observed on microscopic scales in cuprate compounds for compositions close to the high-T_c superconductors, and the relevance of the results for these materials is briefly discussed.

I. INTRODUCTION

The rich phenomenology associated with spin glasses has motivated the study of a large variety of theoretical models, in an effort to understand the effect of such parameters as the nature of the spins, the distribution of the interaction strengths, the underlying lattice, etc. In particular, the case of classical, planar spins with both ferro- and antiferromagnetic interactions has been considered by many authors, following the initial work of Villain[1] who showed the existence in this frustrated XY model of a local discrete degeneracy ("two-level systems") due to the breaking of a chiral symmetry absent in the pure XY model. Most of the work has concentrated on periodically frustrated systems,[2-9] which are models for Josephson junction arrays in an external field, or on the effect of disorder and the extra chiral symmetry on the Kosterlitz-Thouless-Berezinskii transition,[10-20] often for interactions of the simple $\pm J$ type.

In the present work we concentrate our attention on the *ground states* of a disordered XY model, with nearest-neighbor interactions either antiferromagnetic (AF, strength K) or ferromagnetic (strength J). We point out that the nature of the ground states in that case depends crucially on the ratio $\lambda=|K|/J$. Our approach is "anatomical": First one AF impurity in a perfect periodic lattice is studied, for XY or Heisenberg spins, showing that the ground state remains perfectly aligned below a critical value λ_c and Villain states with a finite dipolar moment appear only above the threshold, via a second-order transition. For the square lattice, $|K_c|=J$, so the usual $\pm J$ model is doubly special on that lattice: it corresponds to a transition point for ground-state properties, in the dilute limit, in addition to having the Toulouse gauge invariance[21] under the local transformation ($\mathbf{S}_i \rightarrow -\mathbf{S}_i$, $J_{ij} \rightarrow -J_{ij}$ for site i). Then the interaction of two impurities is considered for XY spins and exact results are given for the dependence of the instability on their relative position. When these results are incorporated in a Landau-type expansion of the energy, one finds that the interaction is short range below the threshold and decays like a power law above, in agreement with numerical results.

The situation when a finite density x of impurities is present is studied numerically on the square lattice in Sec. IV. The nature of the ground states is found to change profoundly when the ratio $|K|/J$ varies. For small ratios the ground states retain long-range order, at least on the scale of the samples studied, while for large ratios they are disordered on short scales. A calculation based on a coherent-potential-approximation-(CPA) type approach is presented for the location of the separation line, as a function of x. Above that line structure remains observable, under the form of locally ordered domains separated by grain boundaries associated with fluctuations in the local density of frustrated plaquettes.

Most of these results were in fact obtained some time ago but remained unpublished, except for a presentation at a conference.[22] An incentive to publish them now, in addition to their intrinsic interest for XY spin glasses,[23] comes from the recent discovery of the high-T_c cuprate superconductors.[24] Spin-glass-type effects are observed in these materials, at the level of relatively large domains in the superconducting phase,[25,26] but also at a more microscopic level in nonsuperconducting samples, as seen in various muon precession experiments on compounds of the family $La_{2-x}Sr_xCuO_{4-y}$ (Refs. 27 and 28) and on $YBa_2Cu_3O_{6+\delta}$ (Ref. 29). Aharony *et al.*[30] have argued that doping introduces frustration-type disorder in these compounds and that spin-glass behavior can then be expected by analogy with other materials, at least within a classical, localized spin description for the copper ions. This approach is in a sense orthogonal to the standard Hubbard-Anderson model approach, where frustration also arises, but from purely quantum-mechanical effects rather than from the disorder.[31] Because of the complexity of the real materials, the theoretical situation is still quite confused so that different lines of thought are worth investigating, even if their starting point is oversimplified. The random frustrated XY model plays an important part in the arguments of Aharony *et al.* and we discuss in Sec. V some of its features which might be relevant to the interpretation of the spin-glass properties observed in La_2CuO_{4-y} and other copper-oxide compounds.

II. ONE ISOLATED ANTIFERROMAGNETIC BOND

We consider the Hamiltonian

$$H=-\sum_{i,j} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j \ , \tag{1}$$

where the $\mathbf{S}_i$ are N classical unit vector spins on a periodic lattice and the J_{ij} are nearest-neighbor interactions which may be either ferromagnetic (strength $J>0$) or antiferromagnetic (strength $K=-\lambda J$). Suppose only one AF bond is present, between spins at nodes A and B of coordinates $\mathbf{R}_A=(0,0)$ and $\mathbf{R}_B=(0,1)$, respectively. All spins remain *strictly parallel* in the ground state of the system unless K is large enough to overcome the effective exchange stiffness J_{eff} due to all the other interactions. This can be simply seen by noting that there is a direct relation between J_{eff} and a quantity studied in the problem of conduction in regular resistor networks—namely, the conductance between nodes A and B when the direct connection between them is removed (for a derivation see Kirkpatrick[32]). Translating back to the exchange problem we obtain for the critical AF interaction

$$K_c=-\left[\frac{z}{2}-1\right]J \tag{2}$$

with z the number of nearest neighbors of each site. Thus, for either planar or Heisenberg spins, $\lambda_c=|K_c|/J=1$ for the 2D square lattice and $\lambda_c=2$ for the 3D simple cubic lattice. The same critical value has been obtained independently by Feigelman and Tsvelik[33] as the threshold for the appearance of a localized magnon bound to an AF bond. The electrical analogy has the merit of simplicity, and it also suggest a direct extension to a finite concentration of AF bonds (see below).

Above the threshold ($\lambda>1$) the ferromagnetic state is unstable and the ground state is a canted Villain state. By treating the AF bond as a perturbation one may expand the energy as a function of the spin deviations from perfect alignment, supposed to be small near K_c. For planar spins on the square lattice this expansion takes the form

$$H=H^{(0)}+H^{(1)}+H^{(2)}+\cdots \ , \tag{3}$$

where

$$H^{(0)}=\frac{J}{2}\sum_{i,j}(\theta^{(i)}-\theta^{(j)})^2 \ , \tag{4a}$$

$$H^{(1)}=-\frac{J}{2}(1+\lambda)(\theta^{(A)}-\theta^{(B)})^2 \ , \tag{4b}$$

$$H^{(2)}=\frac{J}{24}\left[\lambda(\theta^{(A)}-\theta^{(B)})^4-\sum_{i,j}{}'(\theta^{(i)}-\theta^{(j)})^4\right] . \tag{4c}$$

The prime in (4c) indicates that the summation excludes the bond AB and $\theta^{(i)}$ (equivalently θ_{mn}) denotes the deviation of the spin located at site i of coordinates (m,n). By Fourier transforming one obtains

$$H^{(0)}=\frac{J}{2}\sum_{\mathbf{q}} V_{\mathbf{q}}\theta_{\mathbf{q}}^*\theta_{\mathbf{q}} \ , \tag{5a}$$

$$H^{(1)}=-\frac{J}{2N}(1+\lambda)\sum_{\mathbf{q},\mathbf{q}'} U_{\mathbf{q}}^* U_{\mathbf{q}'}\theta_{\mathbf{q}}^*\theta_{\mathbf{q}'} \ . \tag{5b}$$

In these expressions

$$V_{\mathbf{q}}=2\sum_{\{\mathbf{u}_n\}}\sin^2(\tfrac{1}{2}\mathbf{q}\cdot\mathbf{u}_n) \ , \tag{6a}$$

$$U_{\mathbf{q}}=2\sin(\tfrac{1}{2}\mathbf{q}\cdot\mathbf{u}_0)\exp[i\tfrac{1}{2}\mathbf{q}\cdot(\mathbf{R}_A+\mathbf{R}_B)] \ , \tag{6b}$$

where $\{\mathbf{u}_n\}$ denotes the set of the nearest-neighbor displacements and $\mathbf{u}_0=\mathbf{R}_A-\mathbf{R}_B$. Since the perturbation $H^{(1)}$ is separable it is straightforward to minimize $H^{(0)}+H^{(1)}$ with respect to $\theta_{\mathbf{q}}^*$. This yields for the Fourier components of the critical mode

$$\theta_{\mathbf{q}}\propto U_{\mathbf{q}}^*/V_{\mathbf{q}} \ ,$$

and the self-consistency condition on $(\sum\theta_{\mathbf{q}}U_{\mathbf{q}})$ implies

$$(1+\lambda_c)^{-1}=\sum_{\mathbf{q}}(|U_{\mathbf{q}}|^2/NV_{\mathbf{q}})=2/z \ .$$

One obtains finally the deviation in real space for the square lattice

$$\theta_{mn}=\Theta\,\alpha_{mn} \ , \tag{7a}$$

$$\alpha_{nm}=\left[\frac{1}{2\pi}\right]^2\int_{-\pi}^{\pi}dq_1\int_{-\pi}^{\pi}dq_2\frac{2\sin(q_2/2)}{\sin^2\frac{q_1}{2}+\sin^2\frac{q_2}{2}}\times\cos mq_1\sin(n-\tfrac{1}{2})q_2 \ , \tag{7b}$$

where the normalization factor Θ is the deviation of the spins adjacent to the AF bond ($\theta_{0,1}=-\theta_{0,0}=\Theta$). The integral in (7b) can be evaluated for finite (m,n) as a sum of

hypergeometric functions.[34] For large distances the integral is dominated by the region $q \to 0$ and the expression reduces to

$$\alpha_{mn} \simeq \frac{2}{\pi} \frac{n-\frac{1}{2}}{m^2+(n-\frac{1}{2})^2} , \tag{8}$$

showing that the spin deviation is asymptotically a dipolar field with moment $\mu=(2\Theta/\pi)$ centered on the AF bond. The value of Θ is fixed by higher-order terms in the energy, contained in $H^{(2)}$, which for $K=K_C=-J$ have the form

$$H^{(2)}=J\Theta^4(\tfrac{2}{3}-\delta) ,$$
$$\delta=\tfrac{1}{24}\sum_{i,j}{}'(\alpha^{(i)}-\alpha^{(j)})^4 \simeq 0.0620 . \tag{9}$$

The coefficient δ represents the softening by the ferromagnetic bonds of the dominant quartic term due to the AF bond and its numerical value has been obtained using Katsura and Inawashiro's formulas.[34] It is convenient to express the results through a Ginzburg-Landau (GL) energy functional, parametrized by the asymptotic strain field dipole moment μ:

$$F(\mu)=2AJ(1-\lambda)\mu^2+B\lambda J\mu^4+O(\mu^6) \tag{10}$$

with $A=(\pi/2)^2$ and $B=(\pi/2)^4(\frac{2}{3}-\delta)$. This expression for F is valid for $(1-\lambda)$ small, and it shows that the transition is second order and that for $1 \gg \lambda-1>0$ the distortions which minimize F have an asymptotic moment $\mu=\pm(A|K+J|/BJ)^{1/2}$, the two signs corresponding to the two possible Villain states. For larger μ higher-order nonlinear terms in the GL functional must be taken into account. The ground-state spin distortions obtained numerically are shown in Fig. 1, for $K/J=-1.1$ and for $K \to -\infty$.

For large values of $|K|$ the dipole moment μ increases more slowly than $(K_c-K)^{1/2}$ and it saturates as $K \to -\infty$ (Fig. 2), but the numerical evaluation of the saturation value turned out to be uncertain due to strong size effects on the lattices we studied (up to 20×20). Let us note that the reduction in the total magnetic moment from the fully aligned state is given by

$$\Delta M=\sum_{m,n}(1-\cos\theta_{mn}) \cong (\mu^2/4)\ln N \tag{11}$$

and diverges logarithmically with the size of the system, though the magnetization per spin is unchanged. This shows that the effect of an impurity is much more pronounced for vector spins than for Ising ones: in the latter case the distortion is always localized and ΔM is finite, whatever the impurity bond strength.

III. INTERACTION OF TWO AF BONDS

A. Exact results for the instability threshold

When two AF bonds of the same strength $K=-\lambda J$ are present, the threshold for instability of the perfectly aligned ferromagnetic state is shifted to a weaker value, which depends on the relative location of the two bonds. The quadratic term $H^{(1)}$ in the perturbative expansion is now, in Fourier space

$$H^{(1)}=-\frac{J}{2N}(1+\lambda)\left[\left|\sum_{\mathbf{q}}\theta_{\mathbf{q}}S_{\mathbf{q}}\right|^2+\left|\sum_{\mathbf{q}}\theta_{\mathbf{q}}T_{\mathbf{q}}\right|^2\right] \tag{12}$$

with

$$S_{\mathbf{q}}=2\exp[i\tfrac{1}{2}\mathbf{q}\cdot(\mathbf{R}_A+\mathbf{R}_B)]\sin\tfrac{1}{2}\mathbf{q}\cdot(\mathbf{R}_A-\mathbf{R}_B) , \tag{13a}$$

$$T_{\mathbf{q}}=2\exp[i\tfrac{1}{2}\mathbf{q}\cdot(\mathbf{R}_C+\mathbf{R}_D)]\sin\tfrac{1}{2}\mathbf{q}\cdot(\mathbf{R}_C-\mathbf{R}_D) , \tag{13b}$$

for two AF bonds located between points (A,B) and (C,D), respectively. One obtains an equation for the (un-

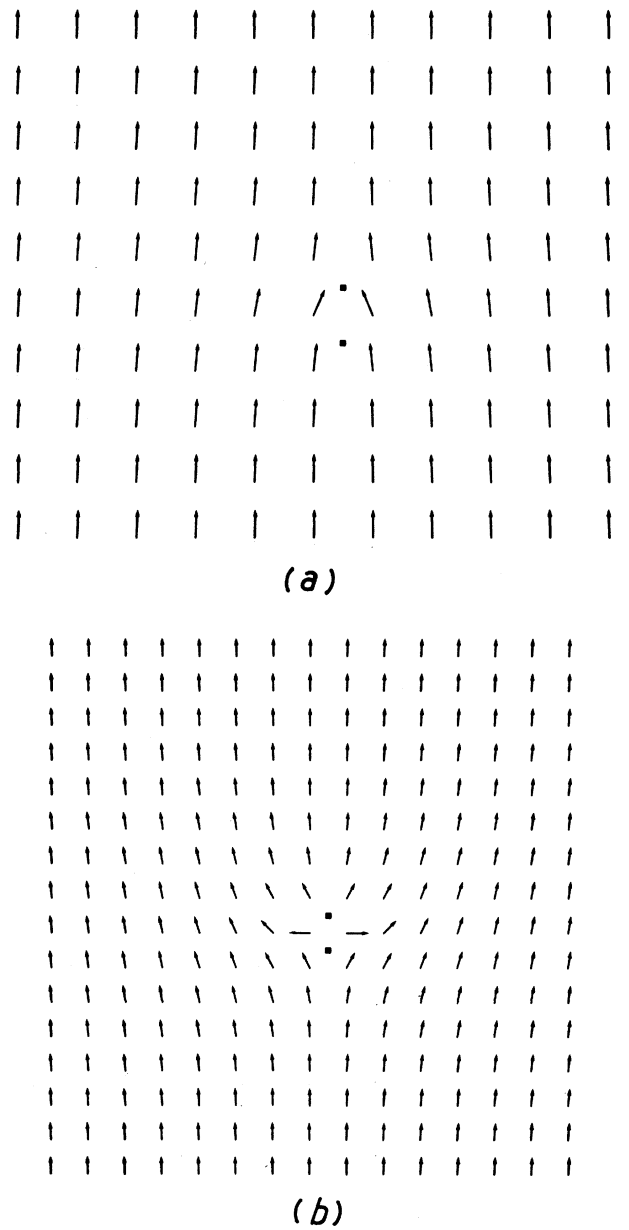

FIG. 1. Ground state of a square lattice of XY spins, with one antiferromagnetic bond of strength K: (a) $K/J=-1.1$, (b) $K=-\infty$. The filled squares indicate frustrated plaquettes.

normalized) eigenmode of $H^{(0)}+H^{(1)}$ in Fourier space,

$$\theta_{\mathbf{q}}=\frac{1+\lambda}{NV_{\mathbf{q}}}(S_{\mathbf{q}}^{*}Y+T_{\mathbf{q}}^{*}Z) \tag{14}$$

with $Y=\sum_{\mathbf{q}}\theta_{\mathbf{q}}S_{\mathbf{q}}$, $Z=\sum_{\mathbf{q}}\theta_{\mathbf{q}}T_{\mathbf{q}}$, which implies in turn two linear relations between Y and Z. The compatibility condition yields finally a simple expression for the threshold, using the fact that $\sum_{\mathbf{q}}(|S_{\mathbf{q}}|^2/NV_{\mathbf{q}})=\frac{1}{2}$ on the square lattice:

$$\lambda_c=\frac{1-2|\Delta|}{1+2|\Delta|}\ , \tag{15}$$

where for nonadjacent AF bonds,

$$\Delta=\sum_{\mathbf{q}}(S_{\mathbf{q}}T_{\mathbf{q}}^{*})/NV_{\mathbf{q}} \tag{16a}$$

$$=\left[\frac{1}{2\pi}\right]^2\int_{-\pi}^{\pi}dq_1\int_{-\pi}^{\pi}dq_2 e^{i\mathbf{q}\cdot\mathbf{R}}\frac{\sin(\mathbf{q}\cdot\mathbf{p}_1/2)\sin(\mathbf{q}\cdot\mathbf{p}_2/2)}{\sin^2(q_1/2)+\sin^2(q_2/2)}\ . \tag{16b}$$

In these expression $\mathbf{R}$ denotes the vector joining the centers of the two AF bonds, $\mathbf{p}_1$ and $\mathbf{p}_2$ the vectors AB and CD, respectively. For two parallel bonds on the opposite sides of an elementary square one finds, for instance, $\Delta=2/\pi-\frac{1}{2}$ and $\lambda_c=\pi/2-1$, showing that two such bonds are less effective for spin canting than a single bond of strength $2K$.

Explicit analytic expressions may be obtained when the distance between the two bonds is large

(i) If the two bonds are parallel, $\mathbf{R}=(m,n)$ with m and n integers and one has

$$\Delta_{\parallel}\cong\frac{1}{\pi}\frac{m^2-n^2}{(m^2+n^2)^2}=\frac{\cos2\Phi}{2\pi R^2}\ , \tag{17}$$

where Φ is the angle between $\mathbf{R}$ and the x axis: $\tan\Phi=n/m$, $R=(m^2+n^2)^{1/2}$. The sign of $\Delta_{\parallel}$ changes when $\Phi=\pi/4$; this just reflects the intuitive fact that it is energetically favorable to have two dipoles of opposite sign when they lie side by side, and of same sign when they lie on top of each other.

(ii) If the two bonds are orthogonal, m and n are half-integers and one has

$$\Delta_{\perp}\cong\frac{1}{\pi}\frac{m^2n^2}{(m^2+n^2)^2}=\frac{\sin2\Phi}{2\pi R^2}\ . \tag{18}$$

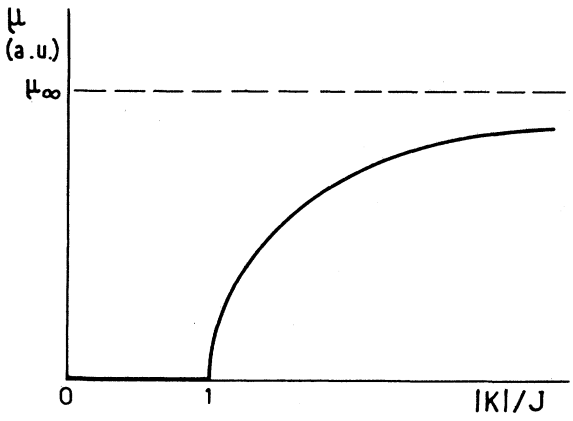

FIG. 2. Schematic variation of the dipole moment μ of the magnetic strain field induced by an isolated AF bond in a square ferromagnetic lattice, as a function of the impurity strength.

In both cases the instability threshold decreases as R^{-2}:

$$|K_c(\mathbf{R})|/J\cong1-4|\Delta|\cong1-g(\Phi)/R^2\ ,\quad R\gg1 \tag{19}$$

where $g(\Phi)=(2/\pi)|\cos2\Phi|$ for parallel bonds ($|\sin2\Phi|$ for orthogonal bonds). Conversely, there is *no* interaction energy at all if $R\geq R_{\min}$, when $\lambda<1$, with

$$R_{\min}\cong\left[\frac{g(\Phi)}{1-\lambda}\right]^{1/2}\ . \tag{20}$$

For $\lambda>1$ there is a long-range interaction between the dipolar distortions, and numerical calculations show that their interaction energy decreases as R^{-2}. The case $\lambda=\lambda_c=1$ gives a weak long-range interaction, with a higher power law, because the Villain dipoles do not preexist in the unperturbed medium. As a consequence the effective interaction will be strongly temperature dependent and may be viewed as a Van der Waals force between thermally fluctuating dipoles. Examples of ground states with two bonds, obtained by a conjugate gradient method, are given in Figs. 3 and 4.

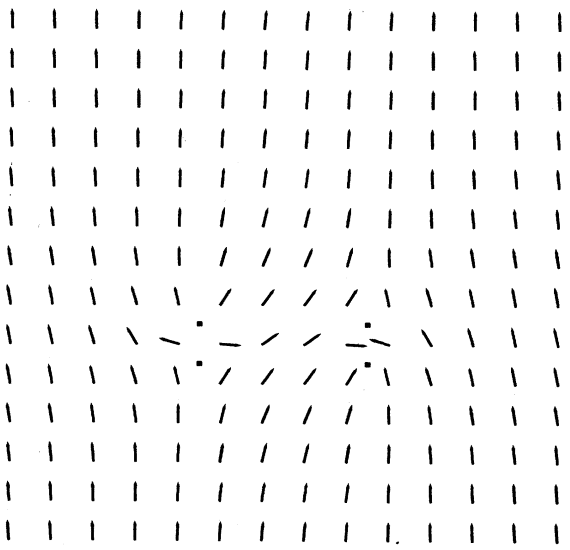

FIG. 3. Ground state with two parallel AF bonds on the same row ($K=-10J$), showing the pairing of opposite dipoles.

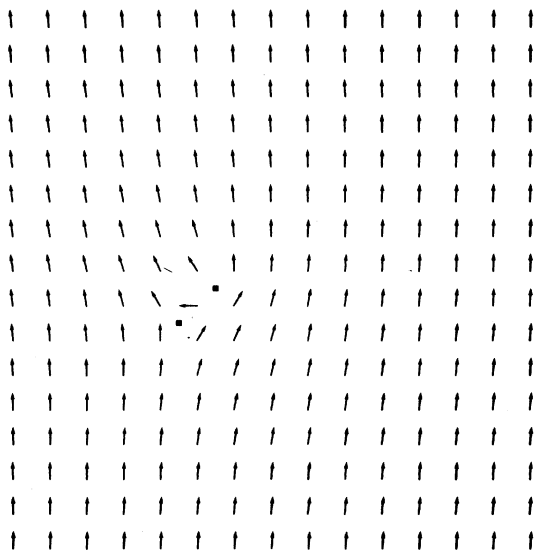

FIG. 4. Ground state with two adjacent orthogonal bonds ($K=-J$).

Another interesting consequence of the perturbation analysis is the existence of a distinct threshold K_m for the metastability of the state where the two dipoles have the opposite relative orientation,

$$K_m(\mathbf{R})=J^2/K_c(\mathbf{R}) .$$

The barrier height between the two states is just given by the ferromagnetic configuration.

B. Ginzburg-Landau functional

The explicit calculation of the quartic terms, which fix the magnitude of the deviations $\theta^{(i)}$ and the ground-state energy, is cumbersome but a simple energy functional may be written, assuming that a single variable for each bond is sufficient to parametrize the total energy. This assumption is reasonable for two parallel AF bonds, since for large distances the two dipoles can be aligned along the same far field direction; for orthogonal bonds the angle between the dipoles has also to be determined and it should be included as a third variable. We restrict here our attention to parallel bonds and, taking as variables the mean relative deviations of the spins adjacent to the AF bonds,

$$\phi_1=(\theta^{(A)}-\theta^{(B)})/2, \quad \phi_2=(\theta^{(C)}-\theta^{(D)})/2 ,$$

we write

$$F(\phi_1,\phi_2)=\epsilon(\phi_1^2+\phi_2^2)+b(\phi_1^4+\phi_2^4)+C_i\phi_1\phi_2+\cdots . \quad (21)$$

In this expression $\epsilon\rightarrow 2(K+J)$ when $R\rightarrow\infty$ and is supposed to be small, and we have omitted terms of the form $\phi_1^2\phi_2^2$ which just renormalize the value of the coefficient b. The interaction coefficient $C_i=C_i(\mathbf{R})$ vanishes when $R\rightarrow\infty$ and has to be chosen so as to reproduce the exact results of the previous section. The minimum of F with respect to ϕ_1 and ϕ_2 is obtained for the following.

(i) $\phi_1=\phi_2=0$, if $|C_i|<2\epsilon$.

(ii) $\phi_1=-\phi_2=[(C_i-2\epsilon)/4b]^{1/2}$, if $C_i>0$ and $C_i>2\epsilon$. The two dipoles point in opposite directions and the ground-state energy is $E_0=-(C_i-2\epsilon)^2/8b$.

(iii) $\phi_1=\phi_2=[(-C_i+2\epsilon)/4b]^{1/2}$, if $C_i<0$ and $C_i<-2\epsilon$. The dipoles point in the same direction, with a ground-state energy $E_0=-(C_i+2\epsilon)^2/8b$.

Comparison with the results of the previous section for the threshold therefore implies the choice

$$C_i(R)\cong 4J\cos 2\Phi/(\pi R^2) , \quad (22)$$

and for $\epsilon<0$ the interaction energy of the two impurities

$$E_{\rm int}(\mathbf{R})=E_0(\mathbf{R})-E_0(\infty)\approx|C_i(\mathbf{R})|\epsilon/(2b) ,$$

decays as R^{-2}.

For $K=-J$, a similar calculation yields $\phi_1\cong c^t/R$ and $E_{\rm int}\cong -c^t/R^4$, but our numerical calculations seem to indicate that the interaction energy decays faster than R^{-4}, so it is likely that the single-parameter assumption leading to Eq. (21) is not valid in that case.

IV. FINITE CONCENTRATION OF AF BONDS

A. CPA approximation

In the previous section we observed that the presence of a nearby negative bond decreases the critical value $|K_c|$ at which stable spin deviations are first induced. The threshold is lowered because the nearby AF bond diminishes the magnetic stiffness felt between sites A and B, even when J_{AB} is set equal to zero. Next we want to understand the consequences of a finite concentration of AF bonds. The equivalence between the magnetic stiffness of an XY spin system and the macroscopic conductivity of a resistor network,[35] for which self-consistent effective medium theories can be constructed,[32] makes this possible.

An effective medium consisting of a uniform exchange strength, J_m, per bond can be defined to describe the result of any distribution $p(J')$ of bond strengths. To determine J_m we require that

$$\int dJ' p(J')\frac{(J_m-J')}{(d-1)J_m+J'}=0 . \quad (23)$$

The content of this equation is simply that J_m be chosen so that the averaged response of the system to long-wavelength strains is uniform across local regions which are described exactly but embedded in the effective medium J_m. For the distribution

$$p(J')=(1-x)\delta(J'-J)+x\,\delta(J'+\lambda J) \quad (24)$$

we find

$$(d-1)(J_m/J)^2 - (J_m/J)\{(1+\lambda)(1-2x) + (d-2)[1-x(1+\lambda)]\}+\lambda=0 . \quad (25)$$

In $d=2$ this means that

$$J_m/J=(1+\lambda)(\tfrac{1}{2}-x)+\tfrac{1}{2}[(1-\lambda)^2-4(x-x^2)(1+\lambda)^2]^{1/2}, \quad (26)$$

where the sign in front of the radical is determined by continuity from the pure case $x=0$ (the other branch is obtained when starting from the AF state, $x=1$). We notice that for $\lambda=1$, which was previously shown to be the threshold bond strength for $2D$, J_m is complex for $0<x<1$, with its imaginary part proportional to $[x(1-x)]^{1/2}$. Thus the instability towards forming spontaneous spin deviations is signaled by the appearance of a complex stiffness. Solving for the condition that the imaginary part vanishes in Eq. (26) we can obtain an expression for the concentration $x_c(\lambda)$ at which widespread spin deviations should appear:

$$x_c(\lambda)=\frac{1}{2}\frac{(1-\sqrt{\lambda})^2}{1+\lambda}, \quad \text{for } d=2. \quad (27)$$

This relation is plotted in Fig. 5. Notice that as $\lambda\to 0$, $x_c\to\frac{1}{2}$, i.e., the percolation threshold concentration x_p, given exactly in this approximation. Thus, as x approaches x_p, AF bonds of any strength give rise to extended spin deviations. Notice, too, that the critical bond strength is a very rapidly decreasing function of concentration. For example, at $x=0.05$, $\lambda_c\cong 0.4$.

Results of the analogous instability calculation for 3D are also plotted in Fig. 5. The CPA solution in that case is

$$4J_m/J=(1+\lambda)(1-3x)+1+\{[1+(1-3x)(1+\lambda)]^2-8\lambda\}^{1/2} \quad (28)$$

and

$$x_c(\lambda)=\tfrac{1}{3}(\sqrt{2}-\sqrt{\lambda})^2/(1+\lambda), \quad \text{for } d=3. \quad (29)$$

Note that $\lambda_c=2$ when $x=0$, so the calculation agrees with the exact result for an isolated impurity, as it should, and in this approximation the percolation threshold is $x_p=\frac{2}{3}$ for $\lambda=0$, close to the correct value $x_p\cong 0.69$ for bond percolation on the cubic lattice.

The stiffness we calculate via J_m is observable as the coefficient of q^2 in the spin-wave dispersion relation. We predict within CPA that long-wavelength spin waves become strongly damped, with a linewidth proportional to their energy, for $x>x_c(\lambda)$. The real part of J_m does not become soft before this happens: at the instability boundary it is found to be

$$J_m[x_c(\lambda)]=J\lambda^{1/2}, \quad \text{for } d=2$$
$$=J(\lambda/2)^{1/2}, \quad \text{for } d=3. \quad (30)$$

B. Numerical simulations

We have performed numerical calculations for various values of x and λ, using both a conjugate gradient method and a Monte Carlo cooling algorithm, in order to confront the predictions of the simple CPA theory. Some typical ground-state spin configurations so obtained for a 2D system are displayed in Figs. 6–8, showing that two very different situations are encountered. For values of the parameters below the line $\lambda_c(x)$ local deviations exist

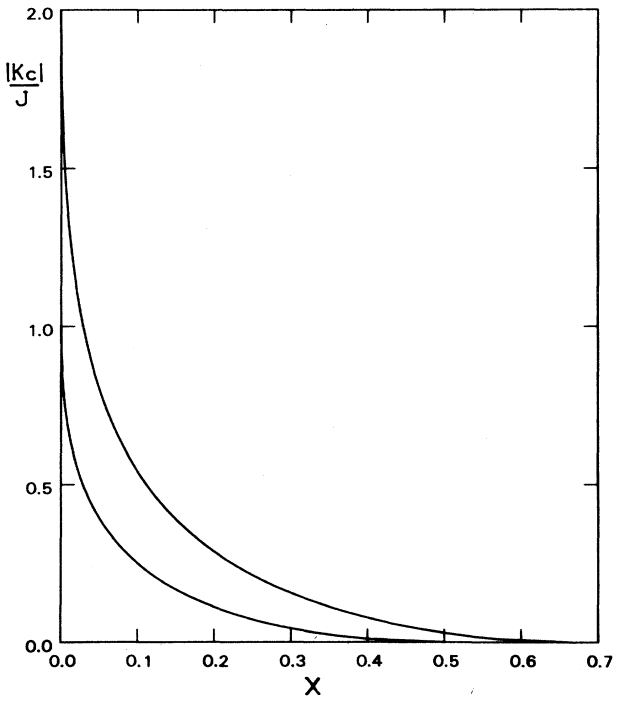

FIG. 5. CPA calculation of the critical AF impurity bond strength $\lambda_c=|K_c|/J$ at which a finite density of extended spin defects appears for vector spins, as a function of the impurity concentration x. Lower curve, $d=2$; upper curve, $d=3$.

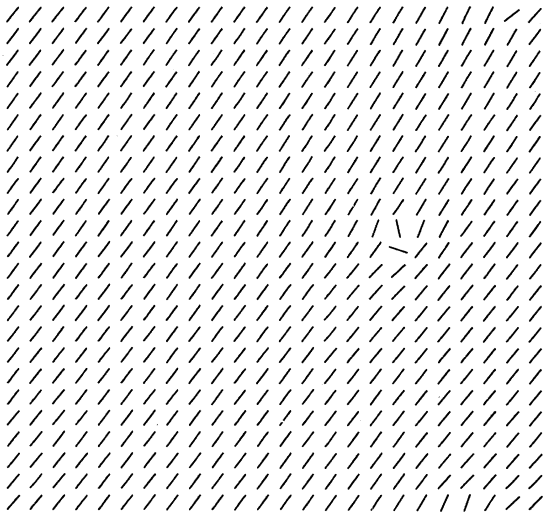

FIG. 6. Ground state of a 2D XY spin system, for $x=0.06$, $K/J=-0.3$ (arrows omitted for clarity).

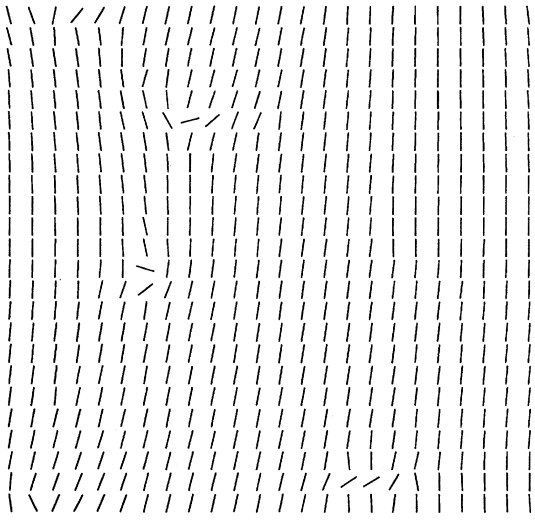

FIG. 7. Ground state for $x=0.09$, $K/J=-0.3$.

but are not sufficient to destroy correlations on the scale of the samples studied. On the contrary, well above the line, the spins are strongly disordered. The agreement with the CPA results is only qualitative, though: for $\lambda=0.3$, Eq. (27) predicts $x_c=0.08$, whereas very little disorder is in fact observed for $x=0.09$ (Fig. 7). A more detailed study will be necessary to obtain the precise location of the line. Anyway, the question of whether long-range order may indeed be present at zero temperature for finite x is subtle, and a conservative interpretation of our results is in terms of a crossover line rather than a true transition—but note that Berge *et al.*[8] have found that in a fully frustrated XY model the ground state remains perfectly ferromagnetic if the AF bond strength $|K|<J/3$.

In the region $\lambda>\lambda_c(x)$, locally ordered regions are still observable in the simulations, for, say, $x<0.1$ (Figs. 9 and 10). Inspection of the pictures reveals that

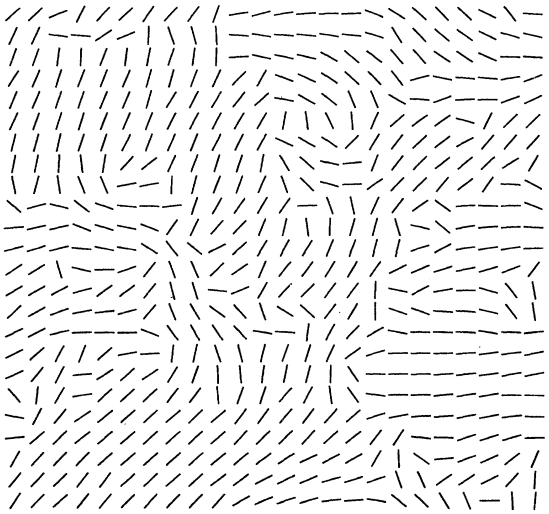

FIG. 8. Ground state for $x=0.20$, $K/J=-0.3$.

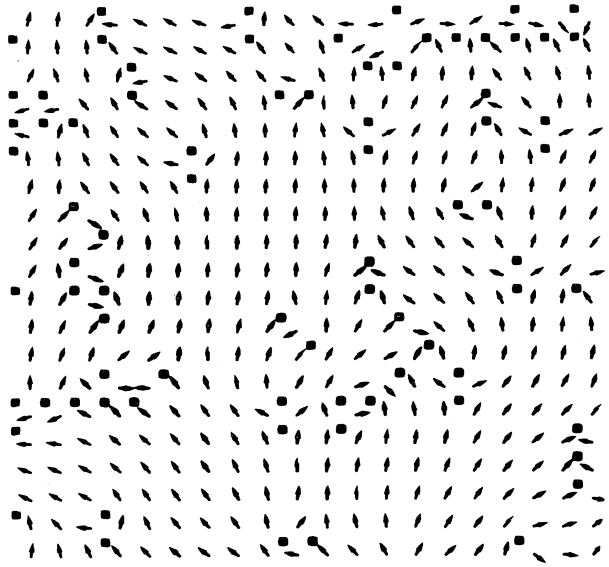

FIG. 9. Ground state for $x=0.05$, $K/J=-2$ (the solid squares indicated frustrated plaquettes).

"domains" ordered along different directions exist in regions that are relatively free of frustration, because of fluctuations in the local density of AF bonds—which may be important for small x. These domains are separated by "grain boundaries" associated with regions of higher frustration. We have not performed a detailed study of the size of these domains, to see whether it diverges close to the line $\lambda_c(x)$.

V. REMARKS ON SPIN-GLASS EFFECTS IN La_2CuO_{4-y} AND RELATED COMPOUNDS

The high-T_c cuprate superconductors are rather complicated materials for solid-state physics, with many

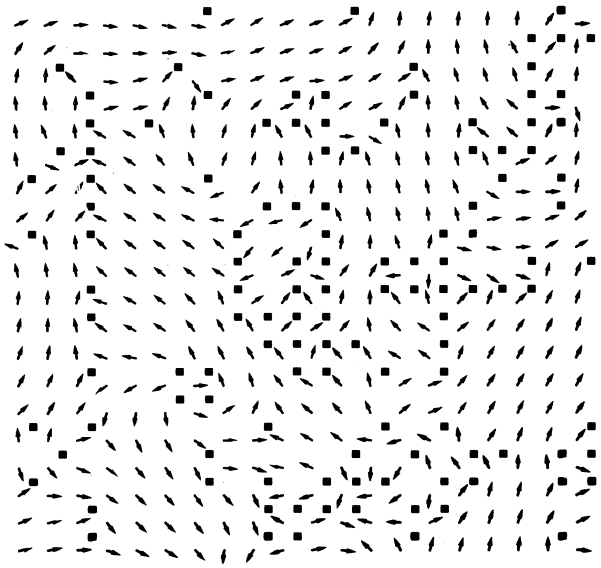

FIG. 10. Ground state for $x=0.10$, $K/J=-1$.

features possibly relevant for the superconductivity mechanism. The study of the phase diagram for families of related compounds, such as $La_{2-x}Sr_xCuO_{4-y}$ or $YBa_2Cu_3O_{7-\delta}$, brings important information on the magnetic and structural properties, as well as constraints on the actual mechanism. Spin-glass-type effects on a microscopic scale (e.g., spin freezing associated to a broad distribution of local fields) have been observed in these compounds, mainly by muon spin relaxation,[27–29] for compositions intermediate between systems with long-range AF order (close to La_2CuO_4 or $YBa_2Cu_3O_6$), and the superconducting range, where no magnetic ordering is observed.

Aharony *et al.*[30] and Harshman *et al.*[28] have proposed that the origin of these effects lies in disorder-induced frustration, as in classical spin glasses. For the ordered parent material (La_2CuO_4 or $YBa_2Cu_3O_6$) the Cu ions may be treated as $S=\frac{1}{2}$ quantum spins, interacting via oxygen-mediated AF bonds ($-J$). In the picture of Aharony *et al.* for the materials at small doping, a localized hole sitting on an oxygen site between two Cu ions in the CuO_2 planes generates an effective ferromagnetic interaction K_F between these spins, giving rise to frustration around an elementary square of Cu ions. For classical spins, by a simple gauge transformation[21] on one of the two Néel sublattices, this is equivalent to the problem of an AF bond ($-K_F$) in a ferromagnetic lattice (J). The anisotropy effects in the basal plane are very weak[36] and as a first approximation, neglecting quantum effects, one recovers the model of vector spins in the presence of random impurity bonds studied in the previous sections.[37] In view of the complexity of the materials and of the difficulty to treat disorder in a quantum-mechanical calculation, this classical model is a reasonable starting point—at least as long as the quantum fluctuations do not destroy the AF order in the ground state.

The correspondence between the concentrations p of holes and x of wrong bonds is not direct, however, because the holes have a localization length of a few lattice spacings, so in a classical approximation their effect should be spread out on several bonds. Aharony *et al.* argue that the ferromagnetic coupling should be spread typically on ten Cu—Cu bonds at low p, but it is much stronger than the AF ones as it is due to direct exchange. If we bluntly identify K and x in the frustrated XY model with $K_F/10$ and $10p$, respectively, the experimental systems should still lie above the critical curve $\lambda_c(x)$ for long-range disorder obtained in Sec. IV, because of the large value of K_F/J and the fast decrease of λ_c with x.

In fact, the net resultant effect is somewhat subtle, because spreading the impurity coupling can relieve frustration. Indeed, if one lattice site has its four bonds of the wrong sign there is no frustration at all.[21] A possible way to distribute the ferro coupling due to the hole between a "cloud" of nine neighboring bonds is shown in Fig. 11: only two plaquettes are frustrated and if all the ferro bonds have equal strength $K=-J$, the system is equivalent, up to gauge transformations, to a string of only three wrong bonds (Fig. 12). For Ising spins the threshold for a nontrivial, degenerate ground state is then $K_c=-2J$, corresponding to a total impurity strength

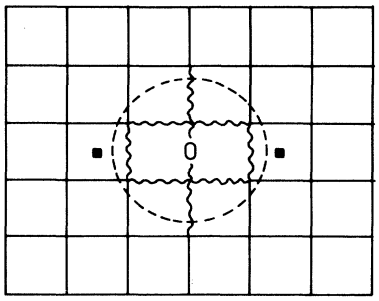

FIG. 11. "Cloud" of nine ferromagnetic bonds (wiggly lines), representing the effect in an AF lattice of a hole localized on an oxygen vacancy (empty circle). Only two plaquettes are frustrated.

$K_F=-18J$ (instead of $-3J$ in the one-bond case). Other ways to spread the hole would give different results but the strong reduction of frustration is a quite general effect. Note that below the threshold the ground state may be imperfectly ordered: what changes at K_c is the degeneracy of the ground state and, for continuous spins, the existence of noncollinearity and of a long-range distortion.

At very low concentrations ($p \ll 1\%$, say), the large distance effect of one impurity remains similar to that of one wrong bond, with a reduced overall strength, but when p increases the situation becomes more intricate. If two nearby impurities with their clouds are considered the spins in the intermediate region are strongly tilted but the outside perturbation is relatively small, because of the compensation of the two dipole fields. Figure 13 shows the interaction of two strings of five negative bonds, of strength $K=-J$, for comparison with Fig. 3 (two bonds of strength $-10J$). Using the nine-bond cloud of Fig. 11

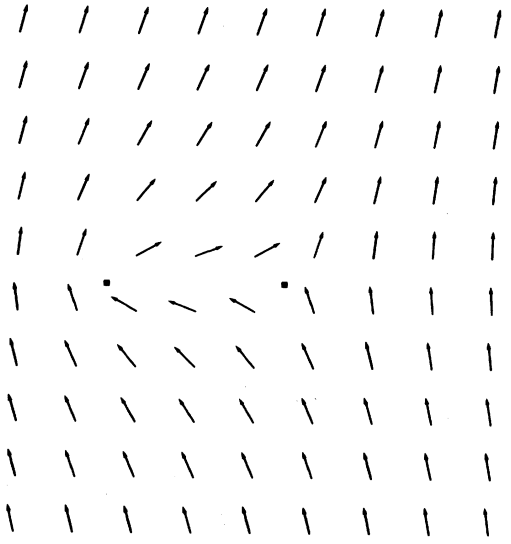

FIG. 12. Ground-state spin configuration around the string of three AF bonds obtained from the bond pattern of Fig. 11 through gauge transformations ($K=-J$).

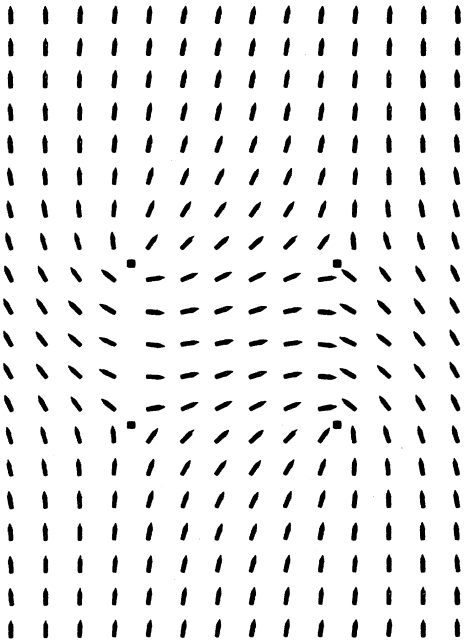

FIG. 13. Interaction of two strings of five AF bonds ($K=-J$).

one can even easily find an arrangement of four impurities that creates no frustration at all, though 36 bonds have the wrong sign. Extensive numerical simulations on a specific model are clearly necessary to take into account the correlated disorder introduced by the hole and to determine the corresponding threshold $K_c(p)$ for long-range disorder.

Let us note that a reduction of frustration in the plane bringing the system below the critical line $\lambda_c(x)$ would not mean that its classical ground state cannot have spin-glass behavior. The local loss of 2D AF order destroys the quasicompensation which is at the origin of the weak interplanar AF coupling in the cuprate compounds, thus creating competing interactions between spins in neighboring planes.[28,30] This leaves open the possibility of 3D spin-glass ordering, even if (quasi-) long-range order exists within the planes.

Another situation where the above considerations may be relevant is found at the twin boundaries in the orthorhombic phase of the cuprate compounds. The accompanying lattice distortion, in the CuO_2 planes, is likely to bind holes or oxygen vacancies, favoring ferromagnetic coupling between the two domains. The structural details of the boundary may have crucial influence on its magnetic behavior if local disorder induces frustration, which will result in noncollinearity between the spin directions in the two domains. This could play a role in the internal Josephson effects observed in the superconducting materials.[26,38]

VI. CONCLUSION

When combined with other work on the random-bond frustrated XY model,[10–20] the present results for the ground-state properties indicate that the complete phase diagram as a function of impurity strength, concentration, and temperature is richer than previously assumed. It deserves a more detailed study, in particular to elucidate the nature of the critical line $\lambda_c(x)$ at finite temperature. Apart from numerical simulations, it would be extremely interesting to perform experiments on materials representative of this model for various values of the ratio K/J, e.g., by generalizing the work of Katsumara *et al.*[23] through suitable chemical substitutions.

The relevance of disorder-induced frustration effects for high-T_c superconductors and related materials is another motivation for future work. The realistic situation, where Coulomb interactions, disorder, and quantum effects all play a role, is intractable at the present time and clearly the quantum aspects are essential for the superconductivity mechanism. The study of the nonsuperconducting phases is nonetheless necessary to assess the relative importance of the various factors and there the classical spin approximation may help to single out important effects due to the disorder. Various extensions of the present work may be considered in that spirit, e.g., introduction of weak 3D couplings and of correlated disorder, and would be worth undertaking if further experiments confirm the existence of a spin glass region between the AF and superconducting compositions of the cuprate compounds.

ACKNOWLEDGMENTS

The collaboration at the origin of the present work began as three of us visited the IBM Thomas J. Watson Research Laboratory. One of us (J.V.) is indebted to his colleagues in Grenoble—especially M. Gordon, M. Lavagna, B. Barbara, and R. Calemczuk, for many discussions about the various facets of the cuprate compounds and the vast relevant literature. As the manuscript was in proof, we received copies of unpublished work by W. Saslow and G. Parker,[39] who have independently considered the ground-state properties of the frustrated XY model. The basic results for the one- and two-impurity case are of course identical to ours, but the details of the calculations, the scope of the papers, and the discussion of experimental relevance are different and the two works are complementary in many respects. As these authors point out, the critical value for the creation of a local distortion by an impurity had already been obtained by de Gennes in 1960.[40]

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[1]J. Villain, J. Phys. C **10**, 1717 (1977); **10**, 4793 (1977).
[2]S. Teitel and C. Jayaprakash, Phys. Rev. B **22**, 598 (1983).
[3]M. Yosefin and E. Domany, Phys. Rev. B **27**, 1778 (1985).
[4]M. Y. Choi and S. Doniach, Phys. Rev. B **31**, 4516 (1985).
[5]T. C. Halsey, J. Phys. C **18**, 2437 (1985).
[6]P. Minnhagen, Phys. Rev. B **32**, 7548 (1985).

[7]D. H. Lee, J. D. Joannopoulos, J. W. Negele, and D. P. Landau, Phys. Rev. B **33**, 450 (1986).
[8]B. Berge, H. T. Diep, A. Ghazali, and P. Lallemand, Phys. Rev. B **34**, 3177 (1986).
[9]E. Granato and J. M. Kosterlitz, J. Phys. C **19**, L59 (1986).
[10]J. V. Jose, Phys. Rev. B **20**, 2167 (1979); Phys. Rev. Lett. **46**, 1591 (1981).
[11]B. S. Shastry, J. Phys. C **12**, L405 (1979); **15**, 931 (1982).
[12]V. S. Dotsenko, Pis'ma Zh. Eksp. Teor. Fiz. **31**, 301 (1980) [JETP Lett. **31**, 276 (1980)].
[13]D. L. Huber and W. Y. Ching, J. Phys. C **13**, 5579 (1980).
[14]C. Kawabata, J. V. Jose, and S. Kirkpatrick, J. Phys. C **14**, L633 (1981).
[15]M. Rubinstein, B. Shraiman, and D. R. Nelson, Phys. Rev. B **27**, 1800 (1983).
[16]S. Jain and A. P. Young, J. Phys. C **19**, 3913 (1986).
[17]H. Kawamura and M. Tanemura, J. Phys. Soc. Jpn. **55**, 1802 (1986); Phys. Rev. B **36**, 7177 (1987).
[18]W. M. Saslow and G. Parker, Phys. Rev. Lett. **56**, 1074 (1986).
[19]B. W. Morris, S. G. Colbourne, M. A. Moore, A. J. Bray, and J. Canisius, J. Phys. C **19**, 1157 (1986).
[20]G. G. Batrouni and E. Dagotto, Phys. Rev. B **37**, 9875 (1988).
[21]G. Toulouse, Commun. Phys. **2**, 1151 (1977).
[22]F. D. M. Haldane, C. Jayaprakash, S. Kirkpatrick, and J. Vannimenus, Bull. Am. Phys. Soc. **25**, 210 (1980).
[23]An experimental realization of a frustrated XY model is provided by the material $Rb_2Mn_{1-x}Cr_xCl_4$. See D. Sieger *et al.*, Solid State Commun. **64**, 1413 (1987); S. Higgins and R. A. Cowley, J. Phys. C **21**, 2215 (1988); K. Katsumara, J. Tuchendler, Y. J. Uemura, and H. Yoshizawa, Phys. Rev. B **37**, 356 (1988); and references therein.
[24]K. A. Müller and J. G. Bednorz, Science **237**, 1133 (1987).
[25]K. A. Müller, M. Takashige, and J. G. Bednorz, Phys. Rev. Lett. **58**, 1143 (1987).
[26]G. Deutscher and K. A. Müller, Phys. Rev. Lett. **59**, 1745 (1987).
[27]J. I. Budnick, B. Chamberland, D. P. Yang, Ch. Niedermayer, A. Golnik, E. Recknagel, M. Rossmanith, and A. Weidinger, Europhys. Lett. **5**, 651 (1988).
[28]D. R. Harshman, G. Aeppli, G. P. Espinosa, A. S. Cooper, J. P. Remeika, E. J. Ansaldo, T. M. Riseman, D. L. Williams, B. Ellma, and T. F. Rosenbaum, Phys. Rev. B **38**, 852 (1988).
[29]N. Nishida *et al.*, J. Phys. Soc. Jpn. **57**, 597 (1988).
[30]A. Aharony, R. J. Birgeneau, A. Coniglio, M. A. Kastner, and H. E. Stanley, Phys. Rev. Lett. **60**, 1330 (1988).
[31]P. W. Anderson, Science **235**, 1196 (1987); M. Inui, S. Doniach, and M. Gabay, Phys. Rev. B **38**, 6631 (1988).
[32]S. Kirkpatrick, Rev. Mod. Phys. **45**, 570 (1973).
[33]M. V. Feigelman and A. M. Tsvelik, Zh. Eksp. Teor. Fiz. **76**, 2249 (1979) [Sov. Phys.—JETP **49**, 1136 (1979)].
[34]S. Katsura and S. Inawashiro, J. Math. Phys. **12**, 1622 (1971).
[35]A. B. Harris and S. Kirkpatrick, Phys. Rev. B **16**, 542 (1977).
[36]G. Shirane *et al.*, Phys. Rev. Lett. **59**, 1613 (1987). In the presence of a weak anisotropy energy Δ the threshold K_c is slightly shifted and the dipolar distorsion field around an impurity has a cutoff at a distance $R \approx a(J/\Delta)$. Experimental bounds on the gap of the spin-wave spectrum indicate that this cutoff is always much larger than the typical distance between impurities for representative materials, so the power-law interaction between two impurities, Eq. (19), remains valid for practical purposes.
[37]Let us emphasize that the present model is very different from the XY model used by I. Morgenstern, K. A. Müller, and J. G. Bednorz [Z. Phys. B **69**, 33 (1987)] to study the "superconductive glass," where the spins represent the superconducting order parameter of semimacroscopic regions coupled by Josephson junctions and the frustration arises from the effect of an external field.
[38]I. Morgenstern, Z. Phys. B **70**, 299 (1988).
[39]G. N. Parker and W. M. Saslow (unpublished); W. M. Saslow and G. N. Parker (unpublished).
[40]P. G. de Gennes, Phys. Rev. **118**, 141 (1960).