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Phase diagram for a random mixture of competing Ising anisotropies

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We study a ferromagnetic system in which each bond can be either of the Ising type ($\sigma^z\sigma^z$) or of anisotropic Heisenberg (Ising $\sigma^x\sigma^x$-like) type, at random with respective concentrations $(1-p)$ and p. A global phase diagram in the temperature-anisotropy-concentration space is obtained within the Migdal-Kadanoff approximation. For the paramagnetically ordered transitions, our results for the critical temperature as a function of p agree very well with those obtained experimentally for $Fe_{1-p}Co_pCl_2 \cdot 2H_2O$.

Magnetic systems with random anisotropies have attracted a great number of experimental[1,2] and theoretical[3] investigations over recent years. In these systems the coupling between any pair of neighboring spins can have $O(n)$ symmetry ($n=1$, 2, 3 correspond to Ising, XY, and Heisenberg models, respectively) with n being either n_1 or $n_2 \geq n_1$ at random. When the order parameters for the pure $O(n_2)$ and $O(n_1)$ phases are not orthogonal [e.g., a random mixture of Heisenberg and Ising or of XY ($S^xS^x+S^yS^y$) and Ising (S^xS^x) couplings] there is a critical line separating the paramagnetic from *a single* ordered phase for any finite concentration of less symmetric bonds [$O(n_1)$ symmetry] and accordingly, the critical exponents are those of the pure $O(n_1)$ system.[4] Also, the critical temperature increases as the concentration of $O(n_1)$ bonds is increased from zero, since the concentration plays the role of an effective anisotropy parameter. These results agree[5] with those obtained from birefringence measurements[2] on the random mixture $Mn_pFe_{1-p}F_2$, which can be approximated by a random Heisenberg-Ising mixture.

On the other hand, when the order parameters for the pure $O(n_2)$ and $O(n_1)$ phases are orthogonal [e.g., a random mixture of Ising (S^xS^x) and Ising (S^zS^z) couplings; or of XY ($S^xS^x+S^yS^y$) and Ising (S^zS^z) couplings] there is a critical line separating the paramagnetic from *three* ordered phases which meet at a decoupled tetracritical point.[6] As the concentration p of one of the components of the mixture, say that of $O(n_1)$ bonds, increases one finds the following low-temperature phases: $O(n_2)$, oblique or mixed (in which the order parameter is at an angle, different from 0 or $\pi/2$, with respect to the pure order parameters) and $O(n_1)$. For this reason, one says these anisotropies *compete*. Also, the critical temperature $T_c(p)$ displays a (sharp) minimum at the tetracritical point (see, e.g., Ref. 6). Several measurements on the competing antiferromagnetic Ising-Ising mixture (Ref. 7) $Fe_{1-p}Co_p$- $Cl_2 \cdot 2H_2O$ agree with the above qualitative predictions, especially with respect to the sharpness of the transitions from both Ising phases to the oblique (mixed) phase. In the competing random XY-Ising mixture, however, the low-temperature transitions involving the mixed phase are smeared in some cases,[8-10] which is attributed to random-field effects[9(b)] or to a residual spin-orbit interaction.[11]

The purpose of this work is to investigate the problem of competing random anisotropies of the Ising-Ising type by a position-space renormalization-group (PSRG) method. In this way, one is able to study the phase diagram when one of the components of the mixture is described by anisotropic Heisenberg couplings. This approach is then complementary to previous[6,11] ϵ expansion[12] studies in the sense that more direct comparison with experimental data is possible.

We consider the following Hamiltonian (in units of $-kT$):

$$\mathcal{H}=\sum_{\langle i,j\rangle} K_{ij}[(1-\Delta_{ij})\sigma_i^x\sigma_j^x + (1-|\Delta_{ij}|)\sigma_i^y\sigma_j^y+(1+\Delta_{ij})\sigma_i^z\sigma_j^z] , \tag{1}$$

where the sum runs over nearest-neighbor pairs of spins on a simple-cubic lattice and the σ's are Pauli matrices. K_{ij} and Δ_{ij} are the exchange-coupling and anisotropy parameter, respectively, both taken to be random variables governed by the following distribution

$$P(K_{ij},\Delta_{ij})=[p\delta(\Delta_{ij}-\Delta)+(1-p)\delta(\Delta_{ij}-1)]\delta(K_{ij}-K) , \tag{2}$$

without correlation between bonds. One should note that if only $\sigma^x\sigma^x$ and $\sigma^z\sigma^z$ couplings were considered in (1) the parameter space would not be invariant under renormalization-group (RG) iterations, since $\sigma^y\sigma^y$ couplings would be generated.

Within the Migdal-Kadanoff (MK) bond-moving approximation[13,14] in three dimensions, a RG transformation by a scaling factor $b=2$ is generated by first combining two bonds "in series" (decimation), and then combining four decimated bonds in parallel, in such a way that the partition function is preserved, that is,[14]

$$\exp(\mathcal{H}_{13}^{(s)})=\mathrm{Tr}_2\exp(\mathcal{H}_{123}) , \tag{3}$$

where $\mathcal{H}_{13}^{(s)}$ and $\mathcal{H}_{123}$ correspond to the Hamiltonian (1) being written (with $j\equiv i+1$) for chains with 2 and 3 spins with respective pairs of couplings $(K^{(s)},\Delta^{(s)})$ and (K_l,Δ_l; $l=1,2$) as given by (2); $\mathcal{H}_{13}^{(s)}$ also contains the usual[14] additive constant $K_0^{(s)}$; Tr_2 stands for the trace over the $\boldsymbol{\sigma}_2$ variables and the superscript (s) refers to "series" combination. The use of $b=3$, while making the process of configurational averaging much more time consuming in numerical calculations, does not improve the results substantially.

The recursion relations are obtained[15] by first expanding the left-hand side of Eq. (3)

$$\exp\mathcal{H}_{13}^{(s)}=a'+b'_{13}\sigma_1^x\sigma_3^x+c'_{13}\sigma_1^y\sigma_3^y+d'_{13}\sigma_1^z\sigma_3^z\ , \tag{4}$$

and comparing the two matrix forms of $\exp\mathcal{H}_{13}^{(s)}$ [one obtained from (1) and the other one from (4), expressed on the basis that diagonalizes $\mathcal{H}_{13}^{(s)}$; see Ref. 15 for details] we relate analytically $K_0^{(s)},K^{(s)}$, and $\Delta^{(s)}$ to a', b'_{13}, c'_{13}, and d'_{13}:

$$K_0^{(s)}=\tfrac{1}{4}\ln\{[(a'-b'_{13})^2-(c'_{13}+d'_{13})^2]\times[(a'+b'_{13})^2-(c'_{13}-d'_{13})^2]\} \tag{5a}$$

$$\left.\begin{matrix}K^{(s)}\\ \Delta^{(s)}\end{matrix}\right\}=\tfrac{1}{4}\ln\left[\frac{(a'+b'_{13})\pm c'_{13}\mp d'_{13}}{(a'-b'_{13})\mp c'_{13}\mp d'_{13}}\right]\ . \tag{5b}$$

On the other hand, we also expand $\mathcal{H}_{123}$ as

$$\exp(\mathcal{H}_{123})=a+\sum_{\substack{i,j\\ i<j}}(b_{ij}\sigma_i^x\sigma_j^x+c_{ij}\sigma_i^y\sigma_j^y+d_{ij}\sigma_i^z\sigma_j^z)\ , \tag{6}$$

where the sum runs over *all* sites of the three-site chain. The relations between a, b_{ij}, etc., and $(K_l,\Delta_l;l=1,2)$ can be obtained following the same procedure outlined above for $\exp\mathcal{H}_{13}^{(s)}$ but in this case it can only be done numerically.[15] Thus, taking (4) and (6) into (3) and performing the partial trace one gets $a'=2a$, $b'_{13}=2b_{13}$, $c'_{13}=2c_{13}$, and $d'_{13}=2d_{13}$, which, through (5), defines the desired recursion relations $K^{(s)}(K_l,\Delta_l;\ l=1,2)$ and $\Delta^{(s)}(K_l,\Delta_l;\ l=1,2)$ for the decimated bond.

The next step consists in combining four decimated bonds in parallel:[15] the $K^{(s)}$'s simply add, giving rise to a renormalized bond $\tilde{K}$ for a given configuration of original bonds $(K_l,\Delta_l;\ l=1,8)$; the renormalized anisotropy $\tilde{\Delta}$ turns out to be an "average" of the decimated $\Delta^{(s)}$ weighted by the $K^{(s)}$'s.

The above steps are followed for each configuration of the eight original pairs (K_l,Δ_l) in the cluster. Then, the renormalized distribution, as given by[16]

$$\bar{P}(\bar{K},\bar{\Delta})=\int\prod_{l=1}^{8}[dK_l d\Delta_l P(K_l,\Delta_l)]\delta(\bar{K}-\tilde{K})\delta(\bar{\Delta}-\tilde{\Delta})\ , \tag{7}$$

is no longer of binary form, and gets more complicated as the number of RG iterations increases. To avoid this uncontrollable proliferation of δ functions, one usually resorts to a truncation scheme[17] that keeps the renormalized distribution in binary form,

$$P'(\bar{K}-\bar{\Delta})=[p'\delta(\bar{\Delta}-\Delta')+(1-p')\delta(\bar{\Delta}-1)]\delta(\bar{K}-K')\ , \tag{8}$$

with p', Δ', and K' chosen in such a way that the following averages are preserved:

$$\langle\bar{K}^{\mu}(1-\bar{\Delta}^{\mu})\rangle_{\bar{P}}=\langle\bar{K}^{\mu}(1-\bar{\Delta}^{\mu})\rangle_{P'},\ \ \mu=1,2\ , \tag{9a}$$

$$\langle\bar{K}(1+\bar{\Delta})\rangle_{\bar{P}}=\langle\bar{K}(1+\bar{\Delta})\rangle_{P'}\ , \tag{9b}$$

where the subscripts refer to averages weighted by the distribution functions given by Eqs. (7) and (8). Equations (9) then define K', Δ', and p' as (implicit) functions of K, Δ, and p. There is certainly a degree of arbitrariness in the choice (5); other choices were tried[5] without major qualitative changes in the resulting phase diagrams.

The RG equations (9) are solved numerically for fixed points and exponents in the usual way,[12] and the critical surface can be obtained by iterating the RG transformation. We found the following fixed points $(1/K^*,\Delta^*,p^*)$ and exponents: (a) Ising-*ZZ* at (7.66, 1, 0) with $\nu_T=1.07$ (cf. 0.63 by series[18]) and a negative crossover exponent $\phi\equiv\nu_T/\nu_\Delta$, (b) Ising-*XX* at (7.66, −1, 1) with the same exponents, and (c) Heisenberg at (2.9, 0,1) with $\nu_T=1.39$ (cf. 0.72 by series[19]) and $\phi=1.56$ (cf. 1.25 by series[20]). Figure 1 shows the resulting phase diagram in the temperature-anisotropy-concentration space. As one crosses the critical surface of Fig. 1, the Ising fixed points $I(X)$ and $I(Z)$ determine the critical behavior at each side of the line *CH*, which in turn is dominated by the Heisenberg fixed point *H*.

Cross sections of Fig. 1 for several values of the anisotropy parameter are shown in Fig. 2. Near each "pure" limit, the behavior is similar to ordinary dilution[21] in the sense that the critical temperature decreases upon dilution. We can understand this by noting that a small amount of, say Ising-*XX* bonds embedded in a sea of Ising-*ZZ* bonds, will inhibit the spread of *ZZ* correlations, just as if they were absent. When *XX* and *ZZ* bonds are present in comparable proportions, however, competition sets in and the behavior is different from dilution. This competition is marked by sharp minima in Fig. 2 (i.e., the point where, for a given Δ, the three curves meet) corresponding to the line *CH* in Fig. 1. While the temperature

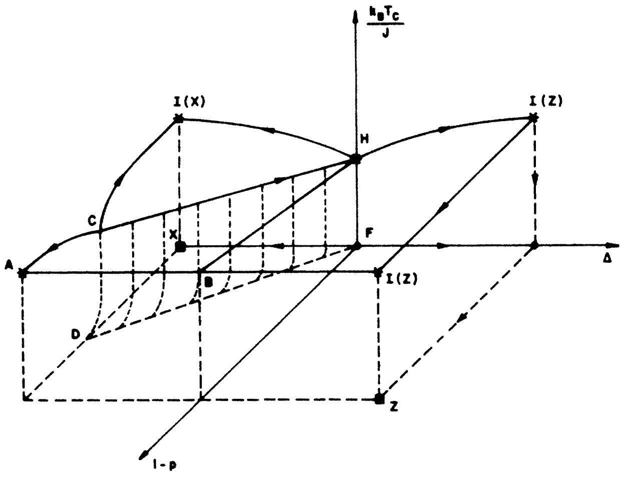

FIG. 1. Phase diagram (schematic) in the temperature (k_BT/J) anisotropy. (Δ), concentration; p, space for a competing random Ising-Ising mixture. Critical fixed points are denoted by (∗), and phase attractors by (■).

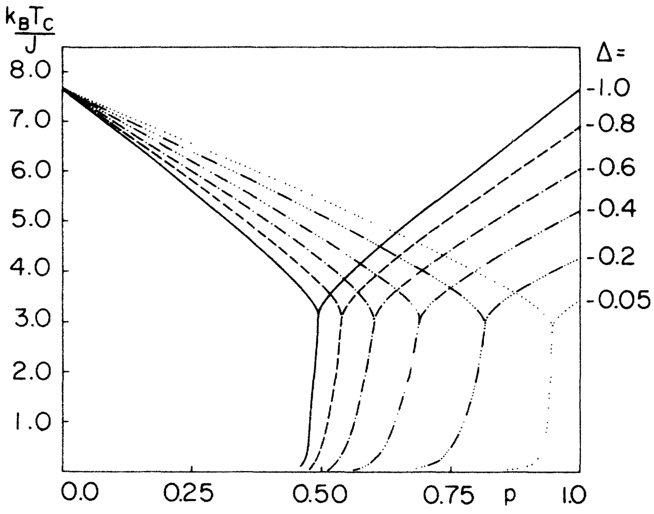

FIG. 2. Sections of the phase diagram (Fig. 1) for fixed values of the anisotropy Δ. Numbers on the right-hand side represent the values of Δ for each curve.

at which these minima occur hardly varies with Δ, there is a strong dependence of their location with the concentration: mixtures of Ising (ZZ) and weakly anisotropic systems (i.e., small $|\Delta|$, $\Delta<0$) only sustain anisotropic ordering up to a few percent of Ising (ZZ) bonds.

In Fig. 3 we compare our results with experimental data from susceptibility and specific-heat measurements[7(a)] on the antiferromagnetic system $\mathrm{Fe}_{1-p}\mathrm{CO}_p\mathrm{Cl}_2\cdot 2\mathrm{H}_2\mathrm{O}$; the comparison is valid in this case, since there are no frustration effects in the latter. The transition between paramagnetic and ordered phases is very well described by our approach, indicating that no other mechanisms are responsible for this transition apart from those included in the model. Since the experimental and theoretical curves are normalized at $p=0$ (Ising-ZZ limit) one can attribute the discrepancy in the opposite limit ($p=1$) to different values of the exchange couplings in these two limits.

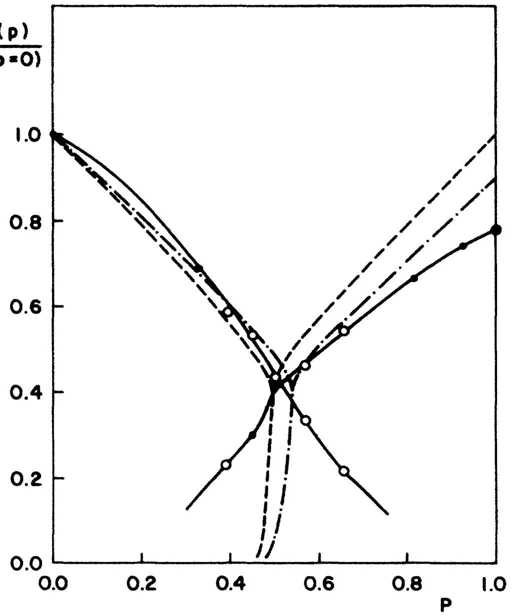

FIG. 3. Reduced critical temperature as a function of the concentration of Ising-XX bonds: full curve, experimental results for $\mathrm{Fe}_{1-p}\mathrm{Co}_p\mathrm{Cl}_2\cdot 2\mathrm{H}_2\mathrm{O}$ (Ref. 7); dashed curve, present results with $\Delta=-1$; dash-dotted curve, present results with $\Delta=-0.8$.

Our results fail to agree with available predictions for the low-temperature transitions. We did not find any mixed phase separating the two Ising regions, which are separated by a single curve instead. This unsatisfactory result of our calculations can be traced back to the clusters used, and *not* to the MK approximation or to the truncation of the renormalized distributions. As pointed out by Castellani, di Castro, and Ranninger[22] in the context of the MK approximation, when three- and four-spin clusters are decimated into a two-spin cluster (scaling factors $b=2$ and 3, respectively), the XY symmetry of the ground state is lost; this behavior persists in a different cluster approximation,[23] reinforcing the idea that this drawback is due to the scaling into a two-spin cluster and not to the MK approximation. It is well established,[14,22,23] however, that this drawback only affects the low-temperature behavior, while critical surfaces attracted by finite temperature fixed points are very reliable, as is the case of the upper boundary in Fig. 3. Since the mixed phase in the present case should be governed by a zero-temperature fixed point corresponding to the *simultaneous* ordering along X and Z (spin) directions, one cannot expect a fair description of such an XZ ordering, similarly to what happens for the usual XY ordering. With respect to the truncation of the renormalized distributions, we would like to stress that the resulting phase diagram is rather insensitive to which averages were preserved;[5] this indicates that the truncation scheme plays no significant role in the absence of the mixed phase.

To sum up, we obtained a phase diagram for the competing Ising-Ising random mixture which agrees very well with experimental data for $\mathrm{Fe}_{1-p}\mathrm{Co}_p\mathrm{Cl}_2\cdot 2\mathrm{H}_2\mathrm{O}$ in what concerns the paramagnetic-ordered transitions; this indicates that these transitions are not influenced by random-field effects or by off-diagonal couplings. Possibly the presence of a mixed phase governed by a zero-temperature fixed point could only be detected by a PSRG framework that (i) distinguishes XY from isotropic Heisenberg ordering at $T=0$, which as far as we know, has not been set up yet and (ii) incorporates geometrical features such as the "percolation" of XX and ZZ clusters. We hope this work stimulates efforts along these directions. Similar results were obtained[5] for an XY-Ising mixture, and will appear elsewhere.

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