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Ising model with short-range correlated dilution

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We consider a diluted Ising model in which the absence of a spin affects the exchange coupling of a nearest-neighbor pair along the line joining the three spins; that is, it acquires the value αJ, where α is a phenomenological parameter $\epsilon[0,1]$. This model has been proposed to explain the experimental phase diagram for $\mathrm{KNi}_x\mathrm{Mg}_{1-x}\mathrm{F}_3$. A position-space renormalization-group analysis clearly distinguishes two percolation thresholds depending on whether $\alpha=0$ or $\alpha>0$, though both cases seem to be in the same universality class. Further, thermal fluctuations dominate over the geometrical ones as in the uncorrelated case, and the critical curve (critical temperature versus concentration of magnetic sites) displays an upward curvature for intermediate degrees of correlation $0<\alpha<1$, as experimentally observed.

The cluster structure properties of quenched dilute magnets are usually described by a simple percolation model. Here, a site on a lattice is considered occupied (magnetic) or unoccupied (nonmagnetic) at random, with the single global constraint that the percentage of occupied sites must equal the concentration of the "magnetic" species present in the sample being modeled. However, it has been found experimentally that in some circumstances a (potentially) magnetic atom may fail to display a magnetic moment, depending on its local environment. Clearly, the simplified picture given above cannot account for these effects; thus, more sophisticated ("correlated percolation") models have been proposed, in which one tries to get hold of the essential environmental aspects, in addition to the purely random ones.

This seems to be the case for $\mathrm{KNi}_x\mathrm{Mg}_{1-x}\mathrm{F}_3$: nuclear magnetic resonance (NMR) data for this system[1] show striking differences from those for the isostructural compound $\mathrm{KMn}_x\mathrm{Mg}_{1-x}\mathrm{F}_3$, which have been interpreted as signaling that a specific correlated percolation model applies to the former substance,[1,2] whereas the latter is properly described by an uncorrelated dilution picture.[3]

The authors of Refs. 1 and 2 recall that, while in Mn^{2+} the electronic configuration is such that the Mn ions can form both π and σ bonds with the fluorine ligands, the corresponding configuration for Ni^{2+} allows only the formation of σ bonds. The directionality of σ bonds then implies that, if an Ni^{2+} ion is replaced by a nonmagnetic atom, this must have a strong effect on the exchange coupling of a nearest-neighbor magnetic pair situated along the line joining the three atoms. For Mn^{2+} the directional effect should be less drastic, owing to the existence of π bonds. Those authors then proposed[2] a model in which the exchange between atoms located at nearest-neighboring sites is

$$J_{\mathrm{i},\mathrm{i}+\boldsymbol{\delta}}=J\epsilon_{\mathrm{i}}\epsilon_{\mathrm{i}+\boldsymbol{\delta}}[(1-\alpha)\epsilon_{\mathrm{i}-\boldsymbol{\delta}}+\alpha]\,, \qquad (1)$$

where $\boldsymbol{\delta}$ denotes an elementary lattice vector, ϵ_{i} is a site occupation variable, with the ensemble average $\langle\epsilon_{\mathrm{i}}\rangle=x$ (magnetic atom concentration), and α gives the strength of the correlation; while for $\alpha=0$, the existence of the bond between i and $\mathrm{i}+\boldsymbol{\delta}$ is entirely dependent on the occupancy of $\mathrm{i}-\boldsymbol{\delta}$, the uncorrelated limit is recovered for $\alpha=1$. For $0<\alpha<1$, the absence of a magnetic ion at $\mathrm{i}-\boldsymbol{\delta}$ only weakens the bond between i and $\mathrm{i}+\boldsymbol{\delta}$, proportionally to α, but does not destroy it.

At zero temperature, for any $\alpha>0$ the problem is the same as that for $\alpha=1$ (uncorrelated); for $\alpha=0$, it can be described by the following geometric prescription: Two neighboring magnetic sites are considered to be in the same cluster only if their nearest-neighbor sites along the same direction of the line joining them are also magnetic.[4] With this rule for the formation of clusters, the authors of Ref. 4 found, by large-cell Monte Carlo renormalization-group calculations on the square lattice, the critical concentration $x_c=0.741\pm0.002$ (significantly higher than the corresponding value 0.5931 ± 0.0006 for the uncorrelated site problem on the same lattice[5]). They also found the critical scaling power $y_p=0.75\pm0.02$; comparison with the (presumably exact) $y_p=\frac{3}{4}$ for uncorrelated percolation in two dimensions[6] indicates that the two problems are in the same universality class, with regards to the percolation transition.

For finite temperatures, the authors of Ref. 2 apply an effective-field theory[7] to a dilute spin-$\frac{1}{2}$ Ising model on a square lattice, with the nearest-neighbor interaction term given by Eq. (1) above. They find qualitative trends, such as an increase in the slope $(1/T_c)(dT_c/dx)$ at the pure point $x=1$ (relative to the uncorrelated case), and an upward curvature in the $T_c\times x$ phase diagram, which are consistent with the experimental data for $\mathrm{KNi}_x\mathrm{Mg}_{1-x}\mathrm{F}_3$ (although the latter is a three-dimensional Heisenberg magnet rather than a two-dimensional Ising system, these trends are interpreted as being essentially correlation effects, expected to be present regardless of spin structure). However, they find *three* different percolation thresholds at zero temperature: $x_c(\alpha=1)=0.428$ for the uncorrelated problem, $x_c(\alpha=0)=0.765$ for full correlation, and $x_c(\alpha)=0.381$ for $0<\alpha<1$. This, as noted by those authors, is not consistent with their model Hamiltonian, from which one should obtain only *two* distinct thresholds: one for $\alpha=0$ where correlation can erase a bond, and another for intermediate or zero correlation $0<\alpha\leq1$. Further, they find different values of T_c

$(x=1)$ for different values of α, which is clearly an undesirable feature [this does not show in their figures, where only the normalized quantity $T_c(x)/T_c(1)$ is plotted]. These two unphysical characteristics stem from the approximations implicit in the Honmura-Kaneyoshi formalism.[7] Although on the Bethe lattice an exact solution of this correlated dilution problem is free from such difficulties,[8] it must be recalled that this kind of lattice is itself a pathological structure; specifically in the present case, where directional effects are all important, the fact that it is only the "radial" direction that is uniquely defined for the Bethe lattice may introduce an undesired bias, which is hard to gauge.

Having this in mind, we have studied the above-mentioned correlated dilution problem for Ising spins on a square lattice, by means of a position-space renormalization-group (PSRG) procedure. As shown below, our results do not display the unphysical features just mentioned; further, they provide an additional insight into the relevance [(in the renormalization-group (RG) sense] of correlation, which is not obtainable through other calculational methods. Thus, we feel that the picture coming from our study complements and improves upon what is already known about the subject.

We have made use of a PSRG transformation which is depicted, for a rescaling parameter $b=2$, in Fig. 1. For the scaled probability $(x')^2$ of the two renormalized sites in Fig. 1(b) being both present *and* joined by an active bond, we count all paths in Fig. 1(a) which lead from A or A' to B or B' and are formed by active bonds. In the extremely correlated limit $\alpha=0$, where a bond can actually be destroyed by correlation [see Eq. (1)], two magnetic sites are considered as joined by an active bond only if both their nearest neighbors along the line joining them are occupied as well. For $0<\alpha\leq 1$, a bond is considered to exist between any two occupied nearest-neighbor sites; this reflects the fact that, no matter how weakened a bond is, it will fully transmit information at zero temperature as long as its strength is not exactly zero. We thus have two different probability recursion relations, one for $\alpha=0$ and another for $\alpha\neq 0$; this will give different percolation thresholds in either case, in agreement with physical intuition. The thermal aspects are incorporated as follows. For each connected configuration of sites which enter for x', if the sites at the bottom of the cell are connected to those at the top through at least one path made up entirely of unaffected bonds (i.e., exchange J, or transmissivity[9] $t\equiv \tanh J/k_BT$), then the renormalized bond is considered to be J'; if this connection necessarily includes a weakened bond (i.e., exchange αJ or transmissivity $u\equiv \tanh \alpha J/k_BT$), then the renormalized bond is taken as $\alpha'J'$. Though somewhat arbitrary, this criterion is justified by the fact that, for a path with one weak bond, magnetic order propagates with lower intensity than it would along one totally made up of strong bonds. One should note that this prescription has the overall effect of grouping together all disorder configurations that do not percolate in the extremely correlated $(\alpha=0)$ limit; as a consequence, in this limit one has $u'=u=0$. With this criterion, we can average t and u over the disordered configurations to get two other recursion relations: $t'(t,u,x)$ and $u'(t,u,x)$, which give the renormalized quantities J' and α'. In a three-dimensional (x,T,α) parameter space, the flow of the PSRG recursion relations gives the approximate phase diagram. In what follows, we shall display only constant-α sections of the critical surface, in order to compare our results to experimental and other theoretical data.

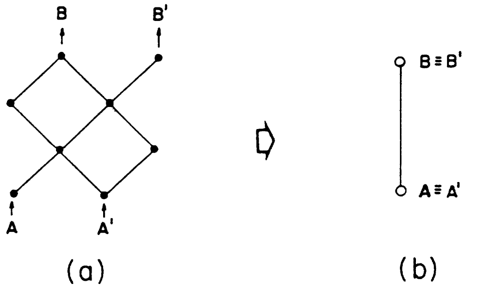

FIG. 1. (a) Cell used in our PSRG transformation (here the scaling factor $b=2$). (b) The cell in (a) is transformed into the two-site, one-bond simpler structure depicted by summing over internal degrees of freedom.

Two technical remarks are worth making. First, we have used the "tilted" cells of Fig. 1, instead of the traditionally used H-shaped cells for the square lattice[5] because they are more suitable for the inclusion of directional effects;[10] second, for small cells one needs suitable boundary conditions imposed on the cell perimeter in order to simulate environmental effects properly; we have tested both free boundary conditions (counting sites along and outside the cell boundaries as occupied) and periodic boundary conditions (which have been successfully employed in PSRG treatments of other correlated dilution problems[11]). The results obtained in either way were qualitatively similar, showing that our approach is essentially stable relative to calculational details.

For the zero-temperature (percolation) transition, we have used scaling parameters $b=2$ and 3, as well as a cell-to-cell renormalization with $b'/b=\frac{3}{2}$, which is believed[5] to give accurate results as $b'/b\rightarrow 1$; this is indeed what happens in our case, as shown below. For the inclusion of thermal aspects, we have performed calculations only for $b=2$.

Owing to the structure of our recursion relations, we have found only two percolation thresholds: one for $\alpha=0$, and another (lower) for $\alpha\neq 0$, as it should be (see Table I). Note that the percolation threshold obtained for the uncorrelated case is compared with the critical probability for *site* percolation, while the authors of Ref. 2 refer their results to the *bond* percolation problem. Although, for the five-site, crosslike cell used in their calculations there is indeed a one-to-one correspondence between sites and bonds, this is purely coincidental; for the actual physical problem, the relevant quantity is the *site* percolation threshold. The general agreement between our results and other available estimates is rather good (however, the closeness of our percolation critical probability with $b'/b=\frac{3}{2}$ and free boundary conditions to the value quoted in Ref. 4 is to be deemed as somewhat fortuitous). Note that the estimates for the percolation correlation-length exponent ν_p are consistent with the correlated and un-

TABLE I. Critical parameters: concentration (x_c) and the correlation-length exponent $\nu_p = y_p^{-1}$ at the zero-temperature fixed point obtained from our PSRG. For $\alpha \neq 0$, the results are the same both for free and periodic boundary conditions.

$\alpha \neq 0$	x_c	ν_p
$b=2$	0.533	1.750
$b=3$	0.537	1.655
$b=\frac{3}{2}$	0.542	1.511
Best estimate	0.5931 ± 0.0006 [a]	$\frac{4}{3}$ [b]
$\alpha=0$	x_p	ν_p
	Periodic boundary conditions	
$b=2$	0.841	1.586
$b=3$	0.827	1.479
$b'/b=\frac{3}{2}$	0.809	1.427
	Free boundary conditions	
$b=2$	0.692	1.672
$b=3$	0.718	1.571
$b'/b=\frac{3}{2}$	0.743	1.421
Best estimate	0.741 ± 0.002 [c]	1.33 ± 0.03 [c]

[a] Reference 5.
[b] Reference 6.
[c] Reference 4.

correlated problems being both in the same universality class, as proposed in Ref. 4.

At the pure limit $x=1$, we obtain the same critical temperature for *all* values of α; further, owing to the self-duality properties of the cells employed,[12] this is the exact critical temperature $k_B T_c/J = 2.269\ldots$ for Ising spins on a square lattice. As depicted in Fig. 2, the initial slope $[1/T_c(1)][dT_c(x)/dx]_{x=1}$ increases gradually with the degree of correlation, varying from 1.82 for $\alpha=1$ for both periodic and free boundary conditions (BC's) to 3.12 (periodic BC) and 2.55 (free BC) for $\alpha=0$. Although, to our knowledge, no accurate estimates are available for the uncorrelated *site* dilution problem (see a discussion of this point in Yeomans and Stinchcombe[9]), it is clear that the exact value[13] 1.329 for the *bond* problem must be a lower bound to the initial slope for $\alpha=1$ in the present case (this is because removal of a site tends to have more drastic effects than removal of a bond). As the values of 1.345 and 2.438 are obtained, respectively, for $\alpha=1$ and $\alpha=0$ in Ref. 2, our general picture is in qualitative agreement with the results of Albino de Aguiar, Brady Moreira, and Engelsberg[2], and also with experimental data on $KNi_xMg_{1-x}F_3$. Further, as can be seen from Fig. 2, our $T_c \times x$ curves for intermediate correlation $0 < \alpha < 1$ tend to have an upward curvature, though perhaps not as markedly as in the corresponding cases of Ref. 2. It is interesting to note that the shape of the phase diagrams obtained are somewhat insensitive to the RG prescription used: Similar ones were obtained by keeping α fixed under scaling (thus following the evolution of x and t only).

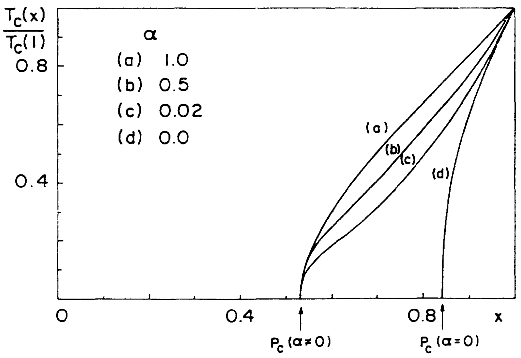

FIG. 2. Phase diagram obtained from our PSRG transformation; here $b=2$ and periodic boundary conditions were used. Use of free boundary conditions implies only slight quantitative variations.

As a final remark, we note that the PSRG flow lines (not depicted in Fig. 2) along the critical surface are directed from the zero-temperature percolation point to the pure Ising fixed point, both for $\alpha=0$ and $\alpha\neq 0$. This is coincident with corresponding results obtained by PSRG for ordinary (uncorrelated) dilution problems, and is related to the existence of two relevant eigenvalues of the PSRG transformation at the percolation point. Since it has been found[14] that, for a different type of correlation (the so-called "bootstrap dilution" problem) the temperaturelike eigenvalue is zero at the percolation threshold (meaning that concentration fluctuations tend to dominate over thermal ones), we interpret the present result as signaling that the correlation studied here is "weak." This means that the overall picture of two competing diverging lengths, one thermal and the other geometric,[15] close to the percolation point, is valid for the present problem as in the case of ordinary dilution: correlation effects are not enough to reverse the situation, as happens for the "strongly correlated" case of bootstrap dilution. Thus, in addition to the result that the geometric transition at zero temperature is in the same universality class as ordinary percolation (consistently with the findings of Ref. 4), we obtain that the behavior against thermal fluctuations (and the interplay between thermal and geometric phenomena) is qualitatively the same in both cases. In other words, the type of correlation discussed here is irrelevant (in the RG sense) regarding both geometric *and* thermal aspects.

Overall, in our PSRG study of correlated dilution we have obtained the qualitative features of upward curvature (for intermediate degree of correlation) of the $T_c \times x$ critical line, as well as the gradual increase (with correlation) of the initial slope of this line at the pure (undiluted) point. From our approach, one naturally obtains only two distinct percolation thresholds: one for $\alpha=0$ and another for $\alpha\neq 0$, as well as a constant (correlation-independent) value of T_c for the pure system. Further, the very structure of the PSRG approach has allowed us to establish that the correlation effects discussed here are irrelevant (as regards universality class of the transition) with respect to both geometric and thermal aspects.

At present, we are discussing the inclusion of antiferromagnetic correlations (that is, $\alpha < 0$) for Ising spins on the square lattice (for which the cells used here are specially suitable[16]), as well as an extension of our method to Heisenberg spins on the cubic lattice, which is closer to the experimental situation in $KNi_xMg_{1-x}F_3$.

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