Mean-field renormalization group: Approach to the diluted site-bond-correlated Ising model

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(Received 4 August 1993)

We study the diluted site-bond-correlated (SBC) Ising model within the scheme of the mean-field renormalization group. The SBC Ising model has been proposed to describe the phase diagram for $KNi_pMg_{1-p}F_3$. One treats the square ($Z=4$) and simple cubic ($Z=6$) lattices by using two different exchange interactions (denoted by models *A* and *B*). In the present paper, the phase diagram for some values of the correlation parameter α, which range from zero to unity, is studied. We obtain two critical concentrations $p_c(\alpha=0)$ and $p_c(\alpha\neq 0)$ in agreement with results from Monte Carlo methods. In addition, an interesting universal relation between the initial slope $\Delta^{(\mu)}(\alpha=1)$ and $\Delta^{(\mu)}(\alpha=0)$ is obtained (μ denotes model *A* or *B*). From this relation, we can estimate the possible exact values to the initial slope on the completely correlated case. Our approach is valid for lattices with any coordination number Z.

I. INTRODUCTION

Randomly diluted magnetic systems have been extensively investigated in both theoretical and experimental aspects.[1] For various reasons, the effect of diluting a magnetic system with nonmagnetic impurities has attracted the attention of many researchers for at least the past two decades. The uncorrelated diluted model[1] is well suited to describe the critical properties of certain magnets. In these models, some magnetic atoms on a lattice are randomly replaced by nonmagnetic atoms, and a bond connecting each pair of occupied magnetic first neighbors is modified. In this context, the diluted magnetic systems are usually associated with an uncorrelated percolation problem[1,3] at $T=0$. Particular interest has been given to the phase diagram for the critical temperature versus concentration. When $T_c\rightarrow 0$, we obtain the critical percolation concentration p_c.[2,3] This value is independent of the model, only providing a dependence with the lattice structure. On the contrary, the initial slope $\Delta=K_c\partial K_c^{-1}/\partial p|_p$ depends on the model in question, since $\Delta(\text{Ising})=\infty$ and $\Delta(\text{Heisenberg or } XY)>0$ (Refs. 4–6) (finite), at $p=p_c$. On the other hand, the experiments have shown that the introduction of nonmagnetic species in some magnetic materials, displays effects not predicted by the usual dilution model. Thus, other models have been proposed to account for correlation effects. Examples of the new approach of alternative site-dilution models are the bootstrap percolation and dilution,[7–9] high-density percolation,[9,10] and the site-bond-correlated (SBC) dilution models.[11,12]

Experimental results from nuclear magnetic resonance (NMR) present striking differences between the randomly diluted magnetic $KNi_pMg_{1-p}F_3$ (Ref. 11) and the isostructural system $KMn_pMg_{1-p}F_3$ (Ref. 13). As an example, for the compound (randomly diluted Heisenberg magnet) $KNi_pMg_{1-p}F_3$, T_c decreases faster than for isostructural $KMn_pMg_{1-p}F_3$, with decreasing concentration. This happens because the latter system is well described by an uncorrelated site-dilution picture. Furthermore, the phase diagram $T_c\times p$ for $KNi_pMg_{1-p}F_3$ displays an upward curvature in contrast to the compound $KMn_pMg_{1-p}F_3$ and the uncorrelated theoretical model. In the pure materials mentioned above, the Ni^{2+} ions can form only σ bonds, while the Mn^{2+} ions, on the contrary, can form both σ and π bonds. The symmetry of the σ bonds suggests that the substitution of a Ni^{2+} ion in $KNi_pMg_{1-p}F_3$ by a nonmagnetic one has a stronger effect on the exchange interaction of a nearest-neighbor magnetic pair situated along the line joining the three atoms than the same effect induced by substitution of a Mn^{2+} ion in $KMn_pMg_{1-p}F_3$. Attempting to describe these differences for the phase diagrams $T_c\times p$, de Aguiar *et al.*[11,12] proposed the site-bond-correlated model for the material $KNi_pMg_{1-p}F_3$. In their model, the coupling between two nearest-neighbor magnetic atoms is assumed to be dependent upon the occupancy of the other nearest-neighbor sites. The Hamiltonian introduced by de Aguiar *et al.*[11,12] to the nearest-neighbor Ising model is given by

$$\mathcal{H}=-\sum_{i,\delta} J_{i,i+\delta}\sigma_i\sigma_{i+\delta}\ , \tag{1}$$

where $J_{i,i+\delta}$ is the exchange interaction between the ions at site i and $i+\delta$, and is given by (denoted model *A*)

$$J_{i,i+\delta}^{(A)}=J\epsilon_i\epsilon_{i+\delta}[(1-\alpha)\epsilon_{i-\delta}+\alpha],\quad J>0 \tag{2}$$

and δ denotes an elementary lattice vector. ϵ_i is a random variable that corresponds to the following probability distribution:

$$P(\epsilon_i)=p\delta(\epsilon_i-1)+(1-p)\delta(\epsilon_i)\ , \tag{3}$$

where p is the concentration of magnetic atoms. The parameter α is the strength of the correlation. The limiting values $\alpha=1$ and $\alpha=0$ correspond to the case of uncorrelated site dilution and to the completely correlated site-bond model, respectively.

The exchange of Eq. (2) was initially proposed by the authors of Ref. 12 to treat the SBC Ising model within

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the scheme of effective-field theory on a square lattice. At first, de Aguiar, Brady Moreira, and Engelsberg[12] incorrectly obtained three values for the critical concentration: $p_c(\alpha=0)=0.765$ for the completely correlated case, $p_c(\alpha=1)=0.428$ for the uncorrelated case, and $p_c(0<\alpha<1)=0.381$. However, da Silva and Brady Moreira[14] found $p_c(\alpha=0)=0.765$ and $p_c(0<\alpha\leq 1)=0.428$, by considering a periodic condition among the active sites $i-\delta$ and $i+2\delta$ that participate in the correlation. We will return to this question later on in this paper.

The authors of Ref. 15 proposed a generalization to the D-vector model on the Bethe lattice by the introduction of the exchange (denoted model B),

$$J^{(B)}_{i,i+\delta}=J\epsilon_i\epsilon_{i+\delta}[(1-\alpha)\epsilon_{i-\delta}\epsilon_{i+2\delta}+\alpha],\quad J>0\ . \tag{4}$$

They found $p_c(\alpha>0)=(Z-1)^{-1}$ for the exchange interactions given by Eqs. (2) and (4). In addition, they obtained only two different values for critical concentration: $p_c(\alpha=0)$ and $p_c(0<\alpha\leq 1)$ providing again evidence of the spurious results of de Aguiar, Brady Moreira, and Engelsberg.[12]

II. FORMALISM AND RESULTS

In the present paper, we treat the SBC Ising model within a scheme of the mean-field renormalization-group (MFRG) method, introduced in the literature by Indekeu, Maritan, and Stella.[16] This approach is based upon a comparison of the behavior of clusters of different sizes (N and N',$N<N'$) in the presence of symmetry-breaking boundary conditions. The magnetizations per spin $M_{N'}(K',b')$ and $M_N(K,b)$ for each case are obtained. From a mean-field point of view, b' and b simulate the effect of surrounding spins in the infinite system. Therefore, b' and b are the symmetry-breaking fields. Following the ideas of Indekeu, Maritan, and Stella,[16] we impose the same scaling relation between the magnetizations and symmetry-breaking fields. Hence, one obtains

$$\left.\frac{\partial M_{N'}}{\partial b'}\right|_{b'\to 0}=\left.\frac{\partial M_N}{\partial b}\right|_{b\to 0}, \tag{5}$$

which is independent of the scale factor. Equation (5) gives a recursion relation involving the coupling constants; i.e., $K'=K'(K)$, where in the fixed point K^* we have $K=K'=K^*$. In the case a nontrivial fixed point we obtain the critical coupling K_c system by solving the fixed-point equation $K^*=K(K^*)$ when the symmetry-breaking occurs. The Hamiltonian of the clusters with $N=1$ and $N'=2$ spins are given by

$$\mathcal{H}_{\{1\}}=-b\sum_{1,\delta}J_{i,1+\delta}\sigma_1\ , \tag{6}$$

$$\mathcal{H}_{\{1,2\}}=-J'_{1,2}\sigma_1\sigma_2-b'\left[\sum_{1,\delta}J'_{1,1+\delta}\sigma_1+\sum_{2,\delta}J'_{2,2+\delta}\sigma_2\right]\ . \tag{7}$$

The magnetizations per spin associated with the clusters N and N' are defined by $M_N\equiv(\langle\sigma_1\rangle_t)_c$ and $M_{N'}\equiv\frac{1}{2}(\langle\sigma_1+\sigma_2\rangle_t)_c$, with t and c indicating thermal and spin-configurational averages. Using M_N and $M_{N'}$ in Eq. (5) and noticing that in the vicinity of the critical temperature $b'(b)\to 0$, we find the transition critical line,

$$(1-p^2)+2p^2G^{(\mu)}(p,K_c,\alpha)=\frac{Z}{Z-1}\ , \tag{8}$$

where $\mu(=A$ or $B)$ denotes the models given by exchanges (2) and (4), respectively. Now, $G^{(\mu)}(p,K_c,\alpha)$ is given by

$$G^{(\mu)}(p,K_c,\alpha)=p^nF(K_c)+(1-p^n)F(\alpha K_c)\ , \tag{9}$$

where $F(\alpha K_c)=e^{\alpha K_c}/[2\cosh(\alpha K_c)]$ and, $n=1$ for model A and $n=2$ for model B. The critical concentrations for each model are obtained from Eq. (8). Therefore, one obtains

$$p_c^{(\mu)}(\alpha)=(Z-1)^{-\phi}\ . \tag{10}$$

For $\alpha=0$ we find $\phi=\frac{1}{3}$ and $\phi=\frac{1}{4}$ for models A and B, re-

TABLE I. Values of the $p_c^{(\mu)}(\alpha)$ and K_c^{-1} on the square and simple cubic lattices obtained by means of various methods for the models A and B.

Method	$p_c^{(A)}(\alpha=0)$	$p_c^{(A)}(\alpha\neq 0)$	$p_c^{(B)}(\alpha=0)$	$p_c^{(B)}(\alpha\neq 0)$	K_c^{-1}	Z
Monte Carlo[a]		0.593	0.741	0.593	2.269	4
		0.312		0.312		6
Effective field[b]	0.765	0.428	0.765	0.428	3.090	4
	0.639	0.293	0.639	0.293	5.039	6
Renormalization group[c]		0.542	0.743	0.542		4
	0.580	0.496		0.496		6
Present work	0.693	0.577	0.760	0.577	2.885	4
	0.585	0.447	0.669	0.447	4.993	6
Exact value[d]		0.590		0.590	2.269	4
		0.307		0.307	4.511	6

[a]References 17 and 21.
[b]References 12 and 14.
[c]References 18 and 19.
[d]Reference 1.

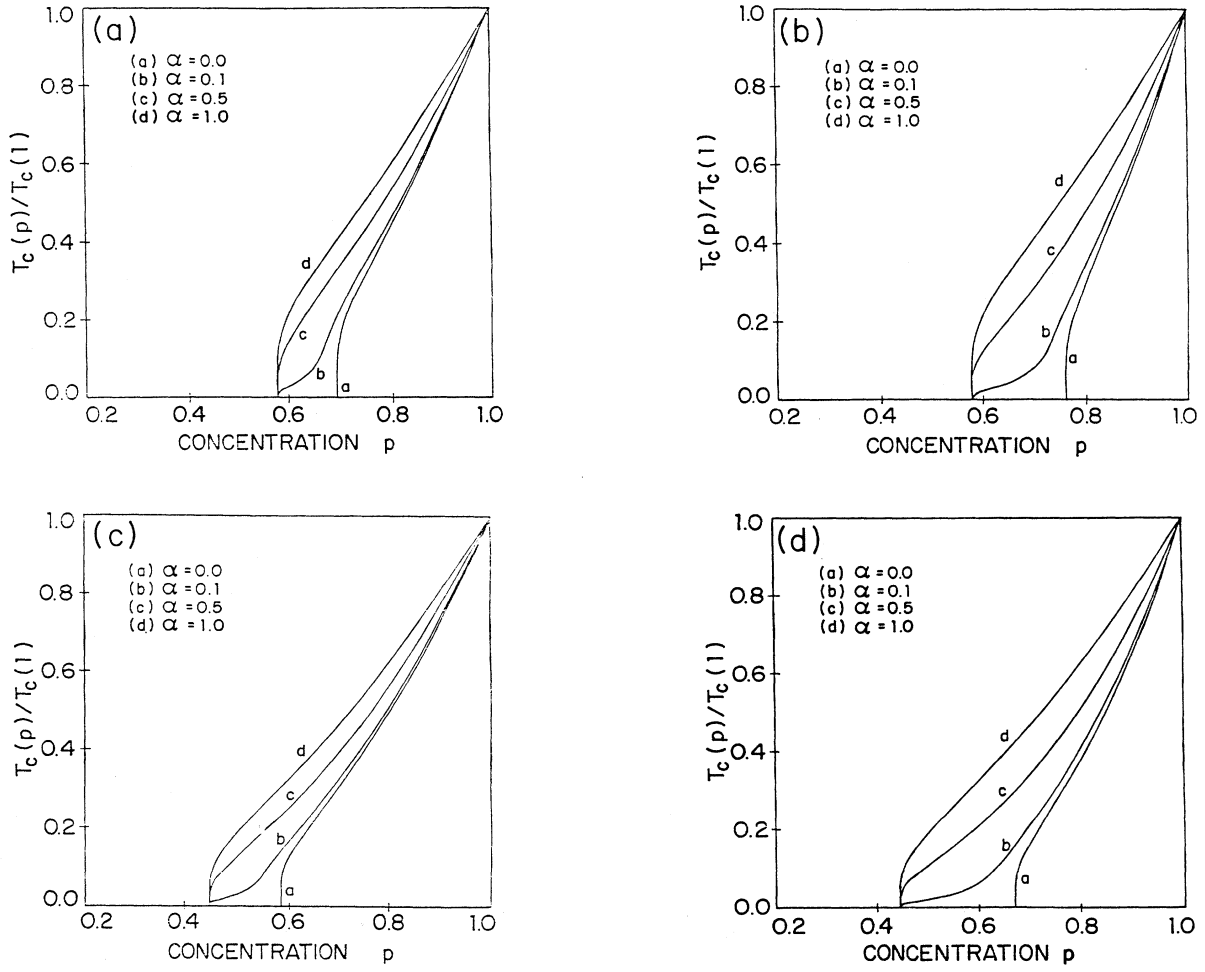

FIG. 1. Phase diagrams in the plane $T-p$ for the SBC Ising model with some typical values of the parameter α on the square (a,b) and simple cubic (c,d) in models A and B, respectively.

TABLE II. Values of the initial slope $\Delta^{(\mu)}(\alpha)$ for $\alpha=0$ and $\alpha=1$ on the square and simple cubic lattices found by employing various methods for models A and B. The superscript a indicates our estimate in the present work by means of relations $\Delta^{(A)}(0)=\frac{3}{2}\Delta^{(A)}(1)$ and $\Delta^{(B)}(0)=2\Delta^{(B)}(1)$.

$\Delta^{(\mu)}(\alpha)$	Monte Carlo[b]	Effective field[c]	Renormalization group[d]	Present work	Exact value (Ref. 1)
$\Delta_{sq}^{(A)}(0)$	2.830	2.483	2.550	3.246	1.994[a]
$\Delta_{sq}^{(A)}(1)$	1.886[a]	1.345	2.820	2.164	1.329
$\Delta_{sq}^{(B)}(0)$	3.773[a]	2.690[a]		4.328	2.659[a]
$\Delta_{sq}^{(B)}(1)$	1.886[a]	1.345		2.164	1.329
$\Delta_{sc}^{(A)}(0)$				3.081	1.56[a]
$\Delta_{sc}^{(A)}(1)$				2.054	1.04
$\Delta_{sc}^{(B)}(0)$				4.107	2.08[a]
$\Delta_{sc}^{(B)}(1)$				2.054	1.04

[b]References 17 and 21.
[c]References 12 and 14.
[d]Reference 18.

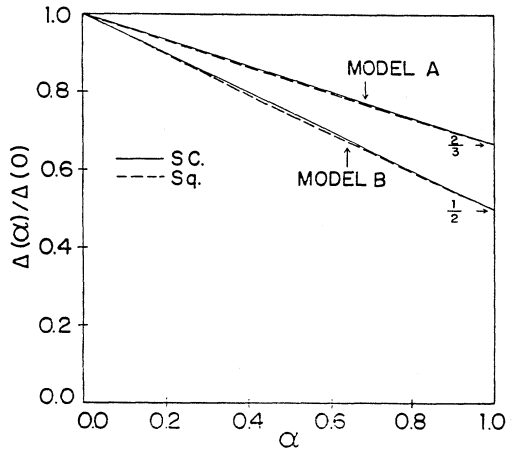

FIG. 2. Behavior of the initial slope $\Delta(\alpha)$ in the models A and B. Dashed lines correspond to the square lattice and solid lines to the simple cubic lattice, respectively.

spectively. However, for $0<\alpha\leq 1$, $\phi=\frac{1}{2}$ in both models. On the other hand, Eq. (8) gives $K_c^{-1}=-2/\ln(1-2/Z)$, which is independent of the parameter α at $p=1$. Table I shows the various values of the $p_c^{(\mu)}(\alpha)$ and K_c^{-1} on the square ($Z=4$) and simple cubic ($Z=6$) lattices. Also in Table I, one observes that there are only two critical concentrations to the values of the parameter α, $p_c(\alpha=0)$ and $p_c(0<\alpha\leq 1)$. Figure 1 shows the phase diagrams in the plane $T-p$ for $Z=4$ and $Z=6$ on models A and B. For the case $0<\alpha<1$ (intermediate correlation) the phase diagrams present an upward curvature while α decreases. This effect is more accentuated for model A. However, when $\alpha=1$ and $\alpha=0$, the upward curvature does not occur.

At this point, we will consider an analytical treatment which can be done without great difficulty. Thus, instead of carrying on numerical calculations, we preserve the simplicity of the MFRG method to show results which represent a remarkable improvement of this scheme.

The initial slope $\Delta(\alpha)=K_c\partial K_c^{-1}/\partial p|_{p=1}$ is, as well, directly obtained from Eq. (8), i.e.,

$$\frac{\Delta^{(\mu)}(\alpha)}{\Delta^{(\mu)}(0)}=\frac{2}{2+n}\left[1+n\frac{F(\alpha K_c)-F(K_c)}{1-2F(K_c)}\right], \qquad (11)$$

where $n=1$ corresponds to the model $A(\mu=A)$ and $n=2$ to model $B(\mu=B)$. By inspection, it is easy to verify according to Eq. (11) that $\Delta^{(\mu)}(1)=2/(2+n)\Delta^{(\mu)}(0)$, which is universal, and independent of the lattice structure. On the other hand, $\Delta^{(\mu)}(1)$ and $\Delta^{(\mu)}(0)$ ($\mu=A$ or B) depend strongly on the lattice structure.

Since one knows the initial slope $\Delta^{(\mu)}(1)$ for the case of the dilution site, which is independent of the model, one can estimate $\Delta(0)=2\Delta(1)\simeq 2.690$ for model B in Ref. 14. Following this same reasoning, it is reasonable to estimate the exact result[1] for the initial slope $\Delta(\alpha)$ for the strongly correlated limit ($\alpha=0$) for models A and B. Therefore, one obtains for $Z=4$, $\Delta^{(A)}(0)\simeq 1.994$ and $\Delta^{(B)}(0)\simeq 2.659$; and $\Delta^{(A)}(0)\simeq 1.56$ and $\Delta^{(B)}(0)\simeq 2.08$ for $Z=6$. Table II contains the various values of $\Delta^{(\mu)}(1)$ and $\Delta^{(\mu)}(0)$ obtained by employing different techniques. The behavior of the initial slope versus the parameter α for $Z=4$ and $Z=6$ on models A and B is displayed in Fig. 2. We perceive that the initial slope decreases gradually when the parameter α increases. This is verified implicitly in Refs. 12, 14, 17–19.

III. CONCLUSIONS

The mean-field renormalization-group method is shown to be appropriate enough to approach the diluted SBC Ising model when employing its simplest version. The phase diagrams and the results obtained depend on the coordination number Z, and the MFRG method is used. The qualitative behavior of the phase diagrams are well in accordance with the characteristic features of the considered Hamiltonian. In addition, we find an interesting relation between the initial slope $\Delta^{(\mu)}(1)$ and $\Delta^{(\mu)}(0)$ for each model: $\Delta^{(A)}(1)=\frac{2}{3}\Delta^{(A)}(0)$ and $\Delta^{(B)}(1)=\frac{1}{2}\Delta^{(B)}(0)$, with $\Delta^{(A)}(1)=\Delta^{(B)}(1)$ and $\Delta^{(A)}(0)<\Delta^{(B)}(0)$. Employing these relations, one can estimate the possible exact values for $\Delta(0)$ in both models. The computing of p_c was explicitly obtained from Eq. (10) for each model. In particular, there are only two critical concentrations $p_c(\alpha=0)$ and $p_c(\alpha\neq 0)$, with $p_c^{(A)}(\alpha=0)>p_c^{(B)}(\alpha=0)$ and $p_c^{(A)}(\alpha\neq 0)=p_c^{(B)}(\alpha\neq 0)$. We perceive that the condition employed by the authors of Ref. 14 is only a device, maybe an ansatz, to simplify their calculus. This happens because, eventually, the ϵ_i random variable may or may not satisfy the periodic condition. Therefore, it is reasonable to think of such a question as a purely statistical problem. The device used by the authors of Ref. 12 and 14 does not permit one to distinguish between either model. However, the results of the above-mentioned authors are in better accord with model B, as is indicated by our arguments. Our aim, later on, is to extend the approach of the MFRG method to treat antiferromagnetic correlations ($\alpha<0$).[14,15,17,20,22] Another case of interest to be studied is the Heisenberg[19,20] model which is more adequate to describe the experimental results of $KNi_pMg_{1-p}F_3$ (Ref. 11).

ACKNOWLEDGMENTS

The authors would like to thank Professor I. P. Fittipaldi and Professor Fernando Moraes for a critical reading of the manuscript. Our work was partially supported by CAPES and CNPq (Brazilian Agencies).

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