Site-bond–correlated D-vector model on the Bethe lattice

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The site-bond–correlated D-vector spin model for randomly diluted magnetic systems is studied on the Bethe lattice with general coordination number. The ferromagnetic critical lines in the temperature-concentration (T_c,p) space are obtained exactly for the Ising $(D=1)$, Heisenberg $(D=3)$, and $D=\infty$ cases, and for both directed and nondirected correlation models. For the antiferromagnetic correlation regime, the (T_c,p) diagram shows the appearance of several zero-temperature critical concentrations and the presence of reentrant phases. The uncorrelated critical line and the percolation concentration are recovered.

I. INTRODUCTION

The critical temperature dependence of the concentration at which the magnetic order vanishes is of great interest for the study of randomly diluted magnetic systems. This dependence is associated with the topological properties of the lattice and also with the symmetry of the interaction Hamiltonian or the spin variables. For instance for randomly diluted Heisenberg magnets like $KNi_pMg_{1-p}F_3$ the decreasing of the critical temperature with the reduction of the concentration is faster than for the isostructural $KMn_pMg_{1-p}F_3$. Further the critical temperature curve for the latter has a downward curvature while the former has an upward one.[1] A new dilution model namely the site-bond–correlated diluted model has been proposed by de Aguiar *et al.*[2] in order to explain these differences. For example in the pure $(p=1)$ related materials mentioned above the Ni^{2+} ions can form only σ bonds, while the Mn^{2+} ions can form both σ and π bonds. Therefore 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 the substitution of a Mn^{2+} ion in $KMn_pMg_{1-p}F_3$. The randomly site-bond–correlated diluted Ising model on the square lattice has been studied by de Aguiar *et al.*[2] within the mean-field approximation. They have considered both the standard mean-field approximation as well as the effective-field theory developed by Honmura and Kaneyoshi.[3]

In this paper we study the randomly site-bond–correlated diluted D-vector spin model within the Bethe-Peierls approximation by solving the model Hamiltonian in the Bethe lattice with general coordination number. We investigate the exact concentration dependence of the ferromagnetic critical temperature of the local magnetization of the Bethe lattice for Ising $(D=1)$, Heisenberg $(D=3)$ and $D=\infty$ cases. In the present model Hamiltonian the site-bond correlation means that the strength and the sign of the exchange interaction between a given pair of nearest-neighbor magnetic atoms are also dependent upon the presence of magnetic atoms on their neighboring sites. We consider two types of topological site-bond correlation, namely, the directed and the nondirected correlation. Furthermore, we assume both ferromagnetic and antiferromagnetic correlation, and we distinguish two particular cases, that is, the strongest correlation situation and the uncorrelated one. The latter case recovers previous results[4] for the standard bond diluted Ising model on the Bethe-Peierls approximation. We expect that the present site-bond–correlated model can exhibit a spin-glass-like phase for the case of antiferromagnetic correlation, since we can have a randomly diluted distribution of ferromagnetic and antiferromagnetic bonds. The stability of this spin-glass-like phase is now being studied.

This paper is organized in the following way. In Sec. II we present the model Hamiltonian and discuss the directed (model A) and the nondirected (model B) site-bond–correlated models. Section III is devoted to the evaluation of the ferromagnetic transition temperatures and to the discussion of the phase diagrams for both models and for the $D=1$, 3, and ∞ cases. Finally the conclusions are summarized in Sec. IV.

II. THE MODEL HAMILTONIAN: DIRECTED AND NONDIRECTED CORRELATION MODELS

We consider a site diluted spin system on the Bethe lattice with general coordination number $z=q+1$ (q is the connectivity). The Bethe lattice can be constructed by connecting z sites to a central site to form the first generation and by connecting successively q sites to form the next generations. The result is an infinite lattice in which every site has z nearest neighbors and there are no closed paths (loops). The sites are randomly occupied by magnetic atoms following a given probability distribution. The magnetic atoms are represented by D-vector spin variables coupled by a nearest-neighbor exchange interaction.

The directed site-bond correlation on the Bethe lattice means that the exchange interaction between two nearest-neighbor magnetic atoms is correlated only with their nearest-neighbor spins belonging to the neighboring

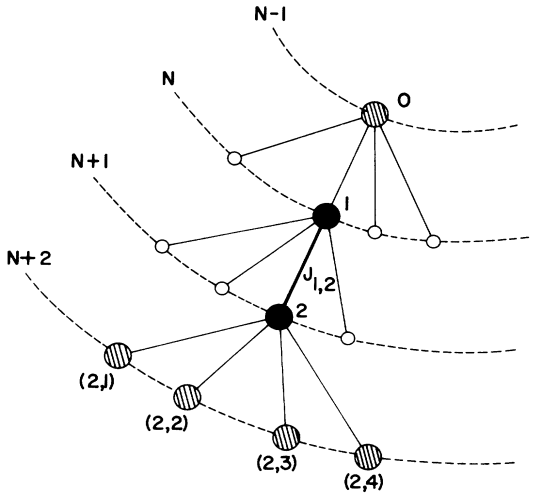

FIG. 1. Model A: Directed correlation. A portion of a Bethe lattice ($q=4$) is shown, where ● are the actual present spins and ◍ are the active correlated sites for a given bond ($J_{1,2}$) between the Nth and the $(N+1)$th generations.

generations. In Fig. 1 the active sites for a given bond are shown for the directed correlation model (model A, hereafter). In this model the correlation is restricted along the radial direction from the central site. On the other hand, in the nondirected correlated model (model B, hereafter) all neighboring sites of a given pair of nearest-neighbor spins are active sites. Therefore, all sites of the lattice are equivalent and there is no hierarchy between the generations. The active sites for a given bond for the model B are shown in Fig. 2. The former model takes into account the directionality effects pointed out by de Aguiar *et al.*,[2] while the latter can be regarded as the appropriated isotropic version of this model.

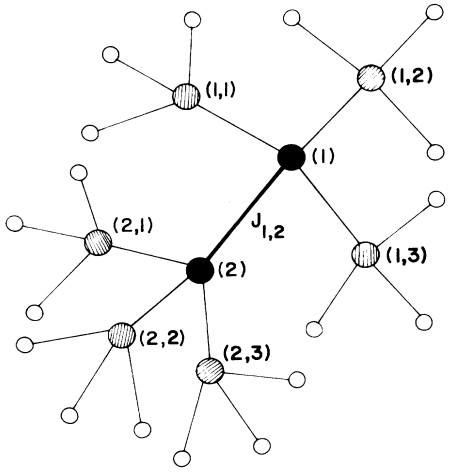

FIG. 2. Model B: Nondirected correlation. A portion of a Bethe lattice ($q=3$) is shown, where ● are the actual present spins and ◍ are the active sites for a given bond $J_{1,2}$.

The general Hamiltonian can be written as

$$H=-\sum_{\langle ij\rangle}{}' J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j-B\sum_i S_i^1 , \tag{1}$$

where J_{ij} is the coupling constant of the exchange interaction between the pair of nearest-neighbor spins $\langle i,j\rangle$, B is the external magnetic field, and S^ν is the νth component of the D-vector spin variables $\mathbf{S}$ which are subjected to the normalizing condition

$$\sum_\nu (S^\nu)^2=\lambda^2 . \tag{2}$$

In what follows we will assume that $\lambda^2=D$, in order to renormalize the exchange interaction coupling constant relative to the spin dimensionality.

A. Model A: Site-bond directed correlation

In this model the correlated sites acting on a given bond (active sites) are those belonging to the inner and the outer nearest-neighbor generations as shown in Fig. 1. Furthermore the nearest-neighbor spin belonging to the inner generation has a much stronger effect than the other active sites, that is, if this site is occupied by a nonmagnetic atom the strength of the exchange interaction is changed by a factor α independently of the occupation number of the other active sites. We note that there is no correlation between the bond exchange and the nearest-neighbor sites belonging to the same generations. Therefore the site-bond correlation is assumed to be active only along the radial direction of the Bethe lattice. The coupling constant for this model for the bond specified in Fig. 1 can be given by

$$J_{1,2}^A=J\epsilon_1\epsilon_2\left[\alpha+(1-\alpha)\epsilon_0\frac{1}{q}\sum_{l=1}^{q}\epsilon_{2,l}\right] , \tag{3}$$

where ϵ_i and $\epsilon_{i,l}$ are independent randomly disordered variables, J ($J>0$) is the ferromagnetic exchange-coupling constant, and α is a parameter governing the correlation. From Eq. (3) we can see that the q outer active neighboring sites contribute to the correlation only if the inner active neighboring site is occupied by a magnetic atom ($\epsilon_0=1$). Therefore in model A the hierarchy between the generations of the Bethe lattice is preserved, and the correlation is directed along the radial direction from the root of the tree.

B. Model B: Site bond nondirected correlation

In this model we do not distinguish the generation structure of the Bethe lattice by assuming that all nearest-neighbor sites of a given bond are equivalent active sites. The coupling constant for the bond specified in Fig. 2 can be given by

$$J_{1,2}^B=J\epsilon_1\epsilon_2\left[\alpha+(1-\alpha)\frac{1}{2q}\sum_{l=1}^{q}(\epsilon_{1,l}+\epsilon_{2,l})\right] . \tag{4}$$

We note that there are $2q$ active sites per bond in this model while there are only $(q+1)$ active sites per bond in the model A.

III. THE TRANSITION TEMPERATURES: (T_c,p)—PHASE DIAGRAMS

The ferromagnetic transition temperature T_c for the pure classical D-vector spins in the Bethe lattice is given by the following equation:[5]

$$1-qt_D(DK)=0 , \tag{5}$$

where $K^{-1}=k_BT_c/J$ is the normalized critical temperature, k_B is the Boltzmann constant and $t_D(x)$ is the generalized hyperbolic tangent defined by

$$t_D(x)=\frac{I_{D/2}(x)}{I_{(D/2)-1}(x)} , \tag{6}$$

where $I_n(x)$ is the modified Bessel function of the first kind of order n. For $D=1$ (Ising), $D=2$ (XY), and $D=3$ (Heisenberg) spins we have, respectively, $t_1(x)=\tanh x$, $t_2(x)=I_1(x)/I_0(x)$, and $t_3(x)=L(x)$, $L(x)$ being the Langevin function.

For quenched random disordered systems in the Bethe lattice the exact critical temperature is given by a straightforward generalization of Eq. (5),[6] that is,

$$1-q\langle t_D(DK_{ij})\rangle_{cc}=0 , \tag{7}$$

where $\langle\cdots\rangle_{cc}$ means the conditional configurational (cc) average over a given distribution of the occupational variables ϵ and $K_{ij}=J_{ij}/k_BT_c$, J_{ij} being defined in the present work by Eqs. (3) and (4).

To perform the cc average in Eq. (7) we assume independent random variables according to a discrete probability distribution given by

$$P(\epsilon)=p\delta(\epsilon-1)+(1-p)\delta(\epsilon) , \tag{8}$$

where p $(0\le p\le 1)$ is the concentration of magnetic atoms. Note that for the cc average considered here the concentration of connected bonds for $\alpha\neq 0$ must be interpreted as the concentration of magnetic atoms. By substituting Eqs. (3) and (4) in Eq. (7) we get the polynomial equation in the concentration. The solution of this equation gives the phase diagram in the temperature-concentration (T_c,p) space. For models A and B we obtain, respectively,

$$1-qp\left[(1-p)t_D(\alpha DK)+p\sum_{n=0}^{q}\binom{q}{n}p^{q-n}(1-p)^n t_D[DK(q-n(1-\alpha))/q]\right]=0 \tag{9}$$

and

$$1-qp\sum_{m=0}^{2q}\binom{2q}{m}p^{2q-m}(1-p)^m t_D[DK(2q-m(1-\alpha))/2q]=0 , \tag{10}$$

where $\binom{a}{b}=a!/(a-b)!b!$. In both models two kinds of correlation can be distinguished: the ferromagnetic correlation for $\alpha>0$ and the antiferromagnetic one for $\alpha<0$. Moreover, we point out two particular cases: $\alpha=0$ which corresponds to the strongest correlation situation and $\alpha=1$ which describes the standard uncorrelated bond diluted spin system.

For $0<\alpha<1$ the system can be regarded as a distribution of ferromagnetic bonds with several strengths weakened by the correlation. Furthermore at $T\to 0$ limit both Eqs. (9) and (10) recover the exact usual (uncorrelated) bond percolation concentration of the Bethe lattice $p_c=1/q$.[7] This is an expected result since in this range of values of α the site-bond correlation acts only in order to weaken the strength of the exchange interaction and therefore does not change the ground-state long-range order.

In the case of strong correlation ($\alpha=0$) the strength of the exchange can vanish due to the action of the site-bond correlation. In this case for both models the ferromagnetic ordered phase at $T\neq 0$ occurs for concentrations higher than the percolation threshold $p_c=1/q$. These concentrations are given by the following equations:

$$1-qp^2[1-(1-p)^q]=0 \quad \text{(model } A) , \tag{11}$$

$$1-qp[1-(1-p)^{2q}]=0 \quad \text{(model } B) . \tag{12}$$

The solutions p_0 of Eqs. (11) and (12) are given in Table I for several values of the coordination number z, where we also include the corresponding values of the percolation threshold. We emphasize that the p_0 concentrations must not be interpreted as a new percolation concentration since the site-bond correlation in the Bethe lattice is irrelevant for the formation of the infinite cluster at the percolation threshold. Nevertheless for the directed correlated model in hypercubic lattices these p_0 values correspond to the critical percolation concentrations in the Bethe-Peierls approximation. For instance, the value of $p_0=0.5971$ for $z=4$ (Table I) should be compared with those ones obtained within effective field approximation $p_0=0.765$,[2] and Monte Carlo calcula-

TABLE I. Percolation concentration $p_c=1/q$ and the p_0 values (see text) for the directed (A) and nondirected (B) models, and for several values of the coordination number z.

	p_0		p_c
z	Model A	Model B	Both models
3	0.7336	0.5264	0.5000
4	0.5971	0.3583	0.3333
5	0.5144	0.2715	0.2500
6	0.4580	0.2185	0.2000
∞	0 as $1/\sqrt{z}$	0 as $1/z$	0 as $1/z$

tions $p_0=0.741$.[8] On the other hand, for the model B the correlation does not affect the percolation concentration, since all percolative clusters are the same as for uncorrelated limit.[9] This is another characteristic feature of the directionality of the directed site-bond correlation.

Now we consider the case of $\alpha<0$ (antiferromagnetic correlation). In this situation the exchange interaction of a given pair of nearest-neighbor magnetic atoms can vanish or have its sign changed depending on the number of magnetic atoms present in its active neighboring sites. Therefore, for a given concentration the system can be regarded as a random mixed distribution of ferromagnetic and antiferromagnetic bonds with several strengths. The critical concentrations at $T=0$ will be dependent on the magnitude of α and are given by the solutions of the following polynomial equations ($\alpha<0$):

$$1-qp\left[(p-1)+p\sum_{n=0}^{q}\binom{q}{n}p^{q-n}(1-p)^n\mathrm{sgn}[q-n(1-\alpha)]\right]=0 \quad \text{(model } A\text{)}, \tag{13}$$

$$1-qp\sum_{m=0}^{2q}\binom{2q}{m}p^{2q-m}(1-p)^m\mathrm{sgn}[2q-m(1-\alpha)]=0 \quad \text{(model } B\text{)}. \tag{14}$$

In the above equations, $\mathrm{sgn}(x)\geq 0$ or <0 for $x\geq 0$ or <0. Since $n=0,1,\ldots,q$ and $m=0,1,\ldots,2q$ in Eqs. (13) and (14), we can identify the existence of $(2q-1)$ critical concentrations for the model A and $(4q-1)$ critical concentrations for the model B when

$$\left.\begin{aligned}&\frac{n-1-q}{n-1}<\alpha<\frac{n-q}{n}, \quad n=1,2,\ldots,q\\ &\alpha=\frac{n-q}{n}, \quad n=1,2,\ldots,(q-1)\end{aligned}\right\}\ \text{model } A\ , \tag{15}$$

$$\left.\begin{aligned}&\frac{m-1-2q}{m-1}<\alpha<\frac{m-2q}{m}, \quad m=1,2,\ldots,2q\\ &\alpha=\frac{m-2q}{m}, \quad m=1,2,\ldots,(2q-1)\end{aligned}\right\}\ \text{model } B\ . \tag{16}$$

We note that for each value of α ($\alpha<0$) specified by Eqs. (15) and (16) a different polynomial equation corresponds given by Eqs. (13) and (14), respectively. In Figs. 3 and 4 we plot the $T=0$ critical concentration as a function of α for the models A and B, respectively, for some values of q. We call to the readers' attention that these critical concentrations for $\alpha<0$ no longer have relation with the percolation concentration, since the system is composed of a mixed distribution of ferromagnetic and antiferromagnetic bonds and frustration effects can be present.

Finally, for $\alpha=1$ both models describe the usual uncorrelated site dilute spin systems; that is, in this limit both Eqs. (9) and (10) give the critical temperature for the Bethe lattice given by

$$1-qpt_D(DK_c)=0\ , \tag{17}$$

where $K_c=J/k_BT_c$ which has already been obtained by

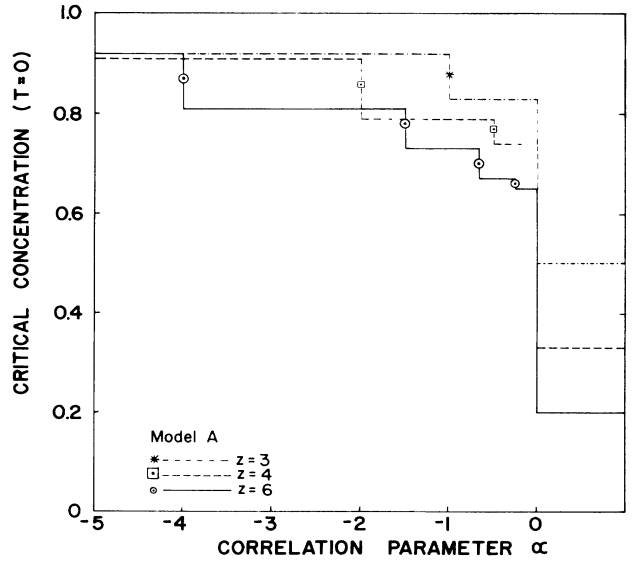

FIG. 3. Critical concentration at $T=0$ for model A, as a function of the correlation parameter for $z=3$, 4, and 6.

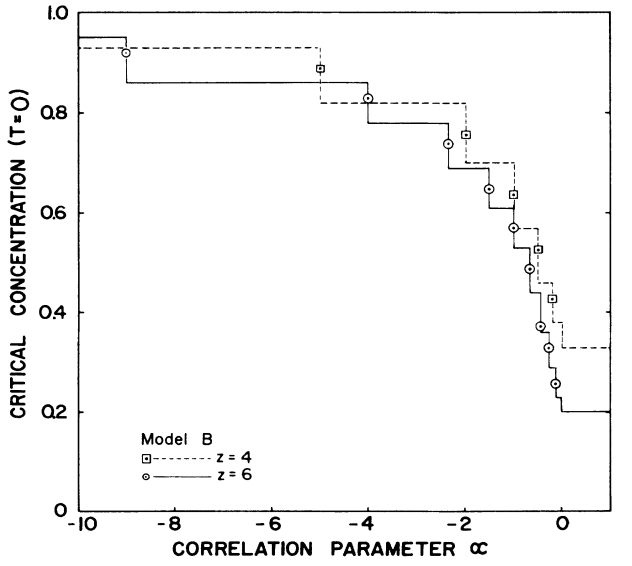

FIG. 4. Critical concentration at $T=0$ for the model B, as a function of the correlation parameter for $z=4$ and 6.

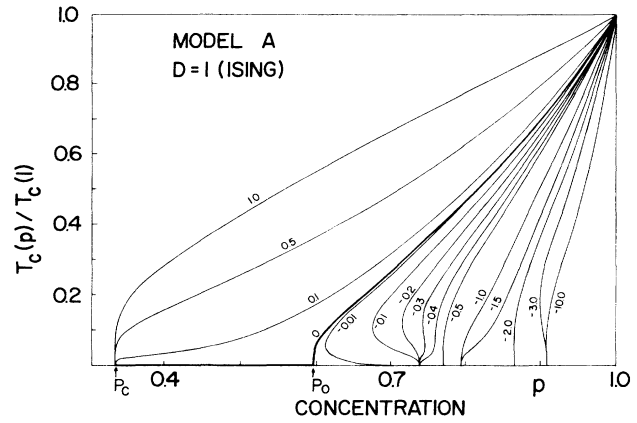

FIG. 5. Ferromagnetic critical temperature vs concentration for model A with Ising spins ($D=1$) and coordination number $z=4$, and for several values of α as indicated. (The thick solid line indicates the critical line for $\alpha=0$.)

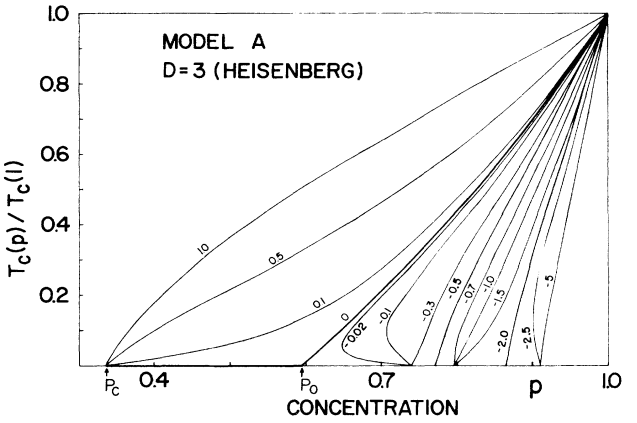

FIG. 7. Ferromagnetic critical temperature vs concentration for the model A with Heisenberg spins ($D=3$) and coordination number $z=4$, and for several values of α as indicated. (The heavy solid line indicates the critical line for $\alpha=0$.)

several authors for $D=1$, 2, and 3 (Ref. 6) and by Stanley (Ref. 5) for general dimensionality. The phase diagrams (T_c,p) for the Ising system ($D=1$) and for both models can be obtained by substituting $t_D(x)$ by $\tanh x$ in Eqs. (9) and (10). In Figs. 5 and 6 we present these diagrams for the case $J>0$, $q=3$ ($z=4$) and for several values of α. For $0<\alpha\leq 1$ all critical lines meet at the same percolation concentration $p_c=1/q$ with an infinite derivative. For $\alpha<0$ we point out the existence of the critical concentrations at $T=0$ obtained by the values of α given by Eqs. (15) and (16) [see also Figs. (3) and (4)]. Furthermore, for some negative values of α, we observe the appearance of reentrant phases which are characteristic of competing interactions systems. We also plot in Fig. 7 the phase diagram (T_c,p) of the model A for the Heisenberg system ($D=3$) which can be obtained from Eq.(9) by substituting $t_D(x)$ by $L(x)$, where $L(x)=(\coth x-1/x)$ is the Langevin function. This diagram shows the same features of the one shown in Fig. 5 for the Ising case, that is, the same critical concentrations at $T=0$, the same percolation concentration for $0<\alpha\leq 1$ and reentrant phases for some values of $\alpha<0$. However, for Heisenberg spins the critical lines have finite derivatives at the critical concentrations at $T=0$.

Finally, the ferromagnetic critical temperature phase diagrams for the infinite spin dimensionality case are obtained by evaluating the $D\to\infty$ limit of the generalized hyperbolic tangent given by Eq. (6), that is

$$\lim_{D\to\infty} t_D(DK)=\lim_{D\to\infty}\frac{I_{D/2}(DK)}{I_{D/2-1}(DK)}=\frac{2K}{1+(1+4K^2)^{1/2}} \tag{18}$$

and by substituting this result in Eqs. (9) and (10). The phase diagram (T_c,p) of the model A and for the $D\to\infty$ case is shown in Fig. 8 for several values of α. The same

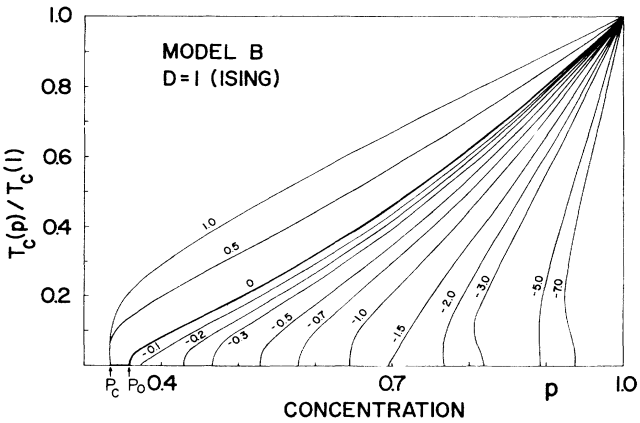

FIG. 6. Ferromagnetic critical temperature vs concentration for model B with Ising spins ($D=1$) and coordination number $z=4$, and for several values of α as indicated. (The thick solid line indicates the critical line for $\alpha=0$.)

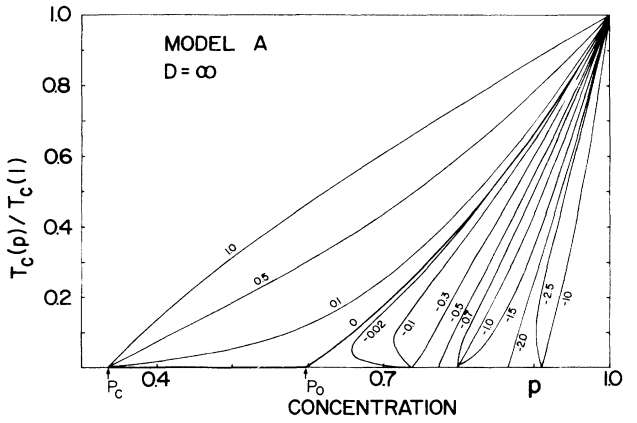

FIG. 8. Ferromagnetic critical temperature versus concentration for the model A with $D\to\infty$ vector spins and coordination number $z=4$, and for several values of α as indicated. (The heavy solid line indicates the critical line for $\alpha=0$.)

features of the previous cases can be observed showing that the physical behavior of the system is not strongly affected by the spin dimensionality for $D > 1$.

IV. CONCLUSIONS

The critical temperatures of the randomly diluted D-vector spin system on the Bethe lattice with general coordination number have been calculated exactly for the directed (model A) and the nondirected (model B) site-bond-correlated models. The results for both models have been analyzed for the entire range of values of the correlation parameter α. For ferromagnetic correlation ($\alpha > 0$) all critical lines meet at the percolation concentration $p_c = 1/(z-1)$ at $T=0$. On the other hand the critical lines for α strictly equal to zero are located in the region $p > p_0$, where p_0, for model A, corresponds to the critical percolation concentration for hypercubic lattices in the Bethe-Peierls approximation. For the antiferromagnetic correlation ($\alpha < 0$) there are $(2q-1)$ and $(4q-1)$ critical concentrations at $T=0$ as α varies, for the models A and B, respectively. The phase diagrams (T_c,p) for the ferromagnetic Ising ($D=1$), Heisenberg ($D=3$), and $D=\infty$ cases have been shown in Figs. 5, 7, and 8 for the model A. The (T_c,p) diagram of the Ising case for the model B is also shown in Fig. 6. All diagrams show almost the same features. We point out the presence of reentrant phases for $\alpha < 0$ which are characteristic of competing interaction systems. For $\alpha < 0$ the system can be regarded as a random mixed distribution of ferromagnetic and antiferromagnetic bonds. In this case we expect that the system presents a spin-glass-like phase, in addition to the paramagnetic and the ferromagnetic phases, due to the frustration and the randomness of the competing interaction introduced by the site-bond correlation. The study of the stability of this spin-glass-like phase is a subject matter of present research.

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