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Critical properties of a random transverse crystal field Ising model with bond dilution

Research Article

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Abstract: Within effective field theory (EFT), the critical properties of a random transverse crystal field Ising model with bond dilution are studied on a square lattice. Under both weak and strong bond dilution conditions, we consider three cases ($\alpha = 0, \pm 0.5$) of a transverse crystal field ratio, obtaining global phase diagrams in $T - D_x$ space for changes in the random transverse crystal field concentration. The phase diagrams obtained for a weak bond dilution are very similar in shape to those of pure bond but with decreases in corresponding ordered phases and critical values. However, the phase diagrams for a strong bond dilution exhibit varieties, including a change in reentrant phenomenon, the occurrence of transverse crystal field degeneration, and the opposite direction crossover of temperature peak value.

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1. Introduction

In past decades, the Blume-Capel model (BCM) has gained in importance [1, 2]. In addition to considering the effect of exchange interaction, the BCM includes a longitudinal crystal field interaction in a Hamiltonian. A variety of techniques have been used to study the BCM [3–10].

Some experiments have revealed macro uniaxial anisotropy in-plane for RE-TM films and Co-M (M = Zr, Nb, Ti) films [11, 12]. Thus, the role of a transverse crystal field becomes evident. In this case, a transverse crystal field is the direction of the hard magnetization axis. Some theoretical researches have dealt with the effect of exchange interaction and with a transverse crystal field in a Hamiltonian. Eddeqaqi *et al.* have studied the spin-1 transverse crystal field Ising model by means of effective field theory (EFT), and have obtained some meaningful results [13]. Jiang *et al.* have investigated a ferromagnetic or ferrimagnetic bilayer Ising system with a transverse crystal field [14]. Htoutou *et al.* have considered a ferromagnetic mixed Ising model with a transverse crystal field [15]. Ekiz *et al.* have dealt with mixed spin-1/2 and spin-1 Ising models with uniaxial and biaxial single-ion

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anisotropy on the Bethe lattice [16]. It is worth noting that the model is a quantum Ising model. Meanwhile, a remarkable problem results from the introduction of randomness. In fact, the presence of randomness may affect the critical properties of systems in a dramatic way. One of the present authors has given the critical properties of the spin-1 random transverse field Ising model and has provided many valuable observations [17]. For the general case, a real spin system may be in two different disorder situations at the same time. Some researches have touched on a complicated disorder (bond and longitudinal crystal field) spin-1 BCM [4, 5]. In the present work, we study the critical properties of a random transverse crystal field Ising model with bond dilution. Our calculations show that, for three cases of a transverse crystal field ratio ($\alpha = 0, \pm 0.5$), the results obtained for weak bond dilution are very similar to those of pure bond in shape but with decreases in corresponding ordered phases and critical values [17]. However, the existence of a strong bond dilution can apparently affect the critical properties and lead to a change in reentrant phenomenon, the occurrence of transverse crystal field degeneration, and the opposite direction crossover of temperature peak value. To our knowledge, certain aforementioned subjects have not yet been studied. Here, we employ effective field theory (EFT) to solve the problem. The results obtained from the EFT were in qualitative agreement with the results of precise numerical solutions [18].

The structure of this work is organized as follows. In Section 2, we outline the theory and make some technical points. The detailed numerical results and discussion of the different disorder conditions are provided in Section 3. Finally, we briefly summarize our results.

2. Theory

The Hamiltonian of a spin-1 random transverse crystal field Ising model with bond dilution can be defined as follows:

$$H = -\sum_{\langle ij \rangle} J_{ij} S_i^z S_j^z - \sum_i D_{x,i} \left(S_i^x\right)^2. \tag{1}$$

Here, S_i^z and S_i^x are spin-1 Pauli matrices associated with the ith site. The first summation only runs over all nearest-neighbor pairs of spins. The second summation involves all sites. J_{ij} is the exchange interaction between the nearest-neighbor sites, taken to satisfy $J_{ij} > 0$. $D_{x,i}$ represents the transverse crystal field parameter with the x-axis. J_{ij} and D_{xi} can satisfy independent probability distributions,

$$P\left(J_{ij}\right) = p\delta\left(J_{ij} - J\right) + (1-p)\,\delta\left(J_{ij}\right), \tag{2}$$

$$P\left(D_{x,i}\right) = t\delta\left(D_{x,i} - D_x\right) + (1-t)\,\delta\left(D_{x,i} - \alpha D_x\right) \tag{3}$$

respectively, where $p_c < p \leqslant 1.0$, $0 \leqslant t \leqslant 1.0$, and $-1 \leqslant \alpha \leqslant 1$. Quantities p and p_c denote the bond dilution concentration and the bond percolation threshold, respectively. Quantity t indicates the concentration of the random transverse crystal field, while α is a tunable parameter of magnitude for the transverse crystal field. Thus, when $t = 1.0$, all of the transverse crystal fields in the lattice have the same positive value, while, when $t = 0$ and $\alpha = -1$, the array has the same negative value. For $0 < t < 1.0$ and $0 < \alpha < 1.0$, the array is an imperfect transverse crystal field distribution, while, for $0 < t < 1.0$ and $-1 < \alpha < 0$, there exists an imperfect mixed positive and negative transverse crystal field in the system. We also take into account the effect of dilution ($\alpha = 0$) in a transverse crystal field.

As pointed out in our previous work [17], we can perform the averaged magnetization m and quadrupolar moment q within the EFT and a cutting approximation,

$$\begin{aligned} m = \langle S_i^z \rangle = \Bigg\langle \prod_{i=1}^{z} \Big[& (S_i^z)^2 \left\langle \cosh\left(J_{ij}\nabla\right)\right\rangle_r \\ & + S_i^z \left\langle \sinh\left(J_{ij}\nabla\right)\right\rangle_r \\ & + 1 - (S_i^z)^2 \Big] \Bigg\rangle F(x)\,|_{x=0}\,, \end{aligned} \tag{4}$$

$$\begin{aligned} q = \left\langle (S_i^z)^2 \right\rangle = \Bigg\langle \prod_{i=1}^{z} \Big[& (S_i^z)^2 \left\langle \cosh\left(J_{ij}\nabla\right)\right\rangle_r \\ & + S_i^z \left\langle \sinh\left(J_{ij}\nabla\right)\right\rangle_r \\ & + 1 - (S_i^z)^2 \Big] \Bigg\rangle G(x)\,|_{x=0}\,, \end{aligned} \tag{5}$$

where

$$\beta = \frac{1}{k_B T}$$

and

$$\nabla = \frac{\partial}{\partial x},$$

while z is the coordination number of the lattice. The functions $F(x)$ and $G(x)$ are written

$$F(x) = \int P(D_{x,i}) f\left(x, D_{x,i}\right) dD_{x,i}, \tag{6}$$

$$G(x) = \int P\left(D_{x,i}\right) g\left(x, D_{x,i}\right) dD_{x,i}, \tag{7}$$

where $f\left(x, D_{x,i}\right)$ and $g\left(x, D_{x,i}\right)$ are

$$f\left(x, D_{x,i}\right) = \sum_{n=1}^{3}\left[\exp\left[2\beta C E_1(n) + \frac{2\beta D_{x,i}}{3}\right]\left[\frac{2x}{3C}E_1(n) + \frac{x^3 D_{x,i}}{27BC}E_2(n)\right]\right]Z^{-1}, \tag{8}$$

$$g\left(x, D_{x,i}\right) = \sum_{n=1}^{3}\left[\exp\left[2\beta C E_1(n) + \frac{2\beta D_{x,i}}{3}\right]\left[-\frac{D_{x,i}}{9C}E_1(n) + \frac{4x^4 + x^2 D_{x,i}^2}{54BC}E_2(n) + \frac{2}{3}\right]\right]Z^{-1}. \tag{9}$$

Here, Z is the partition function,

$$Z = \sum_{n=1}^{3}\exp\left(2\beta C\cos\frac{(n-1)2\pi+\theta}{3} + \frac{2\beta D_{x,i}}{3}\right), \tag{10}$$

and

$$E_1(n) = \cos\frac{(n-1)2\pi+\theta}{3}, \tag{11}$$

$$E_2(n) = \sin\frac{(n-1)2\pi+\theta}{3}, \tag{12}$$

where

$$\theta = \arccos\left(\frac{A}{C^3}\right), \tag{13}$$

$$A = -\frac{1}{27}D_{x,i}^3 - \frac{1}{6}x^2 D_{x,i}, \tag{14}$$

$$B = \frac{1}{9}\left(3x^6 + \frac{3}{4}x^4 D_{x,i}^2\right)^{\frac{1}{2}}, \tag{15}$$

$$C = \frac{1}{3}\left(3x^2 + D_{x,i}^2\right)^{\frac{1}{2}}. \tag{16}$$

From Equation (4), we may easily separate the ferromagnetic state ($m \neq 0$) from the paramagnetic state ($m = 0$). For surpassing Curie temperature, the paramagnetic state ($m = 0$) is the only solution; however, at low temperature, another solution ($m \neq 0$) can be obtained. In order to calculate the ferromagnetic state ($m \neq 0$), we must combine Equations (4) and (5). Then, the self-consistent equation with respect to the averaged magnetization m can be written

$$m = am + bm^3 + cm^5 + \cdots. \tag{17}$$

The magnetization m tends to zero as the temperature approaches a critical value, according to Landau theory. Hence, we consider only the linear term about m in Equation (17) because higher-order terms tend to zero faster than linear terms on approaching the critical temperature. Therefore, the critical ordering frontiers can be obtained from the condition $a = 1$, namely

$$a = z\left\langle\sinh\left(J_{ij}\nabla\right)\right\rangle_r\left[q_0\left\langle\cosh\left(J_{ij}\nabla\right)\right\rangle_r + 1 - q_0\right]^{z-1} F(x)|_{x=0} = 1. \tag{18}$$

When $a = 1$ and $b < 0$, the critical ordering frontiers are identified with the second-order phase transition line. The coefficient b in Equation (17) is given by the following forms:

$$\begin{aligned} b =& z(z-1)q_1\left\langle\sinh\left(J_{ij}\nabla\right)\right\rangle_r\left[\left\langle\cosh\left(J_{ij}\nabla\right)\right\rangle_r - 1\right] \\ &\times\left[q_0\left\langle\cosh\left(J_{ij}\nabla\right)\right\rangle_r + 1 - q_0\right]^{z-2} F(x)|_{x=0} \\ &+ \frac{z(z-1)(z-2)}{3!}\left\langle\sinh^3\left(J_{ij}\nabla\right)\right\rangle_r \\ &\left[q_0\left\langle\cosh\left(J_{ij}\nabla\right)\right\rangle_r + 1 - q_0\right]^{z-3} F(x)|_{x=0} < 0, \end{aligned} \tag{19}$$

where q_0 and q_1 are solutions of

$$q_0 = \left[q_0\left\langle\cosh\left(J_{ij}\nabla\right)\right\rangle_r + 1 - q_0\right]^z G(x)|_{x=0}, \tag{20}$$

$$q_1 = \frac{\frac{z(z-1)}{2!}\left[\left\langle\sinh\left(J_{ij}\nabla\right)\right\rangle_r\right]^2\left[q_0\left\langle\cosh\left(J_{ij}\nabla\right)\right\rangle_r + 1 - q_0\right]^{z-1} G(x)|_{x=0}}{\left\{1 - z\left[\left\langle\cosh\left(J_{ij}\nabla\right)\right\rangle_r - 1\right]\left[q_0\left\langle\cosh\left(J_{ij}\nabla\right)\right\rangle_r + 1 - q_0\right]^{z-1} G(x)|_{x=0}\right\}}. \tag{21}$$

The exchange interaction J_{ij} in the above expressions is given by the bond dilution distribution in Equation (2).

The spin-1 transverse crystal field Ising model has been generalized to two disorder cases (bond dilution and a

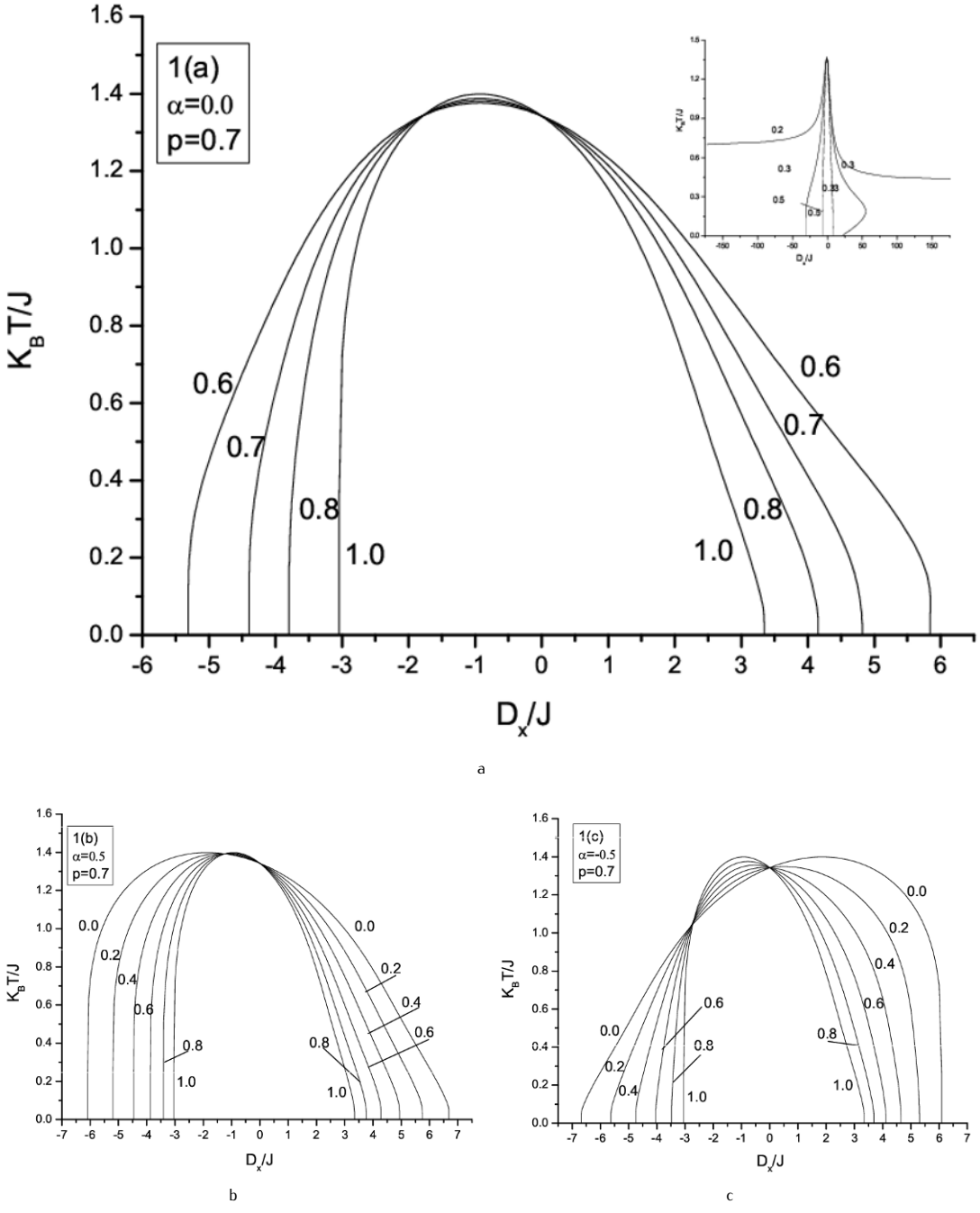

Figure 1. Curie temperatures versus a transverse crystal field with a weak bond concentration of $p = 0.7$ for three transverse crystal field ratios: 1(a) $\alpha = 0$, 1(b) $\alpha = 0.5$, and 1(c) $\alpha = -0.5$. The number accompanying each curve denotes the value of transverse crystal field concentration t.

random transverse crystal field). Obviously, the important physical factors are the disorders in both the bond and the transverse crystal field. Moreover, the expressions are suitable for the lattice with an arbitrary coordination number. In order to avoid too lengthy calculations, we consider only a square lattice as a two-dimensional example. The next step is to solve Equations (18)-(21) numerically.

3. Results and discussion

Firstly, the Curie temperatures versus a transverse crystal field with a weak bond concentration of $p = 0.7$ for transverse crystal field ratio $\alpha(= 0, \pm 0.5)$ are depicted in Figures 1a-1c, respectively, when the value of random transverse crystal field concentration t is changed. We can compare the phase diagrams of a weak bond dilution with the pure bond results of [17]. As can be seen, the curves are very similar in shape. Furthermore, some phenomena have been revealed in [17]. For instance, under crystal field dilution condition $\alpha = 0$, there exists the peak value of critical temperature in the direction of the negative crystal field and there are reentrant phenomena in the direction of the positive crystal field. By choosing ratios $\alpha = \pm 0.5$, the range of the magnetic ordered phase shrinks. With a decrease in crystal field concentration t, the peak value of the critical temperature undergoes a crossover from a negative to a positive direction of the transverse crystal field with ratio $\alpha = -0.5$. Nevertheless, the curves also depict the differences in numerical values. For example, the peak value of the critical temperature is $k_B T/J = 2.316$ in a pure bond state, while the peak value is $k_B T/J = 1.399$ for bond dilution $p = 0.7$. It is evident that the role of the bond dilution weakens the exchange interaction and the transverse crystal field correlation between different sites. This leads to a decrease in corresponding ordered phases and critical values.

Figures 2a-2c express the Curie temperatures dependence of a transverse crystal field with a strong bond concentration of $p = 0.4$ for transverse crystal field ratios $\alpha = 0, \pm 0.5$, respectively, when the value of random transverse crystal field concentration t is changed. By comparing Figures 1a-1c with Figures 2a-2c, the critical properties show marked differences. As seen from Figure 2a ($\alpha = 0$), the peak of the second-order line exists in the positive direction of the D_x/J axis and shows a decline with the decrease of the crystal field concentration. The scope of the ordered phases is almost constant when the crystal field concentration varies in a certain range (*e.g.*, $t = 10$ to 0.6) while the scope magnifies rapidly for small concentrations. We note that there are two intersections for all concentration values. An unusual intersection appears in the positive direction of the D_x/J axis, and indicates the degeneration of the transverse crystal field at the same temperature. An exception is the normal intersection ($D_x/J = 0$). In addition, the reentrant phenomenon appears only in the negative direction because of the non-uniform convergence of negative D_x/J. The case when the transverse crystal field goes to infinity on the transition line ($D_x/J \to \pm\infty$) does not actually occur as a result of the depression of a strong bond dilution. In Figure 2b, we can see different cases from Figure 1b. The region of ordered phases gathers mainly at the scene of positive

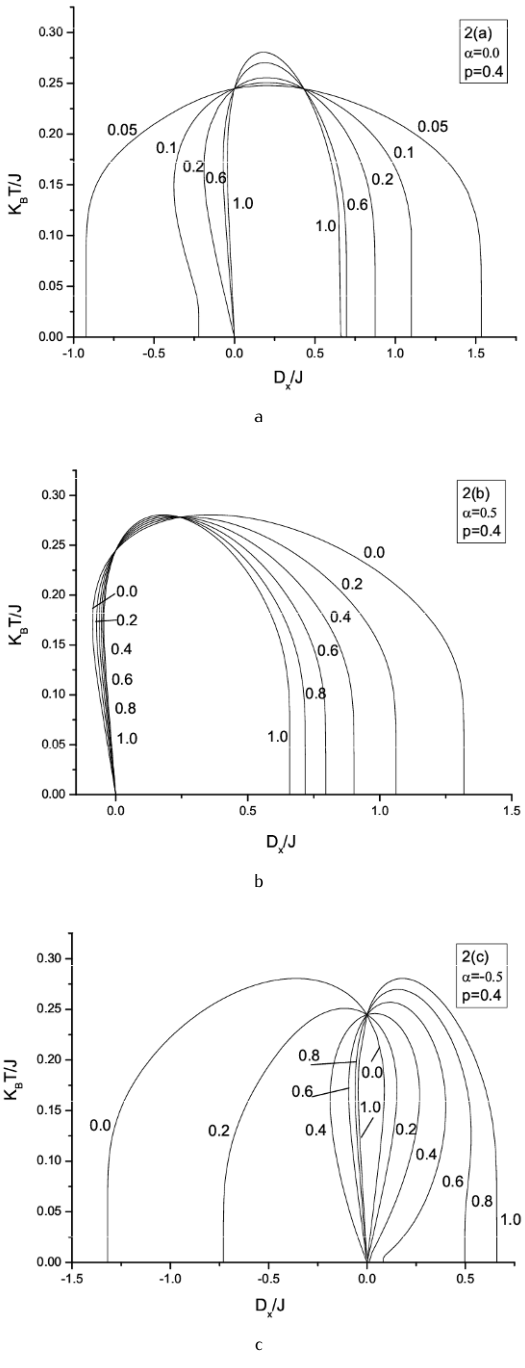

Figure 2. Curie temperatures dependence of a transverse crystal field with a strong bond concentration of $p = 0.4$ for three transverse crystal field ratios: 1(a) $\alpha = 0$, 1(b) $\alpha = 0.5$, and 1(c) $\alpha = -0.5$. The number accompanying each curve denotes the value of transverse crystal field concentration t.

D_x/J. The weak reentrant phenomenon occurs in a narrow area of the negative D_x/J axis. The peak value of critical temperature transfer occurs in the positive direction of the D_x/J axis. Moreover, the values of all transverse crystal fields focus on $D_x/J = 0$ at zero temperature and, hence, $D_x/J = 0$ is a degenerate value at ground state. These values stem from a strong bond dilution and positive ratio $\alpha = 0.5$. Figure 2c ($\alpha = -0.5$) shows that the scope of ordered phases from $t = 1.0$ to $t = 0$ shrinks or expands gradually in the direction of the $+D_x/J$ axis or the $-D_x/J$ axis. It also shows that the peak value of the critical temperature undergoes crossover from the positive to the negative direction of the D_x/J axis. It is obvious that the differences come from the effect of the transverse crystal field ratio for Equation (3) in Figures 1a-1c or Figures 2a-2c, while the corresponding discrepancies between Figures 1a-1c and Figures 2a-2c can be attributed to the magnitude of the bond dilution.

To summarize, we have studied the critical properties of a random transverse crystal field Ising model with bond dilution on a square lattice. For a weak bond dilution where the curves obtained are very similar in shape to those found in [17], some critical values display only the differences in numerical values. Thus a weak bond dilution condition cannot change the basic structure of the phase diagrams. For a strong bond dilution, which is the new structure of phase diagrams, we have shown a deep influence of strong bond dilution on the critical properties and have provided extensive discussion.

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