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The random-mixed-bond spin-1 Ising model with a single-ion anisotropy in a transverse field

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Abstract. In the light of the effective-field theory, the present paper attempts to discuss the investigation done into the phase diagrams of a random nearest-neighbour interaction spin-1 Ising model with a single-ion anisotropy in an applied transverse field on the honeycomb lattice. The interactions are assumed to be independent random variables with distribution $P(J_{ij}) = p\delta(J_{ij} - J_1) + (1 - p)\delta(J_{ij} - J_2)$, where $J_1 > 0$ and $|J_2/J_1| \leqslant 1$. We find a number of interesting phenomena, such as two different types of re-entrant phenomenon due to the competition between the random bond and the negative single-ion anisotropy parameter, as well as the usual frustration of J_{ij}. The influence of a transverse field on the behaviours of the tricritical point and re-entrant transition is also discussed in this paper.

1. Introduction

In the past few decades there has been an increasing number of studies dealing with the phase transition of the spin-1 Ising model [1–6]. In particular, the spin-1 Ising model including the term for a single-ion anisotropy is described by the following Hamiltonian:

$$\mathcal{H} = -\sum_{\langle ij\rangle} J_{ij} S_i^z S_j^z - D\sum_i (S_i^z)^2 \tag{1}$$

where the first summation runs over all pairs of nearest neighbours, and J_{ij} and D are the exchange interaction and the single-ion anisotropy parameter, respectively. The model Hamiltonian, which is often called the Blume–Capel [1, 2] model, has been studied in some detail using a variety of methods [3–8]. It is well known that in the system there exists a tricritical point (TCP) in the phase diagram at which the phase transition changes from second order to first, when the value of D takes a large negative value.

On the other hand, some attention has recently been directed to the Ising model with random interactions [9–11]. The exchange interactions J_{ij} are assumed to be independent random variables with the distribution

$$P(J_{ij}) = p\delta(J_{ij} - J_1) + (1 - p)\delta(J_{ij} - J_2) \tag{2}$$

where $J_1 = J > 0$ and $0 \leqslant p \leqslant 1$. We assume that $J_1 > J_2$ without loss of generality and therefore introduce a parameter $\alpha = J_2/J_1$. As far as we know, however, the effects of an applied transverse field on the phase diagrams (or phase transitions) of the spin-1 Ising model with a crystal-field interaction have not been investigated either experimentally or theoretically, except for the work that we have previously done [12].

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The purpose of this work is to study the effects of a transverse field on phase diagrams in a random-mixed-bond spin-1 Ising model with a negative single-ion anisotropy parameter under the effective-field theory (EFT) introduced by Honmura and Kaneyoshi [13]. Accordingly, the exchange interaction J_{ij} in (1) is assumed to be given by (2). The critical properties including the TCPs and re-entrant phenomena are discussed in detail only for the honeycomb lattice.

2. Formulation

With a spin-1 Ising model within a transverse field considered, the Hamiltonian of the system is given by

$$\mathcal{H} = -\sum_{\langle ij\rangle} J_{ij} S_i^z S_j^z + D\sum_i (S_i^z)^2 - \Omega \sum_i S_i^x \tag{3}$$

where Ω is an applied transverse field, and both S_i^x and S_i^z are components of a spin-1 operator at site i. D is taken to be positive. The starting point for the statistics of our spin system is the relation proposed by Sa Barreto and Fittipaldi [14], within which the thermal average of any spin operator O_i at site i is approximately given by

$$\langle\langle O_i\rangle\rangle_r = \langle\langle \{\mathrm{Tr}_{\{i\}}[O_i \exp(-\beta\mathcal{H}_i)]\}/\mathrm{Tr}_{\{i\}}[\exp(-\beta\mathcal{H}_i)]\rangle\rangle_r \tag{4}$$

where $\langle\cdots\rangle$ indicates the canonical thermal average, $\langle\cdots\rangle_r$ denotes the random-bond average for (2), $\mathrm{Tr}_{\{i\}}$ means the partial trace in respect of the lattice site i, $\beta = 1/k_B T$ and $\mathcal{H}_i = -(\sum_{j\neq i} J_{ij} S_j^z) S_i^z + D(S_i^z)^2 - \Omega S_i^x$. The thermodynamic quantities $m_z = \langle\langle S_i^z\rangle\rangle_r$, $m_x = \langle\langle S_i^x\rangle\rangle_r$ and $q_z = \langle\langle (S_i^z)^2\rangle\rangle_r$ are obtained from equation (4) by substituting S_i^z, S_i^x and $(S_i^z)^2$ for O_i, respectively:

$$m_z = \langle\langle S_i^z\rangle\rangle_r = \left\langle\left\langle \prod_j \Theta_i[S_j^z, (S_j^z)^2; \nabla]\right\rangle\right\rangle_r F(x)|_{x=0} \tag{5}$$

$$m_x = \langle\langle S_i^x\rangle\rangle_r = \left\langle\left\langle \prod_j \Theta_i[S_j^z, (S_j^z)^2; \nabla]\right\rangle\right\rangle_r G(x)|_{x=0} \tag{6}$$

$$q_z = \langle\langle (S_i^z)^2\rangle\rangle_r = \left\langle\left\langle \prod_j \Theta_i[S_j^z, (S_j^z)^2; \nabla]\right\rangle\right\rangle_r H(x)|_{x=0} \tag{7}$$

where

$$\Theta_i[S_j^z, (S_j^z)^2; \nabla] = 1 + S_j^z \sinh(J_{ij}\nabla) + (S_j^z)^2[\cosh(J_{ij}\nabla) - 1]. \tag{8}$$

The functions $F(x)$, $G(x)$ and $H(x)$ are defined by

$$F(x) = \left[\sum_{n=1}^{3} \exp[\![2\beta C\cos\{\tfrac{1}{3}[\theta + (n-1)2\pi]\} - \tfrac{2}{3}\beta D]\!]\left(\frac{2x}{3C}\cos\{\tfrac{1}{3}[\theta + (n-1)2\pi]\}\right.\right.$$
$$\left.\left. - \frac{2}{27}\frac{D^3 x - Dx^3 + \frac{7}{2}D\Omega^2 x}{BC}\sin\{\tfrac{1}{3}[\theta + (n-1)2\pi]\}\right)\right]$$
$$\times\left(\sum_{n=1}^{3} \exp[\![2\beta C\cos\{\tfrac{1}{3}[\theta + (n-1)2\pi]\} - \tfrac{2}{3}\beta D]\!]\right)^{-1} \tag{9}$$

$$G(x) = \left[\sum_{n=1}^{3} \exp[\![2\beta C \cos\{\tfrac{1}{3}[\theta + (n-1)2\pi]\} - \tfrac{2}{3}\beta D]\!] \right.$$
$$\left. \times \left(\frac{2\Omega}{3C} \cos\{\tfrac{1}{3}[\theta+(n-1)2\pi]\} - \frac{2}{27} \frac{\frac{1}{2}D\Omega^3 - 4D\Omega x^2}{BC} \sin\{\tfrac{1}{3}[\theta+(n-1)2\pi]\} \right) \right]$$
$$\times \left(\sum_{n=1}^{3} \exp[\![2\beta C \cos\{\tfrac{1}{3}[\theta + (n-1)2\pi]\} - \tfrac{2}{3}\beta D]\!] \right)^{-1} \tag{10}$$

and

$$H(x) = \left[\sum_{n=1}^{3} \exp[\![2\beta C \cos\{\tfrac{1}{3}[\theta + (n-1)2\pi]\} - \tfrac{2}{3}\beta D]\!] \left(-\frac{2D}{9C} \cos\{\tfrac{1}{3}[\theta + (n-1)2\pi]\} \right.\right.$$
$$\left.\left. + \frac{2}{27} \frac{\frac{1}{2}\Omega^2 x^2 - D^2 x^2 + x^4 - \frac{1}{2}\Omega^4}{BC} \sin\{\tfrac{1}{3}[\theta + (n-1)2\pi]\} - \tfrac{2}{3} \right) \right]$$
$$\times \left(\sum_{n=1}^{3} \exp[\![2\beta C \cos\{\tfrac{1}{3}[\theta + (n-1)2\pi]\} - \tfrac{2}{3}\beta D]\!] \right)^{-1} \tag{11}$$

where

$$\begin{aligned} A &\equiv \tfrac{1}{27}D^3 - \tfrac{1}{3}Dx^2 + \tfrac{1}{6}D\Omega^2 \\ B &\equiv \tfrac{1}{9}[3(D^2x - x^3)^2 + \tfrac{3}{4}D^2\Omega^4 + 15D^2\Omega^2x^2 + 9\Omega^2x^4 + 9\Omega^4x^2 + 3\Omega^6]^{1/2} \\ C &\equiv (A^2 + B^2)^{1/6} = [\tfrac{1}{9}D^2 + \tfrac{1}{3}\Omega^2 + \tfrac{1}{3}x^2]^{1/2} \\ \theta &\equiv \cos^{-1}(A/C^3) \end{aligned} \tag{12}$$

and $\nabla = \partial/\partial x$ is the differential operator. However, if we try to treat the multispin correlation presented in equations (5)–(7) exactly, the performance is mathematically intractable. Therefore, we shall adopt an approximation. The simplest approximation, which is adopted frequently, is the following: $\langle\langle S_i S_j S_k \cdots \rangle\rangle_r = \langle\langle S_i \rangle\rangle_r \langle\langle S_j \rangle\rangle_r \langle\langle S_k \rangle\rangle_r \cdots$, for $i \neq j \neq k \neq \cdots$, with the assumption of the statistical independence of the different bonds. With such a procedure, the longitudinal magnetization m_z, the transverse magnetization m_x and quadrupolar moment q_z can be evaluated from the following coupled equations:

$$m_z = [q_z D_1 + m_z D_2 + 1 - q_z]^z F(x)|_{x=0} \tag{13}$$

$$m_x = [q_z D_1 + m_z D_2 + 1 - q_z]^z G(x)|_{x=0} \tag{14}$$

$$q_z = [q_z D_1 + m_z D_2 + 1 - q_z]^z H(x)|_{x=0} \tag{15}$$

where

$$D_1 = p \cosh(J_1, \nabla) + (1-p) \cosh(\alpha J_1 \nabla) \tag{16}$$

$$D_2 = p \sinh(J_1, \nabla) + (1-p) \sinh(\alpha J_1 \nabla) \tag{17}$$

and z is the lattice coordination number.

Here, we are interested in studying the transition temperature only for the honeycomb lattice with $z = 3$. As discussed in the previous work [12], in the vicinity of the second-order phase transition line, by expanding the right-hand side of equations (13) and (15) with respect to m_z, and retaining only linear terms in m_z, the averaged magnetization can be given by

$$m_z^2 = (1 - a)/b. \tag{18}$$

The second-order transition line can be determined by

$$a = 1 \tag{19}$$

in equation (18). The right-hand side of (18) must be positive. If this is not the case, the transition is of the first order, and hence the point at which

$$a = 1 \qquad \text{and} \qquad b = 0 \tag{20}$$

is the TCP. Here, the parameters a and b are given in the appendix.

3. Phase diagrams

In this section, we shall examine the effect of a transverse field on the phase diagrams of the random-mixed-bond spin-1 Ising model with a negative single-ion anisotropy parameter on the honeycomb lattice by solving equations (19) and (20) numerically.

3.1. The case of $\alpha = 0.5$

Figures 1(a), 1(b) and 1(c) show the phase diagrams in the (T, p) space for three cases corresponding to reduced transverse fields Ω/J of 0.2, 0.8 and 1.2, respectively, for various values of D/J. The full and broken curves denote the second- and first-order phase transitions, respectively; the full circles denote the TCPs. In figure 1(a) the TCP appears in the whole p region from $p = 0.0$ to 1.0 when Ω has a small value. In other words, the second-order transition does not exist in the low-temperature region. On increasing the transverse field the tricritical temperature is depressed when Ω is not too large; the second-order transition could even appear at zero temperature but, when Ω is larger, then at a certain critical value Ω_0 the TCP will disappear. This behaviour of the transverse field can be seen from a comparison between figures 1(a), 1(b) and 1(c). This means that the system with a small value of p easily becomes disordered with $T_c = 0$, if the value of Ω is large. In particular, when the value of Ω equals $2.24J$, the system will be not at all ordered [12]. Additionally, in figures 2(a)–2(c) the change in T_c versus D in the system with $\alpha = 0.5$ is plotted at values of Ω selected to be the same as in figures 1(a)–1(c), and various values of p are used.

In fact, the existence of the TCP is also affected by the negative single-ion anisotropy parameter D besides the transverse field Ω and the randomness of the bonds. This is the result of competition between these three effects. The change in the tricritical temperature T_t as a function of p with $\alpha = 0.5$ for several values of the transverse field Ω is presented in figure 3. As figure 3 shows, on decreasing the random parameter p, the value of T_t decreases. However, T_t displays an interesting behaviour in figure 3. That is T_t instead

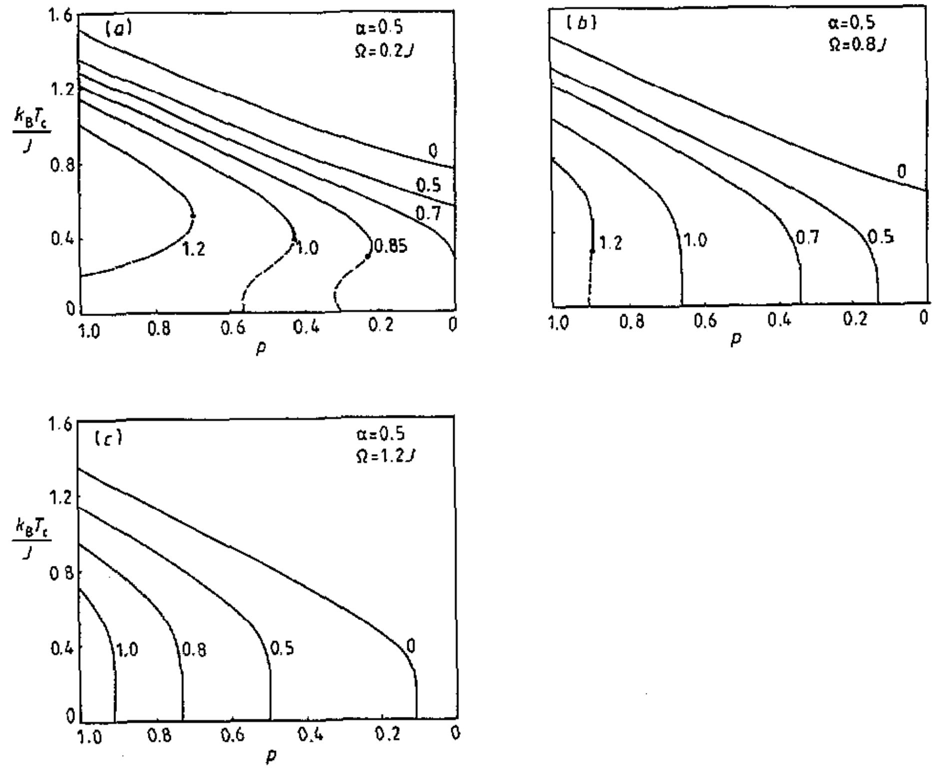

Figure 1. Phase diagrams in (T, p) space for $\alpha = 0.5$ on a honeycomb lattice, for Ω/J-values of (*a*) 0.2, (*b*) 0.8 and (*c*) 1.2: ——, second-order transition; - - - -, first-order transition; ·, TCP. The numbers on the curves are the values of D/J.

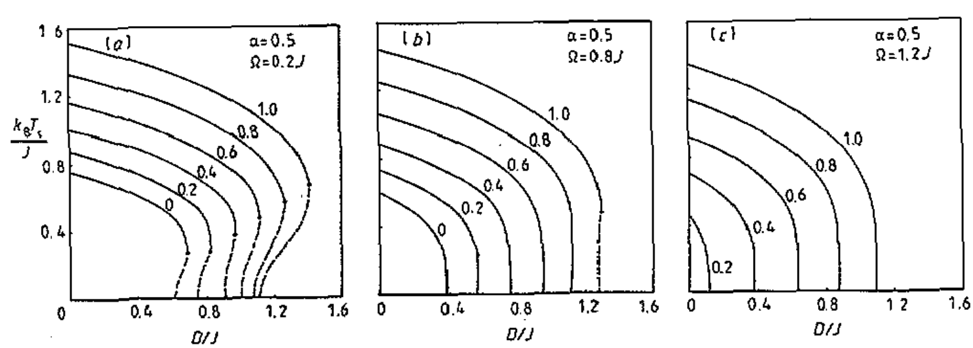

Figure 2. Phase diagrams in (T, D) space.

increases slightly in the range $0.1 > p > 0.0$ when the value of Ω is small. If Ω/J is larger than 0.94, the TCP cannot exist at all.

The re-entrant phenomenon is another interesting problem in phase transition physics. From figures 1 and 2, it can be observed in an appropriate range of parameters (such as the curve labelled 0.85 in figure 1(*a*) or the curve labelled 0.2 in figure 2(*a*)). For the case $\Omega = 0$, Kaneyoshi [9] has discussed the reason for the re-entrant phenomenon in detail.

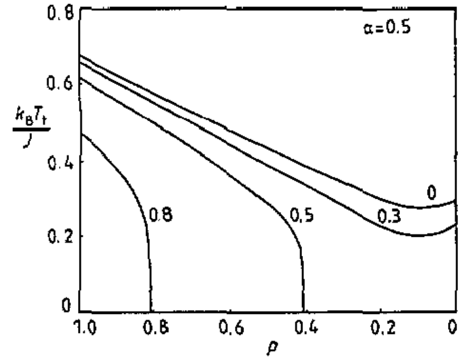

Figure 3. The variations in tricritical temperature k_BT_t/J with p for selected values of Ω/J.

To clarify the effect of a transverse field on the re-entrant phenomenon, the magnetic re-entrant phase diagrams in the T–D plane are given for the two cases $p = 0.2$ and $p = 0.4$ in figures 4(a) and 4(b), respectively, for several values of Ω/J. From figure 4(a) we find that the range of the second-order re-entrant phase transition should decrease with increasing transverse field Ω and should disappear when Ω is larger than a certain value (for example, $\Omega > 0.5J$ in figure 4(b)). However, if a TCP exists in the phase diagrams, the effect of the transverse field on the second-order re-entrant phase transition becomes more complex. With increasing transverse field Ω but not larger than this certain value (in the case of figure 4(b), Ω is not larger than $0.5J$), the TCP should be depressed. This depression may make the second-order re-entrant phase transition appear. These results are highly analogous to those in the quantum transverse Ising model with a random field by use of the MFA [15] and pair approximation [16]. This may be attributed to competition between quantum effects due to the transverse field, the single-ion anisotropy, and the randomness of bonds. In fact, we can see from figures 1 and 2 that the transition in which the randomness of the bonds or the crystal field (or the single-ion anisotropy parameter) dominates has a tendency to be of first order. On the other hand, the transverse field tends to make it second order. We have also observed that the re-entrant phenomenon may occur if D is not large and if Ω is small. When D is large (for example, $D/J = 1.2$) the phenomenon becomes impossible, since most spins are in the $s_j^z = 0$ state rigidly and act like non-magnetic atoms [9]. The three effects (the single-ion anisotropy, the transverse field and the randomness of the bonds) compete in the Ising spin system indeed, and this makes the role of Ω become complex.

3.2. The case of $\alpha = -0.1$

Figures 5(a)–(c) show the changes in T_c with p for $\Omega/J = 0.2$, 0.5 and 0.8, respectively, and for various values of D. The figures clearly show that the tricritical temperature T_t should be depressed on increasing the transverse field Ω, and the TCP disappears for $\Omega > \Omega_0$; the second-order re-entrant phenomenon occurs within the appropriate ranges. In figure 6, the behaviour of T_t is described as a function of p, for values of Ω from 0.0 to $0.8J$. However, for T_t in the region $k_BT/J < 0.03$, in the case of $\Omega = 0.0$, the calculation of numerical values of the TCP will become difficult because of the large numerical overflow as the computer works.

For the system with $\alpha = -0.1$, the re-entrant phenomenon due to the frustration of J_{ij} should occur. To observe the effect of a transverse field on the re-entrant phase diagrams in (T, P) space, in figures 7(a)–(c) we selected the three D/J-values of 0.1, 1.0, and 1.1, respectively. From figure 7(a) we can see clearly that the re-entrant phenomenon is easily

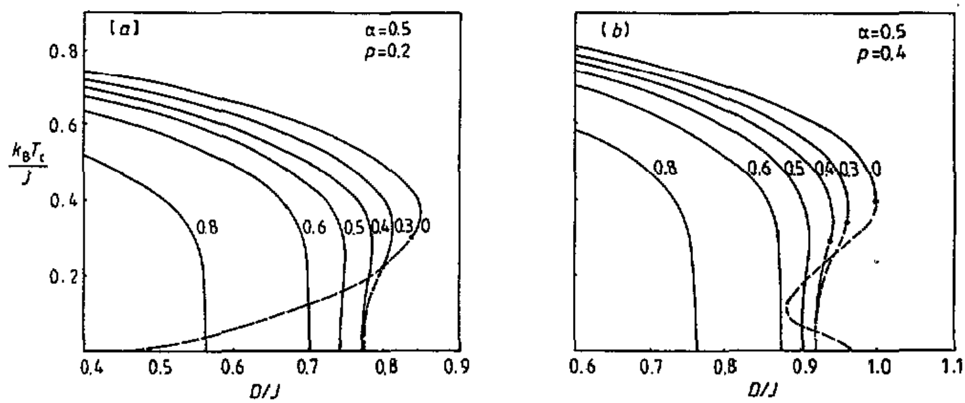

Figure 4. Two examples which exhibit the re-entrant phenomenon for the systems with $z = 3$ and $\alpha = 0.5$ for various values of Ω/J: (*a*) $p = 0.2$; (*b*) $p = 0.4$.

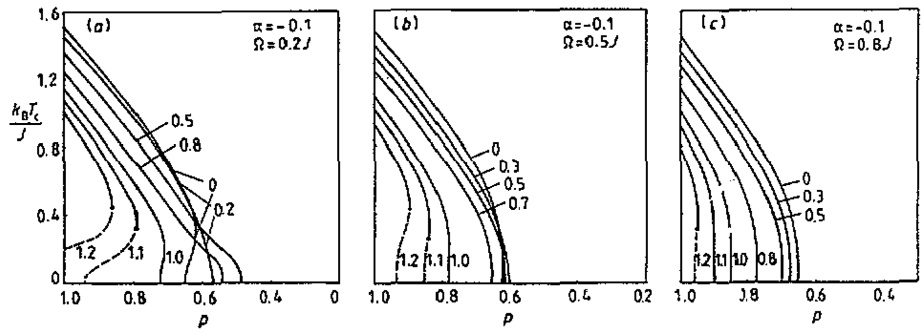

Figure 5. Phase diagrams in (T, p) space for $\alpha = -0.1$ for Ω/J values of (*a*) 0.2, (*b*) 0.5 and (*c*) 0.8. The numbers on the curves are the values of D/J.

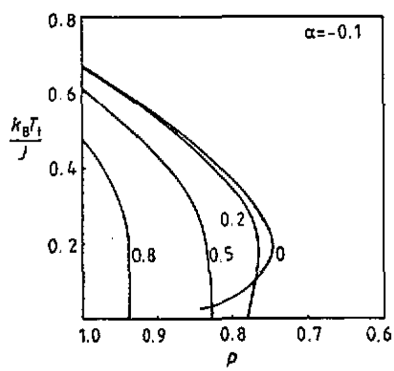

Figure 6. The variations in tricritical temperature k_BT_t/J with p for $\alpha = -0.1$, for selected values of Ω/J.

destroyed by the application of Ω when D/J is small (see the curves labelled 0.3 and 0.5). In figure 7(*b*), D is not small but $D/J = 1.0$; the re-entrant phenomenon is not so easily destroyed by Ω as in figure 7(*a*). Then the role of the transverse field Ω is to destroy the re-entrant phenomenon. However, when $D/J > 1.0$ (for example, $D/J = 1.1$ (figure 7(*c*)), in which the TCP exists, the second-order re-entrant phenomenon occurs with increased Ω. Here the role of Ω is not to destroy but to assist. We think that the mechanism of the effect of Ω on the re-entrant phenomenon in figure 7(*c*), in which TCPs are depressed, is different from that in figures 7(*a*) and 7(*b*). Thus the mechanism of the re-entrant transition is very complex. The origin of the re-entrant transition is not very clear, and maybe it mainly arises from both frustration effects and non-uniform convergence of p_c at $T_c = 0$ axis. Therefore, further investigation into the mechanism of the re-entrant transition is needed.

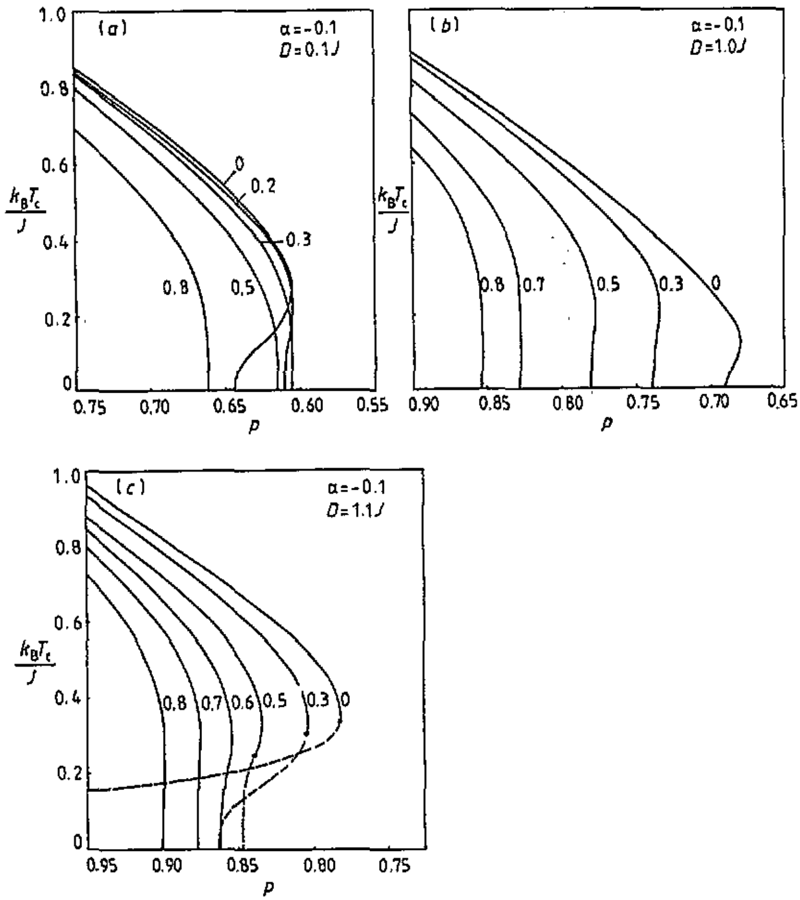

Figure 7. Three examples which exhibit the re-entrant phenomenon for the system with $z = 3$ and $\alpha = -0.1$: (*a*) $D/J = 0.1$; (*b*) $D/J = 1.0$; (*c*) $D/J = 1.1$. The numbers on the curves are the values of Ω/J.

3.3. *The condition for the occurrence of the TCP*

Let us now look at the condition for the existence of TCPs. We can first eliminate D from equation (20) in the limit $T \to 0$ and then solve for the critical transverse field, which can be expressed as $\Omega_0(p, \alpha)$ [17]. The TCP can exist when $\Omega < \Omega_0$ and disappears when $\Omega \geqslant \Omega_0$. The function Ω_0 is calculated numerically for two values of α, and the results are plotted in figure 8. As mentioned above, because of the large numerical overflow as the computer works, the determination of the behaviour of Ω_0 will be difficult in the region in which Ω is very small and $\alpha = -0.1$.

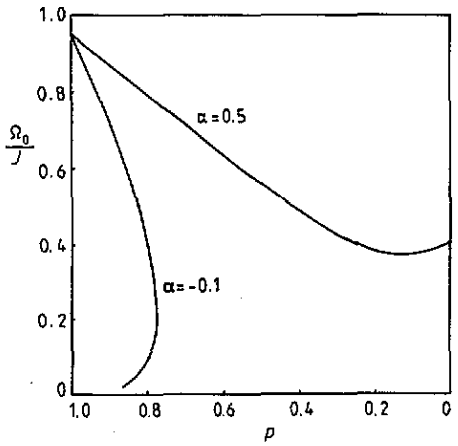

Figure 8. The critical transverse field Ω_0/J plotted against p for two cases: $\alpha = 0.5$ and -0.1.

4. Conclusions

In this work we have calculated phase diagrams for the random-mixed-bond spin-1 Ising model with a single-ion anisotropy in a transverse field for a honeycomb lattice under the EFT. The effects of a transverse field on the phase diagrams have shown a number of interesting phenomena. Moreover, the influence of the transverse field on two different types of re-entrant phenomenon, namely the usual re-entrant phenomenon from the frustration of the exchange interaction J_{ij} and the other due to the competition between the randomness of bonds and the negative single-ion anisotropy, have been discussed. We have also shown the existence of the critical transverse field Ω_0 above which the TCP can no longer occur.

Appendix

The parameter a is defined by

$$a = 3D_2(q_0 D_1 + 1 - q_0)^2 F(x)|_{x=0} \tag{A1}$$

where q_0 is the solution of

$$q_0 = (q_0 D_1 + 1 - q_0)^3 H(x)|_{x=0}. \tag{A2}$$

The parameter b is defined by

$$b = [6q_1 D_2(D_1 - 1)(q_0 D_1 - 1 - q_0) + D_2^3]F(x)|_{x=0} \tag{A3}$$

where

$$q_1 = f/(1 - e) \tag{A4}$$

with

$$e = 3(D_1 - 1)(q_0 D_1 + 1 - q_0)^2 H(x)|_{x=0} \tag{A5}$$

$$f = 3D_2^2(q_0 D_1 + 1 - q_0) H(x)|_{x=0}. \tag{A6}$$

These coefficients can be easily calculated by applying the mathematical relation $\exp(\nu\nabla)\phi(x) = \phi(x + \nu)$.

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