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Ising model with competing random decorating D vector spins†

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Abstract. The Ising model on the square lattice decorated with random annealed diluted competing D vector bond spins is studied. The exact phase diagrams of the critical temperature plotted against the concentration and the critical temperature plotted against the competing parameter are evaluated analytically and presented. Re-entrant behaviour for the ferromagnetic and the antiferromagnetic phases is observed for definite range of values of the concentration. A new bond percolation threshold equal to $p_c^+ = \frac{1}{2}(1+1/\sqrt{2}) = 0.8535\ldots$ is achieved when local competing interactions are present in the system. Moreover p_c^+ is independent of the dimensionality (D) of the decorating spins and therefore independent of the physical origin of the interactions, as it should be. In particular the $D=1$ (Ising), $D=2$ (XY), $D=3$ (Heisenberg) and $D\to\infty$ cases are analysed.

1. Introduction

Disorder and competing interactions are very important ingredients in the current studies of random dilute magnets. Disorder and competing interactions can be introduced by randomly decorating the spin system with competing bond spins. Decorated Ising spin models have been studied for a long time (see, for example, Syozi (1972) for a general reference) but without considering the two ingredients together. For example, the annealed disorder has been considered by Syozi and Miyazima (1966) in the study of the critical temperature of several random diluted decorated Ising models. Kasai *et al* (1969) and Kasai and Syozi (1973) have also investigated the square lattice Ising model decorated with random annealed arrangements of ferromagnetic and antiferromagnetic bonds.

Moreover the phase diagram of the annealed diluted version of the decorated q-state Potts model on the square lattice has also been solved exactly by Wu (1980). Furthermore, Falk (1980) has studied the annealed one- and two-dimensional Ising models decorated with planar XY spins. However, Shukla and Wortis (1980) and Grest (1980), in an attempt to describe the spin-glass behaviour of iron-rich Fe–Al alloys, have studied the quenched disordered spin model, due to Sato and Arrott (1959), by considering the disorder sublattice as decorating the regular one. Also, De'Bell (1980) has proposed a simple annealed bond-decorated Ising model to illustrate the frustation effects found in simple cubic amorphous Ising antiferromagnets, which show a behaviour similar to that discussed in the present paper. On the other hand,

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competing interactions without disorder in decorated models have been considered by several authors. Nakano (1968) and Hattori and Nakano (1968) have introduced the competing interactions in order to study the magnetic and thermal properties of the square lattice antiferromagnetic decorated Ising model in the presence of a magnetic field. Huse *et al* (1981), motivated by the studies of the axial next-nearest-neighbour Ising (ANNNI) model, have investigated the so-called 'mock' ANNNI model by decorating the square lattice Ising model with a finite sequence of competing Ising bond spins along one particular direction. Very recently, Selke and Wu (1986) generalised this latter model replacing the Ising spins by q-state Potts variables. Axial competing interactions in the square lattice Ising model have also been considered by dos Santos *et al* (1986) by decorating the bonds with classical D-dimensional vector spins. The phase diagram and thermodynamic properties of this latter model have been evaluated exactly for a general D-dimensional model even in the $D \to \infty$ limit. The phase diagram of the isotropic version of this model has also been studied by Gonçalves and Horiguchi (1984).

In the present paper we study the square lattice Ising model decorated with randomly annealed D vector bond spins. We assume that the bond vector spins do not interact with each other and only interact ferromagnetically with their nearest-neighbour site Ising spins. Therefore they can be replaced by an effective ferromagnetic interaction between the site spins. Actually, the present model is the general version of the model studied by De'Bell (1980) which corresponds to the $D = 1$ particular case. This effective interaction is temperature and field dependent as has been pointed out by dos Santos *et al* (1986). If we assume that the Ising spins interact antiferromagnetically our model is equivalent to a square lattice antiferromagnetic Ising model with a random annealed distribution of additional effective ferromagnetic bonds. For certain values of the coupling constants this effective ferromagnetic interaction can be compared with the original homogeneous antiferromagnetic one and the competing effects come in to play in the system in a random way. However, for annealed distribution of bond spins these effects do not induce the appearance of the spin-glass phase since the randomness of the decorating bond spins is allowed to adjust itself so that the system achieves genuine thermodynamic equilibrium (Thorpe and Beeman 1976). On the other hand, the phase diagram shows an abrupt change in the stability of the ground-state phases at a given concentration and the appearance of re-entrants in both ferromagnetic and antiferromagnetic lines. The relation of the re-entrant phenomena and the ground-state degeneracy is a consequence of the presence of the competing interactions in the model Hamiltonian as has been studied by Kitatani *et al* (1986) for systems with competing periodic nearest-neighbour interactions. However, in the present model the randomness of the competing interaction introduces a new mechanism for the balance of the stability of the ground-state degeneracy.

In § 2 we present and solve the model Hamiltonian by evaluating exactly the phase diagrams which are discussed in § 3. The conclusions are summarised in § 4.

2. The model Hamiltonian and the solution

We consider a pure antiferromagnetic Ising model on the square lattice with nearest-neighbour exchange interactions of coupling constant J_2 ($J_2 < 0$) which is randomly decorated with classical D vector bond spins $\boldsymbol{S}$ of magnitude λ. When they are present the decorating bond spins interact with their nearest-neighbour site spins σ (Ising spins) by means of a ferromagnetic exchange interaction of coupling constant J_1 ($J_1 > 0$) through the S^1 component along the particular Ising direction, say direction one, where S^ν is the $\boldsymbol{S}$ component along the νth direction ($\nu = 1, 2, \ldots, D$). In figure 1 a portion of the lattice is shown with the sketch of the exchange interactions.

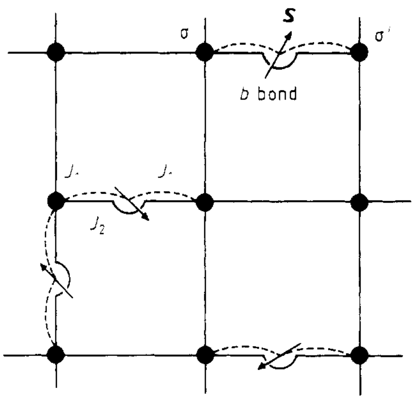

Figure 1. Portion of the square lattice for a given distribution of decorating bond spins with the exchange interactions. ●, Ising spins; ↑, D vector bond spins; (——), antiferromagnetic; (- - - -), ferromagnetic interactions.

The Hamiltonian of the system can be written as $H = \Sigma_b H_b$, H_b being the Hamiltonian for a particular b bond of the lattice, i.e.

$$H_b = -J_1 t_b S_b^1(\sigma + \sigma') - J_2\sigma\sigma' - \delta t_b \tag{1}$$

where t_b is the occupation variable for the decorating bond spin $\boldsymbol{S}_b$, i.e. $t_b = 1(0)$ if the b bond is decorated (undecorated) and δ is the chemical potential related with the annealing dilution of the decorating bond spins.

The partition function of the system is given by

$$Z = \operatorname{Tr} \exp(-\beta H) \tag{2}$$

where $\beta = (K_B T)^{-1}$, T being the temperature and K_B the Boltzmann constant as usual. Tr means the trace (sum) over all configurations allowed by the set of independent variables $\{\sigma, \boldsymbol{S}, t\}$. The sums over the decorating spin bond variables $\{\boldsymbol{S}, t\}$ can be evaluated by using the method of the decoration transformation (Syozi 1972). This can be done for a given bond b, since they are independent, by writing

$$\operatorname{Tr}_{\{S\}} \operatorname{Tr}_{\{t_b\}} \exp(-\beta H_b) = f_b \exp(K_{\text{eff}}\sigma\sigma') \tag{3}$$

where K_{eff} is the reduced effective coupling constant and f_b is the normalising factor to be determined. The sum over the decorating D vector spins $\boldsymbol{S}$ can be performed using the approach of Stanley (1969) (see also dos Santos *et al* (1986) for a more detailed calculation). If we also perform the trace of the occupation number discrete variables t we obtain

$$K_{\text{eff}}(K_1, K_2, \eta) = K_2 + \tfrac{1}{2}\ln\left(\frac{1 + \eta G_n(2\lambda K_1)}{1 + \alpha_n \eta}\right) \tag{4}$$

$$f(K_1, \eta) = \{[1 + \eta G_n(2\lambda K_1)](1 + \alpha_n \eta)\}^{1/2} \tag{5}$$

where $\eta = \exp(\beta\delta)$ is the related fugacity, $K_i = \beta J_i$ $(i = 1, 2)$, $n = (\frac{1}{2}D - 1)$, $\alpha_n = 1 + \delta_{n,-1/2}$ ($\delta_{n,n'}$ being the Kronecker delta function) and

$$G_n(x) = 2^n \Gamma(n+1)\alpha_n x^{-n} I_n(x) \tag{6}$$

$\Gamma(n)$ being the gamma function and $I_n(x)$ being the modified Bessel function of the first kind of order n.

Now the partition function can be written as

$$Z_N = f^{2N}(K_1, \eta) Z_0(K_{\text{eff}}) \tag{7}$$

where N is the lattice number of sites and $Z_0(K_{\text{eff}})$ is the partition function of the isotropic square lattice Ising model with a nearest-neighbour effective exchange interaction of coupling constant $J_{\text{eff}} = \beta^{-1} K_{\text{eff}}$. Therefore the free energy per site has an extra term proportional to $\ln f$. Nevertheless the transition temperatures are not affected since f is an analytical function of T. The transition temperatures are given by the well known Onsager solution (Onsager 1944)

$$\sinh 2K_{\text{eff}}(K_1, K_2, \eta) = \pm 1. \tag{8}$$

The sign $+(-)$ in (8) holds for the ferromagnetic (antiferromagnetic) critical temperature boundaries. The phase diagram $T_c \times p$ (critical temperature plotted against concentration of decorating bonds) can be obtained analytically from (8). The concentration or the fraction of occupied decorating bonds is related to the chemical potential. Since p is the average value of t per bond we can write

$$\begin{aligned} p = \langle t_b \rangle &= \lim_{N\to\infty} \frac{1}{2N} \frac{\partial}{\partial(\beta\delta)} \ln Z \\ &= \frac{\partial}{\partial(\beta\delta)} \ln f + \varepsilon \frac{\partial K_{\text{eff}}}{\partial(\beta\delta)} \end{aligned} \tag{9}$$

where

$$\varepsilon = \langle \sigma\sigma' \rangle = \lim_{N\to\infty} \frac{1}{2N} \frac{\partial}{\partial K_{\text{eff}}} \ln Z_0(K_{\text{eff}}) \tag{10}$$

is the nearest-neighbour pair correlation function. After straightforward calculation we obtain

$$\eta = A[1 + (1 + 4pB/A^2)^{1/2}]/B \tag{11}$$

where

$$A = (2p-1)G_n(2\lambda K_1) - \varepsilon[G_n(2\lambda K_1) - \alpha_n] \tag{12}$$

$$B = 4\alpha_n(1-p)G_n(2\lambda K_1). \tag{13}$$

Finally, eliminating η by substituting (11)–(13) into (8) the phase diagram $T_c \times p$ is given by

$$p = \frac{1}{2}\left(1 - \frac{1}{C}\right) \frac{[G_n(2\lambda K_1)(1+\varepsilon) + \alpha_n C(1-\varepsilon)]}{G_n(2\lambda K_1) - \alpha_n} \tag{14}$$

where

$$C = (\sqrt{2} \pm 1)\exp(2\lambda\alpha K_1) \tag{15}$$

$\alpha = -J_2/\lambda J_1$ being the renormalised competing parameter. On the other hand, the phase diagram $T_c \times \alpha$ (the critical temperature plotted against the competing parameter) can be obtained analytically by inverting (8), i.e.

$$\alpha = \frac{1}{2\lambda K_1} \ln\left(\frac{1+\eta G_n(2\lambda K_1)}{(1+\alpha_n\eta)(\sqrt{2}\pm 1)}\right) \tag{16}$$

with η given by (11). We observe that to get the phase boundary in the $(T_c \times p)$ and $(T_c \times \alpha)$ phase diagrams we have to make use of the critical temperature value of the nearest-neighbour pair correlation function for the square lattice which is given by $\varepsilon = \pm 1/\sqrt{2}$, where the sign $+(-)$ holds for the ferromagnetic (antiferromagnetic) boundary.

3. The phase diagrams

The phase diagrams $(T_c \times p)$ and $(T_c \times \alpha)$ can be plotted from (14) and (16) where G_n is given in the table 1 for the Ising $(D=1)$, XY $(D=2)$, Heisenberg $(D=3)$ and $D \to \infty$ limit cases.

Table 1. Functions $G_n(x)$ for $n = D/2 - 1$ and $x = 2\lambda J_1/K_B T$.

D	$G_n(x) = 2^n\Gamma(n+1)\alpha_n x^{-n} I_n(x)$	
1	$2\cosh x$	
2	$I_0(x)$	
3	$\sinh x/x$	
∞	$\exp(2\bar{x}^2)$	$\bar{x} = J_1/K_B T$

3.1. *Critical temperature against concentration diagrams*

In figure 2 we show the diagram $(T_c \times p)$ for $D = 1, 2, 3$ and ∞ for several values of the competing parameter. We observe the appearance of both the ferromagnetic and the antiferromagnetic phases for $0 < \alpha < 1$. In this range of values of the competing parameter the zero-temperature critical concentration is given by $p_c^{\pm} = \frac{1}{2}(1 \pm 1/\sqrt{2})$ when the sign $+(-)$ gives the ferromagnetic (antiferromagnetic) critical concentration. Moreover the ferromagnetic boundaries for $0 < \alpha < 1$ are bounded by the $\alpha = 0$ line which happens when the homogeneous antiferromagnetic interaction between the site spins vanishes. In this latter case the system behaves like a bond-diluted ferromagnet with the exact $\frac{1}{2}$ critical concentration at $T = 0$ (percolation concentration) for the square lattice. Furthermore, for $\frac{1}{2} < p < p_c^+$, the ferromagnetic boundaries show a re-entrant behaviour with two critical temperatures for a given concentration due to the competing effects introduced by the decoration. However, for $p > p_c^+$ the re-entrant behaviour disappears since the effective interaction becomes strong enough to stabilise the ferromagnetic order at low temperature. On the other hand, the antiferromagnetic boundaries also show the re-entrant behaviour for $0 < \alpha < 1$, but within a D-dependent range of values of p, i.e. $p_c^- < p < p_c^+$ for $D = 1$, $p_c^- < p < 1$ for $D > 1$ and $p_c^- < p < \infty$ for $D = \infty$.

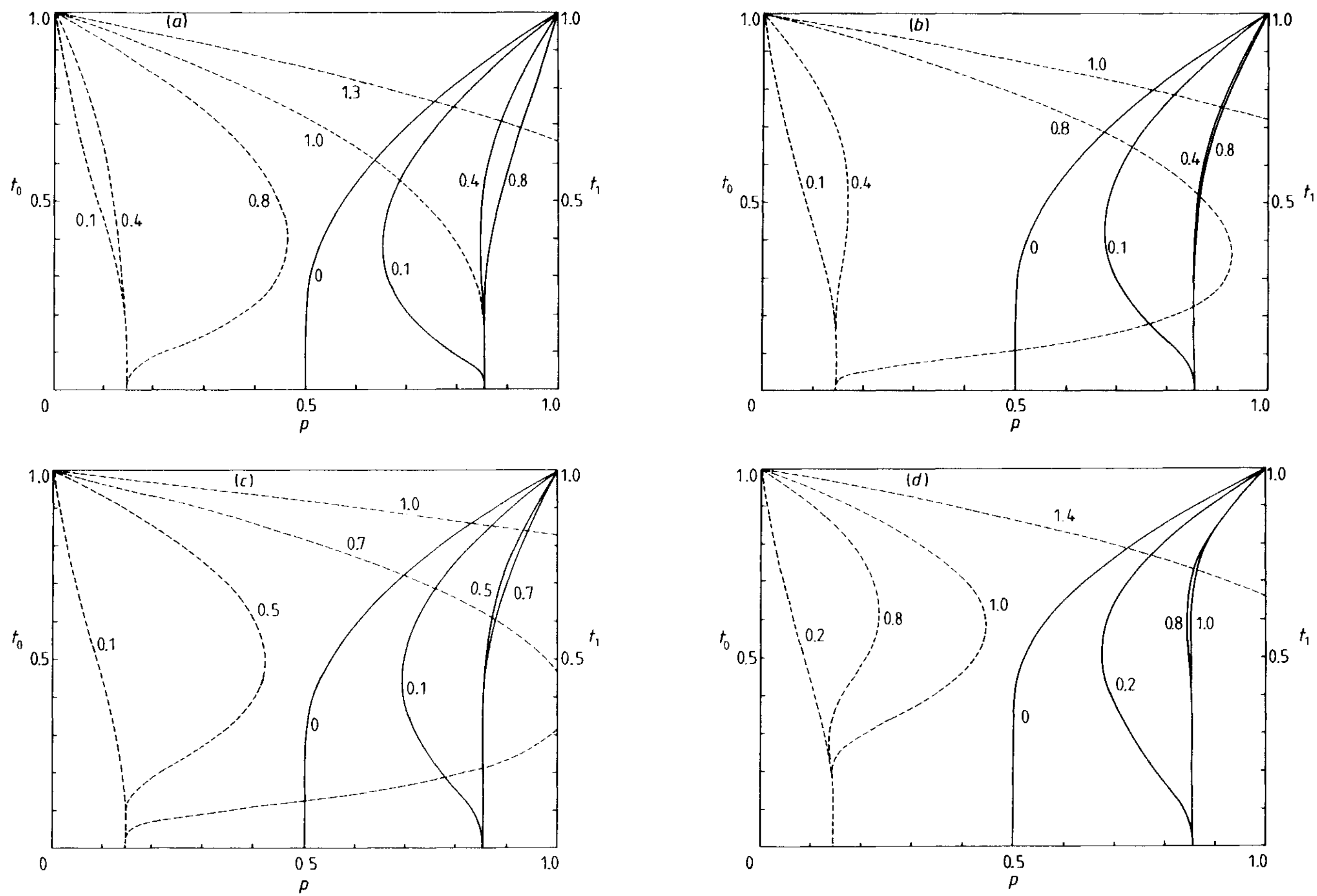

Figure 2. Normalised critical temperatures (t_0, t_1) plotted against concentration p for (a) $D = 1$ (Ising), $\alpha = 0$, 0.1, 0.4, 0.8, 1.0 and 1.3; (b) $D = 2$ (XY), $\alpha = 0$, 0.1, 0.5, 0.8, 1.0; (c) $D = 3$ (Heisenberg), $\alpha = 0$, 0.1, 0.4, 0.7, 1.0, (d) $D = \infty$, $\bar{\alpha} = 0$, 0.1, 0.8, 1.0, 1.4 (- - - -) antiferromagnetic and (——) ferromagnetic boundaries. $t_0 = T_{c\alpha}(p)/T_{c\alpha}(0)$, $t_1 = T_{c\alpha}(p)/T_{c\alpha}(1)$.

For $\alpha \geqslant 1$ the ferromagnetic order is no longer stable since at $T=0$ the Ising spins order antiferromagnetically while the decorating bond spins remain uncorrelated as has been pointed out by dos Santos *et al* (1986).

We observe that all lines shown in figure 2 are normalised with different scaling factors, i.e. with the critical temperature for the α at $p=0(1)$ for the antiferromagnetic (ferromagnetic) lines, respectively. Therefore there is no real cross between the ferromagnetic and antiferromagnetic lines for a given α, as is apparent in figures 2(*b*) and (*c*).

3.2. *Critical temperature against competing parameter diagrams*

The $T_c \times \alpha$ diagrams are shown in figure 3 for several values of p and for $D=1, 2, 3$ and ∞. In these diagrams the abrupt change in the re-entrant behaviour of both the ferromagnetic and the antiferromagnetic lines are evidenced as the concentration approaches to $p_c^{\pm}$ from the left or from the right. For $p=1$ we recover the result of dos Santos *et al* (1986) for the pure isotropic decorated Ising model on the square lattice while for $\alpha=0$ (absence of decoration) we get the pure antiferromagnetic behaviour for the critical temperature. We note that for $D\to\infty$ the antiferromagnetic phase is no longer stable at $T=0$ while the ferromagnetic phase is stable only for $p>p_c^+$.

4. Conclusions

We have studied the critical temperature of the antiferromagnetic Ising model on the square lattice decorated with annealed random diluted D vector bond spins. The analytical expressions of the phase diagrams, critical temperature against concentration ($T_c \times p$) and critical temperature against competing ($T_c \times \alpha$) paiameter have been obtained exactly by mapping the present model with the Onsager solution. These phase diagrams are shown for the Ising ($D=1$), XY ($D=2$), Heisenberg ($D=3$) and the $D\to\infty$ limit cases of the spin dimensionality of the decorating bond spin. The $T_c \times p$ phase diagram is presented in figure 2 showing the appearance of a re-entrant behaviour for both the ferromagnetic and the antiferromagnetic phases for a given α ($0<\alpha<1$) and for a definite range of values of the concentration. For the ferromagnetic phase this range is independent of D, i.e. $\frac{1}{2}<p<p_c^+=0.8535\ldots$, while for the antiferromagnetic phase this range of values is equal to $p_c^-=0.1464\ldots<p<p_c^+=0.8535\ldots$ for $D=1$ and $p_c^-=0.1464\ldots<p<1$ for $D>1$. In figure 3 we have presented the $T_c \times \alpha$ diagrams for several values of p in which is evidenced the abrupt change in the behaviour of the re-entrant boundaries when the concentration becomes greater (smaller) than $p_c^+(p_c^-)$ for the ferromagnetic (antiferromagnetic) phases.

In conclusion we point out that the existence of re-entrant behaviour is a consequence of the presence of local diluted competing effects in the system which has been introduced in the present model by decoration. The same conclusion has also been found by Coutinho *et al* (1987) for another model in which the local competing effects are generated by an antiferromagnetic site-bond correlated random dilution. The quenched diluted decorating version of the present model for hypercubic lattices, which is now being studied by one of us (SC) in the framework of the mean-field-like renormalisation group, shows in addition to the re-entrant behaviour the appearance of the spin-glass phase, as we can anticipate.

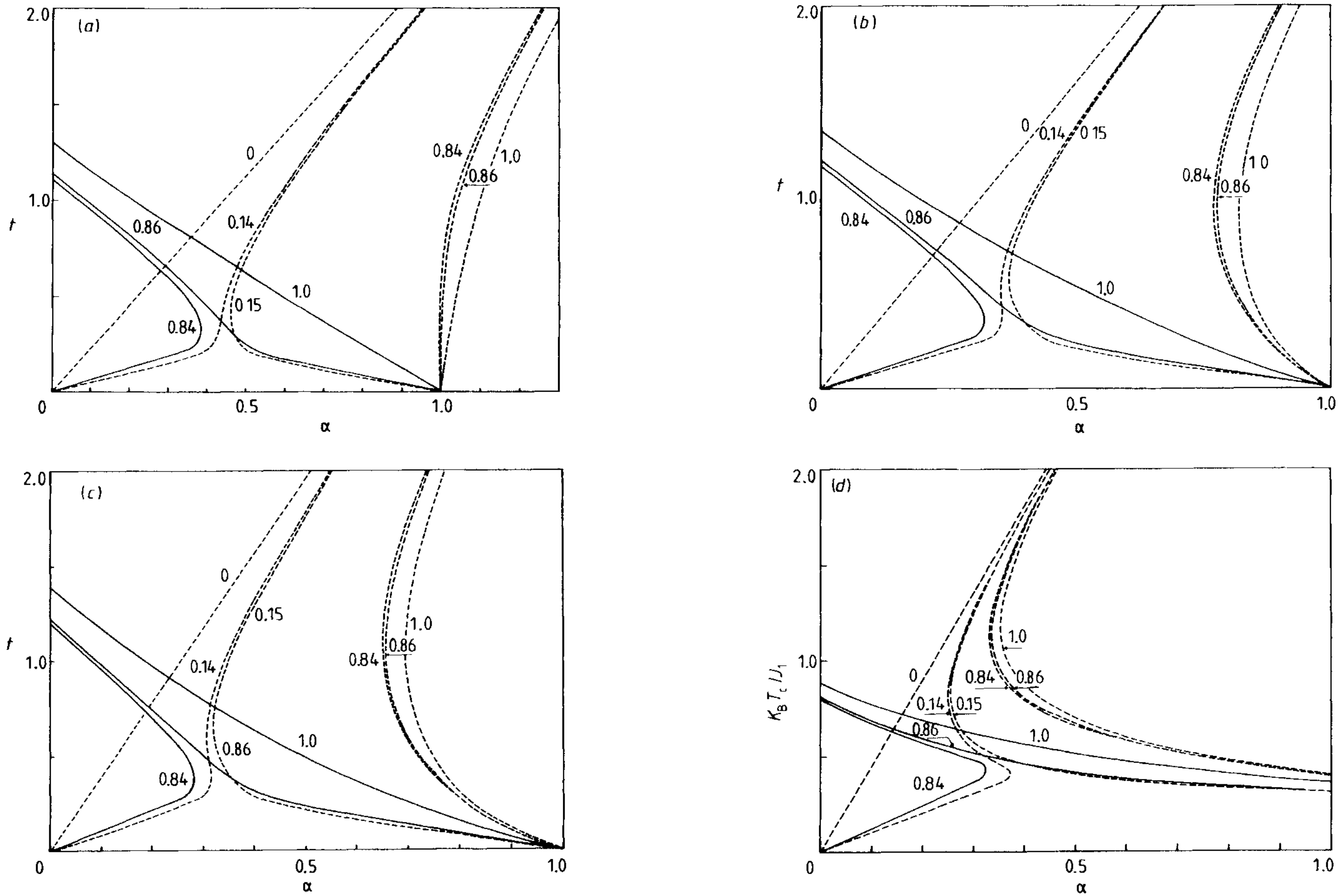

Figure 3. Reduced critical temperature (t) plotted against competing parameter (α, $\bar{\alpha}$) (a) $D=1$ (Ising), (b) $D=2$ (XY), (c) $D=3$ (Heisenberg) and $D=\infty$ for $p=0$, 0.14, 0.15, 0.84, 0.86, 1.0 (----) antiferromagnetic and (——) ferromagnetic boundaries. $t = K_B T_c/J_1$.

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