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The diluted random field mixed spin Ising model: thermodynamical properties

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Abstract

The diluted mixed spin Ising system consisting of spin-$\frac{1}{2}$ and spin-1 with a random field is studied by the use of the finite cluster approximation within the framework of a single-site cluster theory. The state equations are derived using a probability distribution method based on the use of Van der Waerden identities. In this approach, the complete phase diagrams are investigated for the simple cubic lattice, when the random field is bimodally and trimodally distributed. The internal energy, specific heat and susceptibility are also calculated for both kinds of probability distributions.

1. Introduction

The random field Ising model (RFIM) on mono-atomic lattices, where the local quenched random field H_i is assumed to have zero average $\langle H_i \rangle_r = 0$ and is uncorrelated at different sites, has been the subject of much theoretical [1–4] and experimental [5, 6] investigation of the statistical physics of random and frustrated systems. The best experimental realization of a RFIM has been the diluted uniaxial antiferromagnet in a uniform field applied along the spin ordering axis (DAFF), such as $Rb_2Co_xMg_{1-x}F_4$ and $Fe_xZn_{1-x}F_2$ in a magnetic field, which correspond, respectively, to two-and three-dimensional prototypical systems. It has been shown [7, 8] that, in the presence of a uniform field, the random exchange interactions give rise to local random staggered fields and that such a system should be isomorphic to the RFIM. Indeed, many experiments on DAFF's have confirmed some of the theoretical predictions derived for the RFIM [9]. Recently, it has been shown experimentally [10] and through Monte Carlo (MC) simulations [11] that $Fe_xZn_{1-x}F_2$ in an applied uniform field exhibits the equilibrium critical behaviour of the RFIM for a magnetic concentration $x > 0.75$. The RFIM can also be used to describe other processes as the phase separation of a two-component fluid mixture in porous material or gelatine and a solution of hydrogen in metallic alloys [12]. Recent

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experiments on the liquid–vapour transition in aerogel [13] reveal a coexistence curve similar to the pure Ising model but slow dynamics suggestive of random field effects. Because the aerogel creates a random network which attracts the fluid, the RFIM should be an appropriate model [14] for this system.

One of the main points on which attention has been focused is the lower critical dimension d_l. This is the dimension above which long range order ferromagnetic order can exist. It has been shown rigorously that the low temperature phase in $d > 2$ is ferromagnetic [15–17], which means that $d_l = 2$. Also, experiments support the existence of long range order in the three-dimensional RFIM (for instance in $Fe_xZn_{1-x}F_2$) [18–20] while such order does not exist in $d = 2$ RFIM (for instance, in $Rb_2Co_xMg_{1-x}F_4$) [21].

Other important questions concerning the RFIM have been the existence of a tricritical point and the order of low-temperature phase transitions in three dimensions. This seems not to be completely elucidated. Indeed, mean-field theories [22–24] predicted that the existence of a tricritical point depends on the form of the random field distribution. In particular, the bimodal distribution ($\pm H$) yields a tricritical point and the transition was found to be of first order for sufficiently strong random fields, while the Gaussian one led to a second-order phase transition down to $T = 0$. Using renormalization group calculations [25, 26], it has been discussed that, with an appropriate distribution function, it may lead to a tricritical point. Houghton *et al* [27, 28] have performed detailed numerical studies based on the analysis of the high temperature series for the static susceptibility of the RFIM with bimodal and Gaussian distributions. They confirmed the predictions of the mean-field theory for $d \geqslant 4$. In dimensions $d < 4$, however, the analysis suggests that, even for a Gaussian distribution, fluctuation-driven first-order transitions have been observed at low temperatures (sufficiently strong random fields), implying that $d = 4$ is a critical dimension for the RFIM. Furthermore, MC results of RFIM with a bimodal distribution have been either inconclusive (some were interpreted in support of a first-order transition at finite low temperature [29], while others favoured a continuous transition [11, 30]) or suggest an unusual behaviour [31] (jump in the order parameter but with an infinite correlation length at the transition). We have to point out here that the experiments [18–20, 32] on diluted MnF_2 are difficult to clearly interpret but are suggestive of a first-order transition. We note that there is no general consensus, experimentally, on whether the transition is continuous or first order.

On the other hand, some authors [33] have studied the case of a spin-S ($>\frac{1}{2}$) Ising model in a random field within mean-field-like approximations for a bimodal distribution. They have predicted a long-range order at $T = 0$ up to an S-dependent critical value of the field H, and the existence of a tricritical point. Such a model for any S in a random field, which is trimodally distributed, has also been investigated within the mean-field theory [34]. The obtained phase diagram is qualitatively similar to that found earlier [35] for spin-$\frac{1}{2}$ and it exhibits a rich multicritical behaviour. In the limit of very large values of S, the results go asymptotically to ones obtained for the classical ($S \to \infty$) model.

Recently, attention has been directed to the study of the magnetic properties of two-sublattice mixed spin Ising systems. They are of interest for the following main reasons. They have less translational symmetry than their single spin counterparts, and are well adapted for studying a certain type of ferrimagnetism [36]. Experimentally, it has been shown that the MnNi(EDTA)–$6H_2O$ complex is an example of a mixed spin system [37]. The mixed Ising spin system consisting of spin-$\frac{1}{2}$ and spin-1 has been studied by different methods [38–43]. The effect of dilution on the phase diagrams of these kinds of systems are also investigated by various techniques [39, 42, 44].

Since the mono-atomic RFIM exhibits very interesting phase diagrams, it is worth investigating the two-sublattice mixed spin Ising system in a random longitudinal field [45].

This latter system can be described by the following Hamiltonian:

$$H = -\sum_{\langle ij\rangle} J_{ij}\sigma_i S_j - \sum_i H_i\sigma_i - \sum_j H_j S_j \tag{1}$$

where σ_i and S_j are Ising spins of magnitude $\frac{1}{2}$ and S at sites i and j, respectively. J_{ij} is the exchange interaction, H_i and H_j are the random fields and the first summation is carried out only over nearest-neighbour pairs of spins.

The first purpose of this paper is to investigate the effects of site dilution on the phase diagram of the system described by the Hamiltonian (1) when the fields H_i and H_j are assumed to be uncorrelated variables and obey the following symmetric ($Q(H) = Q(-H)$) probability distribution:

$$Q(H_i) = p\delta(H_i) + \frac{(1-p)}{2}[\delta(H_i - H) + \delta(H_i + H)] \tag{2}$$

where the parameter p measures the fraction of spins in the system not exposed to the field. This system can be described by (1) in which we introduce the site occupancy number ξ_i which takes 0 or 1, depending on whether the site is occupied or not. Thus the Hamiltonian of such a system takes the form

$$H = -\sum_{\langle ij\rangle} J_{ij}\xi_i\xi_j\sigma_i S_j - \sum_i H_i\xi_i\sigma_i - \sum_j H_j\xi_j S_j. \tag{3}$$

In the present work, we limit ourselves to the case $S = 1$ and $J_{ij} = J$. One notes that, at $p = 1$ or $H = 0$, the system reduces to the simple diluted mixed spin-$\frac{1}{2}$ and spin-1 Ising model [39, 42]. To this end, we use the finite cluster approximation (FCA) [46] within the framework of a single-site cluster theory. The state equations are derived using a probability distribution method [47] based on the use of generalized Van der Wearden identities [48] that account exactly for the single-site kinematic relations.

The second goal is to examined the internal energy, specific heat and zero-field magnetic susceptibility; especially when the concentration of magnetic sites is changed.

The outline of this work is as follows. In section 2, we give a description of the theoretical framework. In section 3, the phase diagrams of the system are investigated and discussed. In section 4, relevant thermodynamical quantities are presented and analysed. Finally, we comment on our results in section 5.

2. Theoretical framework

The theoretical framework we adopt in the study of the diluted random field mixed spin Ising model described by the Hamiltonian (3) is the finite cluster approximation [46] based on a single-site cluster theory. We have to mention that this method has been successfully applied to a number of interesting pure and disordered spin Ising systems [42, 44, 49]. It has also been used for transverse Ising models [50] and semi-infinite Ising systems [51, 52]. In all these applications, it was shown that the FCA improve qualitatively and quantitatively the results obtained in the frame of the mean-field theory. In this method, we consider a particular spin $\sigma_o(S_o)$ and denote by $\langle\sigma_o\rangle_c(\langle(S_o)^n\rangle_c, n = 1, 2)$ the mean value of $\sigma_o((S_o)^n)$ for a given configuration c of all other spins $\{\sigma_i, S_j; i, j \neq 0\}$ when the site occupational numbers $\{\xi_i, \xi_j\}$ and the random fields $\{H_i, H_j\}$ have fixed values. $\langle\sigma_o\rangle_c$ and $\langle(S_o)^n\rangle_c$ are then given by

$$\langle\sigma_o\rangle_c = \frac{\mathrm{Tr}_{\sigma_o}\,\sigma_o \exp(-\beta H_o^\sigma)}{\mathrm{Tr}_{\sigma_o}\exp(-\beta H_o^\sigma)} \tag{4}$$

and

$$\langle(S_o)^n\rangle_c = \frac{\mathrm{Tr}_{S_o}(S_o)^n \exp(-\beta H_o^S)}{\mathrm{Tr}_{S_o}\exp(-\beta H_o^S)} \tag{5}$$

with

$$H_o^\sigma = -\left(J \sum_{j=1}^{z} \xi_o \xi_j S_j + \xi_o H_o \right) \sigma_o \tag{6}$$

$$H_o^S = -\left(J \sum_{i=1}^{z} \xi_o \xi_i \sigma_i + \xi_o H_o \right) S_o \tag{7}$$

where z is the nearest-neighbour coordination number of the lattice and $\beta = 1/T$. Tr_{σ_o} (or Tr_{S_o}) means the partial trace with respect to the σ-sublattice site o (or S-sublattice site o). $\{S_1, S_2, \ldots, S_z\}$ ($\{\sigma_1, \sigma_2, \ldots, \sigma_z\}$) are the nearest-neighbour spins of $\sigma_o(S_o)$ with which it directly interacts. One notes that, since H_o^σ and H_o^S depend on ξ_o ($\xi_o = 0$ or 1), (4) and (5) can be written in the form

$$\langle \sigma_o \rangle_c = \frac{1 - \xi_o}{2\sigma + 1} \mathrm{Tr}_o(\sigma_o) + \xi_o \frac{\mathrm{Tr}_{\sigma_o} \sigma_o \exp(-\beta \bar{H}_o^\sigma)}{\mathrm{Tr}_{\sigma_o} \exp(-\beta \bar{H}_o^\sigma)} \tag{8}$$

$$\langle (S_o)^n \rangle_c = \frac{1 - \xi_o}{2S + 1} \mathrm{Tr}_o((S_o)^n) + \xi_o \frac{\mathrm{Tr}_{S_o} (S_o)^n \exp(-\beta \bar{H}_o^S)}{\mathrm{Tr}_{S_o} \exp(-\beta \bar{H}_o^S)} \tag{9}$$

which imply

$$\langle \xi_o \sigma_o \rangle_c = \xi_o \frac{\mathrm{Tr}_{\sigma_o} \sigma_o \exp(-\beta \bar{H}_o^\sigma)}{\mathrm{Tr}_{\sigma_o} \exp(-\beta \bar{H}_o^\sigma)} \tag{10}$$

$$\langle \xi_o (S_o)^n \rangle_c = \xi_o \frac{\mathrm{Tr}_{S_o} (S_o)^n \exp(-\beta \bar{H}_o^S)}{\mathrm{Tr}_{S_o} \exp(-\beta \bar{H}_o^S)} \tag{11}$$

where

$$\bar{H}_o^\sigma = -\left(J \sum_{j=1}^{z} \xi_j S_j + H_o \right) \sigma_o,$$

and

$$\bar{H}_o^S = -\left(J \sum_{i=1}^{z} \xi_i \sigma_i + H_o \right) S_o.$$

Performing the partial traces in (10) and (11) and then the thermal average over all spin configurations, we obtain the following exact relations:

$$\langle \xi_o \sigma_o \rangle = \xi_o \langle f(\{\xi_j S_j\}, h_o) \rangle \tag{12}$$

$$\langle \xi_o (S_o)^n \rangle = \xi_o \langle F_n(\{\xi_i \sigma_i\}, h_o) \rangle \tag{13}$$

with

$$f(\{\xi_j S_j\}, h_o) = \frac{1}{2} \tanh\left[\frac{K}{2} \sum_{j=1}^{z} \xi_j S_j + \frac{h_o}{2} \right] \tag{14}$$

$$F_1(\{\xi_i \sigma_i\}, h_o) = \frac{2 \sinh\left[K \sum_{i=1}^{z} \xi_i \sigma_i + h_o \right]}{1 + 2 \cosh\left[K \sum_{i=1}^{z} \xi_i \sigma_i + h_o \right]} \tag{15}$$

$$F_2(\{\xi_i \sigma_i\}, h_o) = \frac{2 \cosh\left[K \sum_{i=1}^{z} \xi_i \sigma_i + h_o \right]}{1 + 2 \cosh\left[K \sum_{i=1}^{z} \xi_i \sigma_i + h_o \right]} \tag{16}$$

where $K = \beta J$, $h_o = \beta H_o$ and $\langle \cdots \rangle$ denotes the canonical thermal average.

The next step is to carry out the configurational averaging over the site occupational numbers ξ_i, to be denoted by $\langle \cdots \rangle_r$.

In order to perform the thermal and configurational averaging on the right-hand side of (12) and (13), we expand the functions $f(\{\xi_i S_i\}, h_o)$ and $F_n(\{\xi_i\sigma_i\}, h_o)$ as finite polynomials of S_j^z and σ_i^z, respectively, that correctly account for the single-site kinematic relations. This can conveniently be done by employing appropriate operators [48]

$$\mathrm{O}^{(\sigma)}(\sigma_i, \xi_i) = [(\sigma_i + \tfrac{1}{2})\delta_{\sigma_i,1/2} + (-\sigma_i + \tfrac{1}{2})\delta_{\sigma_i,-1/2}][\xi_i\delta_{\xi_i,1} + (1-\xi_i)\delta_{\xi_i,o}] \tag{17}$$

$$\mathrm{O}^{(S)}(S_j, \xi_j) = [\tfrac{1}{2}(S_j + (S_j)^2)\delta_{S_j,1} + \tfrac{1}{2}(-S_j + (S_j)^2)\delta_{S_j,-1} + (1-(S_j)^2)\delta_{S_j,o}] \times [\xi_j\delta_{\xi j,1} + (1-\xi_j)\delta_{\xi j,o}] \tag{18}$$

where $\delta_{A,a}$ is a forward Kronecker delta function substituting any operator A on the right by its eigenvalue a. Thus, the expansions of (14)–(16) are then given by

$$f(\{\xi_j S_j\}, h_o) = \prod_j \mathrm{O}^{(S)}(S_j, \xi_j) f(\{\xi_j S_j\}, h_o) \tag{19}$$

$$F_n(\{\xi_i\sigma_i\}, h_o) = \prod_i \mathrm{O}^{(\sigma)}(\sigma_i, \xi_i) F_n(\{\xi_i\sigma_i\}, h_o). \tag{20}$$

In order to carry out the thermal and site disorder configurational averaging, we have to deal with correlation functions. We note that FCA has been designed to treat all spin self-correlations exactly, while mean-field approximation neglects all spin correlations including self-correlations. In this paper, we consider the simplest approximation by neglecting correlations between quantities pertaining to different sites, but we include the correlation between the site disorder and the local configurational-dependent thermal averages [53] of the spin and use the exact identities

$$\langle\langle(1-\xi_o)(S_o)^n\rangle\rangle_r = \frac{1-c}{2S+1}\,\mathrm{Tr}_o((S_o)^n) \tag{21}$$

$$\langle\langle(1-\xi_o)\sigma_o\rangle\rangle_r = \frac{1-c}{2\sigma+1}\,\mathrm{Tr}_o(\sigma_o) \tag{22}$$

which are directly derived from (8)–(11). c denotes the average site concentration defined by $c = \langle\xi\rangle_r$. Doing this we find

$$\langle\langle f(\{\xi_j S_j\}, h_o)\rangle\rangle_r = \prod_{j=1}^{z}\Bigg[\sum_{S_j=-1}^{+1}\sum_{\xi_j=o}^{1} P(S_j, \xi_j)\Bigg] f(\{\xi_j S_j\}, h_o) \tag{23}$$

$$\langle\langle F_n(\{\xi_i\sigma_i\}, h_o)\rangle\rangle_r = \prod_{i=1}^{z}\Bigg[\sum_{\sigma_i=-1/2}^{+1/2}\sum_{\xi_i=o}^{1} R(\sigma_i, \xi_i)\Bigg] F_n(\{\xi_i\sigma_i\}, h_o) \tag{24}$$

with

$$P(S_j, \xi_j) = \sum_{I_1=-1}^{+1}\sum_{I_2=o}^{1} a(I_1, I_2)\delta_{S_j,I_1}\delta_{\xi_j,I_2} \tag{25}$$

$$R(\sigma_i, \xi_i) = \sum_{k_1=-1/2}^{+1/2}\sum_{k_2=o}^{1} b(k_1, k_2)\delta_{\sigma_i,k_1}\delta_{\xi_i,k_2} \tag{26}$$

where

$$a(\pm1, 1) = \tfrac{1}{2}(\pm m_{S1} + m_{S2}), \quad a(0,1) = (c - m_{S2}), \quad a(I_1, 0) = \tfrac{1}{3}(1-c) \tag{27}$$

$$b\left(\frac{\pm1}{2}, 1\right) = \left(\frac{c}{2} \pm \mu_\sigma\right), \quad b\left(\frac{\pm1}{2}, 0\right) = \frac{1}{2}(1-c) \tag{28}$$

where $\mu_\sigma = \langle\langle\xi_i\sigma_i\rangle\rangle_r$ and $m_{Sn} = \langle\langle\xi_j(S_j)^n\rangle\rangle_r$.

Since the field is randomly distributed, we have to perform the random average of H_i according to the probability distribution function $Q(H_i)$ given by (2). The ordering parameters μ and m_n are then defined as $\mu = \overline{\mu_\sigma}$ and $m_n = \overline{m_{Sn}}$, where the bar denotes the random field average. Thus, using (12), (13) and (23)–(26), we obtain the following set of coupled equations for μ and m_n:

$$\mu = c \sum_{I_1=-1}^{+1} \cdots \sum_{I_z=-1}^{+1} \sum_{\xi_1=o}^{1} \cdots \sum_{\xi_z=o}^{1} \left[\prod_{j=1}^{z} a(I_j, \xi_j) \right] \bar{f}(\{\xi_1 S_1(I_1), \ldots, \xi_z S_z(I_z)\}, p, h) \tag{29}$$

$$m_n = c \sum_{k_1=-1/2}^{+1/2} \cdots \sum_{k_z=-1/2}^{+1/2} \sum_{\xi_1=o}^{1} \cdots \sum_{\xi_z=o}^{1} \left[\prod_{i=1}^{z} b(k_i, \xi_i) \right] \bar{F}_n(\{\xi_1 \sigma_1(k_1), \ldots, \xi_z \sigma_z(k_z)\}, p, h) \tag{30}$$

where μ_σ and m_{Sn} in (27) and (28) are replaced by μ and m_n, respectively, and

$$\bar{f}(x, p, h) = \int Q(H_o) f(x, \beta H_o) \, \mathrm{d}H_o$$

$$\bar{F}_n(x, p, h) = \int Q(H_o) F_n(x, \beta H_o) \, \mathrm{d}H_o$$

with $h = \beta H$, $S_j(I) = I$ and $\sigma_i(k) = k$. It is advantageous to carry out further algebraic manipulations on (29) and (30) in order to transform their right-hand sides to an expansion with respect to m_n (or μ) which is suitable for the study of the present system, even in the vicinity of the critical temperature. To this end, we follow the procedure used by two of us (NB and AF) in the case of a mixed spin Ising model [54]. Doing this, we obtain

$$\mu = c \sum_{n_1=o}^{z} \sum_{n_2=o}^{z-n_1} \sum_{i_1=o}^{n_1} \sum_{i_2=o}^{n_2} 2^{-n_1-n_2} C_z^{n_1} C_{z-n_1}^{n_2} C_{n_1}^{i_1} C_{n_2}^{i_2} (-1)^{i_2} (m_1)^{i_1+i_2} (m_2)^{n_1+n_2-i_1-i_2} \times (1-m_2)^{z-n_1-n_2} \bar{f}(K(n_1-n_2), p, h) \tag{31}$$

and

$$m_n = c \sum_{n_1=o}^{z} \sum_{n_2=o}^{z-n_1} \sum_{i_1=o}^{n_1} \sum_{i_2=o}^{n_2} 2^{-n_1-n_2+i_1+i_2} C_z^{n_1} C_{z-n_1}^{n_2} C_{n_1}^{i_1} C_{n_2}^{i_2} (-1)^{i_2} (c)^{n_1+n_2-i_1-i_2} (\mu)^{i_1+i_2} \times (1-c)^{z-n_1-n_2} \bar{F}_n\left(\frac{K}{2}(n_1-n_2), p, h\right) \tag{32}$$

where C_n^p are the binomial coefficients $n!/[p!(n-p)!]$. Relations (31) and (32) are the state equations within the one-spin cluster approximation, which can be called the first-order approximation. Higher-order FCA can be defined as follows: we define the second-order approximation for $\langle\sigma_o\rangle_c(\langle(S_o)^n\rangle_c)$ performing the traces over $\sigma_o(S_o)$ and its first neighbours $\{\sigma_1, \sigma_2, \ldots, \sigma_z\}(\{S_1, S_2, \ldots, S_z\})$, all other spins and all occupational numbers and random fields having fixed values. The obtained expression for $\langle\sigma_o\rangle_c(\langle(S_o)^n\rangle_c)$ in this case will depend only on the external first neighbours of the spins belonging to the border of the cluster $\{\sigma_1, \sigma_2, \ldots.\sigma_z\}(\{S_1, S_2, \ldots, S_z\})$. Following the same procedure for the thermal and configurational averaging as we did for the first-order approximation, and then performing the random average of H_i, we obtain the state equations within the $(z+1)$-spin cluster approximation. Convergence of successive higher approximations has been studied [55] for the two-dimensional site dilute Ising model and it was shown that the critical temperature $T_c(c=1)$ and the site percolation threshold c^* are in better agreement with the exact ones. For our purpose in this paper, we do not need to go beyond the one-spin cluster approximation.

3. Phase diagrams

We are first interested in investigating the phase diagram of the system described by the Hamiltonian (3). Let us first write (31) and (32) for m_1 in the following form:

$$\mu = A_1(K, p, c, h, m_2)m_1 + B_1(K, p, c, h, m_2)(m_1)^3 + \cdots \tag{33}$$

$$m_1 = A_2(K, p, c, h)\mu + B_2(K, p, c, h)(\mu)^3 + \cdots \tag{34}$$

where $A_i, B_i, \ldots (i = 1, 2)$ are obtained from (31) and (32) by choosing the appropriate corresponding combinations of indices $i_j (j = 1, 2)$. Substituting m_1 and m_2 in (31) with their expression taken from (32) we obtain an equation for μ of the form

$$\mu = a\mu + b\mu^3 \cdots \tag{35}$$

where

$$a = A_1 A_2 \tag{36}$$

and

$$b = A_1 B_2 + B_1 (A_2)^3. \tag{37}$$

The second-order transition is then determined by the equation

$$1 = A_1(K, p, c, h, m_2^c)A_2(K, p, c, h) \tag{38}$$

where m_2^c is the solution of equation (32) for $\mu \to 0$, namely

$$m_2^c = c \sum_{n_1=o}^{z} \sum_{n_2=o}^{z-n_1} C_z^{n_1} C_{z-n_1}^{n_2} 2^{-n_1-n_2} (c)^{n_1+n_2} (1-c)^{z-n_1-n_2} \bar{F}_2\left(\frac{K}{2}(n_1 - n_2), p, h\right). \tag{39}$$

The magnetization μ in the vicinity of the second-order transition is given by

$$\mu^2 = \frac{1-a}{b}. \tag{40}$$

The right-hand side of (40) must be positive. If this is not the case, the transition is of first order. In the (T, H) plane and for a given concentration of the magnetic sites, the point at which $a = 1$ and $b = 0$ characterizes the tricritical point.

3.1. The undiluted system

First, let us examine the phase diagram of the undiluted case ($c = 1$) for the simple cubic lattice ($z = 6$). In figure 1, we represent the phase diagram in the (T, H) plane for various values of p. For $p = 1$ (or $H = 0$), the system reduces to the three-dimensional mixed spin-$\frac{1}{2}$ and spin-1 Ising model, which exhibits a transition at a reduced critical temperature K_c. Comparing with the MC value $K_c = 0.526$ [56], the FCA result (0.4736) improves the mean-field approximation value (0.4082). When the random field is bimodally distributed ($p = 0$), the critical temperature decreases gradually from its value $T_c (H = 0)$ in the mixed spin system, to end in a tricritical point. As shown in the figure, when we consider a trimodal random field distribution (i.e. $p \neq 0$), the system keeps a tricritical behaviour for a relatively small range of p ($0 \leqslant p \leqslant 0.2899$). The T component of the tricritical point decreases with increasing values of p and vanishes at $p = 0.2899$. So, a vestigial point which exists in the mono-atomic RFIM [35] does not occur in the random field mixed spin Ising model. When p belongs to the range $0.2899 < p \leqslant 1$, the tricritical behaviour disappears and all transitions are always of second order for any value of the field H. Moreover, we note the existence of a critical value $p^* = 0.5259$, indicating two qualitatively different behaviours of the system which depend on

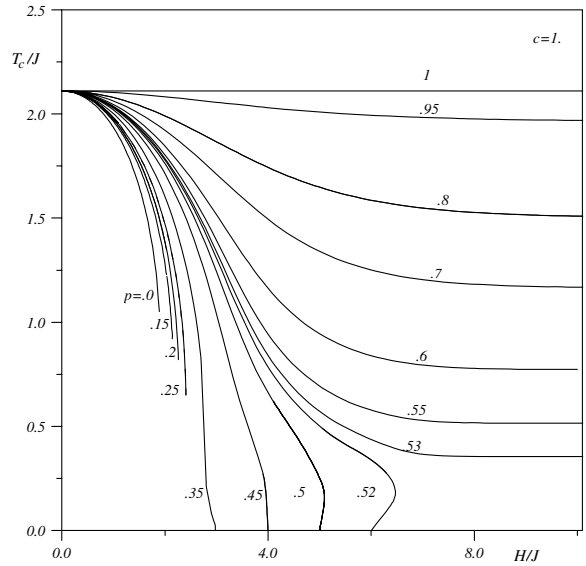

Figure 1. The phase diagram in the T–H plane of the random field mixed spin-$\frac{1}{2}$ and spin-1 Ising system on a simple cubic lattice ($z = 6$). The number accompanying each curve denotes the value of p.

the range of p. Thus, for $p < p^*$, the system exhibits at the ground state a phase transition at a finite critical value H_c of H. But for $p^* < p < 1$, there is no critical field and therefore, at very low temperature, the ordered state is stable for any value of the field strength. This latter behaviour is qualitatively similar to that obtained in the random field spin-$\frac{1}{2}$ Ising model [35]. It is also worth noticing here that such a critical value p^* has been found [54] by two of us (NB and AF) in the study of a mixed spin Ising model in a transverse random field. As expected, we can see in figure 1 that, for a fixed value of H, the critical temperature is an increasing function of p. As clearly shown from the figure, the system exhibits a reentrant behaviour in narrow ranges of H and p. This phenomena is due to the competition between the exchange interaction and frustration induced by quenched local fields. It is interesting to note here that such reentrance does not exist in the spin-$\frac{1}{2}$ RFIM for a trimodal distribution [34, 35].

3.2. The site diluted system

First, let us investigate the system in the absence of the field ($H = 0$ or $p = 1$) by solving numerically (38). For the simple cubic lattice ($z = 6$), the phase diagram is represented in figure 2 and it expresses the known result of a diluted magnetic system [42, 44, 54]. The critical temperature T_c decreases linearly from its value in the mixed Ising system $T_c(c = 1)$, to vanish rapidly at the percolation threshold $c^* = 0.2824$, which is quite good compared with the best value of 0.31 calculated by Sykes and Essam [57]. Secondly, we study the system described by the Hamiltonian (3) when the longitudinal field is bimodally distributed ($p = 0$). Figure 3(a) summarizes the results for the case of the simple cubic lattice. These give the sections of the critical surface $T_c(c, H)$ with planes of fixed values of the dilution parameter c, and therefore they show the influence of c on the critical line of the random field mixed spin Ising model [45]. From the various transition lines plotted when c takes values greater than c^*, it is seen that the system keeps a tricritical behaviour only when at least half of the sites ($0.508 < c \leqslant 1$) of the system are magnetic. The H component of the tricritical point decreases with the value

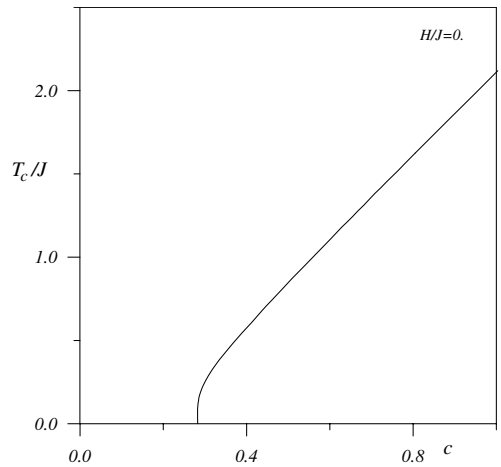

Figure 2. The phase diagram of the diluted mixed spin-$\frac{1}{2}$ and spin-1 Ising system on a simple cubic lattice ($z = 6$) in the absence of the longitudinal field ($H = 0$ or $p = 1$).

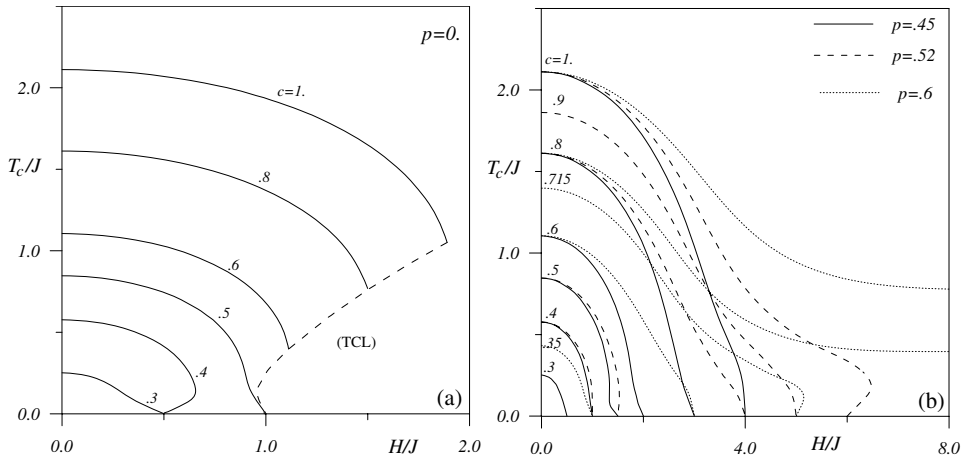

Figure 3. The phase diagram in the T–H plane of the diluted random field mixed spin Ising system on a simple cubic lattice ($z = 6$) with (a) the bimodal distribution ($p = 0$) and (TCL) is the tricritical line. The number accompanying each curve denotes the value of c. (b) Trimodal distributions: $p = 0.45$ (full curves), $p = 0.52$ (broken curves) and $p = 0.6$ (dotted curves). The number accompanying each curve denotes the value of c.

of c and there exists a tricritical line (TCL) which vanishes at $c = 0.508$. When c belong to the range $c^* < c < 0.508$, the tricritical behaviour disappears and all transitions are always of second order for any value of the field. We also note that the phase diagram shows a reentrance in narrow ranges of H and c.

Next, we investigate the phase diagrams of the system when the form of the random field is chosen to be a trimodal distribution ($p \neq 0$). In figure 3(b), we represent the influence of the dilution on the phase diagram of the system when the transition is of second order for any value of H. As illustrated in this figure, three types of effects are shown which depend on the range of p. For the first type (for instance $p = 0.45$), the general behaviour of the critical temperature $T_c(c, H)$ falls with decreasing c and increasing H, and vanishes at a critical value H_c of the field strength which depends on the value of c.

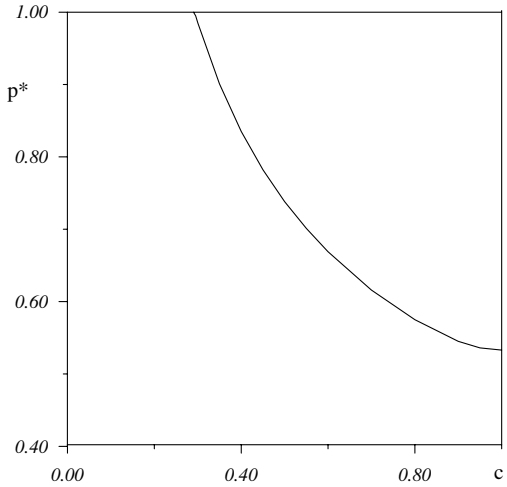

Figure 4. The dependence of the critical value p^* as a function of the dilution parameter c.

Since the undiluted version of the system under study exhibits a reentrant behaviour when the fraction p of spins not exposed to the field H is near p^*, it is worth investigating the effects of the dilution parameter on such reentrance. In figure 3(b), we also represent the variation of the critical temperature with the field H/J, keeping p fixed ($p = 0.52$), for various values of c. Our results indicate that the diluted system exhibits a reentrant behaviour only when the dilution parameter c is very close to 1 ($0.959 < c < 1$ for $p = 0.52$). Thus, for the remaining values of c, the critical temperature decreases gradually from its value T_c/J ($H = 0$) to vanish at some c-dependent critical value H_c of the field.

Now, let us examine the effect of dilution on the system when p is greater than p^* (i.e. there is no critical magnetic field at the ground state). As clearly seen in figure 3(b), the phase diagram plotted in the T–H plane when $p = 0.6$ ($p > p^*(c = 1)$) shows two qualitatively different behaviours which depend on the range of c. For the chosen value of p, when $0.718 < c \leqslant 1$, the system does not exhibit a transition at $T = 0$ and therefore it behaves like the undiluted system. But for $c^* < c \leqslant 0.718$, the system undergoes at the ground state a phase transition at a finite critical value H_c of H. Thus, the dilution may destroy the low temperature ordered state for any H, when it exists in the undiluted system. We have to mention that the properties of the undiluted system ($c = 1$), related to the existence of the value p^*, also appear in the diluted case, but the location of p^* depends on the concentration c of magnetic sites. As shown in figure 4, p^* increases with decreasing values of c which is physically reasonable.

4. Other thermodynamical properties

Next, we evaluate other relevant thermodynamical quantities such as the internal energy U, specific heat C and zero-field magnetic susceptibility χ of the present system.

4.1. Internal energy and specific heat

In the spirit of the FCA, (12) and (13) can be generalized by the following exact relations:

$$\langle g_o \xi_o \sigma_o \rangle = \frac{\xi_o}{2} \left\langle g_o \tanh\left[\frac{K}{2} \sum_{j=1}^{z} \xi_j S_j + \frac{h_o}{2} \right] \right\rangle \tag{41}$$

$$\langle G_o \xi_o S_o \rangle = \xi_o \left\langle G_o \frac{2\sinh\left[K\sum_{i=1}^{z}\xi_i\sigma_i + h_o\right]}{1 + 2\cosh\left[K\sum_{i=1}^{z}\xi_i\sigma_i + h_o\right]} \right\rangle \tag{42}$$

where g_o and G_o represent arbitrary functions of spin variables except for σ_o and S_o, respectively. For a given configuration of the random fields and the site occupational numbers, the internal energy $U_{\sigma S}$ of the system described by the Hamiltonian (3) is given by

$$U_{\sigma S} = -J\frac{N}{2}\left\langle \sum_\sigma \xi_o S_o \right\rangle - \frac{N}{2}\langle H_o \xi_o \sigma_o \rangle - \frac{N}{2}\langle H_o \xi_o S_o \rangle \tag{43}$$

where $\sum_\sigma = \sum_{i=1}^{z}\xi_i\sigma_i$ and N is the total number of sites. In order to calculate $\langle \sum_\sigma \xi_o S_o \rangle$, we substitute $G_o = \sum_\sigma$ in (42). Then it can be written as

$$\left\langle \sum_\sigma \xi_o S_o \right\rangle = \xi_o \left\langle \sum_\sigma \frac{2\sinh\left[K\sum_{i=1}^{z}\xi_i\sigma_i + h_o\right]}{1 + 2\cosh\left[K\sum_{i=1}^{z}\xi_i\sigma_i + h_o\right]} \right\rangle. \tag{44}$$

The second and third terms in (43) can also be calculated by using (41) and (42) with $g_o = H_o$ and $G_o = H_o$.

Following the same procedure as for the evaluation of μ and m_n, namely using the generalized Van der Waerden operators (17), (18) and the single-site probability distributions (25) and (26), we find

$$\left\langle\!\left\langle \sum_\sigma \xi_o S_o \right\rangle\!\right\rangle_r = c \sum_{k_1=-1/2}^{+1/2} \cdots \sum_{k_z=-1/2}^{+1/2} \sum_{\xi_1=o}^{1} \cdots \sum_{\xi_z=o}^{1} \left[\prod_{i=1}^{z} b(k_i, \xi_i)\right] \times \phi_1(\{\xi_1\sigma_1(k_1), \ldots, \xi_z\sigma_z(k_z)\}, h_o) \tag{45}$$

$$\langle\!\langle H_o \xi_o \sigma_o \rangle\!\rangle_r = c \sum_{I_1=-1}^{+1} \cdots \sum_{I_z=-1}^{+1} \sum_{\xi_1=o}^{1} \cdots \sum_{\xi_z=o}^{1} \left[\prod_{j=1}^{z} a(I_j, \xi_j)\right] \times \phi_2(\{\xi_1 S_1(I_1), \ldots, \xi_z S_z(I_z)\}, h_o) \tag{46}$$

$$\langle\!\langle H_o \xi_o S_o \rangle\!\rangle_r = c \sum_{k_1=-1/2}^{+1/2} \cdots \sum_{k_z=-1/2}^{+1/2} \sum_{\xi_1=o}^{1} \cdots \sum_{\xi_z=o}^{1} \left[\prod_{i=1}^{z} b(k_i, \xi_i)\right] \times \phi_3(\{\xi_1\sigma_1(k_1), \ldots, \xi_z\sigma_z(k_z)\}, h_o) \tag{47}$$

where $\phi_1 = \sum_\sigma F_1$, $\phi_2 = H_o f$, $\phi_3 = H_o F_1$, $\sigma_i(k) = k$ and $S_i(I) = I$.

Performing the configurational averaging over the random fields H_i according to the probability distribution function $Q(H_i)$, and further algebraic manipulations [54], the internal energy $U = \bar{U}_{\sigma S}$ is given by

$$-\frac{2U}{NJ} = c \sum_{n_1=o}^{z} \sum_{n_2=o}^{z-n_1} \sum_{i_1=o}^{n_1} \sum_{i_2=o}^{n_2} 2^{-n_1-n_2} C_z^{n_1} C_{z-n_1}^{n_2} C_{n_1}^{i_1} C_{n_2}^{i_2} (-1)^{i_2} [2^{i_1+i_2}(c)^{n_1+n_2-i_1-i_2}(\mu)^{i_1+i_2} \times (1-c)^{z-n_1-n_2}(\bar{\phi}_1 + \bar{\phi}_3) + (m_1)^{i_1+i_2}(m_2)^{n_1+n_2-i_1-i_2}(1-m_2)^{z-n_1-n_2}\bar{\phi}_2]. \tag{48}$$

Using this expression of $U(T, H, c, p)$, we can determine the magnetic contribution to the specific heat via the standard relation

$$C(T, H, c, P) = \frac{\partial U(T, H, c, p)}{\partial T}. \tag{49}$$

For the three-dimensional undiluted system ($c = 1$), figures 5(a), (b) represent a variety of curves showing the temperature dependence of the internal energy U and the specific heat C for the simple cubic lattice in the case of bimodal ($p = 0$) and trimodal ($p \neq 0$) distributions. As seen from these figures, U exhibits a singularity at the transition temperature.

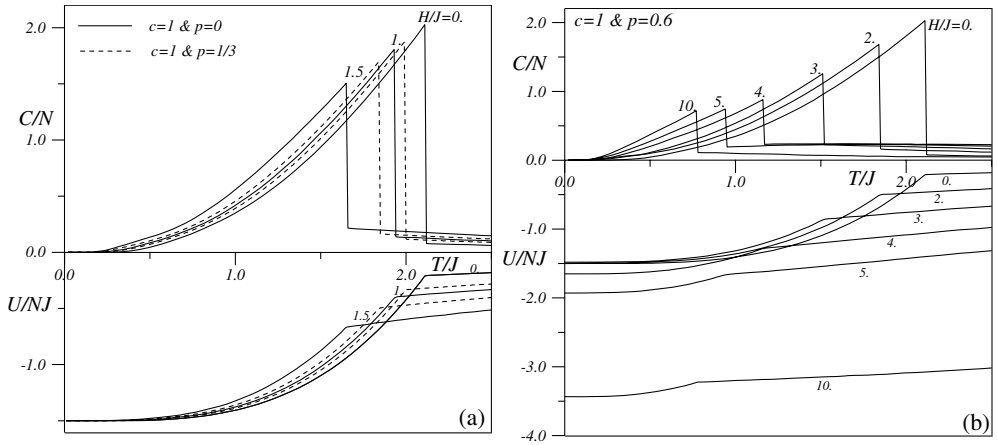

Figure 5. The temperature dependence of the internal energy U and the magnetic specific heat C of the random field mixed spin Ising system on the simple cubic lattice ($z = 6$) for selected values of H/J with: (a) $p = 0$ (full curves), $p = 1/3$ (broken curves) and (b) $p = 0.6$.

At low temperatures, these figures show that

(i) for a given relatively small value of p, the absolute value of the internal energy $|U|$ of the system decreases with increasing strength of the field; and
(ii) for a selected non-zero value of H (less than the critical value), $|U|$ is an increasing function of the concentration p of the site not exposed to the field.

Moreover, we note a remarkable behaviour of the energy $U(T = 0, H, p)$ of the ordered state at zero temperature. Indeed, there exists a critical value $p_c(c = 1) = 0.374$ of p indicating two qualitatively different behaviours of the ground state energy as a function of the field H. Thus, when p belongs to the range $0 \leqslant p < p_c$, the energy of the ordered state, at $T = 0$, does not depend on the value of H (any $H < H_c$); while for $p_c < p < 1$, the ground state energy of the ordered system does not still depend on relatively small values of H, but for larger H it becomes sensitive to the value of the field strength. These behaviours are illustrated in figures 5(a), (b) for selected values of p. On the other hand, we have plotted in the same figures the magnetic contribution C to the specific heat of the system. For both distributions ($p = 0$ and $p \neq 0$), its thermal behaviour shows a discontinuity at the transition temperature $T_c(H, p)$ and the amplitude of the jump gradually decreases with increasing value of H. We also note, from (49), that C is proportional to $1/T^2$ in the limit $T \to \infty$. Moreover, as seen from the figures, C is remarkably depressed by decreasing the field strength H. It is worth noticing here that such a depression has been found recently [58] in the high magnetic concentration Ising antiferromagnet $Fe_{0.93}Zn_{0.07}F_2$ in a magnetic field using optical linear birefringence techniques.

Next, we investigate the effects of dilution on the thermal behaviour of the internal energy and specific heat in comparison with those of the pure system. Results for the case of a simple cubic lattice and for bimodal and trimodal distributions are summarized in figures 6(a), (b) and 7(a), (b). These figures are plotted for two selected values of c: $c = 0.5(c > c^*)$ and $c = 0.2(c < c^*)$ which are, respectively, greater and less than the percolation threshold c^*. For $c^* < c < 1$, and as seen from figures 6(a), (b), the internal energy exhibits qualitatively the same behaviour as the pure system; in particular a singularity at the transition temperature $T_c(p, H)$ when $H < H_c$. But for $H > H_c$, U is an analytic function and therefore no transition occurs.

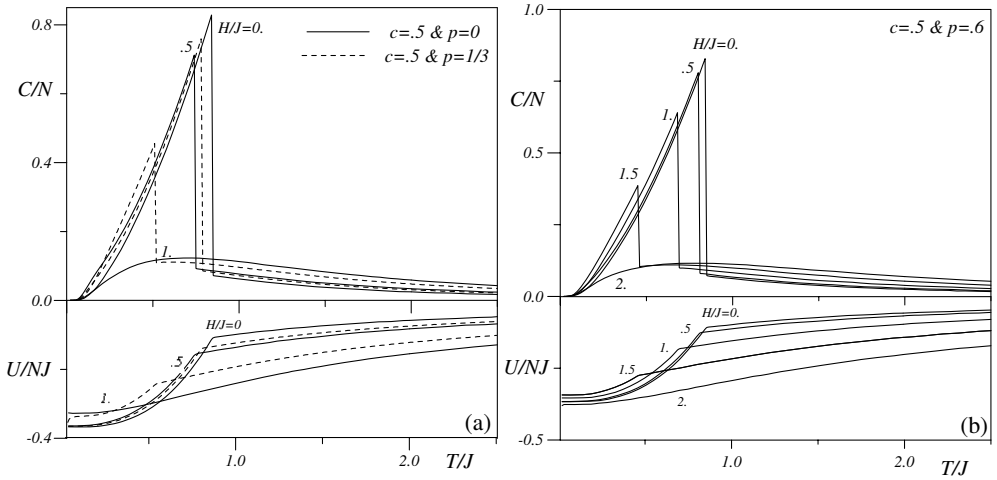

Figure 6. The temperature dependence of the internal energy U and magnetic specific heat C of the diluted ($c = 0.5$) random field mixed spin Ising system on a simple cubic lattice ($z = 6$) for selected values of H/J with: (a) $p = 0$ (full curves), $p = 1/3$ (broken curves) and (b) $p = 0.6$.

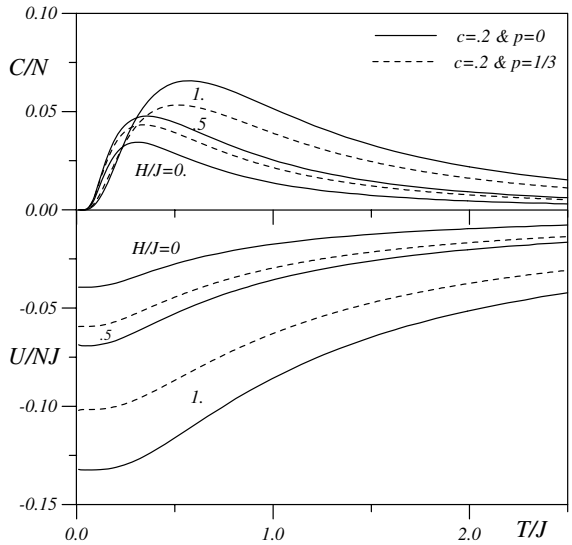

Figure 7. The temperature dependence of the internal energy U and magnetic specific heat C of the diluted ($c = 0.2$) random field mixed spin Ising system on a simple cubic lattice ($z = 6$) for selected values of H/J with $p = 0$ (full curves) and $p = 1/3$ (broken curves).

In the undiluted system, we have defined a critical value of p, namely p_c, below which the ground state energy of the ordered system does not depend on the value of H (any $H < H_c$). As can be expected, such behaviour appears in the diluted case, but only when the impurity concentration is relatively important ($0.805 < c \leqslant 1$). For $c^* < c \leqslant 0.805$, such a value of p_c does not exist and the energy of the ordered system at $T = 0$ becomes sensitive to the value of the field strength for any p.

Concerning the specific heat C, we have to indicate that, for $c^* < c < 1$, two different contributions to C are present: the singular one coming from the unique infinite cluster and the regular one coming from the isolated finite clusters, whereas, for $0 < c < c^*$, the singularity disappears and the specific heat is due exclusively to the finite clusters. In figures 6(a), (b), we have plotted the specific heat of the system for both distributions ($p = 0$ and $p \neq 0$) and they show a discontinuity at the transition temperature and the size of the jump clearly depends on the values of p, c and H. Finally, we note that, when the dilution parameter is less than the percolation threshold ($c < c^*$), the system is always disordered and does not undergo a transition for any value of p and H. Consequently, the internal energy and the specific heat do not exhibit singularities which are shown in figure 7.

4.2. Susceptibility

Let us now investigate the zero-field isothermal magnetic susceptibility. To this end, we add to the Hamiltonian (3) the term $-B(\sum_i \xi_i\sigma_i + \sum_j \xi_j S_j)$, where B is an external magnetic field. Consequently, identities (12) and (13) are generalized into

$$\langle \xi_o \sigma_o \rangle = \xi_o \langle f'(\{\xi_j S_j\}, h_o, b)\rangle \tag{50}$$

$$\langle \xi_o (S_o)^n \rangle = \xi_o \langle F'_n(\{\xi_i\sigma_i\}, h_o, b)\rangle \tag{51}$$

where

$$f'(\{\xi_j S_j\}, h_o, b) = \frac{1}{2}\tanh\left[\frac{K}{2}\sum_{j=1}^{z}\xi_j S_j + \frac{h_o}{2} + \frac{b}{2}\right] \tag{52}$$

$$F'_1(\{\xi_i, \sigma_i\}, h_o, b) = \frac{2\sinh\left[K\sum_{i=1}^{z}\xi_i\sigma_i + h_o + b\right]}{1 + 2\cosh\left[K\sum_{i=1}^{z}\xi_i\sigma_i + h_o + b\right]} \tag{53}$$

$$F'_2(\{\xi_i\sigma_i\}, h_o, b) = \frac{2\cosh\left[K\sum_{i=1}^{z}\xi_i\sigma_i + h_o + b\right]}{1 + 2\cosh\left[K\sum_{i=1}^{z}\xi_i\sigma_i + h_o + b\right]} \tag{54}$$

with $b = \beta B$. To obtain the state equations, we follow the procedure described in the theoretical framework. We find equations similar to those expressed in (31) and (32). Thus, the state equations for the simple cubic lattice are given by

$$\mu = c\sum_{n_1=o}^{6}\sum_{n_2=o}^{6-n_1}\sum_{i_1=o}^{n_1}\sum_{i_2=o}^{n_2} 2^{-n_1-n_2} C_6^{n_1} C_{6-n_1}^{n_2} C_{n_1}^{i_1} C_{n_2}^{i_2} (-1)^{i_2} (m_1)^{i_1+i_2} (m_2)^{n_1+n_2-i_1-i_2} \times (1-m_2)^{6-n_1-n_2} \bar{f}'(K(n_1-n_2),\, p, h, b) \tag{55}$$

$$m_n = c\sum_{n_1=o}^{6}\sum_{n_2=o}^{6-n_1}\sum_{i_1=o}^{n_1}\sum_{i_2=o}^{n_2} 2^{-n_1-n_2+i_1+i_2} C_6^{n_1} C_{6-n_1}^{n_2} C_{n_1}^{i_1} C_{n_2}^{i_2} (-1)^{i_2} (c)^{n_1+n_2-i_i-i_2} (\mu)^{i_1+i_2} \times (1-c)^{6-n_1-n_2} \bar{F}'_n\left(\frac{K}{2}(n_1-n_2),\, p, h, b\right). \tag{56}$$

The initial susceptibility χ per site is defined by

$$\chi = \tfrac{1}{2}(\chi_\mu + \chi_m) \tag{57}$$

where

$$\chi_\mu = \left.\frac{\partial\mu}{\partial B}\right|_{B=0} \qquad \text{and} \qquad \chi_m = \left.\frac{\partial m_1}{\partial B}\right|_{B=0}. \tag{58}$$

To calculate χ, it is advantageous to rewrite (55) and (56) as finite polynomials of m_1 and μ. So they take the following forms:

$$\mu = \sum_{n=o}^{6} \sum_{l=o}^{6-n} C_6^n C_{6-n}^1 m_2^1 m_1^n \bar{A}'_{l,n}(K, h, p, c, b) \tag{59}$$

$$m_1 = \sum_{n=o}^{6} C_6^n \mu^n \bar{B}'_n(K, h, p, c, b) \tag{60}$$

$$m_2 = \sum_{n=o}^{6} C_6^n \mu^n \bar{D}'_n(K, h, p, c, b). \tag{61}$$

The coefficients $\bar{A}'_{l,n}$, $\bar{B}'_n$ and $\bar{D}'_n$ are complicated expressions involving hyperbolic functions and will not be given. Deriving (59)–(61) with respect to B at the point $B = 0$, and eliminating $\frac{\partial m_2}{\partial B}$, the local susceptibilities pertaining to μ and m are given by

$$\chi_\mu = \frac{a_o + a_2 c_o + a_1 b_o}{1 - (a_2 c_1 + a_1 b_1)} \tag{62}$$

$$\chi_m = b_o + b_1 \frac{a_o + a_2 c_o + a_1 b_o}{1 - (a_2 c_1 + a_1 b_1)} \tag{63}$$

where

$$a_o = \sum_{n=o}^{6} \sum_{l=o}^{6-n} C_6^n C_{6-n}^1 m_2^1 m_1^n \frac{\partial \bar{A}'_{l,n}}{\partial B}\bigg|_{B=o}, \qquad a_1 = \sum_{n=o}^{6} \sum_{l=o}^{6-n} C_6^n C_{6-n}^1 n m_2^1 m_1^{n-1} \bar{A}'_{l,n}\bigg|_{B=o},$$

$$a_2 = \sum_{n=o}^{6} \sum_{l=o}^{6-n} C_6^n C_{6-n}^1 1 m_2^{l-1} m_1^n \bar{A}'_{l,n}\bigg|_{B=o}, \qquad b_o = \sum_{n=o}^{6} C_6^n \mu^n \frac{\partial \bar{B}'_n}{\partial B}\bigg|_{B=o},$$

$$b_1 = \sum_{n=o}^{6} C_6^n n \mu^{n-1} \bar{B}'_n\bigg|_{B=o}, \qquad c_o = \sum_{n=o}^{6} C_6^n \mu^n \frac{\partial \bar{D}'_n}{\partial B}\bigg|_{B=o}, \qquad c_1 = \sum_{n=o}^{6} C_6^n n \mu^{n-1} \bar{D}'_n\bigg|_{B=o}.$$

For the three-dimensional undiluted system ($c = 1$), figures 8(a), (b) show the temperature dependence of χ for both distributions. For the bimodal ($p = 0$) and trimodal ($p = 1/3$) cases, $\chi(T)$ is plotted in figure 8(a) for selected values of H when the latter is less than the critical value $H_c(p)$. When H_c does not exist, namely $p > p^*$, the system can exhibit a transition for any value of H. The corresponding thermal behaviour of χ is shown in figure 8(b) for $p = 0.6$. As expected, χ diverges at the critical point $T_c(p, H)$ and presents the $1/T$ behaviour in the limit $T \to \infty$. Here again, it is worth noting that the behaviours of χ with H at low and high temperatures are similar to those obtained recently [59] in $Fe_{0.93}Zn_{0.07}F_2$.

In order to study the effects of dilution on the above zero-field isothermal magnetic susceptibility χ, we represent in figures 9(a), (b) and figures 10(a), (b) the temperature dependence of χ for two selected values of c: $c = 0.5$ ($c > c^*$) and $c = 0.2$ ($c < c^*$). From these figures, we observe that χ vanishes in the limit $T \to 0$ only for $c = 1$, which corresponds to the absence of finite clusters in the system. In the case $c^* < c < 1$ χ diverges twice, one at the critical point $T_c(p, c, H)$ and the other at $T = 0$, which correspond, respectively, to the infinite cluster and finite cluster contributions. In other words, we observe the coexistence of a Curie–Weiss-type law with a Curie-type one. As in the pure case, the susceptibility of the diluted system also presents the $1/T$ behaviour in the limit $T \to \infty$. Finally for $c < c^*$, the thermal behaviour of χ is plotted in figure 10 ($c = 0.2$). As seen from this figure, the divergence remains only at $T = 0$ for any values of H and p.

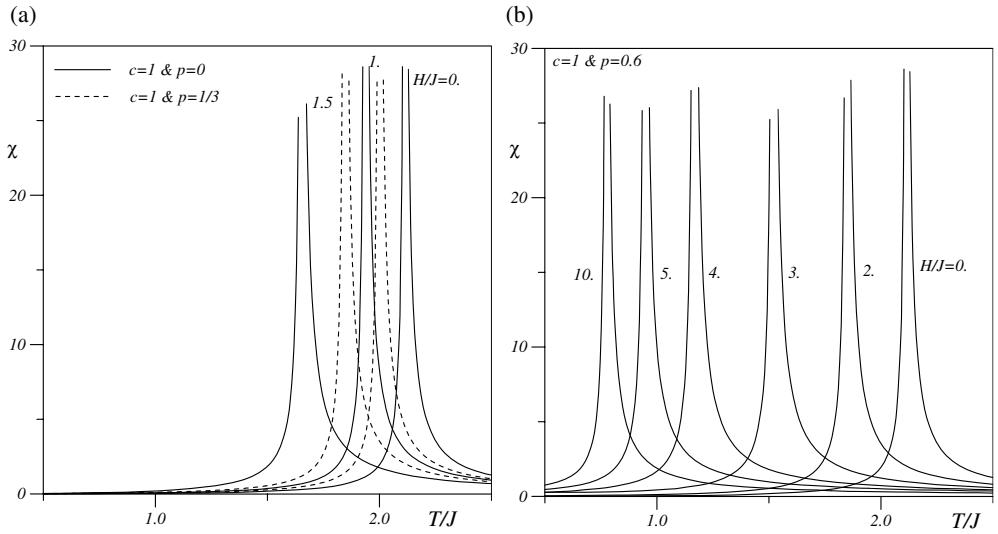

Figure 8. The temperature dependence of the initial magnetic susceptibility χ of the random field mixed spin Ising system on a simple cubic lattice ($z = 6$) for selected values of H/J with: (a) $p = 0$ (full curves), $p = 1/3$ (broken curves) and (b) $p = 0.6$.

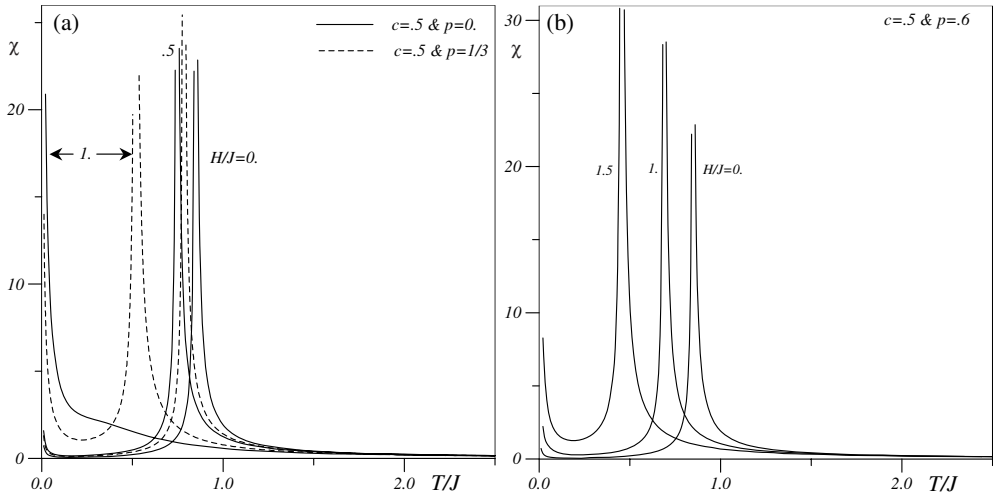

Figure 9. The temperature dependence of the initial magnetic susceptibility χ of the diluted ($c = 0.5$) random field mixed spin Ising system on a simple cubic lattice ($z = 6$) for selected values of H/J with: (a) $p = 0$ (full curves), $p = 1/3$ (broken curves) and (b) $p = 0.6$.

5. Conclusions

In this paper, we have studied thermodynamical properties of the three-dimensional diluted random field mixed spin-$\frac{1}{2}$ and spin-1 Ising model. The random fields are assumed to be uncorrelated variables and obey the bimodal and trimodal distributions. We have used the FCA within the framework of a single-site cluster theory. In this approach, we have derived the state equations using appropriate distributions accounting exactly for the single-site kinematic relations. Let us summarize by stating the main results of this investigations.

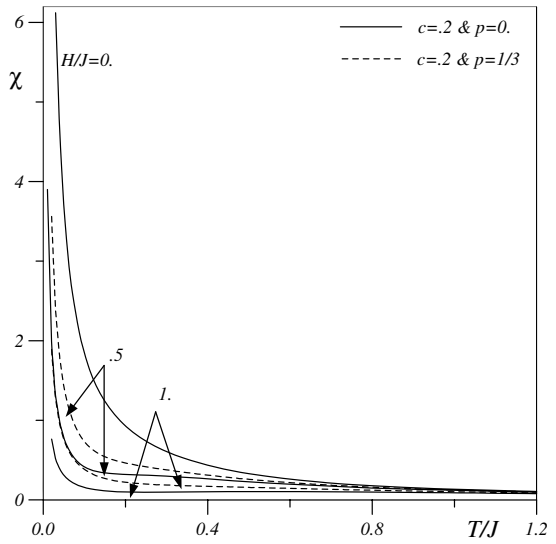

Figure 10. The temperature dependence of the initial magnetic susceptibility χ of the diluted ($c = 0.2$) random field mixed spin Ising system on a simple cubic lattice ($z = 6$) for selected values of H/J with $p = 0$ (full curves) and $p = 1/3$ (broken curves).

First, we have examined the phase diagram of the undiluted system for various values of p (p measures the fraction of spins not exposed to the longitudinal field H). For the bimodal distribution (i.e. $p = 0$), we have found that the system undergoes a second phase transition for low random field, which ends in a tricritical point. For the trimodal case (i.e. $p \neq 0$), the system keeps this behaviour for relatively small values of p ($0 \leqslant p < 0.289$). We note that the T component of the tricritical point vanishes at $p = 0.289$, which means that the vestigial point existing in the mono-atomic RFIM [35] does not occur in the random field mixed spin Ising model. On the other hand, we have define a critical value p^* separating two qualitatively different behaviours of the system: for p less than p^*, the system exhibits, at the ground state, a phase transition at a finite critical value H_c. However, for p greater than p^*, H_c does not exist and the ordered state is stable at very low temperatures for any value of the field strength H. It is also worth noting here that the system exhibits a reentrant behaviour in narrow ranges of H and p. This reentrance does not exist in the mono-atomic spin-$\frac{1}{2}$ RFIM [34, 35].

Secondly, we have investigated the influence of site dilution on the obtained phase diagrams. In bimodal distribution ($p = 0$), we have found that the system exhibits a tricritical behaviour only when at least half of the sites are magnetic. In the trimodal case, we have shown that the system keeps its reentrance behaviour only when the impurity concentration c is close to 1. Furthermore, we have found that the above critical value p^* depends on the value of c and then we have plotted, in the p^*–c plane, the curve which separates the two domains corresponding, respectively, to the existence and absence of the finite critical field H_c.

Other relevant thermodynamical quantities have been evaluated, such as the internal energy U, specific heat C and zero-field magnetic susceptibility χ. Thus, the temperature dependence of U and C are explored for both distributions and it revealed a number of characteristic features at low temperature. In particular, for the undiluted system, we have defined a second critical value p_c indicating two qualitatively different behaviours of the ground state energy $U(T = 0, p, H)$ as a function of the field H: for $0 \leqslant p \leqslant p_c$, the energy of the ordered state, at $T = 0$, does not depend either on H (any $H < H_c$) or on p. However, for $p_c < p < 1$, the

ground state energy of the ordered system does not still depend on small values of H but for larger H, it becomes sensitive to H. The same behaviour has also been found in the dilution case, but only when the dilution parameter c is relatively important; otherwise, such a critical value p_c does not exist and therefore the ground state energy depends on H for any value of the concentration p. Furthermore, the thermal behaviour of specific heat C has been studied when the random field is bimodally and trimodally distributed. We have shown that the amplitude of the jump of C (at the transition) depends on p, H and c. In particular, for given values of p and H, it gradually decreases with c. We also note that, for the pure case, C is depressed by decreasing H. Such a depression has been found recently [58] in $Fe_{0.93}Zn_{0.07}F_2$ in a magnetic field. Moreover, we have investigated the temperature dependence of the susceptibility χ for both distributions. In the pure system, χ vanishes at $T = 0$, whereas for the diluted case, and above the percolation threshold, we have found that χ diverges twice, namely at the critical point and at $T = 0$, which correspond, respectively, to the infinite cluster and finite cluster contributions. It has also been found that χ presents the $1/T$ behaviour in the limit $T \to \infty$. Finally, it is worth mentioning here that, for $c = 1$, the behaviours of χ with H at low and high temperatures are similar to those obtained in $Fe_{0.93}Zn_{0.07}F_2$ [59].

Finally, we mention that the method (FCA) used in this paper is much less sophisticated than the real space renormalization group (RSRG) and applies to a wide class of disordered systems. In particular, site dilution (which is a more physical situation than bond dilution) is much easier to study within the FCA. This is not the case for RSRG. Another advantage of the FCA is that

(i) it is not necessary to introduce *ad hoc* approximations for the renormalized probability distribution of the Hamiltonian parameters, and
(ii) not to choose in a more or less arbitrary way the 'right' random variable for which there is no clear criterion [60].

References

[1] Imry Y 1984 *J. Stat. Phys.* **34** 841
Grinstein G 1984 *J. Appl. Phys.* **55** 2371
[2] Aharony A 1986 *J. Magn. Magn. Mater.* **54–57** 27
[3] Nattermann T and Villain J 1988 *Phase Transitions* **11** 5
[4] Oliveira S M, Continentino M A and Oliveira P M C 1990 *Physica* A **162** 458
[5] Slanic Z and Belanger D P 1998 *J. Magn. Magn. Mater.* **186** 65
Belanger D P, Rezende S M, King A R and Jaccarino V 1985 *J. Appl. Phys.* **57** 3294
[6] Birgeneau R J, Shapira Y, Shirane G, Cowley R A and Yoshigawa H 1986 *Physica* B **137** 83
[7] Cardy J L 1984 *Phys. Rev.* B **29** 505
[8] Belanger D P 1988 *Phase Transitions* **11** 53
King A R, Jaccarino V, Belanger D P and Rezende S M 1985 *Phys. Rev.* B **32** 503
Fishman S and Aharony A 1979 *J. Phys. C: Solid State Phys.* **12** L729
[9] Slanic Z, Belanger D P and Fernandez-Bacca J A 1998 *J. Magn. Magn. Mater.* **177–181** 171
Birgeneau R J, Cowley R A, Shirane G and Yoshizawa H 1984 *J. Stat. Phys.* **34** 817
[10] Slanic Z, Belanger D P and Fernandez-Bacca J A 1999 *Phys. Rev. Lett.* **82** 426
[11] Barber W C and Belanger D P 2000 *J. Appl. Phys.* **87** 7049
[12] Bruinsma R 1987 *Nonlinearity in Condensed Matter* ed A R Bishop *et al* (Berlin: Springer) p 291 ff
[13] Wong A P Y and Chan M H W 1990 *Phys. Rev. Lett.* **65** 2567
[14] de Gennes P G 1984 *J. Phys. Chem.* **88** 6469
[15] Bricmont J and Kupiainen A 1987 *Phys. Rev. Lett.* **59** 1829
[16] Imbrie J Z 1985 *Commun. Math. Phys.* **98** 145
[17] Imbrie J Z 1984 *Phys. Rev. Lett.* **53** 1747
[18] Belanger D P, King A R and Jaccarino V 1985 *Phys. Rev.* B **31** 4538
[19] Yoshizawa H, Cowley R A, Shirane G and Birgeneau R J 1985 *Phys. Rev.* B **31** 4548

[20] Birgeneau R J, Cowley R A, Shirane G and Yoshizawa H 1985 *Phys. Rev. Lett.* **54** 2147
[21] Ferreira I B, King A R, Jaccarino V, Cardy J L and Guggenheim H J 1983 *Phys. Rev.* B **28** 5192
[22] Galam S, Birman J L and Aharony A 1983 *Phys. Rev.* B **28** 5322
[23] Andelman D and Aharony A 1983 *Phys. Rev.* B **27** 3079
[24] Aharony A 1978 *Phys. Rev.* B **18** 3318
[25] Falicov A and Nihat Berker A 1995 *Phys. Rev.* B **51** 8266
[26] Reed P 1985 *J. Phys. C: Solid State Phys.* **18** L615
[27] Houghton A, Khurana A and Seco F J 1986 *Phys. Rev.* B **34** 1700
[28] Houghton A, Khurana A and Seco F J 1985 *Phys. Rev. Lett.* **55** 856
[29] Young A P and Nonenberg M 1985 *Phys. Rev. Lett.* **54** 2429
[30] D'Angles d'Auriac J C 1986 *PhD Thesis* Grenoble
[31] Rieger H 1995 *Phys. Rev.* B **52** 6659
Rieger H and Young A P 1993 *J. Phys. A: Math. Gen.* **26** 5279
[32] Wong P, Von Molnar S and Dimon P 1983 *Solid State Commun.* **48** 573
[33] Saxena V K 1983 *Solid State Commun.* **45** 93
Dwivedi L N and Bhandari C M 1977 *Phys. Status Solidi* b **84** K125
[34] Sebastianes R M and Figueiredo W 1990 *Phys. Rev.* B **42** 2594
[35] Sebastianes R M and Saxena V K 1987 *Phys. Rev.* B **35** 2058
[36] Néel L 1948 *Ann. Phys., Paris* **3** 137
[37] Drillon M, Coronado E, Beltran D and Georges R 1983 *J. Chem. Phys.* **79** 449
[38] Schofield S L and Bowers R G 1980 *J. Phys. A: Math. Gen.* **13** 3697
[39] Benayad N 1990 *Z. Phys.* B **81** 99
[40] Yousif B Y and Bowers R G 1984 *J. Phys. A: Math. Gen.* **17** 3389
[41] Kun-Fa Tang 1988 *J. Phys. A: Math. Gen.* **21** L1097
[42] Benayad N, Klümper A, Zittartz J and Benyoussef A 1989 *Z. Phys.* B **77** 333
Benayad N, Klümper A, Zittartz J and Benyoussef A 1989 *Z. Phys.* B **77** 339
[43] Zhang G M and Yang C Z 1993 *Phys. Rev.* B **48** 9452
[44] Benayad N, Dakhama A, Klümper A and Zittartz J 1996 *Ann. Phys., Lpz.* **5** 387
[45] Benayad N, Fathi A and Khaya L 2001 *Physica* A **300** 225
[46] Boccara N 1983 *Phys. Lett.* A **94** 185
[47] Tucker J W, Saber M and Peliti L 1994 *Physica* A **206** 497
[48] Tucker J W 1994 *J. Phys. A: Math. Gen.* **27** 659
[49] El Atri A and Saber M 1993 *Phys. Status Solidi* b **176** 485
Benayad N, Benyoussef A and Boccara N 1987 *J. Phys. C: Solid State Phys.* **20** 2053
Benayad N, Benyoussef A and Boccara N 1985 *J. Phys. C: Solid State Phys.* **18** 1899
[50] Benayad N and Zerhouni R 1997 *Phys. Status Solidi* b **201** 491
Benyoussef A and Ez-Zahraouy H 1994 *J. Phys.: Condens. Matter* **6** 3411
[51] Benayad N and Dakhama A 1997 *Phys. Rev.* B **55** 12 276
Benayad N and Dakhama A 1997 *J. Magn. Magn. Mater.* **168** 105
[52] Benyoussef A, Boccara N and Saber M 1985 *J. Phys. C: Solid State Phys.* **18** 4275
[53] Tucker J W 1991 *J. Magn. Magn. Mater.* **102** 144
[54] Benayad N, Dakhama A, Fathi A and Zerhouni R 1998 *J. Phys.: Condens. Matter* **10** 3141
[55] Benyoussef A and Boccara N 1983 *J. Physique* **44** 1143
[56] Fathi A and Benayad N 2002 *Phys. Rev.* B submitted
[57] Sykes M F and Essam J W 1964 *Phys. Rev.* A **133** 310
[58] Slanic Z and Belanger D P 1998 *J. Magn. Magn. Mater.* **186** 65
[59] Slanic Z, Belanger D P and Fernandez-Bacca J A 1998 *J. Magn. Magn. Mater.* **177–181** 171
[60] Benyoussef A and Boccara N 1983 *J. Phys. C: Solid State Phys.* **16** 1901
Dickinson H and Yeomans J 1983 *J. Phys. C: Solid State Phys.* **16** L345
Stinchcombe R B and Watson B P 1976 *J. Phys. C: Solid State Phys.* **9** 3221