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ABSTRACT

Within the framework of an effective field theory beyond Mean Field Approximation, we discuss the ferromagnetic phase stability limit in the temperature-concentration space of a quenched bond-mixed spin-1/2 Ising model in square lattice for both competing and noncompeting interactions J_1 and J_2. Quite reasonable results are obtained in both situations. In particular for the case of competing interactions, numerical estimates of the vanishing temperature critical bond concentrations are predicted for particular values of the ratio J_1/J_2.

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During the last few years quite an amount of theoretical work has been devoted to the analysis of quenched and annealed bond- and site-diluted as well as bond- and site-mixed Heisenberg and Ising magnets (see Thorpe and McGurn 1979 and Levy et al 1980 and references therein). Due to its relative simplicity, the quenched bond-disordered square-lattice spin-1/2 first-neighbour-interaction ferromagnetic Ising model has deserved particular attention, and a certain amount of exact results are now available (mainly in what concerns the phase diagram). The situation is however less clear when ferro- and antiferromagnetic competing interactions are allowed within the model. Most of the available discussions refer to a restricted case, namely the quenched bond-random Ising magnet with nearest-neighbour exchange interactions $J_{ij} = \pm J$ (Domany 1979, Grinstein et al 1979 Katsura et al 1979, Reed 1979 as well as Kolan and Palmer 1980 and references therein). This model was recently treated by de Almeida et al 1980 within the framework of a new-type effective field approximation beyond the mean field (MFA) one; the method is based on a convenient differential operator (Honmura and Kaneyoshi 1979) introduced in Callen identity (Callen 1963), and leads, in spite of its simplicity, to quite satisfactory results (as long as we do not refer to the strict critical phenomenon). The purpose of the present work is to treat within the same approximative procedure an extended model, in which J_{ij} is a random variable allowed to take the values J_1 (with probability (1-p)) and J_2 (with probability p). The Hamiltonian of our system will be given by

$$\mathcal{H} = -\sum_{\langle i,j\rangle} J_{ij}\sigma_i\sigma_j \qquad (\sigma_i, \sigma_j = \pm 1), \tag{1}$$

where $\langle i,j\rangle$ runs over all the first-neighbouring couples of sites of a square lattice and the J_{ij} probability distribution is given by

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

in which we assume $J_1 \lessgtr J_2 > 0$ hence $\alpha \equiv J_1/J_2 \leq 1$ (note that this restriction does not imply in loss of generality if we recall that the ferromagnetic and antiferromagnetic orderings are isomorphic in square lattice).

If we introduce now in Callen 1963 identity $\langle\sigma_i\rangle = \langle\tanh\beta\sum_j J_{ij}\sigma_j\rangle$ the differential operator $D \equiv \partial/\partial x$ we obtain the exact relation

$$\langle\sigma_i\rangle = \langle\prod_j[\cosh(\beta J_{ij}D) + \sigma_j\sinh(\beta J_{ij}D)]\rangle\tanh x\Big|_{x=0} , \tag{3}$$

where $\beta \equiv 1/k_B T$, $\langle\cdots\rangle$ indicates the canonical thermal average and $\prod_j$ is the product over the nearest neighbours of the site i. Equation (3) can be rewritten as follows

$$\langle\sigma_i\rangle = \sum_{j=1}^{4}\{\langle\sigma_j\rangle\sinh(\beta J_{ij}D)\prod_{k(\neq j)}\cosh(\beta J_{ik}D) +$$

$$+ \frac{1}{3!}\sum_{k(\neq j)}\sum_{\ell(\neq j,k)}\sum_{m(\neq j,k,\ell)}\langle\sigma_j\sigma_k\sigma_\ell\rangle\cosh(\beta J_{im}D)\prod_{n(=j,k,\ell)}\sinh(\beta J_{in}D)\}\tanh x\Big|_{x=0} , \tag{4}$$

where we have used the property $f(D)\tanh x|_{x=0} = 0$ valid for any even function $f(D)$. Note that the exact relation (4) provides a set of equations for the magnetisation of the various sites once the bond configuration $\{J_{ij}\}$ is specified.

The main aim of this paper is to estimate, from equation (4) and for arbitrary values of α, the critical frontier (in the (p,T)-space) which separates the ferromagnetic phase from any other (to be more precise we intend to determine the limit of stability of the long range ferromagnetic order). If we try to exactly take into account all spin-spin correlations appearing in equation (4) and properly perform the configurational averages (denoted by $\langle\cdots\rangle_J$) the problem quickly becomes untractable, so some approximations have to be done. A first obvious attempt is the following one:

$$<<\sigma_j>\sinh(\beta J_{ij}D) \prod_{k(\neq j)} \cosh(\beta J_{ik}D)>_J \cong$$

$$<<\sigma_j>>_J<\sinh(\beta J_{ij}D) \prod_{k(\neq J)} \cosh(\beta J_{ik}D)>_J \quad , \tag{5}$$

and

$$<<\sigma_j\sigma_k\sigma_\ell>\cosh(\beta J_{im}D) \prod_{n(=j,k,\ell)} \sinh(\beta J_{in}D)>_J \cong$$

$$<<\sigma_j>>_J<<\sigma_k>>_J<<\sigma_\ell>>_J<\cosh(\beta J_{im}D) \prod_{n(=j,k,\ell)} \sinh(\beta J_{in}D)>_J. \tag{6}$$

Through these approximations and by taking into account the homogeneity of the system, equation (4) can be rewritten as follows:

$$m = \{4m<\sinh(\beta J_{ij}D)>_J[<\cosh(\beta J_{ij}D)>_J]^3 \quad +$$

$$+ \; 4m^3<\cosh(\beta J_{ij}D)>_J[<\sinh(\beta J_{ij}D)>_J]^3\}\tanh x\Big|_{x=0} \quad , \tag{7}$$

where $m \equiv <<\sigma_i>>_J$ and

$$<\sinh(\beta J_{ij}D)>_J = (1-p)\sinh(\beta J_1D) + p\sinh(\beta J_2D) \tag{8a}$$

$$<\cosh(\beta J_{ij}D)>_J = (1-p)\cosh(\beta J_1D) + p\cosh(\beta J_2D). \tag{8b}$$

Equation (7) admits two solutions, namely $m \equiv 0$ and a non-trivial one given by

$$m = [\frac{1 - A^+}{A^-}]^{1/2} \quad , \tag{9}$$

where the coefficients $A^\pm$ have been obtained through a tedious but straightforward calculation (which makes use of the property $e^{\lambda D}\tanh x\,|_{x=0} = \tanh\lambda$, ($\forall\lambda$)) and are given by

$$A^{\pm} = (1-p)^4 K_1^{\pm} + 4(1-p)^3 p K_2^{\pm} + 6(1-p)^2 p^2 K_3^{\pm} + + 4(1-p)p^3 K_4^{\pm} + p^4 K_5^{\pm}\,, \qquad (10)$$

where

$$K_1^{\pm} = \frac{1}{2}\left\{\tanh\frac{4\alpha}{t} \pm 2\tanh\frac{2\alpha}{t}\right\}, \qquad (11a)$$

$$K_2^{\pm} = \frac{1}{2}\left\{\tanh\frac{3\alpha+1}{t} \pm \frac{1}{2}\tanh\frac{3\alpha-1}{t} \pm \frac{3}{2}\tanh\frac{\alpha+1}{t}\right\}, \qquad (11)$$

$$K_3^{\pm} = \frac{1}{2}\left\{\tanh\frac{2\alpha+2}{t} \pm \tanh\frac{2\alpha}{t} \pm \tanh\frac{2}{t}\right\}, \qquad (11c)$$

$$K_4^{\pm} = \frac{1}{2}\left\{\tanh\frac{3+\alpha}{t} \pm \frac{1}{2}\tanh\frac{3-\alpha}{t} \pm \frac{3}{2}\tanh\frac{\alpha+1}{t}\right\} \qquad (11d)$$

and

$$K_5^{\pm} = \frac{1}{2}\left\{\tanh\frac{4}{t} \pm 2\tanh\frac{2}{t}\right\}, \qquad (11e)$$

with $t \equiv k_B T/J_2$ [we note that equation (9) remains, as expected, invariant through the transformation $(p,t,\alpha) \to (1-p,\, t/\alpha,\, 1/\alpha)$]. Consequently the critical frontier (strictly speaking the ferromagnetic phase stability limit) obtained from the condition $m = 0$ is given by

$$A^{+} = 1. \qquad (12)$$

In figure 1 we present our results for the critical reduced temperature $T_c(p)/T_c(1)$ as a function of the J_2-bond concentration for typical values of $\alpha \equiv J_1/J_2$. Equation (12) contains several interesting particular cases which we comment in what follows.

The critical temperature of the pure Ising model [herein recovered by taking $p = 1$ ($\forall\alpha$) or $\alpha = 1$ ($\forall p$)] is, within the present approximation, determined by $\tanh \frac{4}{t_c} + 2 \tanh \frac{2}{t_c} = 2$, hence $t_c \cong 3.0898$ which is already an improvement on the usual MFA [which provides $t_c^{MFA} = 4$; we recall that $t_c^{exact} = 2.2692\ldots$] in spite of the fact that both procedures loose the real dimensionality of the lattice which is seen only through its coordination number. We should also mention that the present value for t_c coincides with those obtained by Mamada and Takano 1968, Honmura and Kaneyoshi 1979 and recently by Mattis 1979, as well as with that obtained by Zernike in early 1940.

The critical frontier associated to the bond-diluted Ising model (herein recovered as the case $\alpha = 0$) is given by

$$8(1-p)^3 p \tanh \frac{1}{t_c} + 12(1-p)^2 p^2 \tanh \frac{2}{t_c} +$$

$$+ 6(1-p)p^3 [\tanh \frac{3}{t_c} + \tanh \frac{1}{t_c}] + p^4 [\tanh \frac{4}{t_c} + 2\tanh \frac{2}{t_c}] = 2. \qquad (13)$$

We immediately obtain, at $t_c = 0$, the pure bond percolation critical probability $p_c(\alpha = 0) \cong 0.4284$ which coincides with that obtained by Matsudaira 1973 within his first approximation [we recall that $p_c^{exact} = 1/2$ (Sykes and Essam 1963)]. Equation (13) also provides $\frac{1}{t_c(1)} \frac{dt_c(p)}{dp}\Big|_{p=1} \cong 1.345$ to be compared with the exact value 1.329 (Harris 1974) and $(1-p_c) \frac{d\, e^{-2/t_c(p)}}{dp}\Big|_{p=p_c} \cong 1.156$ to be compared with the exact value 1.386 (Domany 1978). It should be noted that in the low temperatures region the present approximation is quite more performant than the traditional Virtual Crystal Approximation (see for example

Brady Moreira et al 1977 and references therein) as it provides the correct asymptotic behaviour.

For the cases where $0<\alpha<1$, equation (12) provides a family of curves (see figure 1) which behaves as expected (Levy et al 1980), and which presents, in particular, a typical non-uniform convergences in the limit $\alpha\to 0$.

Let us now discuss the region $\alpha<0$ which is the main scope of the present work. Equation (12) recovers, for $\alpha=-1$ and $T=0$, a recent result (de Almeida et al 198 namely that the breakdown of the ferromagnetic phase occurs at $p_c(\alpha=-1) = 5/6$, i.e. for a concentration of antiferromagnetic bonds equal to $1/6 \cong 0.167$; as pointed out by de Almeida et al 1981, this value is in good agreement with Monte Carlo calculation (0.15-0.20; Kirkpatrick 1977), the replica method (0.166, Domany 1979) and the Bethe method (0.167, Katsura et al 1979), whereas other methods (Gabay and Garel 1978, Vannimenus and Toulouse 1977, Grinstein et al 1979) yield a lower value ($\cong 0.1$). The complete critical frontier in the (p,T)-space is now presented in figure 1. Equation (12) leads also to $p_c(\alpha=-1/3) \cong 0.635$ and $p_c(\alpha=-3) \cong 0.931$; as far as we know these are the first estimates in the literature for the critical concentrations associated with these particular values of α. The values -1/3, -1 and -3 for α have a natural interpretation within the present approximation (where the lattice is seen only through the coordination number) as they can be, for the configurational neighbourhood of a given spin, respectively related to the antiferromagnetic/ferromagnetic bond occupancy ratios 3:1, 2:2 and 1:3. On the other hand the situation is unfortunately less satisfactory for negative values of α other than -1/3, -1 and -3 as, in the limit $T_c\to 0$, equation (12) leads to $p_c(0>\alpha>-1/3) \cong 0.600$, $p_c(-1/3>\alpha>-1) \cong 0.659$, $p_c(-1>\alpha>-3) \cong 0.909$ and $p_c(-3>\alpha) \cong 0.945$. It is clear that these results are physically meaningless as there is no reason for such a complex sequence of non-uniform convergences, which leads, at vanishing temperature, to the collapse of large families of curves into single points. Therefore this is to be seen as a mathematical artifact of the present approach where we have neglected multi-spin correlations.

Let us conclude by saying that the present treatment of the critical frontier can be given a certain degree of qualitative (and to a certain extent quantitative) confidence for $\alpha \geq 0$ and $\alpha = -1/3, -1, -3$ in the whole range of temperatures as well as for the other values of α as long as we are far from the low temperature regime. Nevertheless further comparison with results obtained through other techniques should be convenient in order to clarify (beyond the trivial fact that the strict dimensionality of the system is lost) the accurate degree of influence of the neglectance of correlations.

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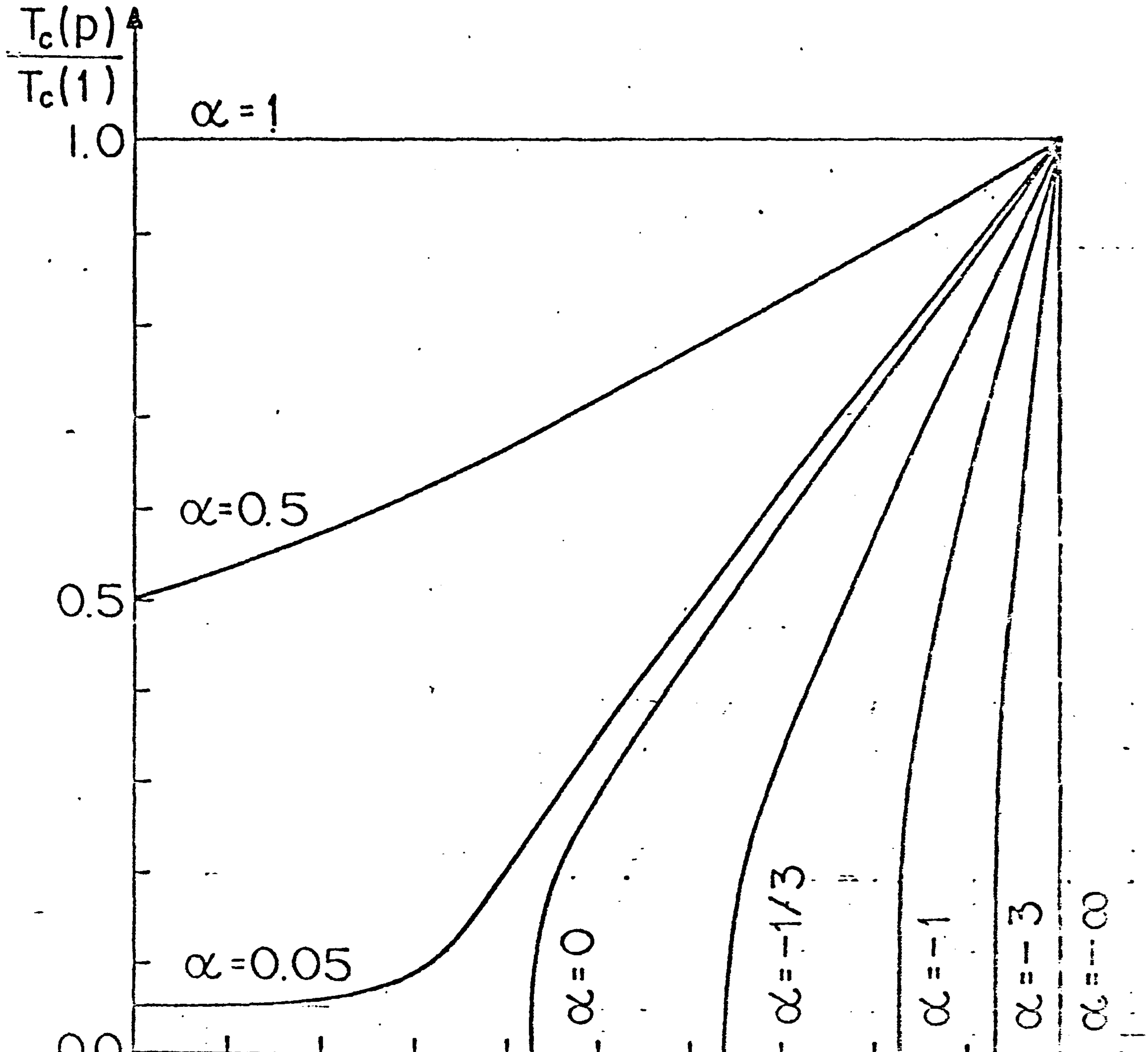
FIGURE CAPTION

FIG.1 The critical temperature (corresponding to the ferromagnetic stability limit) as a function of J_2-bond concentration for typical values of $\alpha \equiv J_1/J_2$.



Tc(p) / Tc(1)
α = 1
1.0
α=0.5
0.5
α =0.05
0.0
α = 0
α = −1/3
α = −1
α = −3
α = −∞
0.0
0.5
1.0
p