Revista Brasileira de Física, Vol. 13, nº 3, 1983

Effective Field Treatment of the Annealed Bond-Dilute Transverse Ising Model

P.R. SILVA and F.C. SÁ BARRETO

Departamento de Física, Universidade Federal de Minas Gerais, Caixa Postal 702, Belo Horizonte, 30.000, MG, Brasil

Recebido em 09 de agosto de 1983

Abstract We study the dilution of the spin-1/2 transverse Ising Model by means of an effective field type treatment based on an extension of Callen's relation (Phys. Lett. 4, 161 (1963)) to the present model. The thermodynamics of the diluted model is obtained and the results are shown to be an improvement over the standard mean field treatment. We also compare the results with the Monte Carlo calculation for the spin-∞ transverse Ising Model.

1. INTRODUCTION

The transverse Ising model has been used to describe phase transitions in ferroelectrics, ferromagnets and cooperative Jahn-Teller systems with an applied external magnetic field. This model hamiltonian was first proposed by de Gennes[1] to represent the basic features of hydrogen-bonded ferroelectrics of the KH_2PO_4 family. In these systems the Ising term corresponds to the interaction between the protons at different lattice sites and the transverse field accounts for the possibility of the protons occupy one of the two minima of a double potential well in a given site. The model can also be applied to study rare-earth compounds with singlet crystal field ground states, as has been done by Wang and Cooper[2]. In these systems there is a competition between the exchange interaction represented by the Ising term and the crystal field represented by the transverse field. There will be magnetic ordering if the ratio between these two terms exceeds a certain value. Cooperative Jahn-Teller systems with an applied external magnetic field is another example where this model hamiltonian works well[3]. Here the phase transition is driven by the interaction between localized orbital electronic states and the crystal lattice. Even at low temperatures sufficiently high applied external magnetic field can retrieve the high temperature phase. We refer to a paper by Stinchcombe[4] which gives a

Work partially supported by CNPq, FINEP (Brazilian Agencies).

more extensive description of the applications and the properties of the model.

The model has been exactly solved in one-dimension by Pfeuty[5] and in high dimensions series expansions results have been obtained by Elliott and Wood[6], Pfeuty and Elliott[7], Yanase et *al*[8] and Yanase[9]. The results of the above works suggested that at a finite temperature the critical behavior of the transverse Ising model is similar to the Ising model with a shift in the critical temperature and that at zero temperature the d-dimensional transverse Ising model behaves critically as d+l -dimensional Ising at T_c. Suzuki[10], Young[11] and Hertz[12] proved latter that the above suggestions were indeed exact statements.

Diluted magnetic systems have received a considerable amount of interest in the last years and we mention theoretical works by Oguchi and Obokata[13] (Ising and Heisenberg diluted), and by Matsudaira[14] and Kaneyoshi, Fittipaldi and Beyer[15] (Ising diluted).

The diluted transverse Ising model was recently studied by Mori[16] using the effective hamiltonian method and renormalization group calculations have been applied to the model by dos Santos[17]. Recently a new effective field theory has been applied to the Ising model[18] and to the transverse Ising model[19].

The work on the diluted Ising model by Kaneyoshi, Fittipaldi and Beyer[15] takes as a starting point an exact relation established by Callen[20] and despite the simplicity of the method they obtain results which are better than the obtained by the molecular fieldapproximation. A paper by Sã Barreto, Fittipaldi and Zeks[19] makes an extention (though not exact) of Callen's relation to treat the transverse Ising model.

It is the purpose of this paper to apply this extension of Callen's relation to study the diluted transverse Ising model. In section 2, we develop a general formalism for the problem, starting froman extension of Callen's relation[19]. In section 3, we get explicit relations for the parallel and the transverse magnetization and discuss some consequences of these results. We obtain in section 4 the critical temperature and the condition for the percolation concentration. In section 5, we analyse the internal energy. Finally in section 6 we discuss our results, as compared with those calculated in the molecular field approximation and also with the results of a Monte Carlo simulation obtained by Prelovsek and Sega[21].

2. FORMALISM OF THE PROBLEM

The hamiltonian for the diluted transverse Ising model can be written as

$$H = -\Omega \sum_i \xi_i \sigma_i^x - \frac{1}{2} \sum_{ij} J_{ij} \xi_i \xi_j \sigma_i^z \sigma_j^z \tag{1}$$

where Ω is the transverse field, J_{ij} is the exchange integral, σ_i^α ($\alpha = x, y$ or z) are the components of the spin 1/2 operators and ξ_i are occupation operators ($\xi_i = 1$ if the site i is occupied and $\xi_i = 0$ otherwise).

The local field at site i is given by

$$E_i = \sqrt{E_{ix}^2 + E_{iz}^2} \tag{2}$$

where

$$E_{ix} = \Omega \tag{3a}$$

and

$$E_{iz} = \sum_j J_{ij} \xi_j \sigma_j^z \tag{3b}$$

Based on references[15,19,20], we can write the following generalized Callen's relations, which are exact only for $\Omega = 0$

$$\langle \sigma_i^z \rangle = \left\langle \frac{\sum_j J_{ij} \xi_j \sigma_j^z}{E_i} \tanh \beta E_i \right\rangle \tag{4a}$$

$$\langle \sigma_i^x \rangle = \left\langle \frac{\Omega}{E_i} \tanh \beta E_i \right\rangle \tag{4b}$$

where E_i is given by eq. (2).

Using the differential operator $e^{\alpha D} f(x) = f(x+\alpha)$, with $D \equiv \frac{\partial}{\partial x}$, in expressions (4) we obtain for $\langle \sigma_i^z \rangle$ and $\langle \sigma_i^x \rangle$

$$\langle \sigma_i^z \rangle = \left\langle e^{(\sum_j J_{ij} \xi_j \sigma_j^z) D} \right\rangle f(x) \Big|_{x=0} \tag{5a}$$

$$\langle \sigma_i^x \rangle = \left\langle e^{(\sum_j J_{ij} \xi_j \sigma_j^z) D} \right\rangle \Gamma(x) \Big|_{x=0} \tag{5b}$$

where

$$f(x) = (x/\sqrt{\Omega^2 + x^2})\tanh \beta \sqrt{\Omega^2 + x^2}$$

$$\Gamma(x) = (\Omega/\sqrt{\Omega^2 + x^2})\tanh \beta \sqrt{\Omega^2 + x^2}$$

Neglecting site correlations we write

$$\langle e^{(\sum_j J_{ij}\xi_j\sigma_j^z)D}\rangle = \langle \prod_j e^{(J_{ij}\xi_j\sigma_j^z)D}\rangle \simeq \prod_j \langle e^{(J_{ij}\xi_j\sigma_j^z)D}\rangle$$

which can be substituted in eq.(5) to give

$$\langle\sigma_i^z\rangle_{\xi_j} = \prod_j \{\cosh(DJ_{ij}) + \langle\sigma_j^z\rangle \sinh(DJ_{ij})\}^{\xi_j} f(x)\Big|_{x=0} \qquad (6a)$$

$$\langle\sigma_i^x\rangle_{\xi_j} = \prod_j \{\cosh(DJ_{ij}) + \langle\sigma_j^z\rangle \sinh(DJ_{ij})\}^{\xi_j} \Gamma(x)\Big|_{x=0} \qquad (6b)$$

3. A. PARALLEL MAGNETIZATION

Taking the configuration average on the expression (6a), we obtain for the equilibrium parallel magnetization defined by $\langle\langle\sigma_i^z\rangle\rangle_c \equiv m_0$, the result

$$m_0 = [\cosh(DJ) + m_0 \sinh(DJ)]^{pz} f(x)\Big|_{x=0} \qquad (7)$$

where $p = \langle\xi_i\rangle_c$ is the average concentration of interacting spins and z is the lattice coordination number (supposing only nearest- neighbor interactions).

In order to further develop expression (7) we introduce the inverse transform of the expression $g_{pz}(y) \equiv [\cosh(y) + m_0 \sinh(y)]^{pz}$, with $y \equiv DJ$, in the following form

$$g_{pz}(y) = \frac{1}{2\pi i}\oint_{c_1} d\alpha'\, G^+_{pz}(\alpha')\, e^{\alpha' JD} + \frac{1}{2\pi i}\oint_{c_2} d\alpha'\, G^-_{pz}(\alpha')\, e^{-\alpha' JD} \qquad (8)$$

where $G^+_{pz}(\alpha')$ ($G^-_{pz}(\alpha')$) is the analytical continuation of $G_{pz}(a)$ defined in the positive (negative) region of the complex a' plane and a is the real part of a'. The direct transforms are given by

$$[G_{pz}(\alpha)]_{\alpha>0} = \int_0^{\infty} e^{-\alpha y}[\cosh y + m_0 \sinh y]^{pz}\, dy \qquad (9a)$$

$$[G_{pz}(\alpha)]_{\alpha<0} = \int_{-\infty}^{0} e^{-\alpha y}[\cosh y + m_0 \sinh y]^{pz}\, dy \qquad (9b)$$

Substituting expression (8) in (7) and performing the calculations indicated by eqs.(9a) and (9b) we obtain (see also Appendix)

$$m_0 = \frac{1}{2^{pz}} \sum_{n=0}^{n'<\frac{pz}{2}} \binom{pz}{n} f[(pz-2n)J]\{(1+m_0)^{pz-n}(1-m_0)^{n}-(1-m_0)^{pz-n}(1+m_0)^{n}\} \qquad (10)$$

Within the approximations used, this expression is general and can be used to describe various situations of dilution. One should notice that it depends on the product pz, and this fact shows the limitation of the results obtained. For example, the results for the undiluted square lattice (p=1, z=4) are the same as for the diluted triangular lattice with p=2/3. And there is no way to distinguish the lattice dimensionality, as for example in the case of pz=6, which is satisfied for the planar triangular lattice and the simple cubic lattice. However, we should stress that those limitations, at this level of approximation, are not a drawback in the method. They can be overcome by the proper treatment of both tharmal and configurational average, where correlations should be taken into account. The method outlined before can be applied to calculate the correlation functions, which although lengthy are simple and straightforward. However we do not intent to show in this paper the modifications caused by the inclusion of the correlation functions. Here, we present the results in its most simple form and show that it goes beyond the mean field results.

Further, we can also make the following coments about expression (10) for the parallel magnetization:

a) It is easy to see that the right hand side of eq.(10) is a polynomial in odd powers of m_0 which is infinite or finite if the product pz is a fractionary or an integral number.

b) m_0 = 0 is always a solution of equation (10), as a consequence of statement (a).

c) m_0 = 1 will be a solution of equation (10) when $\beta \to \infty$ (T=0) and

$\Omega \to 0$ (in this case the function $f[(pz-2n)J] \equiv \tanh[(pz-2n)\beta J]$) .

d) For $pz=2$ the solution of equation (10) is not determined; in order to have solution we must have $pz>2$.

e) Sometimes two solutions satisfy eq. (10); a trivial solution and a finite solution. The way to take the stable solution will be examined in a forthcoming paper where we will be concerned with the dynamics of this system.

f) We show in figure 1 to 3 graphs for the parallel magnetization, as compared with mean field results.

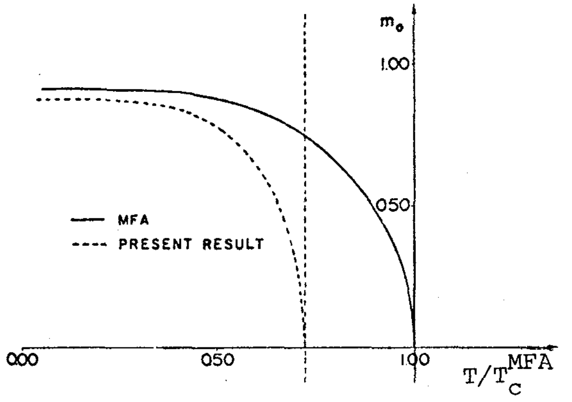


Fig.1 - Parallel magnetization curve for the diluted transverse Ising model, as compared with the mean field result, for $pz=4$ and $\Omega/J=1.6$. (Vertical broken line indicates the transition temperature of the present approximation)

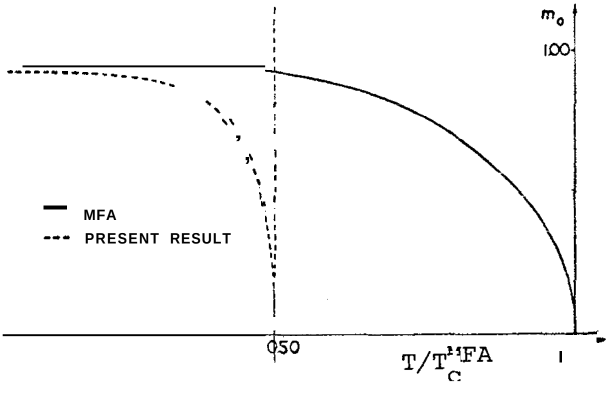


Fig.2 - Parallel magnetization curve for the diluted transverse Ising model, as compared with the mean field result, for $pz=2.5$ and $\Omega/J=0.6$. (Vertical broken line indicates the transition temperature of the present approximation)

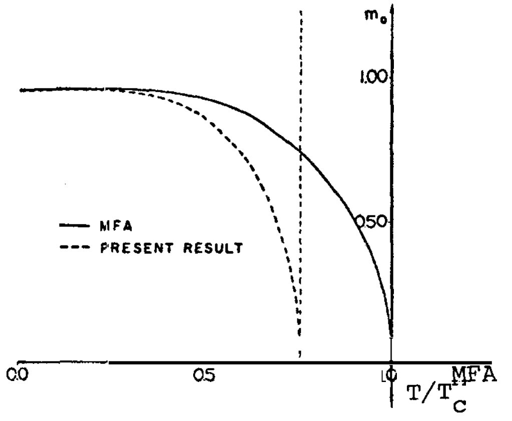


Fig.3 - Parallel magnetization curve for the diluted transverse Ising model, as compared with the mean field result, for pz = = 3.5 and Ω/J = 0.9. (Vertical broken line indicates the transition temperature of the present approximation).

3. B. PERPENDICULAR MAGNETIZATION

Using the same procedure outlined before we get for the equilibrium perpendicular magnetization, $\eta_0 \equiv \langle\langle\sigma_i^x\rangle_{\xi_j}\rangle_c$, the result

$$\eta_0 = [\cosh(DJ) + m_0 \sinh(DJ)]^{pz} \cdot \Gamma(x)\Big|_{r=0} \qquad (11)$$

Let us define the inverse transform of the operator

$$\gamma_{pz}(y) = [\cosh(y) + m_0 \sinh(y)]^{pz}$$

as

$$\gamma_{pz}(y) = \frac{1}{2\pi i}\oint_{c_1} d\alpha'\, \theta^{+}_{pz}(\alpha')\, e^{\alpha' y}$$
$$+ \frac{1}{2\pi i}\oint_{c_2} d\alpha'\, \theta^{-}_{pz}(\alpha') e^{-\alpha' y} + \frac{1}{2\pi i}\oint_{c_3} d\alpha'\, \theta^{0}_{pz}(\alpha') e^{\alpha' y} \qquad (12)$$

where $\theta^{+}_{pz}(\alpha')$ $(\theta^{-}_{pz}(\alpha'))$ is the analytical continuation of θ_{pz}(a) inthe positive (negative) region of the complex α' plane and $\theta^{0}_{pz}(\alpha')$ is the analytical continuation of 8_{pz}(a) in an infinitesimal strip around the imaginary axis.

Substituting this expression into eq. (11) we obtain

$$n_0 = \frac{1}{2\pi i} \oint_{c_1} d\alpha' \, \Gamma(\alpha' J) \, \theta^{+}_{pz}(\alpha') + \frac{1}{2\pi i} \oint_{c_2} d\alpha' \, \Gamma(-\alpha' J) \, \theta^{-}_{pz}(\alpha') + \frac{1}{2\pi i} \oint_{c_3} d\alpha' \, \Gamma(\alpha' J) \, \theta^{0}_{pz}(\alpha') \tag{13}$$

Proceeding in an analogous way as in section 3.A we obtain

$$n_0 = \frac{1}{2^{pz}} \sum_{n=0}^{n'<pz/2} \Big[\binom{pz}{n} \Gamma[(pz-2n)J] \{(1+m_0)^{pz-n}(1-m_0)^n + (1-m_0)^{pz-n}(1+m_0)^n\} + \binom{pz}{pz/2} \Gamma(0) \, (1-m_0^2)^{pz/2}\} \, \delta_{pz,2n} \Big] \tag{14}$$

We see that only if pz is even we have a contribution in $\Gamma(0)$ for the perpendicular magnetization. In the disordered phase, where $m_0=0$, expression (14) reduces to

$$n_0 = \frac{1}{2^{pz}} \sum_{n=0}^{n'<pz/2} \{ \binom{pz}{n} \, 2\Gamma[(pz-2n)J] + [\binom{pz}{pz/2} \Gamma(0)] \delta_{pz,2n} \} \tag{15}$$

About relation (14) for the perpendicular magnetization we can make the following comments:

a) The right hand side of relation (14) is a polynomial in even powers of m_0, which will be finite or infinite whether the product pz is a integral or a fractionary number.

b) At the paramagnetic phase ($m_0=0$) the relation eq.(14) reduces to relation eq.(15).

c) We show in figures 4 to 6 graphs for the perpendicular magnetization, as compared with the mean field result. One should also compare these figures with figure 3 of reference 21. The qualitative behavior is the same in both treatments and totally different from the mean field approach.

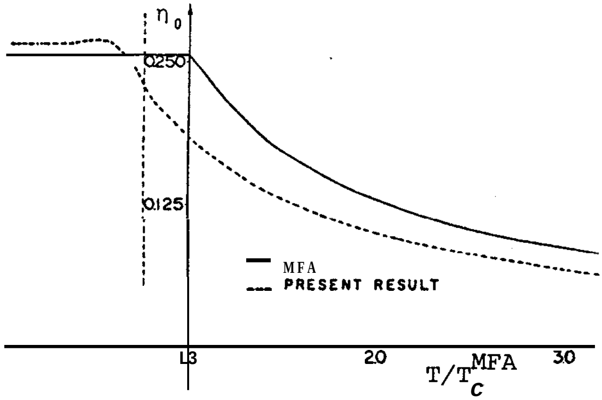


Fig. 4 - Perpendicular magnetization for the diluted transverse Ising model as compared with the mean field result, for $pz = 3.5$ and $\Omega/J = 0.9$. (Vertical broken line indicates the transition temperature of the present approximation).

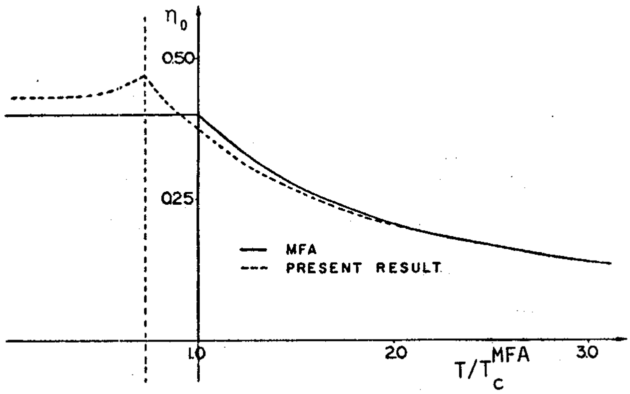
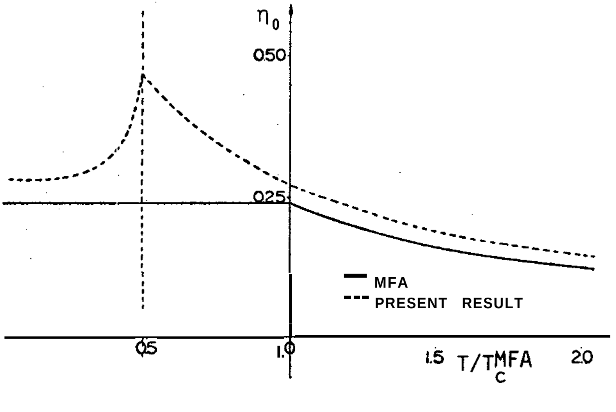


Fig. 5 - Perpendicular magnetization for the diluted transverse Ising model as compared with the mean field result, for $pz = 4$ and $\Omega/J = 1.6$. (Vertical broken line indicates the transition temperature of the present approximation).



Fi'g. 6 - Perpendicular magnetization for the diluted transverse Ising model as compared with the mean field result, for $pz = 2.5$ and $\Omega/J = 0.6$. (Vertical broken line indicates the transition temperature of the present approximation).

4. TRANSITION TEMPERATURE

In order to obtain the transition ternperature we expand expression (7) in a power series around the value $m_0 = 0$.

In the limit of $m_0 \to 0$ we obfain

$$1 = pz\left[\cosh(DJ)\right]^{pz-1} \sinh(DJ) \cdot f(x)\Big|_{x=0,T=T_c} \tag{16}$$

Let us define $\lambda_v(y)$, with $v = pz-1$ and $y = DJ$, by

$$\lambda_v(y) = \left[\cosh(y)\right]^v \sinh(y)$$

The inverse Laplace transforrn of $A_v(y)$ is

$$\lambda_v(y) = \frac{1}{2\pi i}\oint_{c_1} d\alpha' \, L_v^+(\alpha')e^{\alpha' y} + \frac{1}{2\pi i}\oint_{c_2} d\alpha' \, L_v^-(\alpha')\, e^{-\alpha' y} \tag{17}$$

Substituting $\lambda_v(y)$ in eq.(16) we get

$$1 = \frac{pz}{2\pi i}\oint_{c_1} d\alpha' \, L_v^+(\alpha')\, f(\alpha' J)\Big|_{T=T_c} + \frac{pz}{2\pi i}\oint_{c_2} d\alpha' \, L_v^-(\alpha') f(-\alpha' J)\Big|_{T=T_c}$$

where $L_v^+(\alpha')$ ($L_v^-(\alpha')$) is the analytical continuation of $L_v(a)$ in the positive (negative) region of the complex a' plane and a is the real part of a'.

Finally we obtain the relation frorn which we can deduce the transition temperature

$$1 = (pz/2^{pz-1})\left\{ \sum_{n=0}^{n'<(pz)/2} \binom{pz-1}{n} f[(pz-2n)J]_{T=T_c} - \sum_{n=0}^{n''<(pz-2)/2} \binom{pz-1}{n} f[(pz-2n-2)J]_{T=T_c} \right\} \tag{18}$$

The percolation concentration can be obtained from eq.(18) in the limit of T_c=O. Using the definition of $f[(pz-2n)J]$ we get for p_c

$$1 = \frac{pz}{2^{pz-1}} \left\{ \sum_{n=0}^{n'<(pz)/2} \binom{pz-1}{n} \frac{(pz-2n)J}{\sqrt{\Omega_c^2+(pz-2n)^2 J^2}} - \sum_{n=0}^{n''<(pz-2)/2} \binom{pz-1}{n} \frac{(pz-2n-2)J}{\sqrt{\Omega_c^2+(pz-2n-2)^2 J^2}} \right\} \tag{19}$$

For example,applying relation (18) for pz = 3 and 3.2 we obtain

$$\frac{4}{3} = f(3J)\Big|_{T=T_c} + f(J)\Big|_{T=T_c} \qquad \text{for } pz = 3$$

$$\frac{2^{2.2}}{3.2} = f(3.2J)\Big|_{T=T_c} + 1.2\, f(1.2J)\Big|_{T=T_c} \qquad \text{for } pz = 3.2$$

The results of relation (18) can be better understood looking at the graph of figure 7. There, we represent the level lines of the surface $\phi(\Omega/J,\ kT_c/J,\ pz) = 0$, which separates in the space of these three variables, the ordered and disordered regions. We have traced out the level lines for pz going from 2 to 6 in intervals of 0.5. Note that for pz=2 the level line reduces to a point, If we cut the above mentioned surface at the plane $T_c = 0$ we obtain figure 8, which gives us the critical transverse field as a function of pz. We also show in figure 8 the mean field result in order to compare with the present work. Note that for the mean field surface the level line will reduce to a point only at $pz = 0$.

5. INTERNAI. ENERGY AND SPECIFIC HEAT

The interna1 energy is given by

$$U = -\Omega < \sum_i \xi_i \sigma_i^x > - \frac{1}{2} < \sum_{ij} J_{ij} \xi_i \xi_j \sigma_i^z \sigma_j^z > \tag{20}$$

To calculate the correlation function which appears in eq. (20) we use the relation

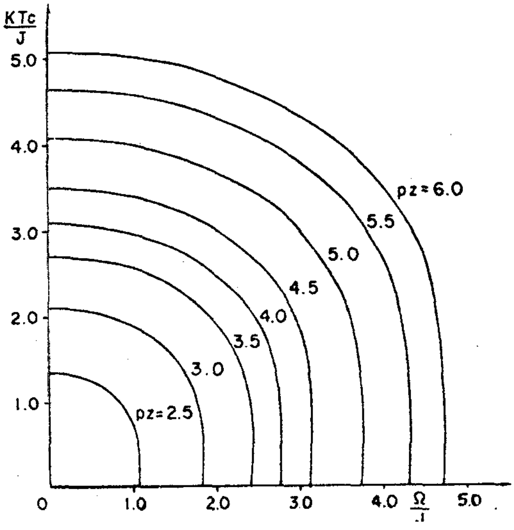


Fig. 7 - Level lines of the section cut of the surface $\phi(\frac{kT_c}{J}, \frac{\Omega}{J}, pz)=0$, which separates the ferromagnetic and paramagnetic phases of the diluted transverse Ising model. From inside we have $pz = 2$ (which coincides with the origin), 2.5, 3.0, 3.5, 4.0, 4.5, 5.0, 5.5 and 6.0.

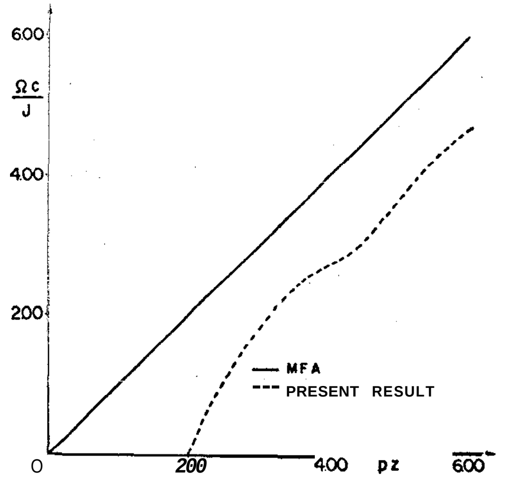


Fig.8 - The percolation curve for the diluted transverse Ising model, as compared with the mean field result (the straight line).

$$\langle\sigma_i^z\ \sigma_j^z\rangle = \langle\sigma_i^z (E_j^z/E_j)\tanh \beta E_j\ \rangle \tag{21}$$

which is valid within the same approximation as relation (4). Using the differentiiil operator defined previously

$$\langle\sigma_i^z\ \sigma_j^z\ \rangle = \langle\sigma_i^z\ e^{DE_j^z}\ \rangle \cdot f(x)\Big|_{x=0}$$

Defining $G_j(x',D) = \langle e^{DE_j^z x'}\rangle$ we obtain for the second term in eq. (20) the following result

$$U_z = -\frac{1}{2}\sum_j \xi_j\ \left(\frac{\partial}{\partial x'}\ G_j(x',D)\,.\ \frac{1}{D}\right).f(x)\Big|_{x=0,\,x'=1}$$

Taking the configuration average

$$\bar{U}_z = -(p/2)\Sigma\ \left(\frac{\partial}{\partial x'}\ \overline{G(x',D)}\,.\ \frac{1}{D}\right).f(x)\Big|_{x=0,\ x'=1} \tag{22}$$

But

$$\overline{G_j(x',D)} = \overline{\langle e^{(\sum_i J_{ij}\ \xi_i\ \sigma_i^z)x'D}\rangle} \approx \prod_i \overline{\langle e^{(J_{ij}\ \sigma_i^z)x'D\ \xi_i}\rangle}$$

$$= [\cosh(x'DJ) + m_0\ \sinh(x'DJ)]^{pz} \tag{23}$$

which gives, after substitution in eq. (22)

$$U_z = -(p^2z/2)NJ\{[\cosh(DJ) + m_0\ \sinh(DJ)]^{pz-1}$$

$$\times[\sinh(DJ) + m_0\ \cosh(DJ)]\}\ .\ f(x)\Big|_{x=0}$$

In order to proceed further we must define the function $h_v(y)$ through

$$h_v(y) = [\cosh y + m_0\ \sinh y]^v\ [\sinh y + m_0 \cosh y]$$

Which gives for $\bar{U}_z$

$$\bar{U}_z = -\frac{p^2 zNJ}{2}\left[\frac{1}{2\pi i}\oint_{C_1} d\alpha' F_v^{+}(\alpha') e^{\alpha' JD}.f(x)\Big|_{x=0} + \frac{1}{2\pi i}\oint_{C_2} d\alpha' F_v^{-}(\alpha') e^{-\alpha' JD}.f(x)\Big|_{x=0}\right]$$

where $F_v^{+}(\alpha')$ $(F_v^{-}(\alpha'))$ is the analytical continuation of $F_v(\alpha)$ in the positive (negative) region of the complex α' plane and a is the real part of α'.

Using $F_V(\alpha)$ we obtain

$$\bar{U}_z = -\frac{p^2 zNJ}{2}\frac{1}{2^{pz}}\Bigg\{\sum_{n=0}^{n'<(pz)/2}\Big[\binom{pz-1}{n} f[(pz-2n)J]$$

$$\cdot\,[(1+m_0)^{pz-n}(1-m_0)^{n} + (1-m_0)^{pz-n}(1+m_0)^{n}]\Big]$$

$$-\sum_{n=0}^{n''<(pz-2)/2}\Big[\binom{pz-1}{n} f[(pz-2n-2)J]\,[(1+m_0)^{pz-n-1}(1-m_0)^{n+1}$$

$$+ (1-m_0)^{pz-n-1}(1+m_0)^{n+1}]\Big]\Bigg\} \qquad (24)$$

The expressions for $\bar{U}_x$ can be immediately obtained from expression (14)

$$\bar{U}_x = -\Omega Np\,\overline{\langle\sigma^x\rangle}$$

$$= -\frac{Np\Omega}{2^{pz}}\sum_{n=0}^{n'<(pz)/2}\Bigg\{\binom{pz}{n}\,\Gamma[(pz-2n)J]\,[(1+m_0)^{pz-n}(1-m_0)^{n}$$

$$+ (1-m_0)^{pz-n}(1+m_0)^{n}] + \binom{pz}{pz/2}\,\Gamma(0)\,(1-m_0^2)^{pz/2}\,\delta_{pz,2n}\Bigg\} \qquad (25)$$

The internal energy is given by,

$$\bar{U} = \bar{U}_x + \bar{U}_z \qquad (26)$$

and the specific heat is obtained from $C_v = d\bar{U}/dT$. For $pz = 3$ we get

$$\bar{U}_z = -\frac{3}{8} NpJ\{[f(3J) + f(J)] + [3f(3J) - f(J)]m_0^2\} \tag{27a}$$

$$\bar{U}_x = -\frac{1}{4} Np\Omega\{[\Gamma(3J) + 3\Gamma(J)] + 3[\Gamma(3J) - \Gamma(J)]m_0^2\}$$

For $pz = 4$ we get,

$$\bar{U}_z = -\frac{NpJ}{4}\{[f(4J) + 2f(2J)] + [6f(4J)]m_0^2 + [f(4J) - 2f(2J)]m_0^4\} \tag{28a}$$

$$\bar{U}_x = -\frac{Np\Omega}{8}\{[\Gamma(4J) + 4\Gamma(2J) + 3\Gamma(0)] +$$

$$[6\Gamma(4J) - 6\Gamma(0)]m_0^2 + [\Gamma(4J) - 4\Gamma(2J) + 3\Gamma(0)]m_0^4\} \tag{28b}$$

(28b)

Looking at relations (27a) and (28a) we see that they give a contribution of the short-range order for the internal energy $\bar{U}_z$. This can be easily verified if we put $m_0 = 0$ at eqs. (27a) and (28a) and represents an improvement over the traditional mean field approximation.

6. CONCLUSIONS

We see that with this new effective field, we have obtained general explicit relations for the thermodynamic quantities of the diluted ti-ansverse Ising model, in all temperature range. In this aspect, this method resembles the traditional mean field approximation. However, there is a difference, even in quality, because this treatment takes into account some of the short range order effects. This evidence is displayed particularly in figure 7, where the present results show no long range order for $pz \leqslant 2$ in contrast to the mean field result and also in the contribution of the two particle parallel spin component correlatlons for the internal energy above T_c. However we must have in mind that this treatment is far from exact and can be used due to its generality as an alternative way to the mean field treatment.

Let us now compare our results with those obtained by Prelovsek and Sega[21] for the S = ∞ transverse Ising model. We can see from figure 1 to 6 that the curves of the present work compare with the curves of Monte Carlo calculations of Prelovsek and Sega[21] for infinite spin, showing a qualitative behavior different from the mean field results. This can be understood, if we look at reference 19, where the generalized Callen's relations for the transverse Ising model were obtained in an approximation which can be understood as treating the neighbors as classical variables, a situation similar to the $S = \infty$ model.

We are grateful to Dr. I.P.Fittipaldi for many valuable discussions.

APPENDIX - TRANSFORM OF THE OPERATORS $g_v(y)$ AND $\gamma_v(y)$

By definition

$$g_v(y) = [\cosh y + m_0 \sinh y]^v \qquad (A.1)$$

where $y = JD = J \frac{\partial}{\partial x}$ and $v = pz$

Then,

$$[G_v(\alpha)]_{\alpha>0} = \int_0^{m} e^{-\alpha y} g_v(y) \, dy \qquad (A.2)$$

Let us introduce a new variable $u = e^{-\alpha y}$

$$[G_v(\alpha)]_{\alpha>0} = (2^{-v}/\alpha)\int_0^1 [(1 + m_0) u^{-1/\alpha} + (1 - m_0)u^{1/\alpha}]^v du \qquad (A.3)$$

Changing again to a new variable $w = u^{2/\alpha}$

$$[G_v(\alpha)]_{\alpha>0} = 2^{-(v+1)} \int_0^1 w^{(1/2)(\alpha-v)-1} (1+m_0)^v [1 + (\frac{1-m_0}{1+m_0})w]^v dw \qquad (A.4)$$

Note that the limits of integration are the same because a is positive. Writing

$$\left[1 + (\frac{1-m_0}{1+m_0})w\right]^v = \sum_{n=0}^{\infty} \binom{v}{n} \left[(\frac{1-m_0}{1+m_0}) w\right]^n \qquad (A.5)$$

we get

$$[G_v(\alpha)]_{\alpha>0} = 2^{-(v+1)} \sum_{n=0}^{\infty} \binom{v}{n} (1+m_0)^v (\frac{1-m_0}{1+m_0})^n \int_0^1 w^{(1/2)(\alpha-v)+n-1} dw$$

$$(A.6)$$

Therefore, after integration

$$[G_v(\alpha)]_{\alpha>0} = 2^{-v} \sum_{n=0}^{\infty} \binom{v}{n} (1+m_0)^{v-n} (1-m_0)^n \frac{1}{\alpha-v+2n} \quad (A.7)$$

Similarly for the other branch, $\alpha < 0$, we get

$$[G_v(\alpha)]_{\alpha<0} = -2^{-v} \sum_{n=0}^{\infty} \binom{v}{n} (1-m_0)^{v-n} (1+m_0)^n \frac{1}{-\alpha-v+2n} \quad (A.8)$$

In order to calculate $[\theta_{pz}(\alpha)]$, $\gtrless 0$ we must proceed in the same way as before and we can show that

$$[\theta_{pz}(\alpha)]_{\alpha>0} \equiv [G_{pz}(\alpha)]_{\alpha>0} \quad (A.9)$$

However, for $\alpha < 0$ we must define $[\theta_{pz}(\alpha)]_{\alpha<0}$ in such way that

$$[\theta_{pz}(\alpha)]_{\alpha<0} \equiv -[G_{pz}(\alpha)]_{\alpha<0} \quad (A.10)$$

because when $m_0 = 0$, in the disordered phase, we must have $\langle\langle\sigma_i^x\rangle\xi_i\rangle_c =$ $= \eta_0 \neq 0$, due to the presence of the transverse field .

The transforms of the operators $\lambda_v(y)$ and $h_v(y)$ can be obtained in a similar way.

REFERENCES

1. P.G.de Gennes, Solid State Commun. *1*, 132 (1963).
2. Y.L.Wang and B.R.Cooper, Phys. Rev. 172, 539 (1968).
3. A.H.Cooke, S.J.Swithenby and M.R.Wells, Solid State Commun. *10*, 265 (1972); see also G.A.Gehring and K.A.Gehring, Rep. Prog. Phys., 38, 1 (1975).
4. R.B.Stinchcombe, J.Phys. C 6, 2459 (1973); see also in Nato Advanced Study Institutes Series: Series B. Physics: Vol. 29 p.209, Ed. Tormod Riste, Plenum Press, New York (1977).
5. P.Pfeuty, Ann. Phys. (NY) 57, 79 (1970).
6. R.J.Elliott and C.Wood, J.Phys. C 4, 2359 (1971).
7. P.Pfeuty and R.J.Elliott, J.Phys. C 4, 2370 (1971).
8. A.Yanase, Y.Takeshige and M.Suzuki, J.Phys.Soc. Japan 41, 1108(1976).
9. A.Yanase, J.Phys. Soc.Japan 42, 1816 (1977).

10. M.Suzuki, Progr. Theor. Phys. 46, 1337 (1971); Progr. Theor. Phys, 56, 1454 (1976).
11. A.P. Young, J.Phys. C 8, L 309 (1975).
12. J.A. Hertz, Phys. Rev. B *14*, 1165 (1976).
13. T.Oguchi and T.Obokata, J.Phys.Soc.Japan 27, 1111 (1969).
14. N.Matsudaira, J.Phys.Soc.Japan 35, 1593 (1973).
15. T.Kaneyoshi, I.P.Fittipaldi and H.Beyer, Phys. Stat. Sol. (b) 102, 393 (1980).
16. K.Mori, J.Phys.Soc.Japan 50, 3688 (1981).
17. R.R. dos Santos, J.Phys. C 15, 3141 (1982).
18. R.Honmura and T.Kaneyoshi, J.Phys. C 12, 3979 (1979).
19. F.C.Sá Barreto, I.P.Fittipaldi and B.Zeks, Ferroelectrics 39, 1103 (1981).
20. H.B.Callen, Phys. Lett. (Netherlands) 4, 161 (1963).
21. P.Prelovsek and I.Sega, J.Phys. C 11, 2103 (1978).

Resumo

A diluição do modelo de Ising num campo transverso é estudada por intermédio de uma aproximaçao do tipo campo efetivo. O trabalho é baseado em uma extensão da relação de Callen (Phys. Lett. 4, 161(1963)) apropriada para tratar o modelo presente. A termodinâmica do modelo diluido é obtida e mostramos que os resultados são melhores quando comparados àqueles obtidos via tratamento convencional do tipo campo medi~. Também comparamos os resultados com cálculos existentes por técnica de Monte Carlo para o modelo de Ising num campo transverso para spin - ∞.