Revista Brasileira de Física, Volume 13, nº 2, 1983

Effective-Field Treatment of an Anisotropic Ising Ferromagnet

E. F. SARMENTO, R. HONMURA*

Departamento de Física, Universidade Federal de Alagoas, Maceió, 57000, AL, Brasil

and

C. TSALLIS

Centro Brasileiro de Pesquisas Físicas, Rua Xavier Sigaud 750, Rio de Janeiro 22290, RJ, Brasil

Recebido em 30 de março de 1983

Abstract We discuss the anisotropic square lattice spin 1/2 Ising ferromagnet. Through this system we illustrate how all relevant thermodynamical quantities (phase diagram, magnetization, short range order parameter, specific heat and susceptibility) can be approximately caiculated within an effective-field unified procedure (which susbtantially irnproves the Mean Field Approximation). Two slightly different approximations for the susceptibility (whose exact computation is still lacking) are presented. The way the extremely anisotropic square lattice recovers the linear chain is exhibited. The present (mathematically simple) procedures could be useful in the study of complex Ising problems.

1. INTRODUCTION

The basic understanding of most magnetic phenomena is presently quite deep. In what concerns theoretical approaches, a great amount of techniques are presently available (series[1], Monte Carlo[2], Renormalization Group[3,4], Coherent Potential Approximation[5] among others; see also references therein); however in practice not all of them are tractable for complex systems, and consequently effective-field theories can be very useful to provide a first insight into these problems. Recently Honrnura and Kaneyoshi[6] have introduced, for the Ising model, a new type of effective-field treatment (based on the use of an appropriate differential operator into the spin correlation function Callen identity[7]) which, without introducing mathematical complexities, has been quite succesfully applied for a large variety of situations (pure systerns[8], bond-randoni magnets[9,10,11] including spin-glass[12] and amorphous[13,14] systems, binary alloys[15], transverse Ising model[16] and surface problems[17]). This approach is quite superior to the standard Mean Field Approximation

---

* Partially supported by CNPq.

(MFA) in several senses; for example, contrarily to MFA, it provides a vanishing critical temperature for the nearest-neighbour linear chain, and exhibits physically expected non uniform convergences (related to various crossovers) in random magnets[9,10]. Up to now most works within this new framework have been exclusively dedicated to the calculation of the phase diagrams and magnetization; the specific heat has been analyzed in two occasions[6,11] in isotropic systems and the magnetic susceptibility in none.

In the present work we study the anisotropic square lattice spin 1/2 Ising ferromagnet. All relevant thermodynamical quantities (namely the phase diagram, spontaneous magnetization, short range order parameter, specific heat and isothermal magnetic susceptibility) are calculated within an unified approximation framework; in particular for the susceptibility (whose exact computation is still to be done) we introduce two slightly different approximations. The fact that we are dealing with an anisotropic system will enable us to exhibit how the d=2 to d=1 crossover ($d \equiv$ dimensionality) occurs.

2. MODEL AND FORMALISM

2.1. Spontaneous magnetization

Let us consider the Hamiltonian

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

where $<i,j>$ run over all the couples of nearest-neighbouring sites on a square lattice, and J equals either J_1 and J_2 ($0 \leqslant J_2 \leqslant J_1 > 0$), respectively corresponding to the x and y axes. The starting point for thestatistics of this system is the following Callen identity[7]

$$<\sigma_i> = <\tanh \beta \sum_j J_{ij} \;\; \sigma_j > \qquad (\beta \equiv 1/k_B T) \tag{2}$$

where j runs over the 4 neighbours of site i, and $<...>$ denotes the canonical thermal average. By introducing [6] the differential operator $D \equiv \partial/\partial x$, Eq. (2) may be rewritten as follows:

$$<\sigma_i> = <e^{\beta D \sum_j J_{ij} \sigma_j}> \tanh x \Big|_{x=0} \tag{3}$$

By introducing the definition

$$G(t,\xi,\eta) \equiv \langle e^{D[\xi(\sigma_1+\sigma_3) + \alpha\eta(\sigma_2+\sigma_4)]/t} \rangle \tanh x \Big|_{x=0} \tag{4}$$

where $t \equiv k_B T/J_1$, $\alpha \equiv J_2/J_1 \in [0,1]$ and σ_1 and σ_3 (σ_2 and σ_4) are the "left" and "right" ("up" and "down") nearest neighbcurs of site i, the spontaneous reduced magnetization will be given by

$$m \equiv \langle\sigma_i\rangle = G(t,\xi,\eta)\Big|_{\xi=\eta=1}$$

$$\simeq \left[\left(\cosh\frac{D}{t} + m\sinh\frac{D}{t}\right)^2 \left(\cos\frac{\alpha D}{t} + m\sinh\frac{\alpha D}{t}\right)^2\right] \tanh x \Big|_{x=0} \tag{5}$$

We have neglected correlations between next-nearest neighbours. By evaluating Eq. (5) we obtain (see also Ref. (9))

$$m = Am + Bm^3 \tag{6}$$

$$A \equiv \left[\tanh\frac{2(1+\alpha)}{t} + \tanh\frac{2}{t} + \tanh\frac{2\alpha}{t}\right]/2 \tag{6'}$$

$$B \equiv \left[\tanh\frac{2(1+\alpha)}{t} - \tanh\frac{2}{t} - \tanh\frac{2\alpha}{t}\right]/2 \tag{6''}$$

which admits the paramagnetic solution $m\equiv0$ and the ferromagnetic one (see fig.1)

$$m = \left(\frac{1-A}{B}\right)^{1/2} \tag{7}$$

The critical line is given by $A=1$, which provides a critical reduced ternperature t_c monotonously increasing from 0 ($d=1$) to 3.0898 ($d = 2$) while α runs from 0 to 1 ($t_c^{\text{exact}}(\alpha=1)=2.2692$; $t_c^{\text{MFA}}(\alpha=1)=4$).

2.2. Short range order parameter and specific heat

The interna1 energy per site $\langle E\rangle$ is given by

$$\langle E\rangle = -J_1\tau_x - J_2\tau_y \tag{8}$$

$$\tau_x \equiv \langle\sigma_i\sigma_1\rangle = \langle\sigma_i\sigma_3\rangle \tag{9}$$

$$\tau_y \equiv \langle\sigma_i\sigma_2\rangle = \langle\sigma_i\sigma_4\rangle \tag{9'}$$

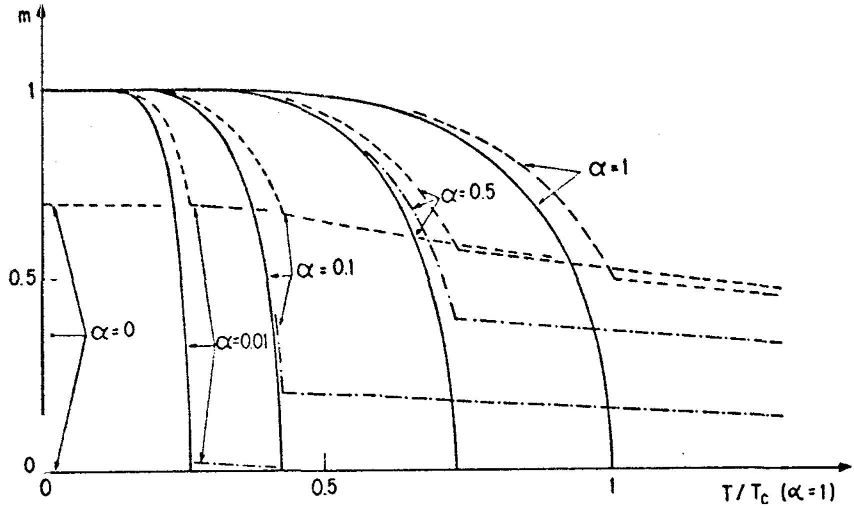

Fig.1 - Thermal behaviours of the spontaneous magnetization (solid line) and the square root of the short range order parameters along the x- (dashed line) and y- (dot-dashed line) directions for selected values of $\alpha \equiv J_2/J_1$.

(τ_x and τ_y are referred hereafter as short range order parameters). By using the two-site Callen identity we can rewrite Eqs. (9) and (9') as follows:

$$\tau_{x,y} = \langle \sigma\, e^{\beta D \sum_j J_{ij} \sigma_j} \rangle \tanh x \Big|_{x=0} \tag{10}$$

or even

$$\tau_x = \frac{1}{2}\frac{t}{D}\frac{\partial}{\partial \xi} G(t,\xi,\eta)\Big|_{\xi=\eta=1}$$

$$= \frac{1}{8}\left\{\tanh\frac{2(1+\alpha)}{t} + \tanh\frac{2(1-\alpha)}{t} + 2\tanh\frac{2}{t}\right\}$$

$$+ \frac{1}{4}\left\{3\tanh\frac{2(1+\alpha)}{t} - \tanh\frac{2(1-\alpha)}{t}\right\} m^2$$

$$+ \frac{1}{8}\left\{\tanh\frac{2(1+\alpha)}{t} + \tanh\frac{2(1-\alpha)}{t} - 2\tanh\frac{2}{t}\right\} m^4 \tag{11}$$

and

$$\tau_y = \frac{1}{2}\frac{t}{\alpha D}\frac{\partial}{\partial\eta}G(t,\xi,\eta)\Big|_{\xi=\eta=1}$$

$$= \frac{1}{8}\left\{\tanh\frac{2(1+\alpha)}{t} - \tanh\frac{2(1-\alpha)}{t} + 2\tanh\frac{2\alpha}{t}\right\}$$

$$+ \frac{1}{4}\left\{3\tanh\frac{2(1+\alpha)}{t} + \tanh\frac{2(1-\alpha)}{t}\right\} m^2$$

$$+ \frac{1}{8}\left\{\tanh\frac{2(1+\alpha)}{t} - \tanh\frac{2(1-\alpha)}{t} - 2\tanh\frac{2\alpha}{t}\right\} m^4 \qquad (11')$$

The temperature dependences of $\sqrt{\tau_x}$ and $\sqrt{\tau_y}$ are depicted in Fig.1. The specific heat per site is given by

$$C = \frac{\partial\langle E\rangle}{\partial T} = -k_B\left[\frac{\partial\tau_x}{\partial t} + \alpha\frac{\partial\tau_y}{\partial t}\right] \qquad (12)$$

The therrnal behaviour of the specific heat is shown in Fig.2 for selected values of α: we remark that, although the well known logarithmic divergence is not reproduced (this is of course typical for effective-field theories), a paramagnetic tail (proportional to $1/T^2$ in the limit of high temperatures) is present, thus improving the standard MFA result.

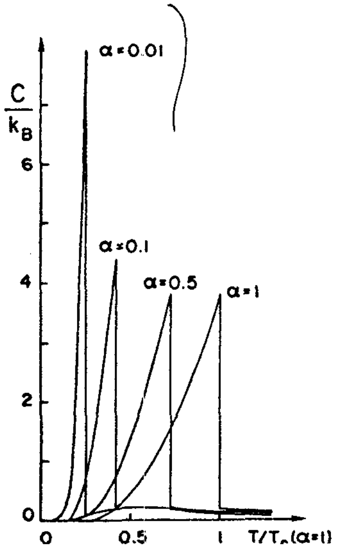

Fig. 2 - Thermal behaviour of the reduced specific heat for selected values of a.

2.3. Susceptibility

In the presence of an external magnetic field H, the term $-g\mu_B H$ must be added to Hamiltonian (1) ($g \equiv$ Landé factor and $\mu_B \equiv$ Bohr magneton); consequently identity (2) is extended into

$$\langle\sigma_i\rangle = \langle\tanh\beta(\sum_j J_{ij}\sigma_j + g\mu_B H)\rangle$$
$$= \langle e^{\beta D \sum_j J_{ij}\sigma_j}\rangle \tanh(x + \beta g\mu_B H)\Big|_{x=0} \tag{13}$$

The zero field isothermal magnetic susceptibility per site is given by

$$\chi_0 = \frac{g^2\mu_B^2}{J_1}\chi \tag{14}$$

$$\chi \equiv \frac{\partial m}{\partial h}\Big|_{h=0} \tag{15}$$

where $h \equiv g\mu_B H/J_1$

The identity (13) can be rewritten as follows:

$$m = \langle e^{D[(\sigma_1+\sigma_3) + \alpha(\sigma_2+\sigma_4)]/t}\rangle \tanh\left(x + \frac{h}{t}\right)\Big|_{x=0} \tag{16}$$

By neglecting next-nearest-neighbour spin correlations, Eq. (16) becomes identical to Eq. (5) except for the transformation $\tanh x \to \tanh(x+h/t)$; differentiation with respect to h on both sides leads to our present first approximation for the susceptibility:

$$\chi^I = \frac{F}{t(1-A-3Bm^2)} \tag{17}$$

where I stands for "first" approximation, A, B and m are given by Eqs. (6'), (6") and (7) respectively, and

$$F \equiv \frac{1}{8}\left\{\left[\operatorname{sech}^2\frac{2(1+\alpha)}{t} + \operatorname{sech}^2\frac{2(1-\alpha)}{t} + 2\operatorname{sech}^2\frac{2}{t}\right.\right.$$
$$\left. + 2\operatorname{sech}^2\frac{2\alpha}{t} + 2\right]$$

$$+ \left[6 \operatorname{sech}^2 \frac{2(1+\alpha)}{t} - 2 \operatorname{sech}^2 \frac{2(1-\alpha)}{t} - 4\right] m^2$$

$$+ \left[\operatorname{sech}^2 \frac{2(1+\alpha)}{t} + \operatorname{sech}^2 \frac{2(1-\alpha)}{t} - 2 \operatorname{sech}^2 \frac{2}{t}\right.$$

$$\left. - 2 \operatorname{sech}^2 \frac{2\alpha}{t} + 2\right] m^4 \Bigg\} \tag{18}$$

The temperature dependence of χ^I is depicted in Fig. 3; remark that, in the limit $t \to \infty$, $\chi^I \sim 1/t$.

Let us now turn onto another type of approximation which will provide our second proposal for the reduced susceptibility, noted χ^{II}.

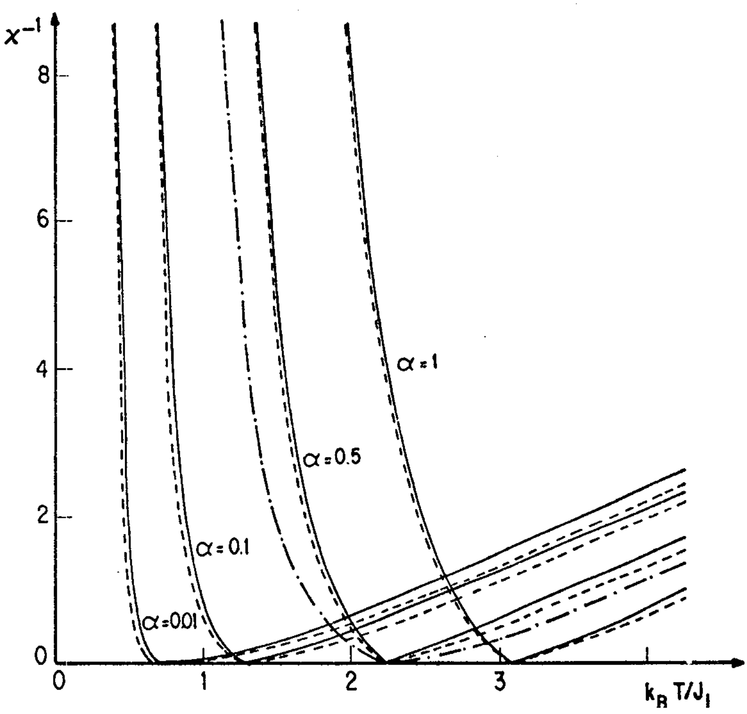

Fig. 3 - Thermal behaviour of the inverse reduced zero field susceptibility within approximations *I* (solid line) and *II* (dashed line) (see the text); the dot-dashed line qualitatively indicates the possible exact result (where, we have taken into account the fact that the exact susceptibility critical exponent γ is known to be larger than one).

Both single-site (Eq.(2)) and two-site Callen identities[7] can be generalized[18] into

$$<f'\sigma_i> = <f' \tanh \beta (\sum_j J_{ij}\sigma_j + g\mu_B H)> \tag{19}$$

where f' is an arbitrary function of all $\sigma_k \neq \sigma_i$ ($f'=1$ and $f'=\sigma_k$ respectively provide the single-and two-site identities). By choosing $f' = f[1 + (\tanh \beta \sum_j J_{ij}\sigma_j)(\tanh \beta g\mu_B H)]$ where f also is an arbitrary function of all $\sigma_k \neq \sigma_i$ we rewrite Eq. (19) as follows:

$$<f\sigma_i> + <f\sigma_i \tanh(\beta \sum_j J_{ij}\sigma_j)> \tanh(\beta g\mu_B H)$$

$$= <f \tanh(\beta \sum_j J_{ij}\sigma_j)> + <f> \tanh(\beta g\mu_B H) \tag{20}$$

By finally choosing $f = 1$ and introducing[19] the differential operator D into this identity, we obtain:

$$<\sigma_i> + <\sigma_i \prod_j e^{\beta J_{ij}\sigma_j D}> \tanh x \Big|_{x=0} \tanh(\beta g\mu_B H)$$

$$= <\prod_j e^{\beta J_{ij}\sigma_j D}> \tanh x \Big|_{x=0} + \tanh(\beta g\mu_B H) \tag{21}$$

By decoupling the nearest-neighbour spin term, i.e. $<\sigma_i \prod_j e^{\beta J_{ij}\sigma_j D}> \simeq <\sigma_i><\prod_j e^{\beta J_{ij}\sigma_j D}>$, and by further decoupling the next-nearest -neighbour spin correlations, i.e. $<\prod_j e^{\beta J_{ij}\sigma_j D}> \simeq \prod_j <e^{\beta J_{ij}\sigma_j D}>$, eq.(21) can be rewritten as follows:

$$m + m \prod_j [\cosh(\beta J_{ij}D) + m \sinh(\beta J_{ij}D)] \tanh x \Big|_{x=0} \tanh(\beta g\mu_B H)$$

$$= \prod_j [\cosh(\beta J_{ij}D) + m \sinh(\beta J_{ij}D)] \tanh x \Big|_{x=0} + \tanh(\beta g\mu_B H) \tag{22}$$

By differentiating (with respect to H) on both sides and explicitly applying the D- operator we obtain the following approximate zero field reduced susceptibility:

$$\chi^{II} = \frac{1 - m^2}{t(1-A-3Bm^2)} \tag{23}$$

We remark that the present denominator coincides with that of Eq. (17); consequently χ^{I} and χ^{II} diverge at one and the same critical point; furthermore, in the limit $t \to \infty$, $\chi^{I} \sim \chi^{II} \sim 1/t$. The temperature dependente of χ^{II} is illustrated in Fig. 3; we remark that in the high temperature region χ^{I} is a better approximation than χ^{II}, whereas at low temperatures χ^{II} tends to be better than χ^{I}.

3. CONCLUSION

The spin 1/2 Ising ferromagnet in anisotropic square lattice has been discussed. All relevant thermodynamlcal quantities (phase diagram in the T - a space with $a \equiv J_2/J_1$, spontaneous magnetization, short range order parameter in both x and y directions, specific heat and zero field isothermal magnetic susceptibility) have been calculated in an effective field unified framework which extends that recently introduced by Honmura and Kaneyoshi[6]. Two slightly different new procedures for approximatively calculating the susceptibility (whose exact computation is still to be done) are presented: one of them tends to be better at high temperatures while the other one tends to be better at low temperatures.

Although the present approach leads to classical (Landau-type) critical exponents (as it is the case for most effective-field theories), and consequently no strict crossover can be observed at the critical exponents level, this framework is quite superior to the standard Mean Field Approximation one as it provides: a) a vanishing critical temperature in the limit $a \to 0$; b) non vanishing tail in the paramagnetic phase specific heat; c) critical temperatures, as function of a, which stand closer to the exact ones (see Ref.(9) for details on this and other types of improvements).

We believe the (mathematically simple) procedures illustrated herein can be useful in order to provide a first insight on a great variety of complex Ising problems.

One of (E.F.S.) acknowledges generous hospitality from Centro Brasileiro de Pesquisas Físicas where part of this work was done; C.T. acknowledges a Gugghenheim Fellowship (USA).

REFERENCES

1. R.V.Ditzian and L.P.Kadanoff, Phys.Rev. B *19*, 4631 (1979).
2. D.P. Landau, Phys. Rev. B *22*, 2450 (1980)
3. C.Jayaprakash, E.K. Riedel and M. Wortis, Phys. Rev. B*18*, 2244(1978).
4. S.V.F. Levy, C. Tsallis and E.M.F. Curado, Phys.Rev.B *21*, 2991(1980).
5. F.G.Brady Moreira, I.P.Fittipaldi and R.B.Stinchcombe, J. Phys. C 14, 4415 (1981).
6. R.Honmura and T.Kaneyoshi, J.Phys. C 12, 3979 (1979).
7. H.B.Callen, Phys. Lett. 4, 161 (1963).
8. T.Kaneyoshi, I.P.Fittipaldi, R.Honmura and T.Manabe, Phys. Rev. B 24, 481 (1981).
9. E.F.Sarmento and C. Tsallis, Phys. Rev. B 27, 5784 (1983).
10. I.P.Fittipaldi, C.Tsallis and E.F.Sarmento, Sol. State Commun. 44, 777 (1982).
11. T.Kaneyoshi, I.P.Fittipaldi and H.Beyer, Phys. Stat. Sol. (b) *102*, 393 (1980).
12. J.R.L. de Almeida, I.P.Fittipaldi and F.C.Sá Barreto, J. Phys.C 14, L 403 (1981).
13. T.Kaneyoshi and H. Beyer, J.Phys.Soc.Japan, 49, 1306 (1980).
14. T.Kaneyoshi and I.P.Fittipaldi, Phys.Stat.Sol. (b) 105, 629 (1981).
15. R.Honmura, A.F.Khater, I.P.Fittipaldi and T.Kaneyoshi, Sol. State Commun. *41*, 385 (1982).
16. F.C.Sá Barreto, I.P.Fittipaldi and B.Zeks, Ferroeletrics 39, 1103 (1981).
17. K.Sakata, E.F.Sarmento, I.P.Fittipaldi and T.Kaneyoshi, Sol. St. Commun 42, 13 (1982).
18. M.Suzuki, Phys. Lett. 19, 267 (1965).
19. T.Tanaka and N. Uryû, Phys. Rev. B 21, 1994 (1980)

Resumo

Discutimos o ferromagneto de Ising de spin 1/2 na rede quadrada anisotrópica. Através deste sistema ilustramos como todas-as grandezas termodinâmicas relevantes (diagrama de fases, magnetizaçao, parâmetro de ordem de curto alcance, calor específico e susceptibilidade) podem ser calculadas aproximadamente com um procedimento unificado de campo efetivo (que melhora substancialmente a Aproximaçao de Campo Médio). Duas aproximações ligeiramente diferentes para a susceptibilidade (cujo cálculo exato ainda está para ser feito) sao apresentadas. O modo através do qual a rede quadrada extremamente anisotrópica reproduz a cadeia linear é exibido. Os presentes procedimentos (matematicamente simples) poderiam ser úteis para o estudo de problemas de Ising complexos.