Revista Brasileira de Física, Vol. 18, nº 2, 1988

Decorated Ising Models with Competing Interactions and Modulated Structures

MARCELO H.R. TRAGTENBERG[+], CARLOS S.O. YOKOI and SILVIO R. SALINAS
Instituto de Física, Universidade de São Paulo, Caixa Postal 20516, São Paulo, 01498, SP, Brasil

Recebido em 28 de outubro de 1987

Abstract We calculate the phase diagrams of a variety of decorated Ising lattices. The competing interactions among the decorating spins may induce different types of modulated orderings. In particular, we consider the effect of an applied field on the phase diagram of the two-dimensional mock ANNNI model, where only the original horizontal bonds on a square lattice are decorated. We then study some Bravais lattices and Cayley trees where all bonds are equally decorated. The Bravais lattices display a few stable modulated structures. The Cayley trees, on the other hand, display a large number of modulated phases, which increases with the lattice coordination number.

1. INTRODUCTION

An Ising model with competing nearest and next-nearest neighbor interactions along one spatial direction, known as ANNNI model (Axial Next-Nearest-Neighbor Ising), has been studied intensively in the last few years[1]. These studies have revealed a very rich phase diagram, displaying Lifshitz[2] and multiphase points[3], and infinitely many commensurate and incommensurate phases[4]. Understandably, the model is very difficult to solve even at the mean-field level[5,6]. Huse, Fisher and Yeomans[7] introduced a simpler model that mimics, so to speak, the true ANNNI model. The model, dubbed mock ANNNI model, is a decorated Ising model with competing interactions restricted to the decorated bonds along one spatial dimension. This model can be solved completely in terms of an anisotropic nearest-neighbor Ising model. In two and three dimensions, in zero field, it exhbits finitely many modulated phases.

In this paper we wish to consider some aspects of the problem that were left out by Huse *et al*[7]. We first study the effect of a mag-

+ On leave from Departamento de Física, Universidade Federal de Santa Catarina, Florianópolis, SC, Brasil netic field on the behavior of the two dimensional mock ANNNI model. Then we consider Bravais lattices and Cayley trees where all the bonds are equally decorated. Although these models are admittedly somewhat removed from known physical systems, we believe that they add to the theoretical understanding of modulated structures.

2. BOND DECORATION AND EFFECTIVE COUPLING

A decorated bond consists of two nodal spins, $S_i = \pm 1$, located on the sites of a lattice, and n decorating spins, $\sigma_i = \pm 1$, located along the bond. The decorating spins interact among themselves with ferromagnetic nearest-neighbor (nn) couplings of strength $J_1 > 0$ and next-nearest-neighbor (nnn) wuplings of strength $J_2 = -\kappa J_1$. The nodal spin, on the other hand, interacts with the nn decorating spin with half strength, $\frac{1}{2} J_1$, and with the nnn decorating spins with the same strength, $J_2 = -\kappa J_1$ (see fig. 1).

The effective couplings between the nodal spins canbeobtained by performing the trace over the decorating spins (dedecoration transformation). The hamiltonian for the decorated bond is

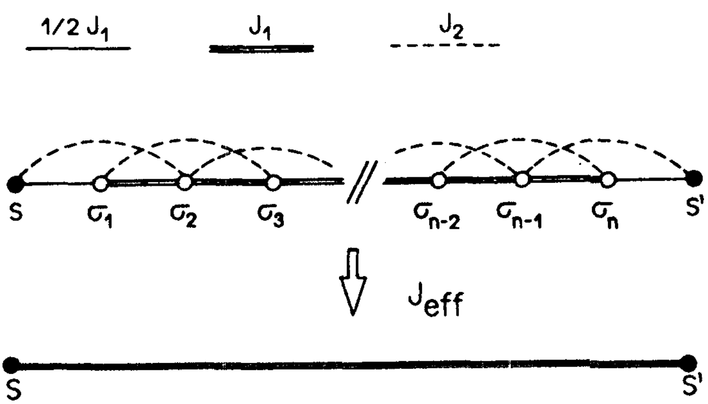

Fig. 1 - Structure of a decorated bond. Solid circles denote nodal spins, S_j, and hollow circles decorating spins, σ_i. The bold line indicates the effective interaction between nodal spins after the dedecoration of decorating spins.

$$H(S,S',\{\sigma\}) = -\sum_{i=1}^{n}\left[\frac{J_1}{2}(\sigma_{i-1}\sigma_i + \sigma_i\sigma_{i+1}) + J_2\,\sigma_{i-1}\sigma_{i+1} + H\,\sigma_i\right] \tag{1}$$

where, for convenience, $\sigma_0 = S$ and $\sigma_{n+1} = S'$. We define the restricted partition function for the decorated bond as

$$Z^{SS'} = \mathrm{Tr}_{\{\sigma\}}\, e^{-\beta H(S,S',\{\sigma\})} \quad . \tag{2}$$

By carrying out the partial trace in eq.(2) we obtain $Z^{SS'}$ in the form

$$Z^{SS'} = C\, e^{K_{\text{eff}}SS' + B_{\text{eff}}(S+S')} \tag{3}$$

Therefore, the effective coupling, K_{eff}, and the effective field, B_{eff}, are given by the expressions

$$e^{4K_{\text{eff}}} = Z^{++}\,Z^{--} \,/\, (Z^{+-})^2 \tag{4}$$

$$e^{4B_{\text{eff}}} = Z^{++} \,/\, Z^{--} \quad . \tag{5}$$

In the case of zero external field, H = 0, we have $Z^{++} = Z^{--}$, so that $B_{\text{eff}} = 0$ and

$$e^{2K_{\text{eff}}} = Z^{++} \,/\, Z^{+-} \tag{6}$$

Using the transfer matrix technique, Huse et al[7] evaluated eq. (6) explicitly for the case of zero external field. For the sake of completeness we reproduce their results below. With

$$K_1 = \beta J_1 = \frac{J_1}{kT} \tag{7}$$

$$\delta = \kappa - \frac{1}{2} \tag{8}$$

$$b(T,\kappa) = (1 + e^{-2K_1})/2e^{2\delta K_1} \tag{9}$$

$$c(T,\kappa) = (1 - e^{-2K_1})/2e^{2\delta K_1} \tag{10}$$

$$\lambda_\pm = b \pm (c^2 + 1)^{\frac{1}{2}} \quad , \tag{11}$$

$$\tilde{\lambda}_\pm = c \pm (b^2 - 1)^{\frac{1}{2}} \quad , \tag{12}$$

$$A_n(T,\kappa) = \lambda_+^n + \lambda_-^n + (\lambda_+^n - \lambda_-^n)/(c^2 + 1)^{\frac{1}{2}} \quad , \tag{13}$$

$$B_n(T,\kappa) = (b-1)^{\frac{1}{2}} (b+1)^{-\frac{1}{2}} (\tilde{\lambda}_+^n - \tilde{\lambda}_-^n) \quad , \tag{14}$$

the effective coupling between the nodal spins in zero field is giver by

$$\tanh K_{\text{eff}} = B_n/A_n \quad . \tag{15}$$

Unfortunately, for the case of non-zero external field, it was not possible to evaluate eqs. (4) and (5) explicitly. Unlike the case of zero field, the σ-τ transformation used by Huse et *al*[7] is of no avail and we have to cope with a 4×4 transfer matrix. The restricted partition function given by eq. (2) can be rewritten in the form

$$Z^{SS'} = \underset{\{\sigma\}}{\mathrm{Tr}} \sum_{i=1}^{n} T(\sigma_{i-1}\sigma_i|\sigma_i\sigma_{i+1})$$

$$= \sum_{\sigma,\sigma'} \langle S\sigma|\underline{\underline{T}}^n|\sigma' S'\rangle \tag{16}$$

where

$$T(\sigma\sigma'|\sigma''\sigma''') = \delta_{\sigma'\sigma''}\, e^{\frac{1}{2}K_1(\sigma+\sigma''')\sigma' + K_2\sigma\sigma''' + B\sigma'} \quad , \tag{17}$$

with

$$K_2 = \beta J_2 = -\kappa K_1 \quad , \tag{18}$$

and

$$B = \beta H = H/kT \quad . \tag{19}$$

Assuming that the 4×4 matrix $\underline{\underline{T}}$ can be diagonalized by a similarity transformation,

$$\underline{\underline{U}}^{-1}\,\underline{\underline{T}}\,\underline{\underline{U}} = \underline{\underline{\Lambda}}\ , \tag{20}$$

where $\underline{\underline{\Lambda}}$ is a diagonal matrix of eigenvalues λ_i, we have

$$Z^{SS'} = \sum_{\sigma\sigma'} \langle S\sigma|\,\underline{\underline{U}}\,\underline{\underline{\Lambda}}^{n}\,\underline{\underline{U}}^{-1}|\sigma' S'\rangle\ . \tag{21}$$

In principle, eq.(21) can be computed without difficulty for arbitrary n using standard mathematical routines. Eqs. (4), (5) and (21) determine the effective coupling constant K_{eff} and the effective field B_{eff} generated by the decorating spins. For small values of n, we have performed explicit calculations to obtain K_{eff} and B_{eff}.

3. 'MIO DIMENSIONAL MOCK ANNNI MODEL IN A FIELD

In the two dimensional mock ANNNI model on a square lattice, only the horizonta! bonds are decorated according to the scheme of fig. 1. The nodal spins in the vertical direction interact ferromagnetically with strength $J_0 > 0$. After the dedecoration transformation discussed in the previous section, the model is transformed into an anisotropic nearest-neighbor Ising rnodel in a fieid. Although there is no exact expression for the transition temperature, there is an approximate expression due to Müller-Hartmann and Zittartz[5]. They estimated the interface free energy between two domains of a square lattice Ising antiferrirnagnet in the presence of a field. The vanishing of the interface free energy determines the critical line. In the presence case, since $J_0 > 0$ and K_{eff} may be negative, we have to consider a two-dimensional Ising metamagnet in a field. The two metamagnetic domains are illustrated in fig. 2. The critical line for a metamagnet with vertical coupling $J_V > 0$ and horizontal coupling $J_H < 0$ in the presence of an external field H is then given by

$$\sinh\left(\frac{2J_V}{kT}\right)\sinh\left(\frac{2J_H}{kT}\right) = -\cosh\left(\frac{H}{kT}\right). \tag{22}$$

The corresponding expression for the mock ANNNI model is

$$\sinh(2K_0)\,\sinh(2K_{eff}) = -\cosh(B+2B_{eff})\ , \tag{23}$$

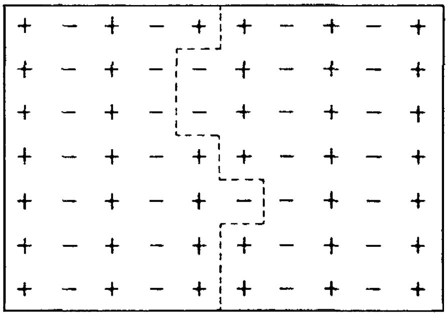

Fig.2 - Two metarnagnetic domains separated by an interface (dotted line).

where

$$K_0 = \beta J_0 = J_0/kT \ , \tag{24}$$

and B, B_{eff} and K_{eff} are given, respectively, by eqs. (19), (5) and (4). The factor 2 in front of B_{eff} comes in because each nodal spinbelongs to twa decorated bonds.

Fig.3 shows the phase diagram of the twa-dimensional mock ANNNI model in zero field for n = 5 and J, = J,. The rnodulated phases are labelled by $\bar{q} = q/2\pi$, where q is the main wave number of the spatially modulated magnetization structure (see section V of Huse et *al.*[7]). Figs. 4 and 5 show the (T,H) phase diagrams corresponding to the cross sections of the global phase diagram for $\kappa = 0.393$ and $\kappa = 0.75$, respectively. Notice that the phases $\bar{q} = 0$ and $1/6$, for which $K_{eff} > 0$, cannot survive in presence of a field.

Huse *et al.*[7] have shown that the principal wave numbers aregiven by

$$\bar{q} = \frac{\ell}{n+1} \qquad \text{if} \qquad K_{eff} \quad 0 \ ,$$

and (25)

$$\bar{q} = \frac{2\ell+1}{2(n+1)} \qquad \text{if} \qquad K_{eff} \quad 0 \ ,$$

where L is any integer. Therefore, for a given n, only the modulated phases with the principal wave number of the form $\bar{q} = (2\ell+1)/2(n+1)$, L = $= 0,1,\ldots, [(n-1)/4]$, will survive in presence of a field. With the exception of the 1/4 phase, these modulated phases display a bubble-like shape in the (T,κ,H) space, and in the (T,H) plane the phase boundaries

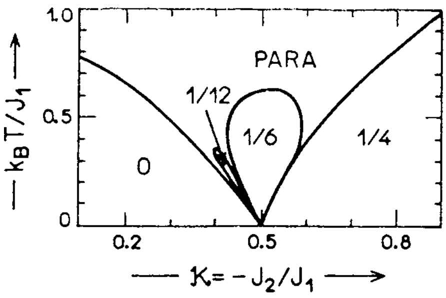

Fig.3 - Zero field phase diagram of the two dimensional mock ANNNI model for $J_0 = J_1$ and $n = 5$.

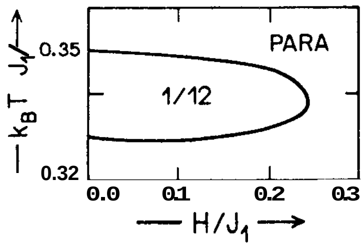

Fig.4 - T vs H phase diagram of the two-dimensional mock ANNNI model for $n = 5$, $J_0 = J_1$ and $\kappa = 0.393$.

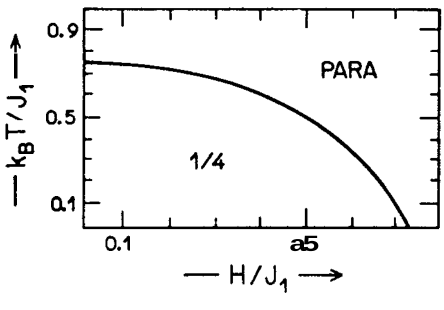

Fig.5 - T vs H phase diagram of the two-dimensional mock ANNNI model for the $n = 5$, $J_0 = J_1$ and $\kappa = 0.75$.

show a reentrant character. These results are reminiscent of the field behavior of the ANNNI model studied in the mean-field approximation[9].

4. ISOTROPICALLY DECORATED BRAVAIS LATTICES

In this section we analyse the behavior of some Bravais lattices where all the bonds are decorated according to the scheme of fig. 1. The critical line in the (T,κ) plane is then given by

$$\tanh K_{eff} = \pm \tanh(J/kT_c) = \pm \omega_c \tag{26}$$

where T_c is the critical temperature of the original (non- decorated) model. The values of ω_c for some representative Bravais lattices are given[10] in table 1. The antiferromagnetic triangular and fcc lattices are frustrated. Therefore, these cases will be discussed separately at the end of this section. Figs. 6 and 7 show the phase diagrams of the model on a sc lattice for $n = 5$ and $n = 6$. We can argue that these two

Table 1 - Values of ω_c for some Bravais lattices.

lattice	ω_c
honeycomb	0.57736
square	0.41421
diamond	0.3538
sc	0.21813
bcc	0.15611
triangular	0.26795
fcc	0.10174

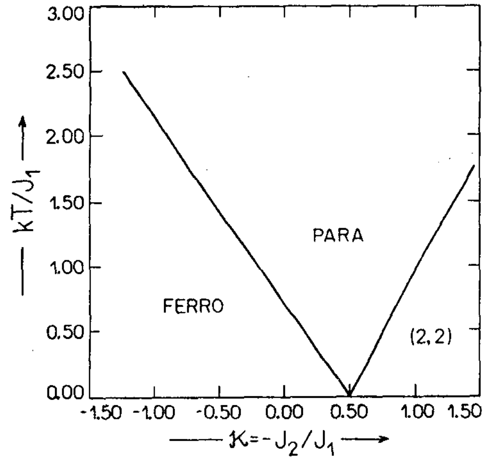

Fig.6 - Phase diagram of the isotropically decorated sc lattice for n=5. No bubbles exist.

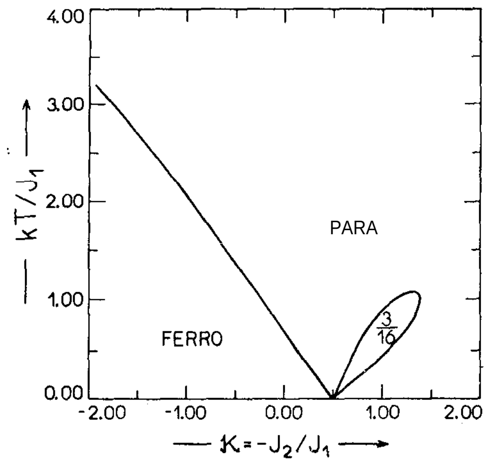

Fig.7 - Phase diagram of the isotropically decorated sc lattice for n=6. Only one bubble exists.

cases essentially exhaust the topologically distinct phasediagrams that are possible for any Bravais lattices and arbitrary n. To this end we examine what happens in the vicinity of the point $T=0$, $\delta=0$, where all the critical lines apparently converge. More precisely, we approach this point with $K_1\delta$ held fixed. Let us define

$$e^{-2K_1\delta} = a \ . \tag{27}$$

Then, in this limit, we have

$$b = c = a/2 \quad , \tag{28}$$

and it is possible to compute eq. (15) as a function of the parameter a. Figs. 8 and 9 show tanh K_{eff} as a function of a for various values of n. It is interesting to observe that all curves meet at the point $K_{eff}=0$ and $a=2$. This implies that the ferromagnetic phase boundary is the same regardless of the number of decorating spins. Obviously, the condition for criticaty is met only at the points where the curves intersect the horizontal lines $\pm\omega_c$. The following conclusions then follow for the sc and bcc lattices. For odd or even values of n the phase diagrams are topologically equivalent to those shown in fig. 6 and 7, respectively. For the diamond, square and honeycomb lattices, on the other hand, we conclude the following. For odd n, the phase diagrams are topologically the same as in fig. 6. For even n, the phase diagrams are the same as in fig. 7 with the absence of bubbles. For the ferromagnetic triangularand fcc lattices the values of ω_c are given in table 1. In the antiferromagnetic case there is no phase transition due to the frustration effects, and we have $\omega_c = \pm 1$. Therefore, for $n = 4\ell+3$ and $4\ell+4$ the phasediagrams are topologically identical to those of figs. 6 and 7, whereas for $n = 4\ell+1$ and $4\ell+2$, where $\ell = 0,1,\ldots,$ no modulated phase is possible.

What is the structure of the ordered phases? In the case of two sublattice systems, the results of eq. (25) of Huse *et al*[7] can still be used to label the different ordered phases, although $\bar{q}$ cannot have the straightforward meaning of a wave number since there is no preferred direction of modulation. Rather, $\bar{q} = 1/\lambda$ is the inverse of the wave number as one progresses from one nodal spin to another in any direction.

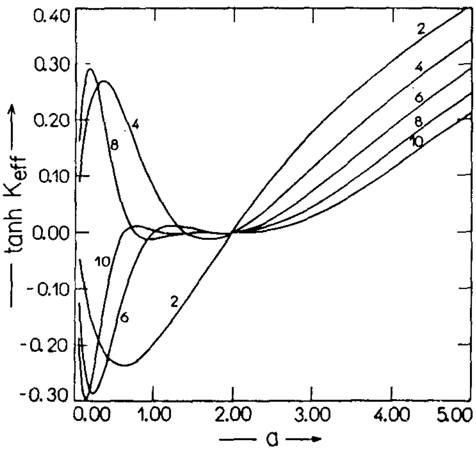

Fig.8 - Graphs of tahn K_{eff} versus $a = e^{-2\delta K_1}$ in the limit δ, $T\to 0$, for even values of *n*.

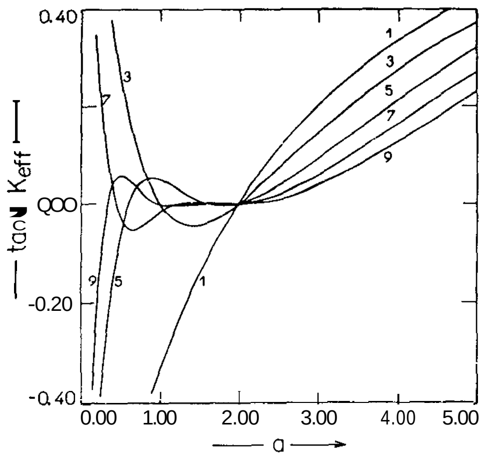

Fig.9 - Graphs of tanh K_{eff} versus $a = e^{-2\delta K_1}$, in the limit δ, $T\to 0$, for odd values of **n**.

5. DECORATED CAYLEY TREES

In this section we examine Cayley trees where all the bonds are decorated according to the scheme shown in fig.1. The critical temperature of the Cayley tree associated with the spontaneous ordering of the innermost region is given by[11]

$$\tanh\left(\frac{J}{kT_c}\right) = \omega_c = \frac{1}{z-1} \quad , \tag{29}$$

where z is the coordination number. The obvious but interesting fact is that the critical temperature can be made arbitrarily large simply by increasing the coordination number. Eqs. (29) and (26), together with the graphs in figs. 8 and 9, show that the increase in the coordination number tends to stabilize a larger number of modulated phases. For particular values of n we can find numerically the minimum coordination number $z_n(\bar{q})$ for the occurrence of the modulated phase $\bar{q}$. For example, we have $z_3(\frac{1}{8}) = 24$, $z_5(\frac{1}{6}) = 21$ and $z_5(\frac{1}{12}) = 283$. It is clear that a quite high coordination number is necessary to produce a phase diagram with many bubbles.

6. SUMMARY

In the case of the two-dimensional mock ANNNI model, only the modulated phases with principal wave numbers of the form $\bar{q} = (2\ell + 1)/2(n + 1)$, $\ell = 0,1,\ldots,[(n-1)/4]$, survive in the presence of a field. These phases exhibit characteristically bubble like forms in the (T,κ,H) space. In the case of isotropically decorated Bravais lattices, only a few modulated structures are stable even for a larger number n of decorating spins. Finally, in the case of the decorated Cayley trees, the number of stable modulated structures is a function of the coordination number z. Larger values of z tend to stabilize a larger number of different modulated structures.

We acknowledge the financial support of Brazilian agencies CNPq and CAPES.

REFERENCES

1. W.Selke, in *Modulated Structure Materials*, T.Tsakalakos ed., p. 23, NATO ASI Series: Martinus Nijhoff, 1984.
2. R.M.Hornreich, M.Luban and S.Shtrikman, Phys.Rev.Lett. *35*, 1678 (1975).
3. M.E.Fisher and W.Selke, Phys.Rev.Lett. 44, 1502 (1980).
4. P.Bak and J.von Boehm, Phys. Rev. B*21*, 5297 (1980).
5. M.H.Jensen and P.Bak, Phys.Rev. 827, 6853 (1983).
6. W.Selke and P.M.Duxbury, Z.Phys. B*57*, 49 (1984).
7. D.A.Huse, M.E.Fisher and J.M.Yeomans, Phys.Rev. 823, 180 (1981).
8. E.Müller-Hartmann and J.Zittartz, Z.Phys. B*27*, 261 (1977).
9. C.S.O.Yokoi, M.D.Coutinho-Filho and S.R.Salinas, Phys. Rev. B *24*, (1981).
10. See, for exarnple, C.Domb in *Phase Transition* and *Critical Phenomena*, C. Domb and M.S.Green, eds., Chap. 3, Academic Press, N.York, 1972.
11. See, for example, R.J. Baxter, *Exactly Solved Models in Statistical Mechanics*, Academic Press, London, 1982, Chap. 4.

Resumo

Calculamos os diagramas de fases de diversas redes de Ising decoradas. As interações competitivas entre os spins de decoração podem induzir diferentes tipos de ordenamentos modulados. Em particular, consideramos o efeito de um campo sobre o diagrama de fases do modelo falso-ANNNI bidimensional, em que apenas são decoradas as ligações horizontais da rede quadrada original. Estudamos logo em seguida diversas redes de Bravais e árvores de Cayley com todas as ligações igualmente decoradas. As redes de Bravais possuem poucas estruturas moduladas estáveis. Por outro lado, as árvores de Cayley possuem um grande número de fases moduladas, que aumenta com a coordenação da rede.