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Reentrant behaviour in two-dimensional Içing models with biquadratic interactions

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Abstract The critica1 behaviour of the spin-1 and spin-2 Ising model with biquadratic interaction is investigated in two dimensions by real space renormalization group. The reentrant behaviour obtained for positive values of the biquadratic coupling occurs for lattices with coordination number $z > 4$.

The spin-1 Ising model with bilinear and biquadratic interactions has been studied by many authors. This models is a particular case of the Blume-Emery-Griffiths (BEG) model', when the crystal field (single ion anisotropy) is absent. The BEG model has been analysed by mean field approximation[1-3], high temperature series expansion[4], Monte Carlo[5] and renormalization group methods[6,7]. The mean field analysis of the spin-1 Ising model with bilinear and biquadratic interactions predicts a second order phase transition for any positive value (antiferromagnetic coupling) of the biquadratic coupling **A.** This prediction is incorrect since one knows from ground state considerations[8] that a phase transítion occurs at $A/J = 1$ (J is the ferromagnetic bilinear coupling). The Bethe lattice calculation[g] and improved mean field treatment[10] predicted a first order transition for large positive values of the biquadratic coupling $A/J > 1$. A recent Bethe lattice treatment of the BEG model'' describes in detaii the phase diagram of the model. **A** new phase, denominated the staggered quadrupolar phase, has been found in the $z = 4$ square lattice, in contrast to other effective field treatments[12]. Also, for the $z = 6$ (triangular lattice) this Bethe calculation finds a reentrance in the ferromagnetic-paramagnetic line. This rich phase diagram also shows first-order transitions lines. Renormalization with increasing A/J with a back bending of

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for the $z = 6$ (triangular lattice) this Bethe calculation finds a reentrance in the ferromagnetic-paramagnetic line. This rich phase diagram also shows first-order transitions lines. Renormalization with increasing A/J with a back bending of this critica1 line ending at $T = 0$ and $A/J = 1$. This reentrant behaviour has been obtained for the simple cubic lattice, in contrast to other approaches as the Bethe lattice calculation of reference 9 which finds this behaviour also for the square lattice. The model has also been investigated by the Monte Carlo technique[14] and its phase diagram for the three-dimensional lattice exhbits a reentrant behaviour for values of $A/J > 1$. As in the renormalization group study[13] no reentrance is found by the Monte Carlo calculation[14] for the square lattice. These authors argue that although no reentrance is found for the model in a square lattice the phase diagram for the triangular lattice may present a reentrant behaviour. One of the objectives of the present work is to look into this comment. As a final remark in this short introduction we mention that while the spin-1 Ising model with bilinear and biquadratic interactions has received much attention, the spin-2 model has to not been studied by any method, as far as we know.

The reentrant phenomenon is observed in a variety of physical systems and has been obtained in different model hamiltonians. Its origin can be traced back to the competition of ferromagnetic and antiferromagnetic couplings, as for example in random bond spin models[15], decorated square lattice Ising models[16], among others. In most systems the disorder mechanism gives rise to the reentrance. It is interesting that this peculiar character of a phase transition is obtained in pure systems, as in the Ising model with bilinear and biquadratic interactions.

In this work, we make use of the mean field renormalization graup (MFRG)[17] treatment to study the spin-1 and spin-2 Ising models with bilinear and biquadratic interactions in two dimensions. We will present numerical results for the honeycomb ($z = 3$), square ($z = 4$) and triangular ($z = 6$) lattices, although other lattices have also been considered. The purpose of the work is to determine the ocurrence of the reentrance in two dimensional lattices with different symmetries and coordination numbers.

The model studied in this publication is described by the Hamiltonian,

$$H = -J \sum S_i S_j + A \sum S_i^2 S_j^2 \ , \tag{1}$$

where the sums run over the z nearest-neighbour paírs of spins for S = 1 and S = 2. The bilinear interaction is taken to be ferromagnetic (J > 0).

The corresponding model defined on a finite lattice of N sites which is disconnected from the infinite lattice by cutting boundary links is given by,

$$H_N = -J \sum S_i S_j + A \sum S_i^2 S_j^2 + hJ \sum p_i S_i + qA \sum p_i S_i^2 \ , \tag{2}$$

where $i = 1, 2, ..., N$ and the sums run over nearest-neighbour pairs. The field hJ and qA are included in order to break the spin flip symmetry, and the weight p_i is the number of cutted boundary links cut at site i (for internal links $p_i = 0$).

Let us define the quantities,

$$M_c = \sum S_i \tag{3.a}$$

$$T_c = \sum p_i S_i \tag{3.b}$$

$$Q_c = \sum S_i^2 \tag{3.c}$$

$$R_c = \sum p_i S_i^2 \tag{3.d}$$

In this model the field h and the corresponding order parameter, to be defined below, vanishes at the critical temperature. At this temperature the other field q and its counterpart, the quadrupolar moment, are finite. Therefore, expanding in first order in the field h we obtain for the finite lattice order parameter M the expression,

$$M =< M_c > - < M_c >_0 = \beta hJ < M_c T_c >_0 \tag{4.a}$$

where $< ... >_0$ denotes the thermodynamical average for h = 0.

The quadrupolar moment is obtained from

$$Q =< Q_c >_0 \tag{4.b}$$

In the mean field approximation, the one-site lattice is used, and the magnetization M and the quadrupolar moment are identifed with the boundary fields h and q, respectively. The mean field results follow from the solution of the coupled equations (4.a) and (4.b). Values for the critical temperature beyond mean field are obtained from lattices with number of sites N > 1 by identifying the magnetization M with the field h. (Yet, the critica1 exponents are still classical).

The MFRG assurnption is that the ratio between the magnetization and the corresponding field h does not depend on the length scale. The assumption is based on the fact that the magnetization of the outside lattice gives origin to the field that acts in the inside lattice. So, M and h scales in the same way, as L^{ϕ}, where L denotes the lattice size. Therefore, the quantity

$$JP_L(J,A) = \beta J < M_c T_c >_0 \quad , \tag{5}$$

scales as $L^0 = 1$, i.e. it does not depend on the lattice size L, as L $\to \infty$. Here, $P_L(J,A)$ is a polynomial in J and A, calculated exactly for a finite lattice of size L, with N sites.

Since the quadrupolar moment is not critica1 it will be treated within a self-consistent way by assuming that Q = q.

The MFRG recursion relation are obtained by equating the values of JP calculated for two different lattice sizes with lengths L' < L (with $N' <$ N sites).

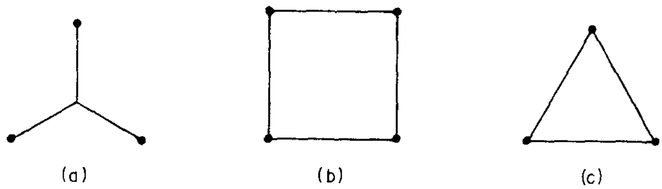
$$J' P_{L'}(J',A') = JP_L(J,A) \ . \tag{6}$$

The fixed point solution of the system is obtained from this relation by imposing the conditions $J' =$ J and $A' = A$.

By solving the coupled equations that result from the above conditions for $K_L = \beta J_L$, q_L and q'_L we obtain the dependence of the critical temperature with the biquadratic coupling for different lattices. As has been shown in a previous publication[13], by using the lattices with $N' = 1$ and $N = 2$ sites in the strong coupling limit $(A/J \to \infty)$ the results for the critical coupling reproduce the Bethe lattice value[8]. For the lattices with coordination number $Z = 3$ and $Z = 4$

a non-reentrant second order phase transition was found, as opposed to the simple cubic lattice ($Z = 6$) where a reentrant behavior was obtained. However the nature of the phase transition in the back-bending region could not be identified by the MFRG approach. Later, a Monte Carlo analysis of the same model[14] showed that the transition is second order and a reentrant behavior is found for the three dirnensional simple cubic lattice.

Although no reentrance was found, by either method, for the two-dimensional square lattice, a reentrant phase could be found in the phase diagram of the triangular lattice ($Z = 6$). In order to analyze the existence of reentrant phases in two dimensional lattices, by MFRG, we use the clusters with $N' = 1$ and $N = 4$ sites for the boneycomb lattice ($Z = 3$) (figure 1.a); $N' = 1$ and $N = 4$ sites for the square lattice Z(= 4) (figure 1.b); $N' = 1$ and N = 3 sites for the triangular lattice ($Z = 6$) (figure 1.c). These clusters have been chosen because they contain all the symmetric properties of each one of these lattices. The two-site cluster, as an example would not contain all the symmetries of each lattice; they would be distinguished only by the coordination number. By calculating the polynomials $P(J, A)$ for the lattices with N' and N sites and making use of relation (6) we obtain the transition temperature k_BT_c/J as a function of A/J. The results are presented in figures 2 and 3. As can be seen in figure 2 for the $S = 1$ rnodel the zero temperature limit is reached for all lattices at the value $A/J = 1$. Moreover, the triangular lattice shows a reentrant ferromagnetic (F) or paramagnetic (P) phase for values of $A/J \approx 1$. For values of $A/J \leq 1$ The ferromagnetic phase is reentrant showing a sequerice of transitions F-P-F-P. A similar sequence of transitions have also been found in the exact solution of a dimer decorated spin 1/2 Ising model[18]. For values of $A/J \geq 1$ the sequence is P-F-P. The $S = 2$ model has also been analysed with the use of the same lattices as shown in figure 1. The results are similar to those obtained for the $S = 1$ model. In figure 3, we show the phase diagram for the triangular lattice for the $S = 1$ and $S = 2$ models. Similar behaviour has been obtained for other two-dimensional lattices with different coordination numbers.



Fia. 1 - Cluster used in the calculation: N=4 sites for the honeycomb lattice (fig.1.a); N=4 sites for the square lattice (fig. 1.b); N=3 sites for the triangular lattice (fig. 1.c). The N'=1 site cluster is not shown.

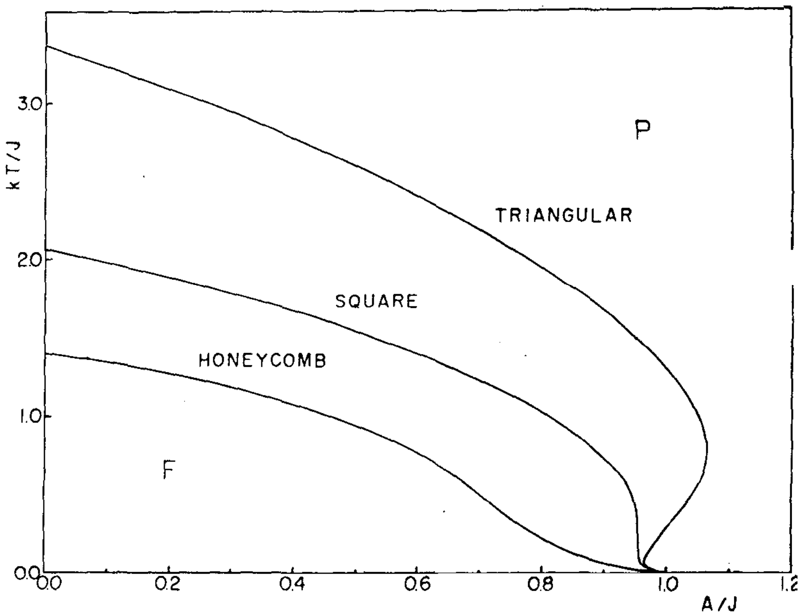


Fig.2 - Critical temperature $(k_B T_c/J)$ as a function of the biquadratic interaction (A/J) for the spin S=1 model in the honeycomb, square and triangular lattice. A reentrant behaviour is observed for the triangular lattice.

Therefore, we may conclude that, by means of the MFRG treatment, reentrant stable phases are found in integer spin-S Ising models with biquadratic interactions in two-dimensional lattices as long the coordination number of the lattice is $Z \geq 6$. This result is in accordance with the Monte Carlo calculation for the $S = 1$

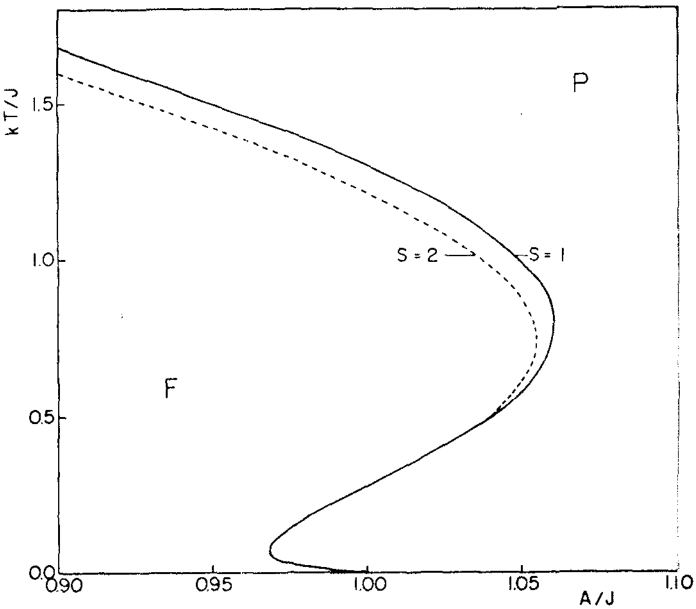


Fig. 3 - Critical temperature (k_BT_c/J) as a function of the biquadratic interaction (A/J) for the spin S=1 and S=2 models in the triangular lattices, showing the reentrant behaviour.

model. The reentrance is a result of the competition of the ferromagnetic bilinear interaction $(J > 0)$ and the antiferromagnetic biquadratic interaction $(A > 0)$, in the pure system.

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Resumo

O comportamento crítico do modelo de Ising de Spin-1 e Spin-2 com interação biquadrática é investigado em duas dimensões por grupo de renormalização do espaço real. O comportamento reentrante obtido para valores positivos do acoplamento biquadrático ocorre para redes com número de coordenação $Z > 4$.