The extended Lipowski-Suzuki method for two-dimensional antiferromagnetic Ising models.

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We present an extension of the Lipowski-Suzuki (LS1) method for studying Ising models with two sublattices ordering. The LS1 method, which was basically built up for investigating Ising ferromagnetic models and yields very accurate results, it gives even the exact T_c for nearest neighbour ferromagnetic Ising model.

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I. INTRODUCTION

The numerical analysis of finite systems, even of very small size, has proven to be an efficient approach in investigating critical properties of two-dimensional spins models.

In a recent paper[1], Lipowski and Suzuki (LS1) have proposed a method for determining critical temperatures of two dimensional ferromagnetic Ising model. This method consists in combining the double cluster approximation(DCA) method[2,3] and the transfer matrix technique[4,5]. It enables them to recover the exact critical temperature for the nearest-neighbour ferromagnetic Ising model on the square, honeycomb and triangular lattices. A first formulation of this method has been presented earlier by the same authors LS2[6]. Results obtained by LS2 are rather poor compared to those of LS1, but a critical comparison between both formulations is beyond the aim of this work. Other works[7,8], have shown that the LS1 method is very accurate in investigating critical behaviour of several two dimensional Ising models, but almost in the ferromagnetic domain.

This paper is a review of studies published in references 9 and 10, we extend the LS1 method for studying the antiferromagnetic Ising models. The models are described by the hamiltonian:

$$H = -\sum_{<i,j>} J_{ij} s_i s_j - h\sum_i s_i \tag{1}$$

Where <i,j> denotes the nearest-neighbour spin pairs and $s_i=\pm 1$. We shall present two models:

* In the first model we take J_{ij} as a constant

This model has been studied by several methods, series-expansion method[11,12], real space renormalization[13,14], phenomenological renormalization[15] and Monte-Carlo simulations[16]. The conjecture of Müller-Hartmann and Zittartz[17] provides an analytic expression for the critical temperature $T_c(h)$,

$$\cosh(h)=(\sinh(2T_c/J))^2 \tag{2}$$

* In the second model , h=0 and J_{ij} take the values: $J_{ij}=J_2<0$ for vertical bonds on odd columns and $J_{ij}=J_1>0$ for all other bonds, as depicted on Fig.1,

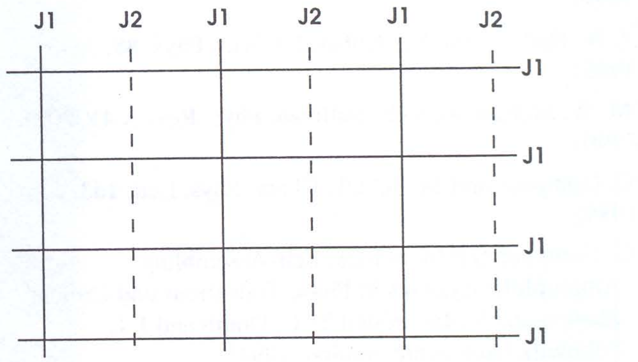

FIG.1: Ising model with nearest-neighbour interaction J_1 and J_2 on the square lattice.

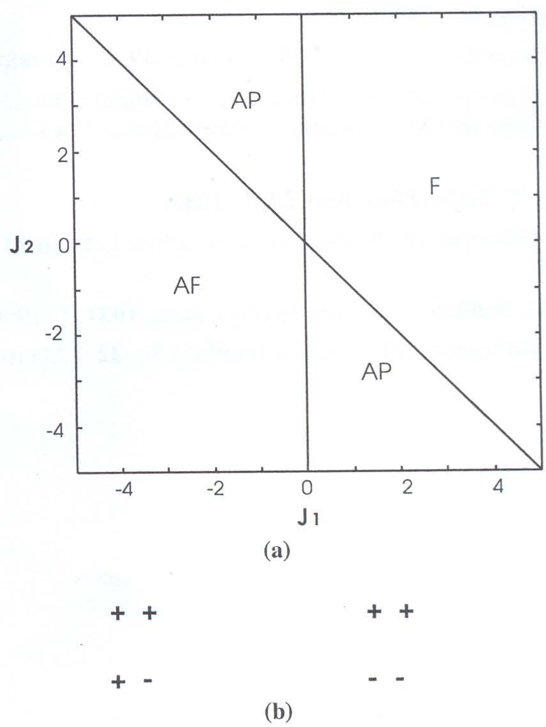

FIG. 2: The ground states phase diagram.(a) and two types of possible antiphase states (b).

where ferromagnetic bonds are denoted by solid lines and antiferromagnetic ones by dashed lines. Hence the special

case J_2=-J_1 is the fully frustrated Ising model proposed by Villain[18].

Depending on the values of the interaction parameters J_1 and J_2, this model has three basic types of ground state: the ferromagnetic (F), the antiferromagnetic (AF) and the antiphase (AP) states (see Fig.2a) where two of the degenerate antiphase states are shown in Fig.2b

II. THE METHOD

We shall recall briefly the principe of the LS1 method for Ising ferromagnetic model, the reader can refer to the original paper[1] for more details.

Let us consider two strips of infinite length and finite width under free boundary conditions. In the spirit of the double cluster approximation[2,3], interactions within each ribbon are treated exactly and boundary spins are merged into an effective magnetic field. The magnetization (m) of the strip is obtained by diagonalizing the corresponding transfer matrix and performing the derivative of the free energy. Suppose that spins on one side of the ribbon are merged into an effective field h_{eff}, and spins of the opposite side are merged into an other auxillary effective field h_{aux}, following LS1 the critical temperature is given by

$$\lambda_n^{-1}\left.\frac{\partial^2\lambda_n}{\partial h_{aux}\partial h_{eff}}\right|_{h_{aux}=h_{eff}=0} = \lambda_{n+1}^{-1}\left.\frac{\partial^2\lambda_{n+1}}{\partial h_{aux}\partial h_{eff}}\right|_{h_{aux}=h_{eff}=0} \tag{3}$$

where λ_n (respectively λ_{n+1}) is the largest eigenvalue of the ribbon of width n (respectively n+1).

It is obvious that for ferromagnetic models, boundary spins are merged into the same effective magnetic field, since the same interactions have been cutted on both sides. However for antiferromagnetic models, one have to choose a transfer which preserve the ground state and take into account the nature of missing boundary interactions. Obviously two types of transfer are possible, the double transfer with staggered effective magnetic field on each boundary (see Fig.3a) or the diagonal transfer with zig-zag rows under homogenous effective magnetic field (Fig. 3b).

The first case leads to the following transfer matrix,

$$T(u,w)=T_1(u,v)*T_2(v,w) \quad , \tag{4}$$

where in the first case:

$$T_1(u,v) = \exp[\beta(J\sum_{i=1}^{n}(u_iu_{i+1}+u_iv_i) + h\sum_{i=1}^{n}u_i - h_{eff}u_1 + h_{aux}u_n)] \quad , \tag{5}$$

$$T_2(v,w) = \exp[\beta(J\sum_{i=1}^{n}(v_iv_{i+1}+v_iw_i) + h\sum_{i=1}^{n}v_i + h_{eff}v_1 - h_{aux}v_n)] \tag{6}$$

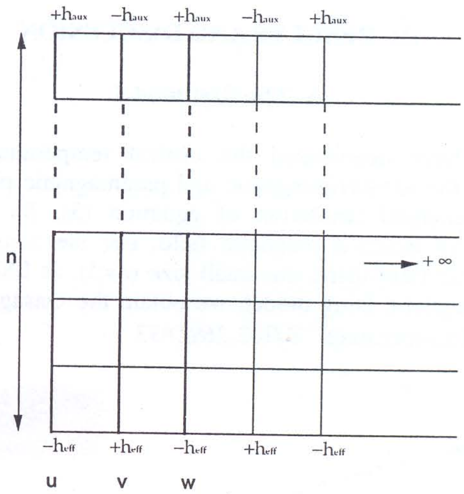

FIG. 3a. Vertical rows of spins u, v and w on the square lattice used to define the double transfer matrix T(u,w) on a strip of width n.

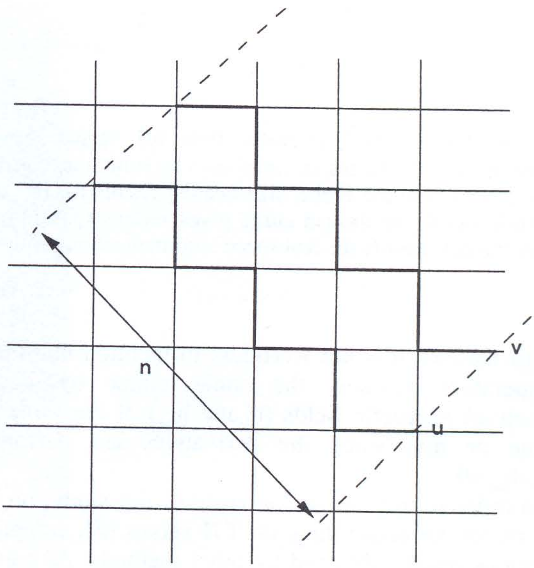

FIG. 3b. Diagonal rows of spins **u** and **v** on the square lattice used in diagonal.

and in the second cas:

$$T_1(v,w) = \exp[\beta J_1\sum_{i=1}^{n}(u_iu_{i+1}+u_iv_i)] \, , \tag{7}$$

$$T_2(v,w) = \exp[\beta\sum_{i=1}^{n}(J_2v_iv_{i+1}+J_1v_iw_i)] \tag{8}$$

u, v and w denote spins configurations of successive vertical rows.$\beta=1/k_BT$ with T the temperature and k_B the Boltzmann constant. For the second case, a simple transfer matrix with the same effective magnetic field on both boundaries is enough.

Both techniques lead to the same results, but from computational point of view the first one is more convenient since the second required even strip's width.

III. RESULTS AND DISCUSSION

A. The first model

We have determined the critical temperature which separe the antiferromagnetic and paramagnetic phases, by the numerical resolution of equation (3), for different values of external magnetic field. For the zero external magnetic field using the small size (n=3), as LS1[1] for the ferromagnetic Ising model, we obtain the Onsager's exact critical temperature[19] $T_c/J \cong 2.2691853$.

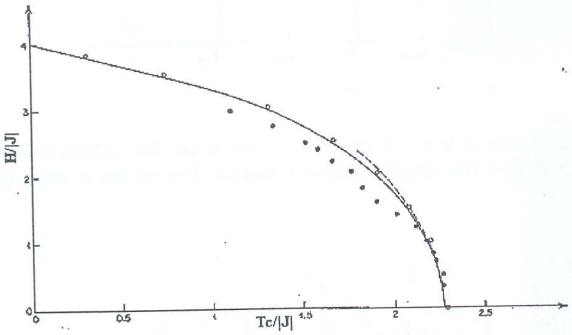

FIG. 4. The external magnetic field h/J versus the critical temperature T_c/J. Our results are shown by solid lines for **n**=3, the open circles give the Finite Size Scaling results for the strips of width 6 and 8, the dashed curve gives series-expansion results, while the dots denote the real space renormalization results.

For the $h \neq 0$ it is not worthless to mention that the critical temperature remains the same either by considering effectives magnetic fields ($h_{ee}$and h_{aux}) of the same absolute value or not, since the derivatives are performed for $h_{chh}=h_{aux}=0$.

In order to test the performance of our study, on Figure 4 we report the phase diagram T_c/J versus h/J, compared with previous results obtained by other methods. As can be seen on Fig 4, the accuracy of the method appears clearly, since very small sizes (hence unsignificant computational effort) enables to obtain critical temperatures of the same order of magnitude as more complicated approaches.

In order to check the accuracy of the method, we analyzed the convergence of the method, and this yields to an exponential convergence. Hence we estimate the exact critical temperature T_{ex} from a three-point power-law fit[5,20] by solving the equality,

$$\left[\left|\frac{T_{n-1}-T_{ex}}{T_n-T_{ex}}\right|\right]^{Ln(n/n+1)} = \left[\left|\frac{T_n-T_{ex}}{T_{n+1}-T_{ex}}\right|\right]^{Ln(n-1/n)} \tag{9}$$

the absolute values are necessary to overcome the oscillatory nature of the convergence. The exponential convergence observed by LS1 is obtained despite small value of the exponent appearing here. In Fig.5, where we have plotted $Ln(|T_n-T_{ex}|)$ versus n for the value of external magnetic field h=1. We conclude that

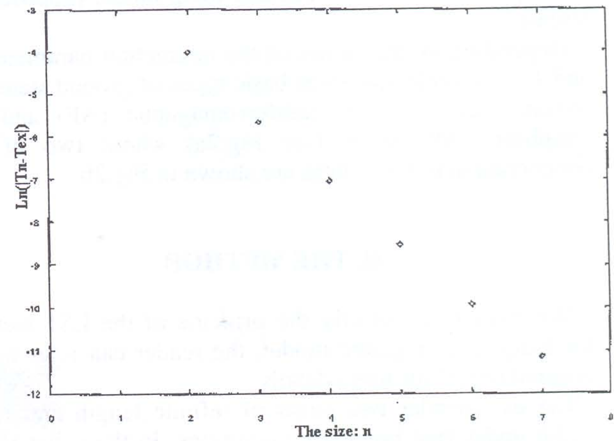

FIG. 5: The values of $Ln(|T_n-T_{ex}|)$ as a function of the size n for the external magnetic field h=1.

$$|T_n - T_{ex}| \propto \alpha^{-n} \tag{10}$$

where $\alpha=-0.14.$, we would like to point out that α is negative because of the oscillatory convergence.

The last interesting result concerns the slop of the $h(T_c)$ in the limit $T_c \to 0$, which is calculated straightforwardly from the phase diagram, and is equal to $\eta=-1.4986$, in good agreement with the known value derived by Baxter[19], say.$\eta=-1.499$.

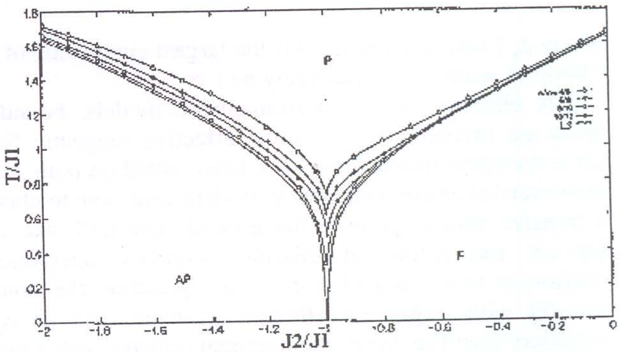

FIG. 6: The critical temperature T/J_1 versus the couplage interaction J_2/J_1 by Finite-Size-Scaling method for n/m=4/6 (triangle), n/m=6/8 (cross), n/m=8/10 (open circle), n/m=10/12 (square) and Lipowski-Suzuki method (full line) for n=3 .

B. The second model

The phase diagram in $(J_2/J_1, T/J_1)$ plane as obtained from LS1 method and compared with those obtained by Finite-Size-Scaling based on transfer matrix calculations (TMFSS) is shown on Fig.6. It consists of two second order transition lines, separating the ferromagnetic ($J_2/J_1>-1.$) and the antiphase ($J_2/J_1<-1.$) from the parramagnetic phase. Again one can see that TMFSS leads $T_c(J_2/J_1=-1) \neq 0$, which decreases with increasing system size. We obtained the extrapolated transition points T_c^* from a three-point power-law fit[5,18] which show very good convergence, unfortunately $T_c(J_2/J_1=-1)$ remains different

of zero, hence for this point more investigation, with large system sizes, are required in order to conclude. We did not found this necessary, since very accurate results are found from LS1 method, in particular $T_C(J_2/J_1=-1)=0$ and this is in good agreement with Monte Carlo simulations[22,23].

IV. CONCLUSION

We have thus presented in this paper a full study of the phase diagram of the two square lattice Ising models with extended Lipowski-Suzuki method. On one hand our results were shown to be completely consistent with previous works concerning both Ising models and on the other hand we found that it was very interesting to show that a simple method (LS1) which does not required too much computational effort, enables to get very accurate result.

ACKNOWLEDGMENT

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