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Spontaneous Magnetization for the Transverse Ising Model in Two and Three Dimensions

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Abstract We calculate the spontaneous magnetization for the transverse Ising model (TIM), in two (2-D) and three dimensions (3-D). The critical indexes of the magnetization at finite temperatures are the same as those of the corresponding Ising model case. We also obtain the critical frontiers which separate the ordered-disordered phases of the TIM in 2-D and 3-D and the critica1 fields compare well with other values available in the literature. As our results are based on extensions of the relations for the magnetization of the pure Ising model, we expect that they will be good estirnates for the spontaneous rnagnetization of the TIM at any finite ternperature.

1. INTRODUCTION

The transverse Ising model (TIM) has been proposed as a model harniltonian to describe the basic features of a list of cooperative systems. For example, this model was proposed by de Gennes[1] to describe the microscopic behaviour of hydrogen-bonded ferroelectrics of the KH_2PO_4 family. Also rnagnetic ordering in rnaterials with singlet crystal -field ground state can be described by the TIM, as reported by Wang and Cooper[2]. Further applications of the model can be found in a paper by Stinchcombe[3].

The hamiltonian of the TIM can be written as

$$H = -\Omega \sum_i \sigma_i^x - \frac{1}{2} J \sum_{ij} \sigma_i^z \sigma_j^z$$

where R is the transverse field, J is the nearest-neighbor exchange interaction and σ_i^α $(\alpha = x, y, z)$ are the components of spin -1/2 operators.

In one-dimension this model was exactly solved by Pfeuty[4] exhi-

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biting long-range order at zero temperature for sufficiently small transverse field intensity. In higher dimensions we have the series expansions results of Elliot and Wood[5], Pfeuty and Elliott[6], Yanase et al[7], Yanase[8] and Oitmaa and Plischke[9]. Among the effective field approaches which represent irnprovements over the mean field calculations for the TIM, we would like to depict the works of Hattori[10] and Sã Barreto et al[11].

Hattori calculations[10] are based on considering a pair of nearest-neighbor spins embedded in the mean field of the remainders, obtaining good results as coinpared with the series.

Sã Barreto et al[11] developed approximated relations for the spontaneous and transverse magnetizations of the TIM. In the case $\Omega = 0$, their relation for the spontaneous magnetization reproduces an exact identity derived by Callen[12]. Also their results can be seen as a lower bound for the critical field, while the mean field approximation (MFA) represents an upper bound for it.

MFA results for the TIM are displayed in a paper by Blinc and Zeks[13] and the comparison between the upper éind lower bounds for the critical field is found in the works of Silva and Sã Barreto[14].

Several renormalization group schemes have been applied to the TIM. We detach the works of dos Santos *et al*[15] and Penson *et al*[16] at zero temperature, and of Friedman[17], Stella and Toigo[18], Plascak[19] and Kolb[20], at finite temperatures.

In this work we intend to obtain the spontaneous magnetization for the TIM in two and three-dimensions based on the known relations for the pure (Ω=0) Ising model. In section 2 we Jiscuss the two-dimensional case. The three-dimensional version is discussed in section 3. Finally, we conclude in section 4, making comparisons of our results with others available in the literature.

2. THE TWO-DIMENSIONAL CASE

Let us pay attention to the following results from the series expansions[5,6,8]: in two or more dimensions the effect of the transverse field on the Ising model is to shift the critical temperature without altering the critical exponents (provided the critical temperature remains finite).

Also we will write the $z = 4$ ($z \equiv$ coordination number) spontaneous magnetization equation for the TIM in the MFA and in the Sá Barreto et *al* approximation[11]. We have

$$M = \frac{4JM}{\sqrt{\Omega^2 + (4JM)^2}} \tanh \beta \tag{2}$$

in the MFA, where M is the spontaneous magnetization, and $\beta \equiv 1/kT$, as usual, and

$$2M = \left[\frac{4J}{\sqrt{\Omega^2 + (4J)^2}} \tanh \beta\sqrt{\Omega^2 + (4J)^2} + 2\frac{2J}{\sqrt{\Omega^2 + (2J)^2}} \tanh \beta\sqrt{\Omega^2 + (2J)^2}\right] M$$

$$+ \left[\frac{4J}{\sqrt{\Omega^2 + (4J)^2}} \tanh \beta\sqrt{\Omega^2 + (4J)^2} - 2\frac{2J}{\sqrt{\Omega^2 + (2J)^2}} \tanh \beta\sqrt{\Omega^2 + (2J)^2}\right] M^3 \tag{3}$$

in the Sá Barreto et *al*[11] approximation.

Putting $R = 0$ in relations (2) and (3), we recover the results for the Ising model in the MFA and in the approximation worked out by Honmura and Kaneyoshi[21], respectively. Moreover, we can see that in these two approximations, the effect of the transverse field is to replace the function

$$\tanh \beta x \quad \text{by} \quad \frac{x}{\sqrt{\Omega^2 + x^2}} \tanh \beta\sqrt{\Omega^2 + x^2}$$

Now consider the exact relation for the spontaneous magnetization of the Ising model in the square lattice, expressed in terms of hyperbolic tangent functions, We can extend this relation to the TIM case, by using the same replacement mentioned above. Doing that we will have:

$$M = 2\left[\frac{2J}{\sqrt{\omega^2 + (2J)^2}} \tanh \beta\sqrt{\omega^2 + (2J)^2}\right]^2 M$$

$$- \left[\frac{2J}{\sqrt{\omega^2 + (2J)^2}} \tanh \beta\sqrt{\omega^2 + (2J)^2}\right]^4 M^9 \tag{4}$$

where o is the "renormalized" transverse field given by

$$\omega \equiv \frac{(z-2)}{(z-1)} \Omega \tag{5}$$

where relation (5) will be explained in the proper occasion.

Putting $\omega = 0$ in equation (4), we recover the exact spontaneous magnetization for the Ising model in a square lattice, as obtained by Yang[22], but expressed in terms of the hyperbolic tangent function[23].

The critical temperature (T_c) is obtained from (4) in the limit as $M \to 0$. We have

$$1 = 2\left[\frac{2J}{\sqrt{w^2 + (2J)^2}} \tanh \beta_c \sqrt{\omega^2 + (2J)^2}\right]^2 \tag{6}$$

Also in the limit as $\beta_c \to \infty$ ($T = 0$) we obtain ω_c (and also Ω_c, using relation (5)). We get

$$1 = 2\left[\frac{2J}{\sqrt{\omega_c^2 + (2J)^2}}\right]^2 \tag{7}$$

Soiving equation (7) we obtaín $R_c/J = 3$.

We compare in figure 1 the line of critical points of the TIM given by relation (6) with the Monte Carlo real space renormalization group calculations of Kolb[20]. Except for a narrow region around the critical transverse field the two curves remain close to each other in a wide range of R. We also compare, in the table 1, the critical field with other available results.

Now let us explain relation (5). In a previous paper[24] we were able to improve the MFA critical points obtained by various versions of the Ising and transverse Ising models, with the imposition of constraints in order to modify the standard mean field approximation. In that work we had to use two constraints: a) one that accounts for the effective transverse field and b) other that accounts for the effect of the correlations in the parallel effective field. However, in this work there is no need for the second constraint (case b), since the exact relation for the spontaneous magnetization contains the exact information about the parallel correlations. With respect to the case a) relation

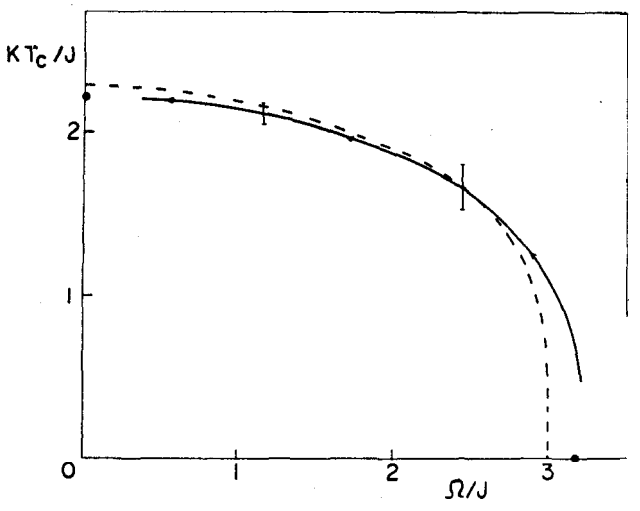

Fig.1 - Critical frontier for the TIM in the square lattice. This calculation (dashed line) is compared with the Monte Carlo renormalization group estimate of Kolb[20] (full line).

Table 1 - Values of the critical field Ω_c/J, for the TIM, accordingto various calculations.

Method / Lattice	Best of dos Santos-Sneddon-Stinchcombe 15	Penson-Julien-PFeuty 16	Hattori 10	Sã Barreto Fittipaldi Zeks 11	Present work	Series
Honeycomb	-	1.97	-	1.83	2.31	-
Square	3.03	2.63	3.3	2.75	3	3.04[5,6]
Triangular	3.74	4.12 4.76	5.4	4.71	4.33	4.77[7]
Simple Cubic	-	-	5.4	4.71	5.30	5.16[5,6]

(5) remains the same as that of the previous paper[24].

In order to pursue further this question let us define the following function

$$f(\alpha,\beta J) = \frac{2}{\sqrt{\alpha^2 + 4}} \tanh \beta J \sqrt{\alpha^2 + 4} \tag{8}$$

where

$$\alpha \equiv \frac{\omega}{J}$$

Then, based in the Potts[25] result for the Ising model in the triangular lattice and using the same argurnent employed in obtaining equation (4), we find

$$M = 2f(\alpha,\beta J)M - \left[2f^3(\alpha,\beta J) - f^4(\alpha,\beta J)\right]M^9 \tag{9}$$

which is the spontaneous magnetization for the TIM in the triangular lattice.

Thecritical temperature isobtained in the limit $M \to 0$, and is given by the equation

$$1 = 2f(\alpha,\beta_c J) \tag{10}$$

Putting a = 0 in eqs. (9) and (10) we recover Potts[25] exact result for the Ising model in the triangular lattice.

The critica1 field is given by the equation

$$1 = \frac{4}{\sqrt{\alpha_c^2 + 4}} \tag{11}$$

obtained by taking the limit $\beta_c \to \infty$ in eq. (10).

The critical field is compared with other available results in the table 1.

Finally, we present the last two-dimensional result of this paper. In an analogous way as we did before we obtain for the TIM in the honeycomb lattice the spontaneous magnetization

$$M = 2\sqrt{1 - f^2(\alpha,\beta J)}M + \{f^2(\alpha,\beta J)\left[2 - f^2(\alpha,\beta J) - 2\sqrt{1 - f^2(\alpha,\beta J)}\right]\}M^9 \tag{12}$$

So, the critical ternperature for the TIM in the honeycomb lattice is given by the equation

$$1 = 2\sqrt{1 - f^2(\alpha, \beta_c J)} \tag{13}$$

and the critical field is given by

$$1 = 2\sqrt{1 - \frac{4}{(\alpha_c^2 + 4)}} \tag{14}$$

Again the critica1 field of (14) is compared with other available results in table 1.

It is worth to mention that the results for the TIM in the honeycomb lattice were obtained based in an extension of Naya's result[26] for the Ising limit (Ω=0). Naturally that case can be reproduced taking a=O in relations (12) and (13).

In figure 2 we present the spontaneous magnetization for the TIM in the square lattice, as a function of the temperature and for various values of the transverse field. We see that the magnetization goes to zero at the critica1 temperature with the critical indexcharacteristic of the two-dimensional Ising model, that is .125.

The results for the other planar lattices look similar to the square lattice case and we do not present plots of them here.

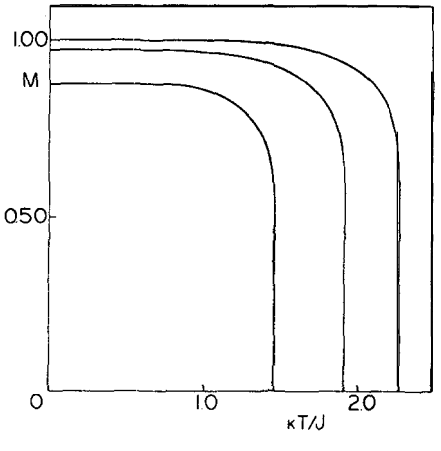

Fig.2 - Spontaneous rnagnetization for TIM in the square lattice, as a function of the ternperature. From inside we have the curves calculated in this work for R/J = = 2.7, R/J = 2 and R = 0, respectively.

3. THE THREE-DIMENSIONAL CASE

In a recent paper[27], we have proposed that the spontaneous magnetization for the Ising model in the simple cubic lattice can be well represented by the equation

$$M = (3 \tanh^2 3\beta J)M - (2 \tanh^3 3\beta J)M^{21/5} \tag{15}$$

The above relatiori gives the critical temperature (T_c) $kT_c/J =$ $= 4.56$ as compared with[28]

$$kT_c/J\Big|_{\text{series}} = 4.51$$

Also relation (15) can be expanded around T_c, as

$$M \approx 1.54 \left(1 - \frac{T}{T_c}\right)^{5/16} \tag{16}$$

a r-esult that can be compared with

$$M\Big|_{\text{series}} \approx 1.57 \left(1 - \frac{T}{T_c}\right)^{5/16} \tag{17}$$

the series result, as quoted by Fisher[29].

Then we can use relation (15) in a similar way as we have used the two-dimensional exact results for Ising model, in order to obtain the spontaneous magnetization for the TIM in the simple cubic lattice. Doing so, we have

$$\begin{aligned} M = {} & 3\left(\frac{3J}{\sqrt{\omega^2 + (3J)^2}} \tanh \beta\sqrt{\omega^2 + (3J)^2}\right)^2 M \\ & - 2\left(\frac{3J}{\sqrt{\omega^2 + (3J)^2}} \tanh \beta\sqrt{\omega^2 + (3J)^2}\right)^3 M^{21/5} \end{aligned} \tag{18}$$

Taking the limit as $M \to 0$, we obtain the critica1 frontier of the TIM in the simple cubic lattice. We get

$$1 = 3\left(\frac{3J}{\sqrt{\omega^2 + (3J)^2}} \tanh \beta_c\sqrt{\omega^2 + (3J)^2)}\right)^2 \tag{19}$$

Finally, we obtain the critical field ($\beta_c \to \infty$) through the equation

$$1 = \frac{27\,J^2}{\omega_c^2 + 9J^2} \tag{20}$$

The critical field obtained from eq. (20) is compared with the other results from the literature, in table 1.

We plot in figure 3 the critical frontiers of the TIM in the two and three-dimensional lattices treated in this paper. Also we compare in tables 2 and 3 the values of the present work with the series results, in the square lattice and in the simple cubic lattice cases. We see that the agreement between the two calculations arenotso good as expected.

In figure 4 we present the spontaneous magnetization for the TIM in the simple cubic lattice, as function of the temperature and for various values of the transverse field. We see that the magnetization goes to zero at the critical temperature with the critical index characteristic of the three-dimensional Ising model, that is .3125 as quoted from series results by Fisher[29].

4. CONCLUSIOMS

In this paper we have obtained the spontaneous magnetization for the TIM in two-dimensions based in extensions of the exactrelations for the pure Ising case, since for the pure Ising (Ω=0) the magnetization can be expressed in terms of hyperbolic tangent functions. Also starting from what we think is a good analytical relation for the Ising model in the simple cubic lattice, we were able to extend the relation for the TIM case.

The spontaneous magnetization obtained for the TIM in two and three-dimensions goes to zero at the critical temperature with the same critical indcx of the pure Ising model (Ω=0) versions, respectively.

The comparison of the critical fields (see table 1) with other results of literature shows that we have obtained results close to the best estimates (close to the series results, in particular).

Also the comparison of the line of critical points, in the square lattiçe case, shows a good match with the Monte Carlo Renormalization Group calculation of Kolb[20], except in a narrow region below Ω_c

Table 2 - Critical temperature for some values of the transverse field, obtained in this work, compared with series results[5,6], for the square lattice case.

Ω/J	KT_c/J (series[5,6])	KT_c/J (this work)
0	2.252	2.269
0.224	2.248	2.265
1.415	2.020	2.106
2.162	1.660	1.840
2.566	1.348	1.584
2.804	1.120	1.330
2.880	0.940	1.204
3	-	0
3.080	0	-

Table 3 - Idem as table 2, for the simple cubic lattice.

Ω/J	KT_c/J (series[5,6])	KT_c/J (this work)
0	4.518	4.556
0.444	4.506	4.546
2.760	3.960	4.133
4.080	3.132	3.497
4.656	2.448	3.005
4.920	1.968	2.665
5.036	1.620	2.463
5.124	1.026	2.268
5.160	0	2.169
5.303	-	0

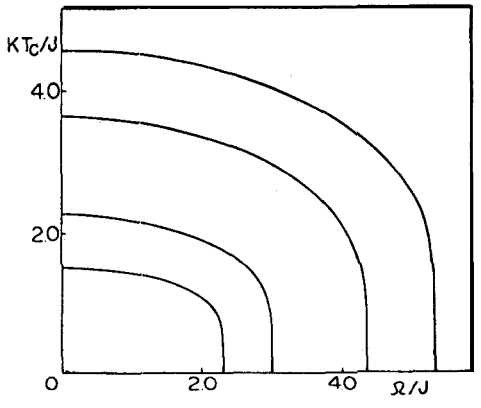

Fig.3 - Critical frontier which separates the paramagnetic and ferromagnetic phases of the TIM, according to this work. From inside we have the curves for the honeycomb, square, triangular and simple cubic lattices, respectively.

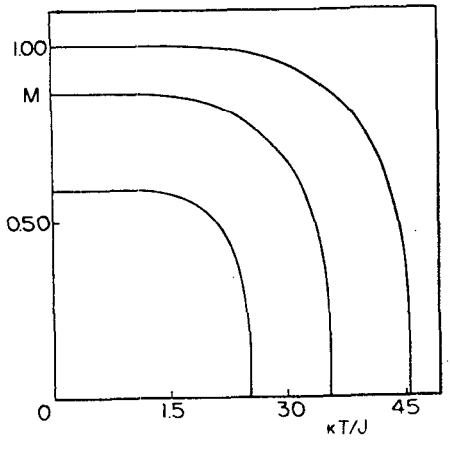

Fig. 4 - Spontaneous magnetization for the TIM in the simple cubic lattice as a function of the temperature, calculated in this work. From inside we have the curves for $\Omega/J = 5$, $\Omega/J = 4$ and $\Omega = 0$, respectively.

as can be seen in figure 1. But the results are not so good, as compared with the series results[5,6] (see tables 2 and 3).

We expect that the results here obtained can be good estimates of the spontaneous magnetization of the TIM far from the quantum behavior at $T=0$.

In particular we expect the results to be quite good near $\Omega=0$, the Ising limit.

Now the method has at least two shortcomnings:

a) The results do not display the correct criticality ($\beta \cong 5/16$) of the TIM in 2-D at zero temperature in terms of the transverse field, which corresponds (see tha papers of Young[30], Hertz[31] and Suzuki[32]) to the criticality of the Ising model one dimension higher (3-D) in terms of the temperature parameter.

b) We can not calculate a quantity such as the transverse magnetization for the TIM, since we do not have the corresponding quantity in the pure Ising model case.

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Resumo

Neste artigo calculamos a magnetização espontânea para o modelo de Ising transverso (TIM) em duas (2-D) e três dimensões (3-D). Os índices críticos da magnetização são os mesmos que os do modelo de Ising nos casos correspondentes. Também obtemos as fronteiras críticas que separam as fases ordenadas e desordenadas do TIM em 2-D e 3-D e os valores dos campos críticos estão próximos dos encontrados na literatura. Devido ao fato de que nossos resultados são baseados em extensões das expressões para a magnetização do mddelo de Ising puro, esperamos que eles sejam boas estimativas para a magnetização espontânea do TIM em temperaturas finitas.