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Correlation Effects in the Ising Model in an External Field

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Abstract The thermodynamic properties of the spin-1/2 Ising Model in an external field are evaluated through the use of the exponential differential operator method and Callen's exact relations. The correlations effects are treated in a phenomenological approach and the results are compared with other treatments.

1. INTRODUCTION

Despite the great variety of papers published on the Ising Model, the number of reports decreases in appreciable amount when the subject is the Ising Model in an external field.

Recently, Gartenhaus[1] applied the method of Kramers- Wannier[2] to evaluate the thermodynamical properties of the spin-1/2 Ising Model in an external field for the square lattice. The results obtained are in excellent agreement with the exact ones in the limit of zero external field. However, this method presents some difficulties when three dimensional lattices are treated.

Here we study the two and three dimensional spin - 1/2 Ising Model in an external field with the use of the exponential differential operatcr technique introduced by Honmura and Kaneyoshi[3,4], in a set of exact relations due to Callen[5].

The differential operator method has been applied to various problems described by Ising hamiltonians (see for example Taggart and Fittipaldi[6] and references therein). The results obtained encourage us to apply the method to the Ising Model in an external field.

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A first approximation, in which we neglect spin correlations, is developed in Sec. 2. In Sec. 3 we develop a second approximation, in which we incorporate the correlation effects as was proposed by P. R. Silva and F.C. Sá Barreto[7]. Finally, in the last section we discuss and comment the results obtained.

2. THERMODYNAMICAL PROPERTIES – I

The hamiltonian that describes the spin 1/2 Ising Model in an external field H is given by

$$\mathcal{H} = -\frac{1}{2} J \sum_{i,j} \sigma_i \sigma_j - H \sum_i \sigma_i \tag{1}$$

where σ_i are z-component Pauli spin operator taking values ± 1, and J is the exchange interaction between two nearest neighboring sites i and j. Callen's identity for the thermal average value of the site magnetization is given by[5,8]

$$< \sigma_i > = < \tanh \beta E_i > \tag{2}$$

where $<\ldots> = (\mathrm{Tr}\, e^{-\beta\mathcal{H}} \ldots)/\mathrm{Tr}\, e^{-\beta\mathcal{H}}$, $\beta = 1/KT$, and $E_i = J \sum_j \sigma_j + H$ is the local field operator at site i.

Applying the exponential differential operator $e^{aD} f(x) = f(x+a)$, (here $D \equiv \partial/\partial x$) into Callen's identity and expanding the exponential in power series we obtain[4,9]

$$< \sigma_i > = < \prod_j \left[\cosh(\beta JD) + \sigma_j \sinh(\beta JD)\right] > \tanh(x+\beta H) \Big|_{x=0} \tag{3}$$

2.1. Magnetization

As a first approximation we neglect spin correlations. According to reference 10 we can write eq. (3) as

$$m = \left[\cosh(\beta JD) + m \sinh(\beta JD)\right]^z \tanh(x+\beta H) \Big|_{x=0} \tag{4}$$

where $m = <\sigma_i> = <\sigma_j>$ and z is the coordination number. Expressing the hyperbolic functions in terms of exponentials and using the definition of the exponential differential operator we get

$$16m = A_4(0) + A_4(1)m + A_4(2)m^2 + A_4(3)m^3 + A_4(4)m^4 \tag{5}$$

for the square lattice (z=4) and

$$64m = A_6(0) + A_6(1)m + A_6(2)m^2 + A_6(3)m^3 + A_6(4)m^4 + A_6(5)m^5 + A_6(6)m^6 \tag{6}$$

for the triangular and simple cubic lattice (z=6), where the coefficients $A_z(n)$ are listed in table 1.

We show in Figure 1 the magnetization, for square lattice, as a function of temperature, for some values of the externa1 field.

2.2. Internal Energy

According to our first approximation and reference 10 we can write the internal energy as

$$U = -\frac{1}{2} NZJ\{[\sinh(\beta JD) + \langle\sigma_j\rangle \cosh(\beta JD)] \, [\cosh(\beta JD) + \langle\sigma_j\rangle \sinh(\beta JD)]^{z-1}\} \tanh(x+\beta H)\Big|_{x=0} \tag{7}$$

which leads to

$$U = -\frac{1}{8} NJ[B_4(0) + B_4(1)m + B_4(2)m^2 + B_4(3)m^3 + B_4(4)m^4] \tag{8}$$

for the square lattice (z=4) and

$$U = -\frac{3}{64} NJ[B_6(0) + B_6(1)m + B_6(2)m^2 + B_6(3)m^3 + B_6(4)m^4 + B_6(5)m^5 + B_6(6)m^6]$$

for the triangular and simple cubic lattice (z=6). The coefficients $B_z(n)$ are listed in Table 1. In Figure 2 we show the internal energy, for the square lattice, as a function of temperature.

2.3. Susceptibility

From equations (5) and (6) we can easily evaluate the susceptibility $\chi = \partial m/\partial H$. In Figure 3 we present graphs of the susceptibility, for H = 0, $0.1J$, 0.25 and $0.4J$, as a function of T. The results are in good agreement with those obtained by other methods[8].

Table 1 - The symbols $A_z(n)$ and $B_z(n)$ denote the coefficients which appear multiplied by the n-th power of the magnetization in equations (5) and (6) and in equations (8) and (9), respectively, for the lattices with a coordination number z. The function $f(x)$ is defined as $f(x) \equiv \tanh(x)$.

$$A_4(0) = f(\beta H+4\beta J)+f(\beta H-4\beta J)+4\left[f(\beta H+2\beta J)+f(\beta H-2\beta J)\right]+6f(\beta H)$$

$$A_4(1) = 4\left[f(\beta H+4\beta J)-f(\beta H-4\beta J)\right]+8\left[f(\beta H+2\beta J)-f(\beta H-2\beta J)\right]$$

$$A_4(2) = 6\left[f(\beta H+4\beta J)+f(\beta H-4\beta J)\right]-12f(\beta H)$$

$$A_4(3) = 4\left[f(\beta H+4\beta J)-f(\beta H-4\beta J)\right]-8\left[f(\beta H+2\beta J)-f(\beta H-2\beta J)\right]$$

$$A_4(4) = f(\beta H+4\beta J)+f(\beta H-4\beta J)-4\left[f(\beta H+2\beta J)+f(\beta H-2\beta J)\right]+6f(\beta H)$$

$$A_6(0) = f(\beta H+6\beta J)+f(\beta H-6\beta J)+6\left[f(\beta H+4\beta J)+f(\beta H-4\beta J)\right]+ \\ + 15\left[f(\beta H+2\beta J)+f(\beta H-2\beta J)\right]+20f(\beta H)$$

$$A_6(1) = 6\left[f(\beta H+6\beta J)-f(\beta H-6\beta J)\right]+24\left[f(\beta H+4\beta J)-f(\beta H-4\beta J)\right] + \\ + 30\left[f(\beta H+2\beta J)-f(\beta H-2\beta J)\right]$$

$$A_6(2) = 15\left[f(\beta H+6\beta J)+f(\beta H-6\beta J)\right]+30\left[f(\beta H+4\beta J)+f(\beta H-4\beta J)\right]- \\ - 15\left[f(\beta H+2\beta J)+f(\beta H-2\beta J)\right]-60f(\beta H)$$

$$A_6(3) = 20\left[f(\beta H+6\beta J)-f(\beta H-6\beta J)\right]-60\left[f(\beta H+2\beta J)-f(\beta H-2\beta J)\right]$$

$$A_6(4) = 15\left[f(\beta H+6\beta J)+f(\beta H-6\beta J)\right]-30\left[f(\beta H+4\beta J)+f(\beta H-4\beta J)\right] - \\ - 15\left[f(\beta H+2\beta J)+f(\beta H-2\beta J)\right]+60f(\beta H)$$

$$A_6(5) = 6\left[f(\beta H+6\beta J)-f(\beta H-6\beta J)\right]-24\left[f(\beta H+4\beta J)-f(\beta H-4\beta J)\right]+ \\ + 30\left[f(\beta H+2\beta J)-f(\beta H-2\beta J)\right]$$

$$A_6(6) = f(\beta H+6\beta J)+f(\beta H-6\beta J)-6\left[f(\beta H+4\beta J)+f(\beta H-4\beta J)\right] + \\ + 15\left[f(\beta H+2\beta J)+f(\beta H-2\beta J)\right]-20f(\beta H)$$

$$B_4(0) = A_4(1)/4$$

$$B_4(1) = 4\left[f(\beta H+4\beta J)+f(\beta H-4\beta J)\right]+4\left[f(\beta H+2\beta J)+f(\beta H-2\beta J)\right]$$

$$B_4(2) = 6\left[f(\beta H+4\beta J) - f(\beta H-4\beta J)\right]$$

$$B_4(3) = 4\left[f(\beta H+4\beta J)+f(\beta H-4\beta J)\right]-4\left[f(\beta H+2\beta J)+f(\beta H-2\beta J)\right]$$

$$B_4(4) = A_4(3)/4$$

$$B_6(0) = A_6(1)/6$$

cont. Table 1

$$B_6(1) = 6[f(\beta H+6\beta J)+f(\beta H-6\beta J)]+16[f(\beta H+4\beta J)+f(\beta H-4\beta J)]+$$
$$+\ 10[f(\beta H+2\beta J)+f(\beta H-2\beta J)]$$

$$B_6(2) = 15[f(\beta H+6\beta J)-f(\beta H-6\beta J)]+20[f(\beta H+4\beta J)-f(\beta H-4\beta J)] -$$
$$-\ 5[f(\beta H+2\beta J)-f(\beta H-2\beta J)]$$

$$B_6(3) = 20[f(\beta H+6\beta J)+f(\beta H-6\beta J)]-20[f(\beta H+2\beta J)+f(\beta H-2\beta J)]$$

$$B_6(4) = 15[f(\beta H+6\beta J)-f(\beta H-6\beta J)]-20[f(\beta H+4\beta J)-f(\beta H-4\beta J)]-$$
$$-5[f(\beta H+2\beta J)-f(\beta H-2\beta J)]$$

$$B_6(5) = 6[f(\beta H+6\beta J)+f(\beta H-6\beta J)]-16[f(\beta H+4\beta J)+f(\beta H-4\beta J)] +$$
$$+\ 10[f(\beta H+2\beta J)+f(\beta H-2\beta J)]$$

$$B_6(6) = A_6(5)/6$$

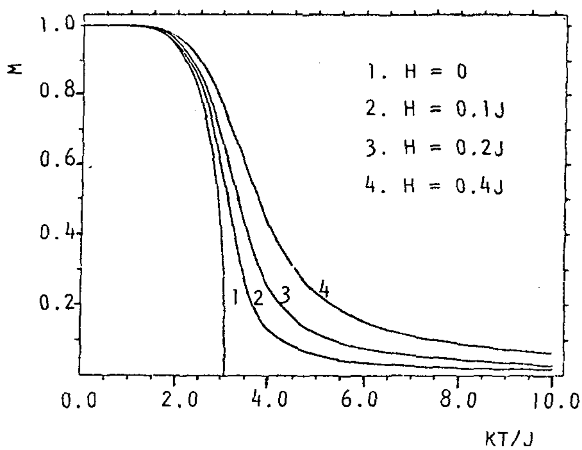

Fig.1 - Magnetization for the square lattice as function of the temperature T in the first approximation, for different values of the external field *H*.

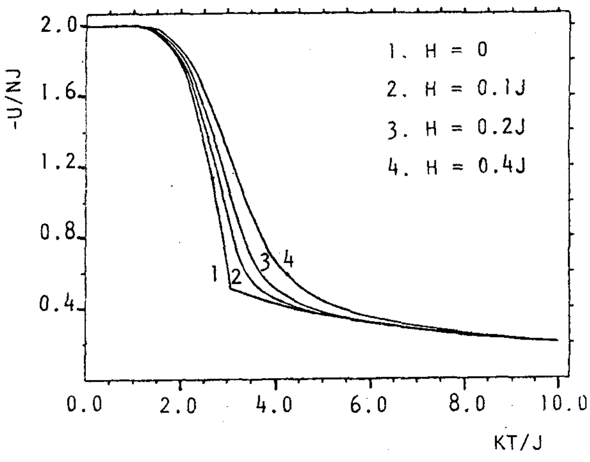

Fig. 2 - The internal energy for the square lattice which is given by equation (9) as function of T, in the first approximation and for various values of the external field H.

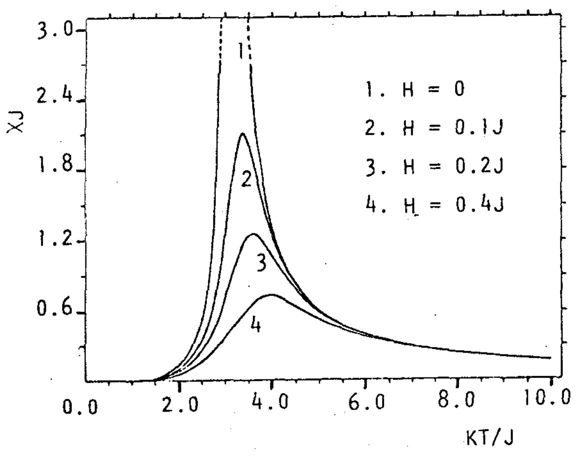

Fig.3 - Susceptibility for the square lattice as a function of T, for various values of H, in the first approximation. The dashed part of the H = 0 curve indicates that the zero-field susceptibility goes to infinite when the temperature goes to T_c.

3. THERMODYNAMICAL PROPERTIES – II

Here we incorporate, following reference 7, the effects of correlations in the effective field acting on the site i due to the neighbor spins j, rewriting eq.(4) as

$$\langle\sigma_i\rangle = \left[\cosh(\beta JD) + \langle\langle\sigma_j\rangle\rangle\sinh(\beta JD)\right]^z \tanh(x+\beta H)\Big|_{x=0} \qquad (10)$$

Notice that $m = \langle\sigma_i\rangle = \langle\sigma_j\rangle \neq \langle\langle\sigma_j\rangle\rangle$; $\langle\langle\sigma_j\rangle\rangle$ is $\langle\sigma_j\rangle$ modified by the correlation effects, which have been neglected in the previous section We suppose that $\langle\langle\sigma_j\rangle\rangle$ is related to m, in the following way[7]

$$\langle\langle\sigma_j\rangle\rangle = \alpha_z^{-1}(H,T)m \qquad (11)$$

where

$$\alpha_4(H,T) = \frac{\tanh(\beta H + 8\beta J\,m)}{\tanh(\beta H + 7\beta J\,m)} \qquad (12)$$

for the square lattice (z=4),

$$\alpha_6(H,T) = \frac{\tanh(\beta H + 6\beta J\,m)}{\tanh(\beta H + 5\beta J\,m)} \qquad (13)$$

for the triangular lattice (z=6) and

$$\alpha_6(H,T) = \frac{\tanh(\beta H + 26\beta J\,m)}{\tanh(\beta H + 25\beta J\,m)} \qquad (14)$$

for the simple cubic lattice (z=6). The present treatment distinguishes the triangular and the simple cubic lattice, a result which has been obtained in reference 7 for the case H=0.

3.1. Magnetization

We can now evaluate the magnetization simply substltuting eqs. (12), (13) and (14) into equation (10). The results for the square lattice are shown in Figure 4 as a function of temperature and Figure 5 as a function of the external field.

As we can see from Figure 4, in the limit H=0 we obtain a first order phase transition which is not correct. However, the results for H = $0.1J$, $0.2J$ and $0.4J$ are in good agreement with reference 1 and for H=O some irnprovement has been achieved for the critical temperature (T_c) over other internal field calculations[6,11,12]. The results o'btained for T_c are listed in Table 2. In order to explain the inconsistency of the present results for T_C with the correspondents appearing in reference 7 (see table 2), we must consider the following points.

a) In the work of reference 7 numerical calculations for the spontaneous magnetization has not been done and the first order transition was not detected.

b) On considering the square lattice case, for example, we have $\alpha(H=0, T=T_C) = 8/7$ (see equation 12) when we take the limit as m goes to zero, as was done in reference 7.

c) In the case of first order transition we can not take the above limit ($m \to 0$) and then $\alpha(H=0, T=T_C)$ will be less than $8/7$ (in the square lattice case) consequently leading to different critical temperature.

In Figure 6 we compare the magnetization for the simple cubic and triangular lattice as calculated in the first and second approximations. For H = $0.1J$, we see that the correlation effects are much less important for the simple cubic lattice than for the triangular lattice.

Also, in Figure 5, we note that at high temperature we can write the magnetization as a linear function of the external field.

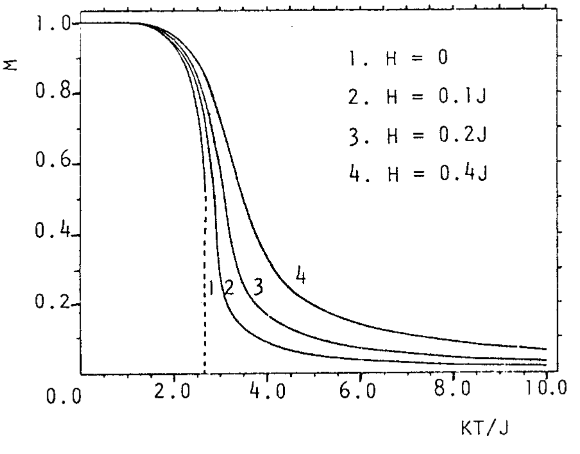

Fig.4 - Magnetization for the square lattice as function of T and for various values of H, in the second approximation. The dashed line is a extrapolation from the calculated values (solid lines).

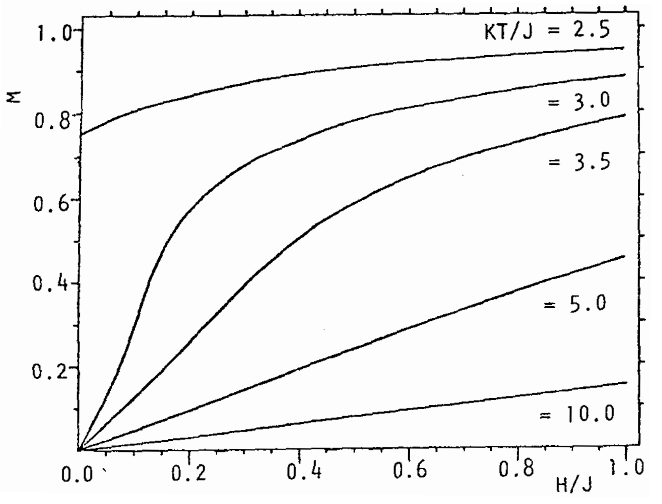

Fig.5 - Magnetization for the square lattice as function of H, in the second approximation, for different values of temperature T.

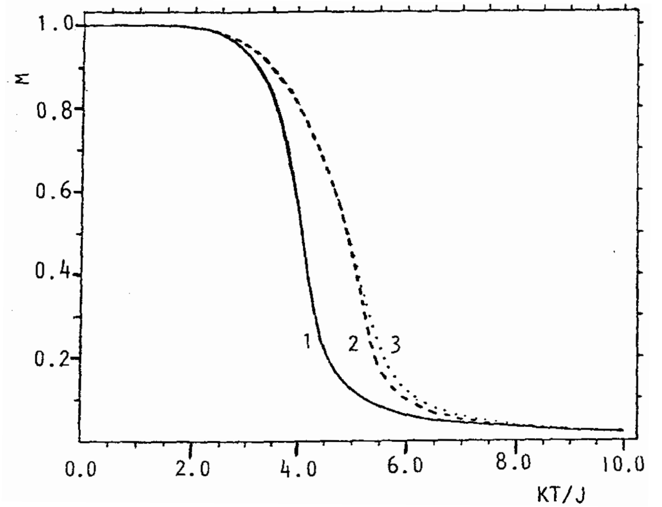

Fig.6 - The magnetization as a function of T, for H = $0.1J$. The second approximation for the triangular and simple cubic lattices is shown in curves 1 and 2, respectively; 3 represents the first approximation for triangular (or simple cubic) lattice.

Table 2 - Comparison of the critical temperature (KT_c/J) with other approximations for the square, triangular and simple cubic lattices.

Approximations	Square	Triangular	Simple Cubic
Weiss (MFA)[11]	4	6	6
Mamada-Takano[12]	3.090	5.073	5.073
Matsudaira[13]	2.622	4.271	4.731
Taggärt-Fittipaldi[6]	2.680	4.890	4.890
Silva-Sá Barreto[7]	2.421	3.861	4.802
Present work (second appr.)	2.665	3.875	4.885
Exact or series[14]	2.269	3.641	4.510

3.2. Internal Energy

To evaluate de internal energy we replace $<<\sigma_3>>$ by $<\sigma_3>$ in equation (7) and make use of equations (12), (13) and (14). The internal energy for the square lattice is plotted in Figure 7. Comparing Figures 2 and 7 we see that for $H=0$ we have improved slightly the short-range order[15]. This is better seen in Figure 8, which shows the internal energy, for $H=0$, for the triangular and the simple cubic lattices, in the first and second approximations. As can be seen the only difference between the first and second approximations, for the simple cubic lattice, occurs in the neighbourhood of T_c, this is just what is expected since near T_c the correlations are more irnportant. The results for the short-range order in the internal energy are presented in Table 3.

3.3. Susceptibility

Proceeding as in section 2.3 and using equations (12), (13) and (14) we obtain the susceptibility. In Figure 9 we present the susceptibility for the square lattice. We see that as H decreases, the peak becornes more and more sharp and the maximum of each curve displaces toward the critical temperature. Note that for $H = 0$ the sosceptibility diverges for $T = T_c$, In this second approximation we obtain better results for the maximum points as compared with those obtained by Gartenhaus[1]. In Figure 10 the susceptibility is shown for the triangular and the simple cubic lattices, for H = $0.1J$ and H = $0.4J$. We can see that the second approximation distinguishes the dimensionality of the lattices (both with z = 6), a result that does not appear in other methods[6,11,12,13]. We must emphasize that the second approximation was first workedout in reference 7, but restricted to the case H = 0.

Table 3 - Values of the internal energy at T_c, in units of $-(NJZ/2)$(the zero temperature value) for the square, triangular and simple cubic lattices.

Approximations	Square	Triangular	Simple Cubic
MFA[16]	0	0	0
Kaneyoshi *et al.*[10]	0.250	0.167	0.167
Present work			
(second appr.)	0.274	0.200	0.171
Exact or series[17]	0.707	0.667	0.536

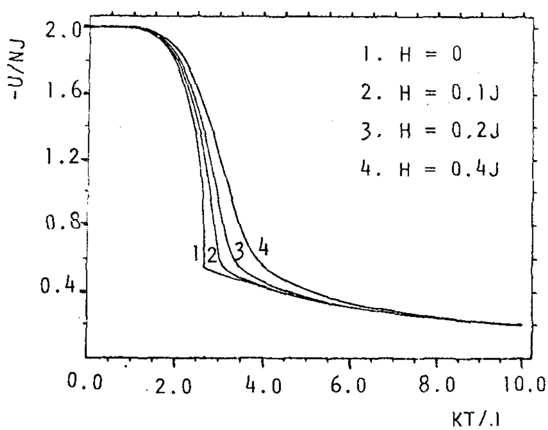

Fig.7 - Internal energy, for the square lattice, as a function of T, in the second approximation, for various values of H.

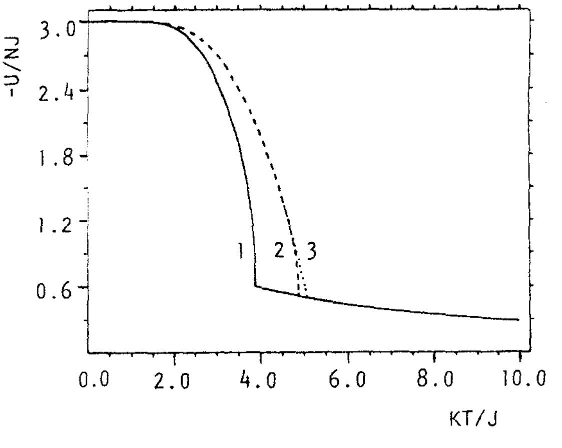

Fig.8 - Internal energy as a function of T, for H = 0. The second approximation for the triangular and simple cubic lattices is shown in curves 1 and 2, respectively; 3 represents the first approximation for triangular (or simple cubic) lattice.

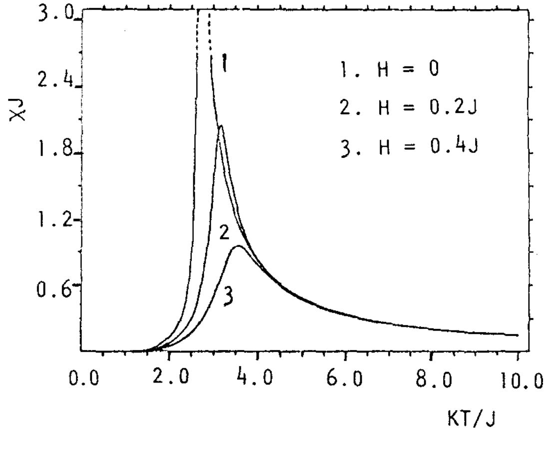

Fig.9 - Susceptibility, for the square lattice, as a function of T, in the second approximatlon, for various values of H.

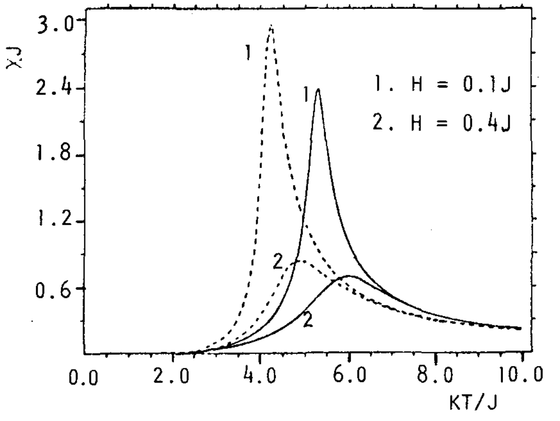

Fig.10 - Susceptibility, for the triangular (dashed curves) and simple cubic (solid curves) lattices, as function of T for $H=0.1J$ and $H=0.4J$, in the second approximation.

4. DISCUSSION AND COMMENTS

Refering to Figure 4 we should note that for the critical temperature we consider the point where the magnetization discontinuously goes to zero in the second approximation. The wrong order of the transition (1st order) is due to the fact that the present treatment overestimates the effect of the correlations.

As is shown in Figure 5, in the region of low fields, the curves for KT/J = 2.5 and KT/J = 3.0 have a slight positive curvature; for higher values, the curvature becomes negative. This is not in agreement with Griffiths and Sherman[18] which conclude that the magnetization should have a negative curvature for all field strengths and for all values of the temperature. Again, this result occurs because, as we have said before, we overestimated the correlations. Thus, in the region where the correlations are more important, i.e., in the region of low fields and low temperatures it seems reasonable to expect this behavior.

With respect to the susceptibility, we note that for the square lattice and in the second approximation (Figure 9), for H = $0.1J$ the maximum occurs at KT/J 2.9, for H = $0.2J$, it occurs at KT/J 3.2 and for H = $0.4J$ it occurs at KT/J 3.6. These results are in close agreement with those obtained by Gartenhaus[1], who predicts that for H = $0.1J$, the maximum occurs at KT/J 2.8, for H = 0.2 at $KT/J \cong$ 3.2 and for H = $0.4J$ at KT/J 3.6.

From Tables 2 and 3 and figures 1 and 2, we see that in the first approximation taking H = 0, we recover the results obtained by Mamada and Takano[12], which coincides with those obtained by Honmura and Kaneyoshi[4,10].

It seems that the most irnportant point in our work is that it distinguishes between planar triangular lattice and simple cubic lattice (both having z = 6), for finite externa1 field, as is shown in Figure 10.

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Resumo As propriedades termodinâmicas do Modelo de Ising em um campo externo para spin-1/2 são estudadas através do método do operador diferencial e de relações exatas devidas à Callen. Os efeitos das correlações são tratados de um ponto de vista fenomenológico. Também comparamos os resultados presentes com outros disponíveis na literatura.