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THE SPONTANEOUS MAGNETIZATION OF TWO-DIMENSIONAL RECTANGULAR ISING MODEL: EFFECTIVE-FIELD THEORY ANALYSIS

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Resumo

Neste artigo de revisão estudaremos o modelo de Ising bidimensional. O modelo consiste de interações ferromagnéticas $J_y = \lambda J_x$nas direções $x(y)$. Para alguns valores do parâmetro λ serão obtidos a magnetização como uma função da temperatura T , usando da técnica do operador diferencial, proposta por Honmura e Kaneyoshi (1979), baseada na teoria de campo efetivo com aglomerado finito de $N = 1$ spins (EFT-1).

Palavras-Chave: Modelo de Ising, Teoria de campo efetivo, rede quadrada.

Abstract

In this paper we have studied the two-dimensional rectangular Ising model. The model consists of ferromagnetic interactions $J_y = \lambda J_x$ in the $x(y)$ direction. For some values λ we obtain the magnetization m as a function temperature T, using the framework of the differential operator technique, proposal by Honmura and Kaneyoshi (1979), based in the effective field theory with finite cluster of $N = 1$ spins (EFT-1).

Key-words: Ising model, effective-field theory, square lattice.

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1. Introduction

The Ising model is a well-known and studied model in the statistical mechanics. Because of its simplicity, this model has attracted the concerted attention for over 80 years. The Ising model was first solved in one-dimensional, where was observed that it have not phase transition at a finite temperature (i.e., $T_c = 0$ (ISING, 1925). In 1944, Onsager (1944) obtained an exact expression for the free energy of the Ising model on a square lattice in zero field, and in 1952 Yang (1952) presented a computation of the spontaneous magnetization. Recently, Zhang (2007) has presented a conjectured expression for the free energy and spontaneous magnetization of the 3d Ising model, but some authors have argued that these conjectures are false (WU et al., 2008). The most reliable estimates for the phase transition temperature T_c in the 3d Ising model were computed by using high-temperature series and Monte Carlo (MC) methods (MCCOY e WU, 1973; BAXTER, 1982). The best estimates rely on finite-size scaling of MC simulations on a simple cubic lattice is $k_B T_c/J = 4.5115240(21)$, while on a square lattice we have an exact value $k_B T_c/J = 2/ln\left(1+\sqrt{2}\right) \simeq 2.269185314$....

Another motivation to study the Ising model is because itcan be used to describe the critical behavior of a broad class of materials, including easyaxis magnets, binary alloys, simple liquids and their mixture, polymer solutions, subnuclearmatter, etc. (ANDREI N. et al., 1983; CHUNG et al.,1983; WHITE, 1993).

It is the purpose of the present paper to calculate the spontaneous magnetization (i.e.,the intensity of magnetization at zero external magnetical field) of a two-dimensional Ising model of a ferromagnet. Van der Waerden (1993) and Ashkin and Lamb had obtained a series expansion of the spontaneous magnetization that converges very rapidly at low temperature (KUZ'MIN, 2005). Near the critical temperature, however, their series expansion cannot be used. We shall here obtain a close expression for the spontaneous magnetization by the matrix method which was introduced into the problem of the statistical of a two-dimensional Ising model by Montroll and Kramers and Wannier (HONMURA e KANEYOSHI, 1979; TUCKER, 1994). Onsager gave in 1944 a complete solution of the matrix problem. His method was subsequently greatly simplified by B. Kaufmam (1993), and the result has been used to calculate the short-range order in the crystal lattice (FISHMAN e VIGNALE, 1991).

This paper will be presented in the following way: in the Section 2, we will develop with details the model of Montroll being used effective-field theory in clusters with one spin (EFT-1) (STRIEB e CALLEN, 1963; FISHMAN e LIU, 1992; IDOGAKI e URYÛ, 1992; JIANG e FISHMAN, 1993; CHAKRABORTY, 1993; DO NASCIMENTO et al., 2012), in the Section 3 the behavior of the magnetization m as a function reduced temperature given by T, varying the exchange ratio J_y/J_x among the directions x and y, and finally in the Section 4 the due conclusions of this paper.

2. Model and formalism

A. Hamiltonian

The model to be studied is the nearest-neighbor (nn) Ising antiferromagnetic in a longitudinal magnetic field, which is described by the following Hamiltonian:

$$H = -J_x \sum_{i,\overrightarrow{\delta_y}} \sigma_i^z \sigma_{i+\overrightarrow{\delta_x}}^z - J_y \sum_{i,\overrightarrow{\delta_y}} \sigma_i^z \sigma_{i+\overrightarrow{\delta_y}}^z \qquad (1)$$

where σ_i^μ is the $(\mu = x, y, z)$ component spin-1/2 Pauli operator at site i,$J_x\left(J_y\right)$ is the exchange coupling along the $x(y)$ axis, $\delta_x(\delta_y)$ denotes the nearest-neighbor vector along the $x(y)$ axis and we define the parameter $\lambda = J_y J_x$.

On the other hand, in the case of J $(y > 0)$ we have the SAF (see Figure 1a) and $J_x < 0$ AF (see figure 1b) states, respectively. The ground-state of the model (1) is characterized by a parallel spin orientation in the horizontal and vertical direction, see Figure 1c. In the absence of magnetic field H, the criticality of the three magnetic states (F, AF and SAF) are equivalent, i.e., $T_c(0) = T_N(0)$. In the presence of the field the F state present not phase transition, while that the AF and SAF states have field induced phase transition with $T_N^{SAF}(H) \leq T_N^{AF}(H)$ (WEISS, 1907).

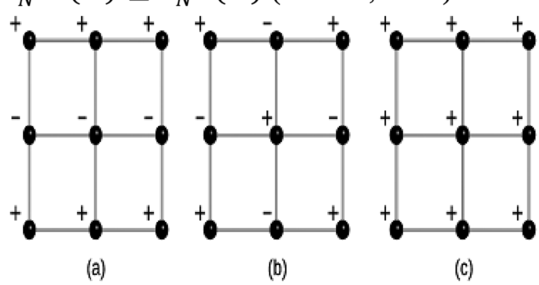

Figure 1: Representations of the SAF (a), AF (b) and F (c) ground states.

The model is exactly solved for $H =$, because the lattice is now composed of independent planes, so the critical temperature may be calculated by using the relation given in Onsager (1944)

$$sinh\left(\frac{2J_x}{k_B T_N}\right)\sinh\left(\frac{2J_{yx}}{k_B T_N}\right) = 1(2) \quad (2)$$

where for the particular isotropic case $J_x = J_y = J(\lambda = 1)$ we have $k_B\, T_N/J = 2/ln\left(1+\sqrt{2}\right)$. Effective-Field Theory To begin with an effective-field treatment, we need the averages of a general function involving spin operator components $O(\{n\})$, these are obtained by effectuating the following operations (WEISS, 1907)

$$(\{n\})\rangle = \langle\frac{Tr_{\{n\}}O(\{n\})e^{-\beta H_n}}{Tr_n e^{-\beta H_n}}\rangle\,(3) \quad (3)$$
$\langle O$

where the partial trace Tr_n is taken over the set n of spin variables (finite cluster) specified by the multi-site spin Hamiltonian H_n and $\langle\cdots\rangle$ indicates the usual canonical thermal average.

The method deals with the effects of the surrounding spins of a finite cluster with N spins through a convenient differential-operator technique in such a way that all relevant selfspin correlations are considered (BETHE, 1935). In contrast, the spin correlations are neglected in the mean-field procedure. The interactions within the cluster are exactly treated and the effect of the remaining lattice spins is dealt by using the random phase approximation (RPA).

In order to treat the model (1) by the EFT approach, we consider a simple cluster on a lattice consisting of a central spin and z perimeter spins being the nearest-neighbors of the central one. The nearest-neighbor spins are substituted by an effective field produced by the other spins, which can be determined by the condition that the thermal average of the central spin is equal to that of its nearest-neighbor ones. The Hamiltonian for this cluster is given by

$$\mathcal{H}_1 = \left(-J_x\sum_{\vec{\delta_x}}\sigma^z_{(i+\vec{\delta_x})} - J_y\sum_{\vec{\delta_y}}\sigma^z_{(i+\vec{\delta_y})}\right)\sigma^z_1. \quad (4)$$

Using the Hamiltonian (4) in the approximate Callen-Suzuki relation we obtain the average magnetization as: $m = \langle\sigma_1^z\rangle$ is given by

$$m = \langle tanh[\beta(\alpha_1 + \alpha_2)]\rangle(5) \quad (5)$$

Where

$$\alpha_1 = J_x\sum_{\vec{\delta_x}}^{z}\sigma^z_{\left(i+\vec{\delta_x}\right)}$$

and

$$\alpha_2 = J_y\sum_{\vec{\delta_x}}^{z}\sigma^z_{\left(i+\vec{\delta_y}\right)}$$

Now using the identity $exp\left(aD_x + bD_y\right)F(x,y) = F(x+y+a+b)$ (where

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$D_\mu = \frac{\partial}{\partial \mu}$ is the differential operator) and the van der Waerden relation for the two-state spin system (KIKUCHI, 1951), i.e./ $exp(a\sigma_I^z) = cosh(a) + \sigma_i^z sinh(a)$, the Eq. (5) can be rewritten as

$$m = \left\langle \prod_{\vec{\delta_x}}^{2} (\alpha_x + \sigma^z_{(1+\vec{\delta_x})}\beta_x) \prod_{\vec{\delta_y}}^{2} (\alpha_y + \sigma^z_{(1+\vec{\delta_y})}\beta_y) \right\rangle F(x,y)|_{x=y=0} \quad (6)$$

with
$F(x,y) = tanh[\beta(x+y)]$, where $\alpha_{\mu=cosh(J_\mu D_\mu)}$ and $\beta_\mu = sinh(J_\mu D_\mu)$.

The magnetizations m in Eq. (6) is expressed in terms of multiple spin correlation functions. The problem becomes unmanageable when we try to treat exactly all boundary spin-spin correlation function present in Eq. (6). Here we use a decoupling of the procedure that ignores all higher-order spin correlations on right-hand sides in Eq. (6), namely

$$\langle \sigma_i^z \sigma_j^z \dots \sigma_i^z \rangle \simeq m.m \dots m$$

where $i \neq j \neq \dots \neq l$ and $m = \langle \sigma_i^z \rangle$. The approximation (8) neglects correlations between different spins but takes relations such as $\langle (\sigma_{iv}^z)^2 \rangle = 1$ exactly into account, while in the usual MFT all the self- and multispin correlations are neglected. We can then rewrite the Eqs. (6) in the form

$$m = (\alpha_x + m\beta_x)^2 (\alpha_y + m\beta_y)^2 F(x,y) \quad {}_{x=y=0}$$
(9)

Expanding the right-hand side of the Eq. (9), one obtains an equation form of the form: In this figure, the transition between the SAF and P phases is invariably of second-order and independent of the longitudinal and transverse fields.

$$m = a_0 + a_1 m + a_2 m^2 + a_3 m^3 + a_4 m^4 \quad (10)$$

where in this work only second-order transitions is observed and the coefficients a_0, a_1, a_2 , a_3 and a_4 are functions of λ, see Appendix A.

3. Results and discussion

In Figure 2, the magnetization curve (m) is presented as function of the reduced temperature for selected values of λ (= 1.0, 0.8, 0.6, 0.4 and 0.2). The two-dimensional rectangular Ising model exhibits a phase transition, with the presence of a second-order transition at $T = T_c(\lambda)$. The numerical determination of the phase boundary (second-order phase transition) is obtained by solving the Eq. (10). Near the critical temperature, the ferromagnetic order parameter for behaves as

$m \sim t^\beta$ and $\chi \sim t^{-\gamma}$ where $\underset{t=}{\overset{c}{T - T}}$ and the critical exponents are classical (i.e., β = 1/2 and γ = 1).

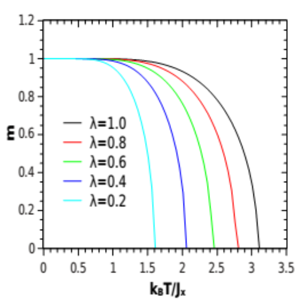

Figure 2: Dependence of the magnetization m as a function of the critical temperature, $k_B T/J_x$, for the two-dimensional rectangular Ising model with several values of λ.

Experimentally, it is also noted that the molar specific heat at vanishes field has singular behavior. This quantity may diverge

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of according with $c \sim \vee T - T_c \ ^{-\alpha}$. An example of this behavior was obtained by Connelly et al. for Ni (YAMAMOTO, 2009). For a singularity classified by α=0 the divergence is like-logarithmic. Some values of the critical exponents α, β and γ were obtained experimentally as: Fe (α=−0.12, β=0.39, γ=1.34) (ETXEBARRIA et al. 2004), Co (KATORI e SUZUKI, 1988) (α=..., β = 0.38, γ = 1.34), EuO (CHUNG, 2006) (α=−0.04, β=0.37, γ=1.40) and EuS (CHUNG,1952) (α=−0.13, β=0.36, γ=1.39).

4. Conclusions

We will discuss in this section the spontaneous magnetization as a function of the critical temperature, for the two-dimensional rectangular Ising model with several values of λ. The behavior of the critical temperature is increasing function of the λ (see Figure 2) in the onedimensional (λ = 0) limit we obtain $T_c = 0$. This result differs from the classical approach that is $k_B T_c / J_x = 2.0$.

For an Ising chain (λ=0), the correlation length at low temperature presents an exponential divergence (CONELLY, 1971) $\xi_T \simeq e^{A/T}$, and for the quasi-one-dimensional limit at T = 0 we expect the critical behavior $\xi_\lambda \simeq \lambda^{-1/\phi}$ (ϕ is the crossover exponent). Therefore, comparing the two correlation lengths, i.e., $\xi_T = \xi_\lambda$ (HELLER, 1967), we can explain the logarithmic divergence of the inverse critical temperature given by $k_B T_c / J_x \simeq A / ln\,(1/\lambda)$. The classical approach presents the linear behavior $k_B T_c / J_x = 2 + 2\lambda$, which shows an incorrect result in the one-dimensional limit (λ = 0) $T_c \neq 0$ (KOUVEL,1968).

Disclosure

This article is unpublished and is not being considered for any other publication. The authors and reviewers did not report any conflict of interest during their evaluation. Therefore, the journal *Scientia Amazonia* owns the copyright has the approval and permission of authors for publication, this article electronically.

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Appendix A

The coefficients a_0, a_1, a_2, a_3 and a_4 are given by

$$a_0 = \alpha_x^2 \alpha_y^2,$$
$$a_1 = 2\left(\alpha_x^2 \alpha_y \beta_y + \alpha_x \alpha_y^2 \beta_x\right),$$
$$a_2 = \left(\alpha_x^2 \beta_y^2 + 4\alpha_x \beta_x \alpha_x \beta_y + \alpha_y^2 \beta_x^2\right),$$
$$a_3 = 2\left(\alpha_x \beta_x \beta_y^2 + \alpha_y \beta_y \beta_y^2\right),$$

and

$$\alpha_4 = \beta_x^2 \beta_y^2$$

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