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Monte Carlo study of the Ising antiferromagnetic with a longitudinal field on the anisotropic square lattice

J. Roberto Viana [a], Minos A. Neto [a], J. Ricardo de Sousa [a,b,*]

[a] Departamento de Física, Universidade Federal do Amazonas, 3000 Japiim, 69077-000 Manaus-AM, Brazil
[b] National Institute of Science and Technology for Complex Systems, Universidade Federal do Amazonas, 3000 Japiim, 69077-000 Manaus-AM, Brazil

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ABSTRACT

The Ising antiferromagnetic in the presence of a magnetic field on an anisotropic square lattice is studied by Monte Carlo simulation. We obtained the phase diagram in the T–H plane investigating the reentrant behavior around of the critical field $H_c = 2J_y$. Using the Binder cumulant we locate the critical temperature T_c as a function of H. In order to test our simulation, for null field we obtain the critical behavior of T_c as a function of $r = J_y/J_x$ and is in excellent agreement with exact solution of Onsager. Our results indicate a second-order transition for all values of H and particular case $r = 1$ (independent of the ratio $r \neq 0$), where not reentrant behavior was observed.

In recent years, the effect of a longitudinal field in the Ising antiferromagnetic on an anisotropic square lattice has been discussed [1–7]. The phase diagram in the temperature longitudinal field plane was obtained by using several approximative methods (for example, effective field theory (EFT), Bethe–Peierls approximation (BP), mean field approximation (MFA), etc.), and the results have been, in some cases, contradictory. This model is described by the following Hamiltonian:

$$\mathcal{H} = -J_x \sum_{i,\vec{\delta}_x} \sigma_i \sigma_{i+\vec{\delta}_x} + J_y \sum_{i,\vec{\delta}_y} \sigma_i \sigma_{i+\vec{\delta}_y} - H \sum_i \sigma_i, \qquad (1)$$

where σ_i are the Ising variables with values ± 1 at site i, J_x (J_y) is the exchange coupling along the x (y) axis, $\vec{\delta}_x$ ($\vec{\delta}_y$) denotes the nearest-neighbor vector along the x (y) axis, and H is the longitudinal magnetic field. We assume positive magnetic field ($H > 0$).

The ground-state of the model (1) is exactly soluble. For $H > 2J_y$ a ferromagnetic (F) state is found with $\sigma_i = 1$ at all sites. On the other hand, for $H < 2J_y$ we have a ground-state which is described as ferromagnetic chains, aligned along the x (or y) axis, ordered antiferromagnetically in the y direction (or x direction). This ordered state is denoted by *superantiferromagnetic* (SAF). This model is also exactly soluble for $H = 0$, and the critical temperature is obtained by solution of the equation [8]:

$$\sinh\left(\frac{2J_x}{k_B T_N}\right) \sinh\left(\frac{2J_y}{k_B T_N}\right) = 1, \qquad (2)$$

where the critical Néel temperature T_N is an increasing function of the ratio $r = J_y/J_x$. In the one-dimensional ($r = 0$) limit we obtain $T_N = 0$, as expected, with the following *exact* asymptotic behavior

$$\frac{k_B T_N}{J_x} \simeq \sqrt{2}\,.\,r^{1/2} \qquad (3)$$

as $r \to 0$. This is different from the logarithmic behavior $\frac{k_B T_N}{J_x} \simeq A/\ln(1/r)$ obtained by EFT [7]. In the particular case $J_x = J_y = J$, we have the exact value $k_B T_N/J = 2/\ln(1+\sqrt{2})$.

The study of the phase diagram in the T–H plane by using the traditional MFA presents qualitative wrong results. It predicts a first-order transition for low temperatures, with the presence of a tricritical point (TCP), and when H/J_x approaches the value 2.0 the first-order transition temperature presents a *negative* slope (i.e., $\Gamma = (\frac{dT}{dH})_{H=H_c} < 0$). Using the linear chain approximation (LCA) [3] only second-order phase transition (no TCP) is observed with a reentrant behavior around of the critical value $H_c = 2.0J_y$ (i.e., *positive* slope, $\Gamma > 0$). Müller and Zittartz [4] developed a new approximation to obtain the critical line by considering an interface free energy for the particular case of the isotropic square lattice. The original application of this method was conjectured to give exact results. Further analysis has shown that the method is not exact for $H \neq 0$, being exact only for the limit of null magnetic field ($H = 0$) [9]. The generalization of this interface method to treat the anisotropic square lattice, Eq. (1), has been presented by Rottman [1]. The critical line obtained for $J_x = J_y = J$ case shows a *negative* slope at $T = 0$ (i.e., $(\frac{dT}{dH})_{H=H_c} < 0$) and a reentrant phase transition does not occur.

Introducing a new approach by considering the zeros of the partition function on an elementary cycle, Wang and Kim [10] have obtained a closed-form formula for the critical line and

* Corresponding author at: Departamento de Física, Universidade Federal do Amazonas, 3000 Japiim, 69077-000 Manaus-AM, Brazil.
E-mail address: jsousa@pq.cnpq.br (J.R. de Sousa).

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showed that at $T = 0$ the slope is *positive*, indicating the presence of a reentrant behavior. The system passes through the super-antiferromagnetic (SAF) ordered for the paramagnetic phase as T is decreased when H is slightly above the critical field $H_c = 2J_y$. This approach in the zero-field limit reduces to the Onsager formula for the critical temperature. Recently, Neto et al. [7] have used two approximative methods, namely the Bethe–Peierls (BP) and the effective-field-theory (EFT) and the results are contradictory. The BP approximation found a reentrant behavior around of the critical field $H_c = 2J_y$, while EFT presents not reentrance. Therefore, the existence or not of the reentrant behavior on the phase diagram in the T–H plane of the model (1) is still an open problem to be considered by a rigorous method, for example, Monte Carlo (MC) simulations [11]. To the best of our knowledge, theoretical works to investigate this phase diagram have never been carried out using a MC simulation.

The main purpose of this Letterr is to study the phase diagram in the T–H plane for $r = 1$ of the model (1) by using Monte Carlo simulations and investigate the existence or not of the reentrant behavior around to the critical field $H_c/J_x = 2.0$. The square lattice of size L having $L \times L$ sites is decomposed into two sublattice (A and B) with opposite spins, corresponding to the SAF ground state. The order parameter (*staggered magnetization*) is defined by $\langle m_s \rangle = \langle (m_A - m_B)/2 \rangle$, where $\langle m_\mu \rangle = \langle \frac{2}{N} \sum_{i \in \mu} \sigma_i \rangle$ is the magnetization of the sublattice $\mu = A, B$ and $N = L^2$ number of spins. In our simulations we have considered lattices with periodic boundary conditions. In addition, samples of $L = 16$, 32 and 64 have been used for finite-size scaling. To locate the critical temperature we performed simulations for each values of the parameters r and H/J_x, with a temperature step $\Delta T = 0.1$ and runs comprising up to 10^4 MCS after equilibration. We used the intersection of the fourth-order cumulant $U_4(L)$, which is defined as [12]

$$U_4(L) = 1 - \frac{\langle m_s^4 \rangle}{3\langle m_s^2 \rangle^2}, \tag{4}$$

where $\langle m_s^2 \rangle$ and $\langle m_s^4 \rangle$ are the canonical averages of the second and fourth moments of magnetization. Thus, we measured $U_4(L)$ for a number of temperatures and systems sizes along the second-order line. The statistical errors of the MC simulations used for the estimation of $T_N(r, H)$ of a particular r and H were found much smaller than the statistical errors coming from the fact that we used. Therefore, the MC errors are not shown in our graphs they are smaller than the symbol sizes.

In order to test our simulations we have calculated the critical temperature as a function of the ratio r for null field $H = 0$, where the cumulants were obtained in the range $r \in [0, 1]$ for each system size with $L = 16$, 32 and 64. In Fig. 1 we show the phase diagram of the anisotropic Ising model in the plane of anisotropy parameter (r) and reduced temperature ($k_B T/J_x$) and we compare with the exact solution, Eq. (2). Our results are in excellent agreement with exact solution. The critical temperature decreases with the decreases of the parameter r, and in the one-dimensional limit ($r = 0$) we obtain the exact value $T_N = 0$ with a critical behavior given by Eq. (3).

The presence of the magnetic field have indicated a qualitative critical behavior independent on the ratio r. Therefore, considering the particular case $r = 1$ we will investigate the existence of the controversial reentrant behavior on the phase diagram in the T–H plane around the critical field $H_c/J_x = 2.0$. The inset in Fig. 2 shows, as an example, the cumulants as a function of the reduced temperature calculated for $H/J_x = 1.0$ for each system size. The common point of intersection for these particular case of field magnetic have been estimated as $k_B T_N/J_x = 2.0196(7)$. In Fig. 2 we show the phase diagram in the T–H plane so obtained. In the region of low (high) temperature (field), the critical temperature is monotonically decreasing with increase of field, and for $H/J_x = 2.0$ we have $T_N = 0$, where a reentrant behavior is not observed. We have compared with results of mean field approximation (MFA) and effective-field theory (EFT). MFA presents a tricritical point, while EFT shows the correct qualitative results with only second-order transition and, as usual in this kind of approach, overestimates T_N in comparison with our MC simulations.

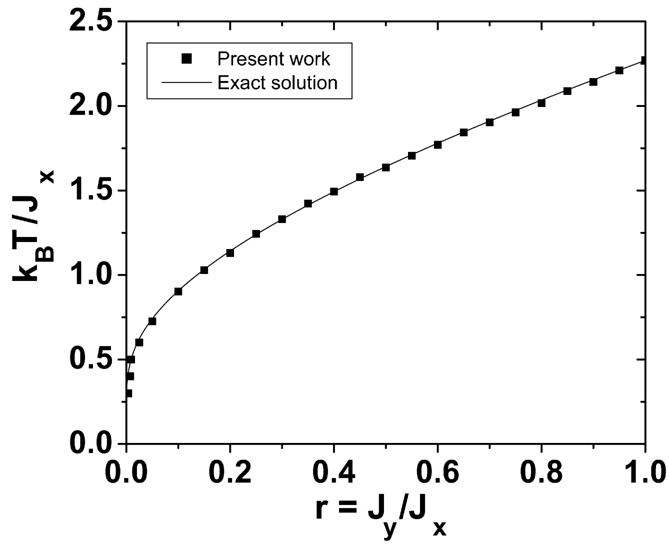

Fig. 1. Dependence of the zero-field reduced critical temperature $k_B T/J_x$ on the ratio $r = J_y/J_x$ for the Ising model on an anisotropic square lattice. The solid curve corresponds to the exact solution, Eq. (2), and square our Monte Carlo simulations.

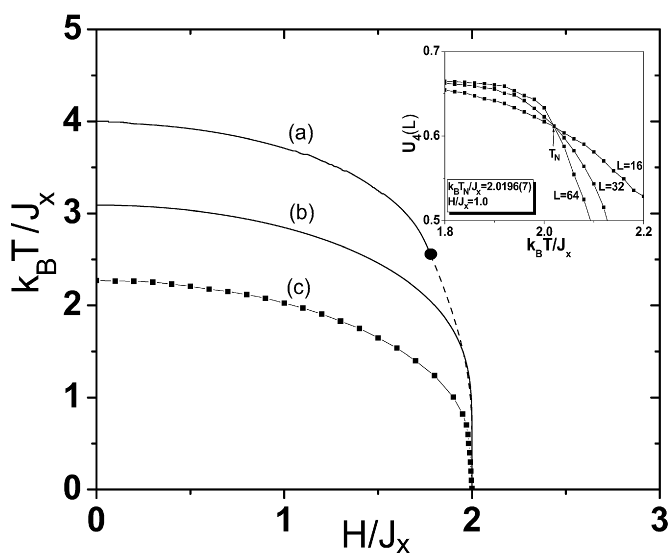

Fig. 2. Phase diagram in the T–H plane of the Ising superantiferromagnetic on an anisotropic square lattice. The curves (a) and (b) corresponds solutions of MFA [2] and EFT [7], respectively. The dashed line corresponds the first-order transition and the solid line the second-order transition. The curve (c) is our results of MC simulations. The inset shows the fourth-order cumulant $U_4(L)$ for particular field $H/J_x = 1.0$ and system sizes $L = 16$, 32 and 64.

In summary, the phase diagram in the T–H plane of the Ising superantiferromagnetic on an anisotropic square lattice was studied by means of Monte Carlo simulations. Using standard finite size scaling techniques, on high accuracy numerical data, we have estimated the critical temperature. A second-order transition is observed for all values of $H/J_x \in [0, 2]$. The most important result of the present work is that the phase diagram observed has no reentrant behavior around of the critical field $H_c/J_x = 2$. Depending of the approximative methods used the reentrance can be observed [7]. Recently, this model have been treated by using renormalization group (RG) approach [13], where the reentrant behavior was not observed. The behavior of the phase diagram at low temperature found using this approach (RG) is not in accordance with our results, in particular, the ground state ($T = 0$, $H = H_c \simeq 1.62 J_x$), where the correct value of the critical field (exact solution) is $H_c = 2 J_x$.

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