Anisotropic Ising model in a magnetic field: Effective-field theory analysis

Minos A. Neto,[1] Rosana A. dos Anjos,[2] and J. Ricardo de Sousa[2]
[1]*Instituto de Física, Universidade Federal Fluminense, Av. Litorânea, 24210-340, Niterói-RJ, Brazil*
[2]*Departamento de Física, Universidade Federal do Amazonas, 3000 Japiim, 69077-000, Manaus-AM, Brazil*
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The anisotropic two-dimensional Ising model in the presence of a magnetic field is studied within two different approaches: the effective-field theory (EFT) with correlation and the Bethe-Peierls (BP) approximation. The model consists of ferromagnetic interaction (J_x) in the x direction and antiferromagnetic interaction (J_y) in the y direction. The phase diagram in the T-H plane is obtained for the particular case $J_x=J_y$. Special focus is given in the low-temperature region of the phase diagram, where a first-order phase transition is observed using the mean-field approximation, which is in disagreement with the linear chain approximation (LCA). Our results indicate a second-order phase transition for all values of $H/J\in[0,2]$, with the presence of a reentrant behavior only observed in the BP approximation in accordance with the results of the LCA and *exact* solution. The null field critical temperature is an increasing function of $r=J_y/J_x$, and in the $r\rightarrow 0$ limit we have found, using BP and EFT, the approximate form $k_BT_N/J_x\simeq A/\ln(1/r)$ in accordance with the exact result of Onsager.

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I. INTRODUCTION

The Ising model is one of the most actively studied models in statistical mechanics. Exact solutions can be obtained for the simple model in one-dimensional (1D) and for certain two-dimensional (2D) lattices.[1] Up to now, no solution or exact value of T_c, the critical temperature, for the antiferromagnetic Ising model has been obtained for 2D in the presence of a magnetic field and three-dimensional (3D) cases

In the absence of exact solutions for many models, the first step in the description of the magnetic properties of solids is usually the application of an effective-field theory (EFT).[2] Because of its simplicity, the mean-field approximation (MFA) has played an important role in the study of cooperative phenomena since the concept of the molecular field was introduced by Weiss in a phenomenological model for ferromagnetism and by Néel for antiferromagnetism. The MFA can be relied on for an appropriate description of the major aspects of the phenomena being studied. However, this MFA approach has some deficiencies due to the neglect of correlations, when results are compared with experiments. The MFA can be shown to be equivalent to having each site interacting equally with all other sites; its prediction of critical temperature is not very accurate. Physically, having a particular spin interacting equally with all others of the system ignores both the presence of a finite correlation length and the strong fluctuations near T_c. The MFA predicts a phase transition at finite temperature in the 1D Ising model, which does not agree with the exact solution.

There has been an increasing number of works dealing with much less sophisticated approximation schemes, which represents a remarkable improvement over the traditional MFA.[2] For example, the Bethe-Peierls (BP) approach[3] includes local spin correlations and fluctuations, and details of the type of lattice, beyond the effects of the coordination number z. To obtain a solution for the critical temperature T_c, a self-consistency condition is imposed: the mean values of the spins in clusters, which are soluble exactly, must all be the same. This condition determines the mean field due to the spins outside the cluster. The BP approach, when applied to the Ising model in small clusters (one and two sites), finds the reduced critical temperature $k_BT_c/J=2/\ln[z/(z-2)]$ better than the MFA for all lattice with a finite value of the coordination number, z. This approximation obtains the exact solution $T_c=0$ for the linear lattice ($z=2$). However, the MFA gives an *incorrect* value, $T_c>0$.

Oguchi[4] developed an approach for correction of the MFA, where he used interacting pairs in the mean field of their surrounding sites obtaining an estimate for the critical temperature, with the value $T_c\neq 0$ for a 1D lattice. We can construct such a series of approximations by increasing the cluster size L of the cluster mean-field shown approaching the true critical temperature T_c^* in the limit of large L for the ferromagnetic Ising model,[5] obtaining the exact value $T_c^*=0$ for the 1D lattice. Recently, a new correction of the MFA was proposed by Wysin and Kaplan[6] and applied in the Ising model. In this approach, called the *self-consistent correlated field* (SCCF), the values of the magnetization of nearest neighbors in the Ising model take two values m^+ and m^-, depending on whether the central site has values $\sigma_i=1$ and -1, respectively. With this correlated neighbor field $h_{\text{eff}}=zJ[\delta_{\sigma_{i'},1}m^+ + \delta_{\sigma_{i'},-1}m^-]$, the neighbor magnetizations m^+ and m^- are determined self-consistently and the critical temperature is given by the expression $k_BT_c/J=(z-1)\text{sech}^2(J/k_BT_c)$. This approach does not lead to a phase transition at the 1D limit ($z=2$), just as in the BP approximation (i.e., $T_c=0$).

On the other hand, the 2D Ising model has been used extensively to study a variety of magnetic compounds.[7–9] In the presence of competing interactions, a richness of structures is observed[10] explaining why many physical systems exhibit complex phase diagrams with periodic and quasiperiodic structures, as, for example, gases adsorbed on surfaces,[11] alloys,[12] polytypes,[13] and intercalated compounds.[14] Theoretically, short-range competing interactions may lead to a variety of commensurate and incommensurate structures. For example, the 2D axial next-nearest-neighbor Ising (ANNNI) model[15] describes reasonably well the (2×1) and (3×1) phases as well as incommensurate

structures observed in the chemisorbed systems O/Pd(100).[16] The phase diagram of the ANNNI model is very interesting in three dimensions (3D), where many commensurate phases are present.[17] In 2D, enhanced fluctuations destroy the long-wavelength commensurate phases, leaving only a few commensurate phases and a floating incommensurate phase.[17]

A new EFT with correlation has successfully been used to study the thermodynamic properties of classical and quantum spin models.[18–24] This EFT is based on the use of rigorous correlation identities as a starting point and utilizes the differential operator technique introduced by Honmura and Kaneyoshi.[25] Even without introducing mathematical complexities, this approach, which is conceptually as simple as the standard MFA, shares with other methods a great versatility. This method may explicitly and systematically include correlation effects.[26]

The purpose of the present work is to investigate the phase boundary using EFT of 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. In this work, we assume $J_x=J_y=J>0$ and positive field ($H>0$).

The Hamiltonian (1) is exactly soluble for vanishing field ($H=0$),[27] and the critical temperature is given by

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

where, for the particular case $J_x=J_y=J$, we have the exact value $k_B T_c/J = 2/\ln(1+\sqrt{2}) \simeq 2.269$.

At zero temperature ($T=0$), the ground state of the Hamiltonian (1) is also exactly soluble. Ferromagnetic states (F) are found for $H>2J_y$, with $\sigma_i=1$ at all sites. For $H<2J_y$, the ground state is described as ferromagnetic chains, aligned along the x (or y) axis, ordered antiferromagnetically in the y direction (or x direction), and is denoted by superantiferromagnetism (SAF).[28]

At finite temperature T, a second-order phase transition is observed for $H \leqslant 2J_y$ between the low-temperature ordered phase (SAF) and the high-temperature ordered phase (F). The usual MFA has been applied in the model (1), whose qualitative results are wrong.[29] It predicts a first-order transition for small temperature (or high-field). Using the linear-chain approximation (LCA),[30] a reentrant second-order transition is observed near $H_c=2J_y$ at low temperature. In this approximation (LCA), the analysis is exact along the chains, while interchain interactions are treated in the mean-field approximation.

However, the study of the criticality of the model (1) by the traditional mean-field method (MFA) cannot give reasonable results. For the isotropic square lattice (i.e., $J_x=-J_y=J$), Müller-Hartmann and Zittartz[31] developed a new approximation to obtain the critical line by considering an interface free energy. The original application of this method was conjectured to give exact results. Further analysis has shown that the method is not exact for $H\neq 0$,[32] being exact only for the limit of null magnetic field ($H=0$). The generalization of this interface method to treat the anisotropic square lattice, Eq. (1), has been presented by Rottman.[28] The critical line obtained in Ref. 28, for the $J_x=J_y=J$ case, shows a *negative* slope at $T=0$ [i.e., $\left(\frac{dH}{dT}\right)_{T=0} < 0$] and a reentrant phase transition does not occur. For the isotropic square lattice also the slope is *negative*.[31,33] On the other hand, introducing a new approach by considering zeros of the partition function on an elementary cycle, using Griffiths' smoothness postulate,[34] Wang and Kim[35] have obtained a closed-form formula for the critical line and showed that at $T=0$ the slope is *positive*, indicating the presence of a reentrant behavior. The system passes through the 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, Eq. (2). Therefore, based on the *exact* solution,[35] we can expect that the critical behavior at low temperature for the model (1) with $J_x=J_y=J$ presents a reentrant behavior. The purpose of this paper is to identify whether there is the reentrant phase transition for the model (1) when analyzed by effective-field theories (EFT and BP).

The paper is organized as follows. In Sec. II, we develop two approaches: the EFT and BP approximation to treat the model (1). The MFA and LCA are also described. In Sec. III, we discuss the results of the phase diagram in the (T-H) plane for the particular case of $J_x=J_y=J$. Our main results are summarized and further problems of interest are mentioned in Sec. IV.

II. EFFECTIVE-FIELD THEORIES

In this section, we apply some approximative methods to treat the phase diagram of the Hamiltonian (1).

A. Differential operator technique

An alternative way to obtain the averages of a general function involving spin operator components $O(\{n\})$ is given by[19]

$$\langle O(\{n\})\rangle = \left\langle \frac{\mathrm{Tr}_{\{n\}} O(\{n\}) e^{-\beta H(\{n\})}}{\mathrm{Tr}_{\{n\}} e^{-\beta H(\{n\})}} \right\rangle, \qquad (3)$$

where the partial trace $\mathrm{Tr}_{\{n\}}$ is to be taken over the set $\{n\}$ of spin variables specified by the multisite spin Hamiltonian $\mathcal{H}(\{n\})$, and $\langle\cdots\rangle$ indicates the usual canonical thermal average.

In order to explain our main idea, we consider a simple example of a finite cluster with one spin. First, we treat the sublattice A. The Hamiltonian (1) for this cluster is given by[22]

$$\mathcal{H}_1^A = \left[-J_x \sum_{\vec{\delta}_x} \sigma_{(1+\vec{\delta}_x)A} + J_y \sum_{\vec{\delta}_y} \sigma_{(1+\vec{\delta}_y)B} - H \right] \sigma_{1A}. \qquad (4)$$

To calculate the magnetization $m_A=\langle\sigma_{1A}\rangle$, one has to effect the inner traces in Eq. (3) over the states of spins

$\sigma_{1A}(=\pm 1)$. In this way, substituting Eq. (4) in Eq. (3), we obtain

$$m_A = \left\langle \tanh\left(K_x \sum_{\vec{\delta}_x} \sigma_{(1+\vec{\delta}_x)A} - K_y \sum_{\vec{\delta}_y} \sigma_{(1+\vec{\delta}_y)B} + L \right) \right\rangle, \quad (5)$$

where $K_\mu = \beta J_\mu$ $(\mu = x, y)$ and $L = \beta H$.

Now using the identity $e^{aD_x} F(x) = F(x+a)$, where $D_x = \frac{d}{dx}$ is the differential operator, and the van der Waerden relation $e^{a\sigma_i} = \cosh(a) + \sigma_i \sinh(a)$, Eq. (5) can be written as

$$m_A = \left\langle \prod_{\vec{\delta}_x}^{2} (\alpha_x + \sigma_{(1+\vec{\delta}_x)A}\beta_x) \cdot \prod_{\vec{\delta}_y}^{2} (\alpha_y - \sigma_{(1+\vec{\delta}_y)B}\beta_y) \right\rangle F(x)|_{x=0}, \quad (6)$$

with

$$F(x) = \tanh(x + L), \quad (7)$$

where $\alpha_\mu = \cosh(K_\mu D_x)$ and $\beta_\mu = \sinh(K_\mu D_x)$.

The magnetization m_A in Eq. (6) is exact and is expressed in terms of multiple spin correlation functions. However, it is clear that if we try to treat exactly all boundary spin-spin correlation functions present in Eq. (6), the problem becomes unmanageable. Here, in the EFT, we use a decoupling procedure that ignores all higher-order spin correlations on both right-hand sides in Eq. (6), namely

$$\langle \sigma_{iA}\sigma_{jB} \cdots \sigma_{lA} \rangle \simeq m_A m_B \cdots m_A, \quad (8)$$

where $i \neq j \neq \cdots \neq l$ and $m_\nu = \langle \sigma_{i\nu} \rangle$ $(\nu = A, B)$. The approximation (8) neglects correlations between different spins but takes relations such as $\langle (\sigma_{i\nu})^2 \rangle = 1$ exactly into account, while in the usual MFA all the self- and multispin correlations are neglected. Using this approximation Eq. (8), Eq. (6) is written as

$$m_A = (\alpha_x + m_A\beta_x)^2 (\alpha_y - m_B\beta_y)^2 \, F(x)|_{x=0}. \quad (9)$$

Following the same procedure to obtain Eq. (9), the expression for the magnetization in sublattice B is given by

$$m_B = (\alpha_x + m_B\beta_x)^2 (\alpha_y - m_A\beta_y)^2 \, F(x)|_{x=0}. \quad (10)$$

To determine the transition (or Néel) temperature, let us introduce two new variables: staggered magnetization $m_s = \frac{1}{2}(m_A - m_B)$ and total normalized magnetization $m = \frac{1}{2}(m_A + m_B)$. Then, it can easily be shown that Eqs. (9) and (10) are equivalent to

$$m_s = A_1(m) m_s + A_3(m) m_s^3 \quad (11)$$

and

$$m = A_0(m) + A_2(m) m_s^2 + A_4(m) m_s^4, \quad (12)$$

where the functions A_p $(p = 0\text{–}4)$ are dependent on m in addition to temperature, magnetic field, and parameter $r = J_y/J_x$ (see the Appendix).

The second-order phase transition $(m_s \to 0)$ is then determined from the condition $A_1(m_o) = 1$ and $A_0(m_o) = m_o$, where m_o is the value of the total magnetization in the critical line $(m_s = 0)$. This critical line occurs for all values of $H \in [0, H_c = 2J_y]$. In the limit of null field $(H = 0)$, we have obtained the value $m_o = 0$ for $r = 1$ and $k_B T_N/J = 3.085$.

We note that the present method is appropriate only to estimate second-order phase boundaries. To treat models that present a first-order phase transition, such as, for example, the Blume-Capel and random-field Ising models, one needs to calculate the free energy for the ordered and paramagnetic phases and to find a point of intersection. Unfortunately, no expression exists for the free energy at finite temperature in the frame of the effective-field theory with correlations. The phase diagram in the T-H plane comprises a SAF phase $(m_s \neq 0)$ at low fields and a paramagnetic phase $(m_s = 0)$ at high fields. In the absence of next-nearest-neighbor interaction, there is only one critical line that separates the paramagnetic (P) and SAF phases by a continuous (second-order) phase transition.

B. Linear chain approximation

The MFA can be extended to strips of finite width in the limit of infinite length using the transfer-matrix methods (TMM).[36] Effective mean field (H_{eff}) is applied at the boundary (or surface) of the half-infinite systems, and the magnetizations on the center line are calculated exactly using TMM and are determined self-consistently. For example, we consider a systematic series of infinite strips to study the critical behavior of the 2D Ising model as a typical demonstration of the convergence to obtain T_c. For one-line, three-line, five-line, and seven-line strips, we have,[37] respectively, $k_B T_c/J = 3.526$, 2.9221, 2.7285, and 2.6294, as compared to $k_B T_c/J = 4$ in the MFA and the exact value $k_B T_c/J = 2.269$. Applying the LCA in the model (1) for one-line strips, we obtain the magnetizations m_A and m_B as[30]

$$m_A = \frac{e^{2K_x} \sinh(L - 2K_y m_B)}{\sqrt{1 + e^{4K_x} \sinh^2(L - 2K_y m_B)}} \quad (13)$$

and

$$m_B = \frac{e^{2K_x} \sinh(L - 2K_y m_A)}{\sqrt{1 + e^{4K_x} \sinh^2(L - 2K_y m_A)}}. \quad (14)$$

Inserting $m_A = m + m_s$ and $m_B = m - m_s$ into Eqs. (13) and (14), self-consistently, the magnetizations (m and m_s) for any temperature, field, and ratio r are obtained. However, as we are interested in the calculation of ordering near the critical point, the usual argument that the staggered magnetization m_s tends to zero as the temperature approaches its critical value allows us to consider only linear terms in m_s. In this case, the phase diagram is obtained if we simultaneously solve the following set of equations self-consistently:

$$m_o = \frac{e^{2K_x} \sinh(L - 2K_y m_o)}{W} \quad (15)$$

and

$$\frac{2e^{2K_x}[W - \sinh^2(L - 2K_y m_o)] K_y \cosh(L - 2K_y m_o)}{W^3} = 1, \quad (16)$$

with

$$W = \sqrt{1 + e^{4K_x} \sinh^2(L - 2K_y m_o)}. \quad (17)$$

By solving Eqs. (15) and (16) numerically, we obtain also a second-order phase transition with the presence of a reentrant behavior (two critical temperatures) near the critical field $H_c = 2J_y$. For null field ($H=0$), we have found $m_o = 0$ and $k_B T_N / J = 3.526$ ($r=1$).

C. Mean-field approximation

The MFA can be made in a great variety of ways. These methods, however, share a common point: the average of a product of variables is replaced by the product of the averages of these variables. A simple method is that which follows from Gibbs-Bogoliubov's variational principle, and this is the most convenient one for our purpose. The variational theorem for a system described by a Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}'$ (where $\mathcal{H}' = \mathcal{H} - \mathcal{H}_0$) states that an upper bound to the exact free energy is given by

$$F(\mathcal{H}) \leqslant \Phi \equiv F(\mathcal{H}_0) + \langle \mathcal{H} - \mathcal{H}_0 \rangle_o, \quad (18)$$

where $F(\mathcal{H}_0) = -k_B T \ln Z_o$ is the free energy associated with a given soluble Hamiltonian $\mathcal{H}_0$ for a finite cluster (Ω) written in the MFA, $Z_o = \mathrm{Tr}\, e^{-\beta \mathcal{H}_0}$, and

$$\langle O \rangle_o = \frac{\mathrm{Tr}_\Omega [O e^{-\beta \mathcal{H}_0}]}{\mathrm{Tr}_\Omega [e^{-\beta \mathcal{H}_0}]}, \quad (19)$$

where $\beta = 1/k_B T$. For clusters with one spin, choosing the noninteracting trial Hamiltonian as

$$\mathcal{H}_0 = -\eta_A \sum_{i \in A} \sigma_i - \eta_B \sum_{i \in B} \sigma_i - H \sum_{i \in A,B} \sigma_i, \quad (20)$$

where η_A and η_B are the variational parameter, the free energy Eq. (18) is given by

$$\frac{\Phi(\eta_A, \eta_B)}{N J_x} = -\frac{t}{2} \ln[4 \cosh \beta(H + \eta_A) \cosh \beta(H + \eta_B)] + r m_A m_B - \frac{1}{2}(m_A^2 + m_B^2) + \frac{\eta_A}{2J_x} m_A + \frac{\eta_B}{2J_x} m_B \quad (21)$$

with

$$m_\mu = \tanh \beta(H + \eta_\mu), \quad (22)$$

where $\mu = A, B$, $t = k_B T / J_x$, and $r = J_y / J_x$. The condition that the right-hand side of Eq. (21) is stationary determines the parameters

$$\frac{\eta_\mu}{J_x} = \begin{cases} 2m_A - 2r m_B & \text{if } \mu = A \\ 2m_B - 2r m_A & \text{if } \mu = B. \end{cases} \quad (23)$$

Substituting Eq. (23) in Eq. (22), we obtain the mean-field state equations

$$m_A = \tanh\left[\frac{1}{t}(h + 2m_A - 2r m_B)\right] \quad (24)$$

and

$$m_B = \tanh\left[\frac{1}{t}(h + 2m_B - 2r m_A)\right], \quad (25)$$

where $h = H / J_x$.

The right-hand side of Eq. (21), at the stationary point, gives the mean-field free energy per spin,

$$f = -t \ln\left[4 \cosh \frac{1}{t}(h + 2m_A - 2r m_B) \cosh \frac{1}{t}(h + 2m_B - 2r m_A)\right] - r m_A m_B + \frac{1}{2}(m_A^2 + m_B^2). \quad (26)$$

Equations (24) and (25) are two coupled transcendental equations for m_A and m_B. Once the fixed values of r, $m_A(T,H)$, and $m_B(T,H)$ are known, Eq. (26) gives the free energy per spin $f(T,H)$ from which all thermodynamic properties, in particular the phase diagram, can be derived. In terms of the new variables $m = \frac{1}{2}(m_A + m_B)$ and $m_s = \frac{1}{2}(m_A - m_B)$, Eq. (26) is rewritten as

$$f = -t \sum_{p=0}^{1} \ln\left\{2 \cosh \frac{1}{t}[h + 2(1-r)m + 2(-1)^p (1+r) m_s]\right\} + (1-r)m^2 + (1+r)m_s^2, \quad (27)$$

with

$$m = \frac{1}{2} \sum_{p=0}^{1} \tanh \frac{1}{t}[h + 2(1-r)m + 2(-1)^p (1+r) m_s] \quad (28)$$

and

$$m_s = \frac{1}{2} \sum_{p=0}^{1} (-1)^p \tanh \frac{1}{t}[h + 2(1-r)m + 2(-1)^p (1+r) m_s]. \quad (29)$$

The results above, Eqs. (27)–(29), are equivalent to that obtained in Ref. 28 using the version of the MFA in the Bragg and Williams approximation. In the MFA, we found a first-order phase transition in the region of low temperature in contradiction with the results of EFT and LCA discussed in Secs. II A and II B, respectively, that obtain a second-order phase transition for all temperature. For null field ($H=0$) and $r=1$, we found the classical value $m=0$ and $k_B T_N / J = 4.0$ discussed above for the square lattice.

D. Bethe-Peierls approximation

The BP approximation has long been used to improve the ordinary mean-field results. It is the simplest mean-field-like approximation that takes into account two-site correlations. There are several alternative ways to present the BP approximation besides the approach given in the original paper.[3] One of these involves a Cayley tree and consideration of the behavior of the spins deep inside the tree. If the tree has a branching ratio of $z-1$, then the behavior of these spins is equivalent to that predicted by the original BP approximation for a system with z nearest-neighbor spins. An even simpler

approach, and one that is more like the cluster mean-field approach,[5] consists of considering a central spin and its z nearest neighbors forming a cluster of $z+1$ spins. One replaces the nearest-neighbor interactions that the z spins on the perimeter of the cluster have with spins outside the cluster with mean-field interactions and then requires that the thermal average of the perimeter of spins is equal to the thermal average of the central spin. The BP method is also equivalent to the pair approximation.[38]

In this BP approximation, a given spin σ_{oA} is regarded as the central member of a group, which consists of this spin and its z nearest neighbors. While writing down the Hamiltonian of this group, the interaction between the central spin and the z neighbors is taken into account. The interaction of these neighbors with other spins in the lattice is considered again through a mean field at sublattice $\mu=A,B$, denoted by H_E^μ. In this scheme of the BP approximation, the Hamiltonian (1) for the sublattice A is written by

$$\mathcal{H}_{oA} = -\sigma_{oA}[H + J_x(\sigma_{1A}+\sigma_{2A}) - J_y(\sigma_{1B}+\sigma_{2B})] - (H+H_E^A) \times(\sigma_{1A}+\sigma_{2A}) - (H+H_E^B)(\sigma_{1B}+\sigma_{2B}), \tag{30}$$

where the molecular fields H_E^A and H_E^B are determined by the conditions of self-consistency,

$$m_{oA} = m_A,$$

$$m_{oB} = m_B, \tag{31}$$

where $m_{o\mu}=\langle\sigma_{o\mu}\rangle$ and $m_\mu=\langle\frac{1}{2}(\sigma_{1\mu}+\sigma_{2\mu})\rangle$ $(\mu=A,B)$. From Eq. (30), we can obtain m_{oA} and m_A by the expressions

$$m_{oA} = \frac{\partial \ln Z_{oA}}{\partial L} \tag{32}$$

and

$$m_A = \frac{1}{2}\frac{\partial \ln Z_{oA}}{\partial L_A}, \tag{33}$$

where $L=\beta H$, $L_\mu=\beta(H+H_E^\mu)$, and the partition function for this group of spins as a whole is given by

$$\begin{aligned} Z_{oA}(L,L_A,L_B) &= 2\{e^{2(L_A+L_B)}\cosh(L+2K_x-2K_y) + 2e^{2L_A}\cosh(L+2K_x) \\ &+ e^{2(L_A-L_B)}\cosh(L+2K_x+2K_y) + 2e^{2L_B}\cosh(L-2K_y) \\ &+ 2e^{-2L_B}\cosh(L+2K_y) + e^{-2(L_A-L_B)} \\ &\times\cosh(L-2K_x-2K_y) + 4\cosh L + 2e^{-2L_A} \\ &\times\cosh(L-2K_x) + e^{-2(L_A+L_B)}\cosh(L-2K_x+2K_y)\}. \end{aligned} \tag{34}$$

Similar results are found for the sublattice B case,

$$m_{oB} = \frac{\partial \ln Z_{oB}}{\partial L} \tag{35}$$

and

$$m_B = \frac{1}{2}\frac{\partial \ln Z_{oB}}{\partial L_B}, \tag{36}$$

where Z_{oB} is the same expression of Z_{oA}, Eq. (34), replacing L_A by L_B [i.e., $Z_{oB}(L,L_A,L_B)=Z_{oA}(L,L_B,L_A)$]. We can rewrite the boundary conditions (31) by

$$m_{os}(L_t,L_s) = m_s(L_t,L_s),$$

$$m_o(L_t,L_s) = m(L_t,L_s), \tag{37}$$

where $m_{os}=\frac{1}{2}(m_{oA}-m_{oB})$, $m_o=\frac{1}{2}(m_{oA}+m_{oB})$, $m_s=\frac{1}{2}(m_A-m_B)$, $m=\frac{1}{2}(m_A+m_B)$, $L_t=\frac{1}{2}(L_A+L_B)$, and $L_s=\frac{1}{2}(L_A-L_B)$.

Equations (37) are two coupled transcendental equations to determine the molecular fields L_t and L_s for fixed values of r, H, and T. When the temperature approaches its critical value, $T_N(H)$, the staggered magnetization m_{os} (or m_s) tends to zero. However, as we are interested in the calculation of the phase diagram (i.e., dependence of T_N with the parameters H and r), we consider only the linear terms in L_s. Using the conditions (37), we obtain the phase diagram if we simultaneously solve the following set of equations:

$$F_1(T_N,H,r,L_o) = 0,$$

$$F_2(T_N,H,r,L_o) = 0 \tag{38}$$

with

$$F_1(T_N,H,r,L_o) = \left\{\frac{\partial[m_{os}(L_o,L_s) - m_s(L_o,L_s)]}{\partial L_s}\right\}_{L_s=0} \tag{39}$$

and

$$F_2(T_N,H,r,L_o) = m_o(L_o,0) - m(L_o,0), \tag{40}$$

where L_o is the total molecular field in the critical line $(m_s=0)$. We have used the MAPLE software to generate the appropriate expressions for the functions above and numerically determined the critical temperature. In particular, for null field $(H=0)$ we obtain $L_o=0$ and $k_BT_N/J=2/\ln 2 \simeq 2.285$ $(r=1)$ in accordance with the result of Ref. 3. In the limit of low temperature, a reentrant behavior is observed, also, near the critical field $H_c=2J_y$.

III. RESULTS AND DISCUSSION

We will discuss in this section the phase diagram in the T-H plane for $r=1$. In Fig. 1, the phase diagrams are plotted using the MFA, LCA, EFT, and BP approximations. In EFT, the staggered magnetization falls smoothly to zero when the temperature increases from zero to $T_N(H)$ for all values of $h\in[0,2]$ characterizing a second-order phase transition. On the other hand, in the MFA we have the presence of first- and second-order phase transitions. Below the tricritical point (TCP) $(h_{ot}\simeq 1.756,\ t_{ot}=8/3\simeq 2.667)$, the magnetization curve may include an unstable solution in addition to the stable solution. In the LCA and BP approaches, the magnetization in the vicinity (below) the critical field $h_c=2$ shows evidence of reentrant behavior with the presence of two critical temperatures. The reentrant behavior in the T_N versus H

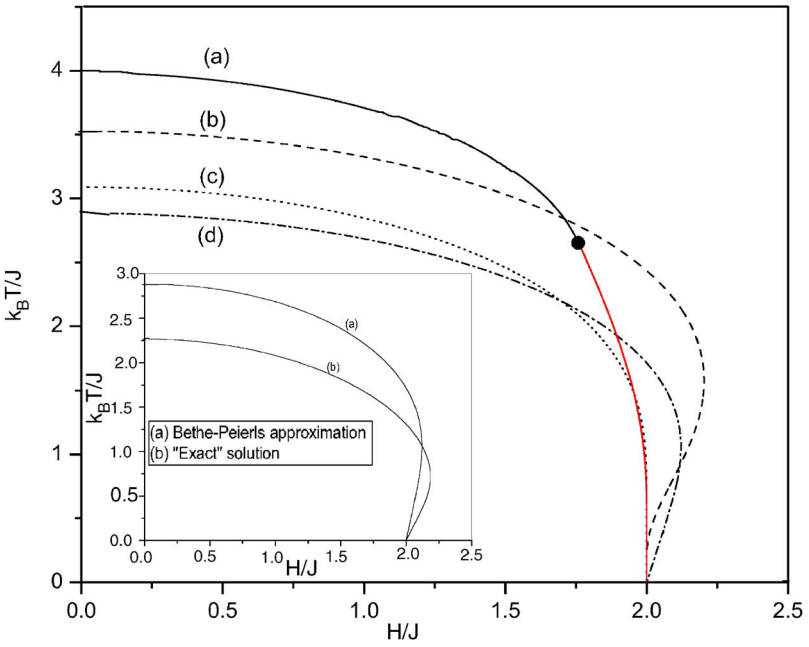

FIG. 1. (Color online) Dependence of the reduced critical temperature, k_BT/J, on the reduced magnetic field, H/J, for the anisotropic two-dimensional Ising model with competitive interactions. The curve (a) derived from the MFA incorrectly leads to a first-order phase transition (red curve) at low temperature. There is a tricritical point at coordinates (1.756, 2.667). The curves (b), (c), and (d) are found using the LCA (Ref. 30) EFT (present work), and BP approximation (present work), respectively. We compare (inset) the results of the reentrant behavior obtained by the BP method with the *exact* solution (Ref. 35).

curve (Fig. 1), predicted here by LCA (Ref. 30) and BP approximations in the low temperature limit, has been observed previously in Ref. 35. For small temperature ($r=1$), we obtain a linear behavior $H \simeq 2J + A(k_BT)$, with a positive slope ($A>0$) obtained by the BP approximation in reasonable agreement with the results of Ref. 35, while the LCA (Ref. 30) presents an exponential behavior $H \simeq 2J + J\left(\frac{k_BT}{2J}\right)^{2/3} \exp(-2J/k_BT)$. To analyze the reentrant phenomena, in Fig. 1 (see inset) we have shown the phase boundaries for $r=1$ in the T-H plane using the BP approximation (present work), and compare the results of Ref. 35 (*exact solution*).

The behavior of the zero-field critical temperature is an increasing function of ratio r (see Fig. 2) in the one-dimensional ($r=0$) limit; we obtain $T_N=0$, with the exception of the incorrect result of the MFA, $k_BT_N/J_x=2.0$. Furthermore, T_N approaches zero when the ratio r decreases, and near $r=0$ we obtain the following law for T_N:

$$k_BT_N/J_x \simeq A/\ln(1/r), \tag{41}$$

where A is a constant that depends on the approximation used.

For an Ising chain ($r=0$), the correlation length at low temperature presents an exponential divergence[1] $\xi_T \simeq e^{a/T}$, and for the quasi-one-dimensional limit at $T=0$ we expect the critical behavior $\xi_r \simeq r^{-1/\phi}$ (ϕ is the crossover exponent). Therefore, comparing[40] the two correlation lengths, i.e., $\xi_T=\xi_r$, we can explain the logarithmic divergence of the inverse critical temperature given by Eq. (41). The MFA presents the linear behavior $k_BT_N/J_x=2+2r$, which shows an incorrect result in the one-dimensional limit ($r=0$) $T_N \neq 0$.

IV. CONCLUSIONS

We study the phase diagram in the T-H plane of the anisotropic two-dimensional Ising model with competing interactions using the EFT and BP approaches. A second-order phase transition is observed for all values of reduced magnetic field $h \in [0,2]$. The most important result of the present work is the possibility of the occurrence of the reentrant phenomenon in the T-H plane depending on the approximation. The early interface method[28] work did not find reentrance near $H_c=2J$, suggesting a phase diagram like the square antiferromagnetic Ising model.[31] For the anisotropic ($J_x=J_y=J$) 2D Ising model, the theoretical calculations show disagreement between different methods. The results obtained by the BP approximation (and also by the LCA) show

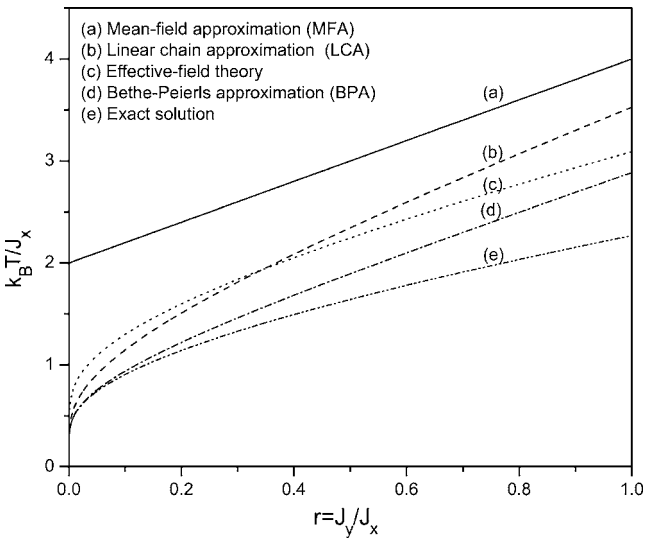

FIG. 2. Dependence of the zero-field reduced critical temperature k_BT_N/J_x on the ratio $r=J_y/J_x$ for the anisotropic two-dimensional Ising model. The results derived from the MFA (a) incorrectly give a phase transition in the 1D ($r=0$) Ising model limit. The curves (b), (c), and (d) are found by the LCA, BP, and exact solution (Ref. 27) Eq. (2), respectively.

a reentrant behavior in low temperature in accordance with the rigorous results of Ref. 35.

The interface method, when applied in the square AF Ising model,[31] presents the null-field critical temperature equivalent to results for the critical line (1% of error) in comparison with the *exact solution* (see Ref. 35). Therefore, these two methods (good approximation) used in the model (1) are identical in the isotropic limit and much different in the case of the anisotropic lattice. In principle, using the EFT a approach in a cluster with one spin, we cannot obtain the reentrant behavior. Rigorous results have shown successive phase transitions in two-dimensional Ising models with competing interactions.[39]

We can apply the EFT approach in the finite-size-scaling (FSS) scheme[22] or include correlations between nearest neighbors.[26] For example, in Ref. 22 the FSS scheme was used for clusters with one (EFT-1) and two (EFT-2) spins to study the phase diagram in the *T-H* plane for the three-dimensional Ising antiferromagnetic model on a simple cubic (sc) lattice and obtained incorrect results (reentrant behavior). On the other hand, results obtained by the EFRG (effective-field renormalization-group) method indicate an absence of reentrant behavior in accordance with the results of the Monte Carlo (MC) simulation.[41] The BP approximation has also been applied to obtain the phase diagram of this model.[42] The Néel temperature decreases with increasing field. For a body-centered-cubic (bcc) lattice (3D) and small range of field above the critical field $H_c = zJ$, there are two transitions (presence of reentrance) corresponding to the appearance and disappearance of the alternating long-range order as temperature is lowered. For the square (2D) and simple cubic (3D) lattices, only one critical temperature is observed (absence of reentrance). These results in 2D and 3D lattices are in accordance with Monte Carlo simulation[41] and the EFRG approach.[22] We have presented a preliminary study of finite-size scaling (EFRG) in the model (1) and verified the presence of the reentrant behavior. Other methods, such as DMRG and Monte Carlo simulation, can be used to give more information on the phenomenon. The occurrence of reentrant phases in the model (1) certainly deserves further attention.

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APPENDIX

The list of coefficients in Eqs. (11) and (12) is defined by

$$A_0(m) = \{\alpha_x^2\alpha_y^2 + 2(\alpha_x\beta_x\alpha_y^2 - \alpha_y\beta_y\alpha_x^2)m + (\alpha_x^2\beta_y^2 + \alpha_y^2\beta_x^2 - \alpha_x\beta_x\alpha_y\beta_y)m^2 + 2(\alpha_x\beta_x\alpha_y^2 - \alpha_y\beta_y\alpha_x^2)m^3 + \beta_x^2\beta_y^2 m^4\}\, F(x)|_{x=0}, \tag{A1}$$

$$A_1(m) = 2\{(\alpha_x\beta_x\alpha_y^2 + \alpha_y\beta_y\alpha_x^2) - (\alpha_x\beta_x\beta_y^2 + \alpha_y\beta_y\beta_x^2)m\}\, F(x)|_{x=0}, \tag{A2}$$

$$A_2(m) = \{\alpha_x^2\beta_y^2 + \alpha_y^2\beta_x^2 + 4\alpha_x\alpha_y\beta_x\beta_y 2(\alpha_x\beta_x\beta_y^2 - \alpha_y\beta_y\beta_x^2)m - 2\beta_x^2\beta_y^2 m^2\}\, F(x)|_{x=0}, \tag{A3}$$

$$A_3(m) = 2(\alpha_x\beta_x\beta_y^2 + \alpha_y\beta_y\beta_x^2)\, F(x)|_{x=0}, \tag{A4}$$

and

$$A_4(m) = \beta_x^2\beta_y^2\, F(x)|_{x=0}. \tag{A5}$$

These coefficients are determined by applying the identity $e^{aD_x}F(x) = F(x+a)$.

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