Three-dimensional Ising model with nearest- and next-nearest-neighbor interactions

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The phase diagram of the Ising model in the presence of nearest- and next-nearest-neighbor interactions on a simple cubic lattice is studied within the framework of the differential operator technique. The Hamiltonian is solved by employing an effective-field theory with finite clusters consisting of a pair of spins. A functional form is also proposed for the free energy, similar to the Landau expansion, in order to obtain the phase diagram of the model. The transition from the ferromagnetic (or antiferromagnetic) phase to the disordered paramagnetic phase is of second order. On the other hand, a first-order transition is obtained from the lamellar phase to the paramagnetic phase, as well as from the lamellar phase to the ferromagnetic (or antiferromagnetic) phase, with the presence of a critical end point. An expected singular behavior of the first-order line at the critical end point is also obtained.

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The occurrence of competing exchange interactions in magnetic materials can give rise to a rich variety of magnetic ordered states, as well as phase transitions between them, with the presence of first- and second-order lines and critical and multicritical phenomena [1]. Of particular interest is the Ising model with nearest-neighbor (J_1) and next-nearest-neighbor (J_2) interactions (denoted by J_1-J_2 Ising model) which can be defined by the Hamiltonian

$$\mathcal{H} = -J_1 \sum_{\mathrm{NN}} \sigma_i \sigma_j + J_2 \sum_{\mathrm{NNN}} \sigma_{i'} \sigma_{j'}, \tag{1}$$

where $\sigma_i = \pm 1$ and the sums run over nearest-neighbor (NN) and next-nearest-neighbor (NNN) pairs of spins, respectively. The one-dimensional version of the model (1) can be exactly solved and has no phase transition for finite temperatures [2]. Apart from an exact solution available on the so-called disorder line for the two-dimensional model [3], in two and three dimensions one has no exact solution and the form of the phase diagram in its parameter space remains a considerable problem. It is known that the system presents a disordered paramagnetic phase (P) at high temperatures and, depending on the ratio $\alpha = J_2/J_1$, two different ordered phases at low temperatures: (i) either a ferromagnetic phase (F) when $J_1 > 0$ or an antiferromagnetic phase (AF) when $J_1 < 0$ and (ii) a lamellar, also called superantiferromagnetic (SAF), phase. In fact, the phase diagram of this system is symmetric regarding to the sign of J_1: for negative values of J_1 one has just to change the F ordering by the AF ordering. In general, $J_1 > 0$ and also $J_2 > 0$ are considered in Eq. (1) in order to explore the richer portion of the phase diagram, since in the case $J_2 < 0$ one has no competing interactions and a simple ferromagnetic phase.

The Hamiltonian (1) has been studied on the square lattice by Monte Carlo (MC) simulations [4,5], the cluster variational method (CVM) [5,6], and an effective-field theory (EFT) employing finite clusters [7]. It has been shown that the phase diagram in the α versus temperature plane exhibits a second-order phase transition between the ferromagnetic (or antiferromagnetic) phase to the paramagnetic phase for $\alpha < 1/2$, with a decreasing critical temperature $T_c(\alpha)$ as α increases, and finally approaching zero when the ratio $\alpha = 1/2$. Due to the exact solution for the disorder line, it is known that there is no finite-temperature transition between the F and SAF phases [3,8]. In the region $\alpha < 1/2$ the critical exponents are the same as those of the pure two-dimensional Ising universality class. For $\alpha > 1/2$ the low-temperature ordered phase corresponds to a lamellar structure, or a superantiferromagnetic phase, composed of alternate single ferromagnetic rows (or columns) of opposite oriented spins. In the range $1/2 < \alpha < \alpha_t$, the transition from the SAF phase to the disordered phase is first order. (α_t, T_t) is a tricritical point. For $\alpha > \alpha_t$ the transition is second order with critical exponents continuously varying with the parameter α (nonuniversal behavior) [4,5].

On the other hand, in three dimensions we do not have so many studies as in its two-dimensional counterpart and the situation seems to be not so clear yet. A study using the CVM [9] has shown that the model has a first-order transition line separating the SAF phase from the disordered paramagnetic phase, as well as from the SAF phase to the ferromagnetic or antiferromagnetic phase, with the presence of a critical end point at (α_{CE}, T_{CE}). In this case, this model has been previously applied to treat random surfaces [10,11] and microemulsions [12] and also as a discretized string action [13].

In this paper we study the criticality of the J_1-J_2 Ising model described by the Hamiltonian (1) on a simple cubic lattice. We only consider $J_1 > 0$ because the phase diagram is symmetric regarding the sign of J_1. We employ the EFT which has been successfully used to treat critical and multicritical phenomena in classical [14–17] and quantum models (for instance, transverse Ising and Blume-Capel and ferromagnetic and antiferromagnetic quantum Heisenberg, as well as frustaded Heisenberg, among others). More recently, the EFT approach has been extended also to the study of first-order transitions through a functional form for the free energy based on a Landau-like expansion [7,18]. When applied

to the two-dimensional version of the model (1) the EFT using a cluster of four spins in a plaquette [7] could account for the phase diagram of the model producing results in better agreement with MC simulations than the CVM approach. For instance, the EFT and MC simulations predict a second-order phase transition for $\alpha=1$ while the CVM gives a first-order character. The same qualitative result is also obtained in this case from the EFT with a two-spin cluster.

The ground state ($T=0$) has an exact solution which depends on the frustration parameter α. For $\alpha<\alpha_M=\frac{z_1}{2z_2}$, where z_1 and z_2 are the NN and NNN numbers, respectively, we have a ferromagnetic state and for $\alpha>\alpha_M$ this frustration parameter induces a new magnetic order that depends on the dimension d of the lattice. As said above, on a square lattice ($d=2$) the SAF state is characterized by alternate single ferromagnetic rows (columns) of opposite oriented spins. In the case of the simple cubic lattice ($d=3$) the model exhibits a lamellar phase which consists of alternate planes of different spin alignments. At $\alpha=\alpha_M$ and $T=0$ we have a multiphase point in which several different ordered phases coexist (contrary to the $d=2$ case where in addition to the ordered phases the disordered paramagnetic phase also coexists at this point).

For finite temperatures we use herein the EFT approach which provides a hierarchy of approximations to obtain the thermodynamic properties of magnetic models. One can continue this series of approximations by considering larger and larger clusters and, as a consequence, better results are obtained. The exact solution would be obtained by considering an infinite cluster. However, by using relatively small clusters one can obtain a reasonable description of the thermodynamic properties of several models.

The EFT method is based on the use of rigorous correlations identities as a starting point and utilizes the differential operator technique developed by Honmura and Kaneyoshi [19]. The thermal expectation value of a general function of spin components Ω_N can be obtained by the relation corresponding to the generalized Callen and Suzuki identity [20], i.e.,

$$\langle \Omega_N \rangle = \left\langle \frac{\mathrm{Tr}_N\, \Omega_N \exp(-\beta \mathcal{H}_N)}{\mathrm{Tr}_N \exp(-\beta \mathcal{H}_N)} \right\rangle, \tag{2}$$

where the partial trace Tr_N is taken over the set of N spins variables specified by a finite-system Hamiltonian $\mathcal{H}_N$, Ω_N is a thermodynamic quantity which is a function of all the N spins of the cluster, and $\langle \cdots \rangle$ indicates the canonical thermal average taken over the ensemble defined by the complete Hamiltonian $\mathcal{H}$. In order to treat the Hamiltonian (1), we use a cluster with two spins on a simple cubic lattice which is illustrated in Fig. 1. The Hamiltonian for this cluster is given by

$$\mathcal{H}_2 = -J_1 S_1 S_2 - a_1 S_1 - a_2 S_2, \tag{3}$$

with

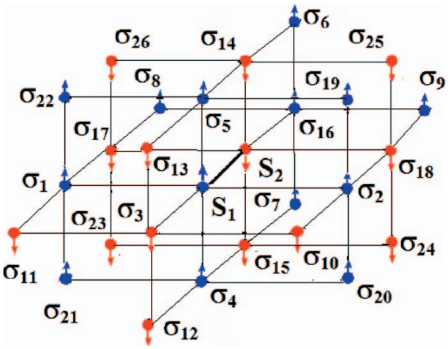

FIG. 1. (Color online) Cluster with two spins S_1 and S_2, and the corresponding 26 nearest- and next-nearest-neighbors σ_i, in the lamellar phase structure.

$$a_1 = -J_1 \sum_{i=1}^{5} \sigma_i + J_2 \left(\sum_{i=10}^{17} \sigma_i + \sum_{i=19}^{22} \sigma_i \right) \tag{4}$$

and

$$a_2 = -J_1 \sum_{i=14}^{18} \sigma_i + J_2 \left(\sum_{i=2}^{9} \sigma_i + \sum_{i=23}^{26} \sigma_i \right), \tag{5}$$

where we adopt $S_i=\pm 1$ for the spins belonging to the cluster and $\sigma_i=\pm 1$ for the 26 spins surrounding the cluster. The quantity Ω_2 is either m_A or m_B, where we have divided the lattice sites into two distinct interpenetrating sublattices A and B, with

$$m_A = \langle S_1 \rangle = \langle \sigma_i \rangle,$$

$$(i = 2,3,4,5,6,7,8,9,18,19,20,21,22)$$

and

$$m_B = \langle S_2 \rangle = \langle \sigma_j \rangle,$$

$$(j = 1,10,11,12,13,14,15,16,17,23,24,25,26).$$

The average magnetization per spin in sublattice A (see, for example, Ref. [18]) is obtained by

$$m_A = \left\langle \frac{\sum_{S_1,S_2=\pm 1} S_1 \exp(-\beta \mathcal{H}_2)}{\sum_{S_1,S_2=\pm 1} \exp(-\beta \mathcal{H}_2)} \right\rangle, \tag{6}$$

which can be written as

$$m_A = \left\langle \frac{\sinh(\tilde{a}_1 + \tilde{a}_2) + \exp(2K_1)\sinh(\tilde{a}_1 - \tilde{a}_2)}{\cosh(\tilde{a}_1 + \tilde{a}_2) + \exp(2K_1)\cosh(\tilde{a}_1 - \tilde{a}_2)} \right\rangle, \tag{7}$$

where $\tilde{a}_i=-\beta a_i$ $(i=1,2)$ and $K_1=\beta J_1$.

Now, using the identity $\exp(aD_x+bD_y)g(x,y)=g(x+a,y+b)$, where $D_\gamma=\frac{\partial}{\partial \gamma}$ $(\gamma=x,y)$ is the differential operator, Eq. (7) can be rewritten as

$$m_A = \langle \exp(\tilde{a}_1 D_x + \tilde{a}_2 D_y) \rangle\, g(x,y)\big|_{x,y=0}, \tag{8}$$

with

$$g(x,y) = \frac{\sinh(x+y) + \exp(2K_1)\sinh(x-y)}{\cosh(x+y) + \exp(2K_1)\cosh(x-y)}. \quad (9)$$

Using the van der Waerden identity for a two-state spin—i.e., $\exp(a\sigma_i) = \cosh(a) + \sigma_i \sinh(a)$ $(\sigma_i = \pm 1)$—Eq. (8) can be *exactly* written in terms of multiple-spin correlation functions occurring on its right-hand side. However, it is clear that if we try to treat exactly all boundary spin-spin correlation functions, the problem becomes unmanageable. In this case we use a decoupling procedure which ignores all high-order correlations on the right-hand side of Eq. (8), i.e.,

$$\langle \sigma_i \cdot \sigma_j \cdots \sigma_l \cdot \sigma_p \rangle \simeq \langle \sigma_i \rangle \cdot \langle \sigma_j \rangle \cdots \langle \sigma_l \rangle \cdot \langle \sigma_p \rangle, \quad (10)$$

where $i \neq j \neq \cdots \neq l \neq p$. Approximation (9) neglects correlations between different spins but takes relations such as $(\sigma_i)^2 = 1$ exactly into account, while in the usual mean-field approximation (MFA) all the self-spin and multiple-spin correlation functions are neglected. Similar expressions are obtained for m_B.

Applying approximation (10) in Eq. (8) and the boundary conditions for the ferromagnetic phase $m_A = m_B = m$ and lamellar phase $m_A = -m_B = m$, we obtain equations of state given by

$$m = \Lambda_\mu(m, \alpha, T) = \sum_{p=0}^{12} a_{\mu p}(T, \alpha) m^{2p+1}, \quad (11)$$

where the coefficients $a_{\mu p}(T,\alpha) = \frac{1}{(2p+1)!}\left(\frac{\partial^{2p+1}\Lambda_\mu}{\partial m^{2p+1}}\right)_{m=0}$ are determined by applying the identity

$$\exp(aD_x + bD_y) g(x,y) = g(x+a, y+b).$$

The corresponding expressions for $a_{\mu p}(T,\alpha)$. are rather lengthy to be reproduced here. In the above equations we have μ=F (ferromagnetic) or SAF (lamellar).

Because close to a continuous transition one has $m \sim 0$, from Eq. (11) one can locate the second-order line through the condition

$$a_{\mu 0}(T, \alpha) = 1. \quad (12)$$

Possible tricritical points can be additionally located when

$$a_{\mu 1}(T, \alpha) = 0. \quad (13)$$

One can note that it is not possible to calculate first-order transition lines on the basis of the equation of state (11) alone because in this case one has $m \neq 0$ at the transition point. To solve this problem one needs to compute the free energies for the ferromagnetic, SAF and paramagnetic phases. First-order transitions correspond then to the locus on the phase diagram where free energies are equal. Although the EFT does not furnish a way to get such a function, we can resort to a different procedure based on the well-known Landau expansion. Assuming that the equation of state (11) can be obtained by the minimization of a given free energy functional like $\Phi_\mu(T, \alpha; m)$—i.e., $\frac{\partial \Phi_\mu}{\partial m} = 0$—we can express such relation as

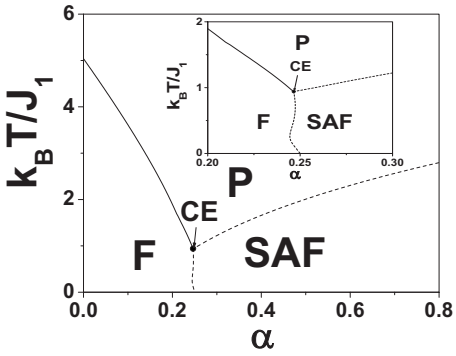

FIG. 2. Phase diagram in the α versus temperature plane of the Ising model with nearest- and next-nearest-neighbor interactions on a simple cubic lattice obtained by the EFT with two-spin cluster. The solid and dashed lines correspond to second- and first-order phase transitions, respectively. CE is the critical end point and the low-temperature first-order line ends at $\alpha_M = 1/4$ (see text) for $T = 0$. The inset shows the region close to the critical end point.

$$\Phi_\mu(T, \alpha; m) = \lambda_0(T, \alpha) + \frac{\lambda_1(T, \alpha)}{2}\left[1 - \sum_{p=0}^{12} \frac{a_{\mu p} m^{2p}}{p+1}\right] m^2, \quad (14)$$

from which one gets equation of state (11) where $\lambda_{r=0,1}(T, \alpha)$ are arbitrary functions which turn out to be irrelevant when searching for the discontinuous transitions. For instance, the boundary between the ordered phases and the disordered paramagnetic phase $m = 0$ is given by

$$\sum_{p=0}^{12} \frac{a_{\mu p}(T, \alpha) m^{2p}}{p+1} = 1. \quad (15)$$

Note that for a second-order transition where $m = 0$ equation above is the same as Eq. (12), as it should be.

Thus, for a given T and α, second-order transitions are obtained when Eq. (12) is satisfied and first-order transitions to the disordered state are obtained by simultaneously solving the two transcendental expressions (11) and (15) for $\mu = \mathrm{F}, \mathrm{SAF}$. The transition between the ordered phases F and SAF is given when

$$\left[1 - \sum_{p=0}^{12} \frac{a_{Fp} m_F^{2p}}{p+1}\right] m_F^2 = \left[1 - \sum_{p=0}^{12} \frac{a_{SAFp} m_{SAF}^{2p}}{p+1}\right] m_{SAF}^2, \quad (16)$$

where m_F and m_SAF are the solutions of Eq. (11) for μ=F and SAF, respectively. The corresponding phase diagram is depicted in Fig. 2. A second-order transition line separates the F (or AF) phase from the P-disordered phase which terminates at the critical end point ($\alpha_{CE} = 0.246\,511$, $k_B T_{CE}/J_1 = 0.940\,00$). A first-order transition is seen for $\alpha > \alpha_{CE}$ between the SAF and P phases. As α increases this transition remains first order. This is indeed an expected result because when $\alpha \to \infty$, the system corresponds to independent fcc antiferromagnetic Ising models which present a first-order behavior. Indeed, this first-order transition has been recently obtained by using Monte Carlo simulations using the Wang-

Landau algorithm [21]. The limiting slope for $\alpha \to \infty$ gives us the transition temperature in units of J_2: namely, $k_B T_N/J_2 = 0.8920$. This value is quite far from the Monte Carlo result [21] $(k_B T_N/J_2)_{MC} = 1.7217(8)$. This discrepancy can be understood because it corresponds to the case $J_1 \to 0$ and the cluster of Fig. 1 has in this case its interacting spins disconnected and asymmetric regarding its neighbors. In fact, the present pair approximation applied directly to the fcc lattice gives $k_B T_N/J_2 = 1.526\,04$, which is indeed comparable to the above Monte Carlo result.

For $T < T_{CE}$ the SAF and the F (AF) phases are also separated by a first-order transition line. However, this transition line is in overall bent to the ferromagnetic phase, in contrast to the positive slope obtained for this line according to the CVM approach [9] and also by low-temperature series expansions [22]. A different critical exponent for the critical end point has also been achieved [9]. It has to be noticed, however, that the widely varying estimates of critical exponents obtained in Ref. [9] are due to the presence of strong crossover effects. We expect to have the same critical behavior at a CEP, as is indeed the case for the double critical end point of the spin-3/2 Blume-Capel model [23].

The inset in Fig. 2 shows the first-order transition line close to the critical end point. One can see that a singularity indeed appears at this point, as predicted by phenomenological scaling and thermodynamic arguments by Fisher and coworkers [24–26]. Although this prediction has been corroborated by analytical calculations on extended spherical models [25,26] and Monte Carlo simulations in symmetrical binary fluid mixtures [27], this is seen here not for the second derivative of the transition line but for the first derivative as well. The kink visible in the inset of Fig. 2 can be a mean-field-like behavior.

Finally, a word should be said about the free energy function (14). It is well known that according to a Landau expansion its validity will be only near the critical end point, where the magnetization is very small. In the present case, however, we are extrapolating its applicability to regions far away from the CE point. In order to justify *a posteriori* such an extrapolation we first note that in fact the function given by Eq. (14) is a polynomial of degree $2+2p_{\max}=26$, meaning that we have a rather long series in m. Nevertheless, at $T=0$ and $\alpha=1/4$, Eq. (16) is satisfied for $m_F=m_{SAF}=1$ in such a way that we recover the exact zero-temperature multiphase point. In addition, the expected first-order transition is obtained in the limit $\alpha \to \infty$. For these reasons we believe that the dashed lines in Fig. 2 are really within the present two-spin approximation (apart from the reentrant behavior at low temperatures and the overall negative slope).

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