Phase transitions in the classical *n*-vector model on the fcc lattice

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The classical *n*-vector model on the face-centered cubic lattice with ferromagnetic and antiferromagnetic interactions is studied by using the framework of an effective field theory approach in cluster with two spins. For $n=1$ (Ising), $n=2$ (*XY*-planar rotator), $n=3$ (Heisenberg), and $n\to\infty$ (spherical) models the ferromagnetic system undergoes a second-order phase transition while the antiferromagnetic system presents a first-order behavior. The first-order character for $n=3$, which is inconclusive in the literature, seems actually to be the case for the isotropic Heisenberg antiferromagnet, and the same is expected to hold for the less studied *XY* and spherical models. In addition, the transition temperatures are quantitatively comparable to the exact one (when available) and to those from Monte Carlo simulations and series expansion.

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I. INTRODUCTION

The study of geometrically frustrated antiferromagnet spin models have attracted both experimental and theoretical interest during the past twenty years. The primary interest emerged as a new class of magnetic materials with uncommon physical properties.[1–4] The effect of frustration leads to nontrivial, highly degenerate ground states, and it can be very difficult to ascertain the correct solution to a given model, even when extreme approximations are used, such as mean-field theory. In particular, geometric frustration does not require adjustment of the magnitude of the coupling constants and the most well-known examples of frustrated systems are the antiferromagnetic triangular and kagomé lattices in two dimensions and pyrochlore and face-centered-cubic (fcc) lattices in three dimensions. In all these lattices, the elementary unit of the magnetic structure is a triangle, which makes it impossible to satisfy all the antiferromagnetic bonds at the same time, with the result of a macroscopically degenerated ground state.

The first nontrivial frustrated model, which has been exactly solved by Wannier, is the Ising antiferromagnet on the triangular lattice.[5] The principal result is that no finite temperature (i.e., $T_N=0$) ordering occurs so that the effect of this frustration is to increase the lower critical dimension beyond two. After the solution of Wannier, other two-dimensional frustrated Ising models have also been exactly treated by various authors.[6] Therefore, these exact solutions can be a good starting point for testing approximate theories prior to application to more complex systems.

In particular, the nature of the ground state and the low-lying excited states in the fcc antiferromagnet (AF) with only nearest-neighbor (nn) interaction continues to be an interesting problem in the field of magnetism.[7–10] For bipartite lattices, such as square and simple cubic ones, the solution of classical, and some quantum (*XY* and transverse Ising), ferromagnetic (F) models, immediately yields the solution of the corresponding antiferromagnetic (AF) model through a gauge symmetry (for the quantum Heisenberg model this symmetry does not exist[11]). However, the fcc lattice is not bipartite. The difficulty experienced in the study of the fcc AF spin model resides in the fact that it is geometrically frustrated, resulting in an infinite ground-state degeneracy and also allows the system to present a first-order phase transition.

Inclusion of next-nearest-neighbor (nnn) interaction in fcc AF spin models can even change the nature of the phase transition from first order to second order (continuous) for certain values of the parameter $\alpha\in[0,\infty)$, where $\alpha=J_2/J_1$ and $J_1(J_2)$ is the nn (nnn) coupling constant. This is so because for small α all known investigations of the system agree with the first-order character of the transition, whereas in the limit $\alpha\to\infty$ the fcc lattice decouples into four independent ferromagnetic simple cubic lattices, which exhibit a continuous phase transition. In fact, three different types of AF orders, denoted by AF-I, AF-II, and AF-III, have been predicted to exist in the fcc AF spin models with nn and nnn interactions,[12] where the types of magnetic orders are dependent on the α parameter. The AF-I magnetic order is composed of ferromagnetic (100) planes antiferromagnetically coupled. The type AF-II can be viewed as defective type AF-I in which the spins in a given cluster (100) plane can be subdivided into at least two interpenetrating antiferromagnetic clusters. All spins in a given cluster are either parallel or antiparallel to the cluster axis. Finally, the AF-III ordering has four degenerate configurations, and it is necessary to divide the fcc lattice into four interpenetrating simple sublattices *A* (corner spins), *B*, *C*, and *D* (three face-centered spins, respectively). In Fig. 1, we have schematically the ground-state configurations of the AF-I [Fig. 1(a)], AF-II [Fig. 1(b)] and AF-III [Fig. 1(c)] magnetic order.

From an experimental viewpoint, the different types of AF ordering discussed above have been observed in magnetic compounds. The sign convention used is one in which an exchange interaction is positive for antiferromagnetic interaction and negative for ferromagnetic interaction. For example, the AF-I order is reported in a number of neodymium systems,[13] such as NdP ($J_1=0.01$ K, $J_2=-0.11$ K, $\alpha=-11.0$,

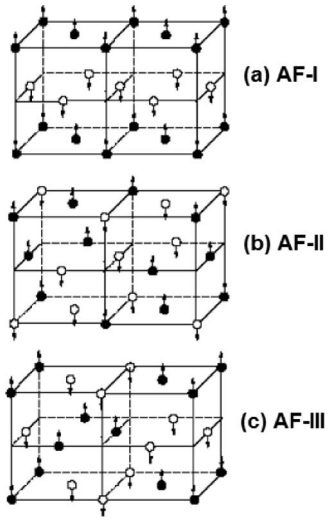

FIG. 1. Schematic structures of the ground-state configurations in an fcc classical antiferromagnet: (a) type AF-I, (b) type AF-II, and (c) type AF-III. The black and white points represent the up and down spins along the z direction, respectively.

T_N=11 K), NdAs (J_1=0.03 K, J_2=−0.10 K, α=−3.3, T_N=13 K), NdSb (J_1=0.07 K, J_2=−0.11 K, α=−1.6, T_N=16 K), and NdBi (J_1=0.09 K, J_2=−0.18 K, α=2.0, T_N=24 K). The AF-II magnetic order has been observed in binary transition-metal oxides MnO (J_1=0.01 K, J_2=−0.11 K, α=−1.1, T_N=118 K),[14] CoO (J_1=5.5 K, J_2=27.5 K, α=5.0, T_N=289 K),[15] NiO(J_1=34.16 K, J_2=202 K, α=8.4, T_N=523 K) (Ref. 16) and the sulfide, viz., α-MnS (J_1=7.0 K, J_2=12.7 K, α=1.8, T_N=152 K).[17] The third kind of antiferromagnetic order, AF-III, has been observed in β-MnS [(J_1=28 K, J_2=2.8 K, α=0.1, T_N=98 K) and some diluted magnetic semiconductors such as $A_{1-x}\mathrm{Mn}_xB$ (where A=Cd,Zn,Hg and B=Se,Te). There are several other known systems in which magnetic ions occupy the fcc lattice. For example, the UO_2 is of type AF-I (Ref. 18) and, instead of a second-order transition, it presents a first-order transition. Therefore, the nature of the phase transition is also an interesting problem to be experimentally treated and theoretically explained.

Extensive theoretical studies have been made to treat the criticality of the fcc antiferromagnetic Ising model with only nn interaction.[19–22] There appears to be a consensus among the authors that the transition is of first order with the associated spin ordering being of type AF-I. The most recent study on this system which we are aware of is the Monte Carlo simulation of Beath and Ryan,[7] where a precise value of the transition temperature (Néel temperature) has been estimated k_BT_N/J=1.7217. This value is very small in comparison with the second-order phase transition temperature of the ferromagnetic case,[23] i.e., k_BT_c/J=9.7943.

On the other hand, in the case of the fcc antiferromagnetic Heisenberg model the nature of the phase transition remains less clear. Previous linear spin-wave calculation[12] indicates diverging spin reduction at finite temperature. It has been argued that this model (classical and quantum) has no long-range order. Similarly, the Green's-function approach[24] predicts no phase transition when $T>0$. In addition, other procedures such as series expansion, Green's-function, and spin-wave-based methods cannot offer further clarification on the particular point either (i.e., the nature of transition), since these three methods are suited to treat second-order transition in magnetic models. Monte Carlo simulations of classical fcc Heisenberg antiferromagnet[25–29] have shown, however, that thermal fluctuations stabilize a type-I structure (AF-I order) in the absence of nnn interactions. The authors have concluded that the transition is of first order, in contrast with the results of Fernandez *et al.*[25] who found a second-order character. The latter conclusion of a continuous transition may be due to rather small lattice size (L=8), large temperature interval, and rather short runs, as was pointed out in Monte Carlo (MC) simulations by Diep and Kawamura.[26] Therefore, one can say that MC simulations have confirmed, for the classical fcc Heisenberg antiferromagnet, a first-order phase transition[28] at k_BT_N/J=1.3377, which is also smaller than the second-order temperature for the ferromagnetic case,[30] i.e., k_BT_c/J=8.6705.

For planar models, preliminary results have also indicated the collinear AF-I-type order at low temperature for the nearest-neighbor XY antiferromagnet on a fcc lattice. But there is, up to now, no estimate for the (possible) first-order transition temperature.[26] The scenario is still less clear in the case of the spherical model.

At this stage, it is then natural to ask the question of what would happen if one treats this lattice by considering the more general model with an n-component vector spin on its sites, where n=1,2,3, and ∞ corresponds to the Ising, XY, Heisenberg, and spherical models, respectively. It is clear that some studies have been made only for the case of n=1 and 3. However, no attention has been paid to the nature of the phase transition in the more general case of the fcc n-vector antiferromagnet. This fact has motivated the present investigation, where the approximate properties have been studied by employing the effective-field theory.

The organization of the present paper is as follows. The effective-field theory is formulated and applied to the nearest-neighbor fcc classical n-vector model in Sec. II. The formalism is constructed using a finite cluster with two spins and the Zernike approximation. Results of the transition temperature for the system with ferromagnetic (T_c) and antiferromagnetic (T_N) interaction are shown in Sec. III. We also discuss the criticality of the Ising (n=1), XY or planar (n=2), Heisenberg (n=3), and spherical ($n=\infty$) models. In particular, the results for the Ising and Heisenberg models are compared with MC simulations discussed previously in the literature. Some concluding remarks are given in Sec. IV.

II. MODEL AND EFFECTIVE-FIELD THEORY

The three-dimensional n-vector model, or O(n) model, is quite studied in the literature due to the fact that many real magnetic materials show large values of spin ($S>1/2$) in which the classical limit ($S\rightarrow\infty$) can be a good approximation, mainly above the transition temperature. The classical spin approximation consists of replacing the quantum mechanical spin operator by a classical vector fixed in length,

but free to orient itself in any direction. The classical partition function $\mathcal{Z}_{cl}$ is an integral over the phase space defined by the solid angle available to each spin vector. For nonfrustrated classical systems (and some quantum systems as, for example, the quantum XY and transverse Ising models) there is a unitary operator in which the partition function of the F case is simply mapped into the partition function of the AF case by redefining the spin direction on one sublattice (i.e., $J \rightarrow -J$, J being the nn exchange coupling) of the AF system. This fact implies the same transition temperature for the F or AF system. Such a unitary operator, however, does not apply to the quantum Heisenberg model[11] and to frustrated systems, as the ones studied herein.

A. Hamiltonian

We consider the classical n-vector model defined on the fcc lattice with a unit cell shown in Fig. 1, which can be given by the following Hamiltonian:

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j, \tag{1}$$

where J is the exchange coupling for all bonds ($J>0$ and $J<0$ correspond to the AF and F system, respectively), $\langle i,j \rangle$ denotes nearest-neighbor pairs of spins, and $\vec{S}_i = (S_i^1, S_i^2, \ldots S_i^n)$ is a vector spin of n components at site i with

$$|\vec{S}_i| = \sqrt{\sum_{p=1}^{n} (S_i^p)^2} = n^{1/2}. \tag{2}$$

In particular, the model (1) for $n=0,1,2,3$ and $n \rightarrow \infty$ corresponds, respectively, to the self-avoiding walk, Ising, classical XY (or planar), and classical isotropic Heisenberg and spherical models.

The ground state of the classical fcc Heisenberg ($n=3$) antiferromagnet is more degenerate than the corresponding Ising ($n=1$) one. It has been shown that the average energy value,[31] i.e., $E_0 = \langle \mathcal{H} \rangle$, at $T=0$ for the fcc O(3) (Heisenberg) is identical to the case of the Ising model. With the inclusion of nnn interaction J_2 ($\alpha = J_2/J_1$) in the Hamiltonian (1), the nature of the ground state changes as a function of α. Considering the fcc lattice as made up of four simple-cubic lattices, the ground state for $\alpha<0$ consists of three pairs of configurations in which two sublattices are occupied by *up* spins (sublattice A) and the other two by *down* spins (sublattice B) as in Fig. 1(a) (AF-I order). The corresponding average energy per spin in units of J is $\mathcal{E}_0^{\mathrm{I}} = -2+3\alpha$. In the intermediate region $0<\alpha<0.5$ there are again six ground states (three pairs) consisting of configuration type AF-III order as shown in Fig. 1(c) with $\mathcal{E}_0^{\mathrm{III}} = -2+\alpha$. Finally, for $\alpha>0.5$ the ground state has AF-II order as shown in Fig. 1(b) with $\mathcal{E}_0^{\mathrm{II}} = -3\alpha$. The points at $\alpha=0$ and $\alpha=0.5$ correspond to first-order phase transitions between the AF-I $\rightarrow$ AF-III and AF-III $\rightarrow$ AF-II states, respectively. For $\alpha=0$ the AF-I state dominates at low temperature, while at $\alpha=0.5$ the AF-III state dominates.

These conclusions of several magnetic phases (AF-I,II,III) in the fcc antiferromagnet as a function of the α parameter (not the nature of the order of the transition) have been confirmed in the fcc Ising ($n=1$) (Ref. 20) and classical Heisenberg ($n=3$) (Ref. 8) antiferromagnets. Therefore, at least in principle, such an hypothesis can be extended for all values of n in the fcc O(n) antiferromagnet. On the other hand, the order of the transition of the AF-I state at finite temperature depends on the value of α. In particular, Monte Carlo simulations in the fcc Ising antiferromagnet[20] have indicated a second-order transition for $\alpha \leq -0.25$ and a first-order for $-0.25 < \alpha \leq 0$. In this paper we will restrict the analysis only on the nature of the phase transition of the fcc O(n) antiferromagnet in the absence of nnn interaction ($\alpha=0$) as a function of the number (n) of the spin components.

B. Formalism

Some years ago, a simple and versatile scheme, denoted by effective-field theory (EFT) has successfully been used to treat second-order phase transitions of classical and quantum models.[32–36] Recently, EFT also was applied to study first-order phase transitions in frustrated models.[36] The EFT provides a hierarchy of approximations to obtain 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 that contain the topology of the lattice, one can obtain a reasonable description of thermodynamic properties as will be shown below. The EFT method is based on the use of rigorous correlation identities as a starting point and utilizes the differential operator technique developed by Honmura and Kaneyoshi.[37]

The thermal expectation value of a general function involving spin operator components in finite cluster Ω_N can be obtained by the relation corresponding to the generalized Callen and Suzuki identity,[38] i.e.,

$$\langle \Omega_N \rangle = \left\langle \frac{\mathrm{Tr}_N \Omega_N e^{-\beta \mathcal{H}_N}}{\mathrm{Tr}_N e^{-\beta \mathcal{H}_N}} \right\rangle, \tag{3}$$

where the partial trace Tr_N is taken over the set of N spin variables specified by a finite-system Hamiltonian $\mathcal{H}_N$ and $\langle \cdots \rangle$ indicates the canonical thermal average taken over the ensemble defined by the complete Hamiltonian $\mathcal{H}$.

For a cluster with two spins, de Sousa and de Albuquerque[39] have developed an EFT to treat the criticality of the ferromagnetic n-vector model on a lattice with arbitrary coordination number z. Using a two-spin Hamiltonian for the finite system $\mathcal{H}_{N=2}$ in Eq. (3), the magnetization per spin $m = \left\langle \frac{S_1+S_2}{2} \right\rangle$ was found. Applying the differential operator technique and EFT an approximate expression for m is obtained for all values of z. Later, de Sousa[40] generalized this approach to treat the antiferromagnetic case. The lattice sites are divided into two distinct interpenetrating sublattices A and B, where the corresponding magnetizations are given by $m_{A(B)} = \langle S_{1(2)} \rangle$ on a simple lattice ($z=6$). The Curie (Néel) temperature associated to the second-order phase transition is obtained by using the boundary conditions $m_A = m_B \rightarrow 0$ ($m_A = -m_B \rightarrow 0$) for the F (AF) case.

Contrary to the mean-field approximation (MFA), where all the self-spin and multiple-spin correlation functions are neglected, EFT neglects correlations between different spins but takes relations such as $S_i^2=1$ exactly, which is critical for incorporating frustration. According to Netz and Berker,[41] the failure in the case of a triangular Ising model by using MFA is due to a violation of the hard-spin condition $S_i^2=1$. The two different methods, EFT and the recursive lattice technique,[42] exactly treat the hard-spin constraint and correctly reproduces the one-dimensional result (i.e., $T_c=0$) and exhibits a nonzero critical temperature for the three-dimensional frustrated Ising model. Recently, EFT[43] and hard-spin mean-field theory[44] have been used to study frustrated Ising systems with competitive interactions.

Following the same procedure developed by de Sousa [40] and assuming an ordered state of the AF-I type shown in Fig. 1(a), the average magnetization in sublattice A (m_A) is given by the following expression:

$$m_A = \hat{\Omega}\,(m_A, m_B) g_n(x,y)\big|_{x,y=0}, \tag{4}$$

with

$$\hat{\Omega}(m_A,m_B) = \prod_{\mu=x,y} (\alpha_\mu - m_B\beta_\mu)^5(\alpha_\mu - m_A\beta_\mu)^2 \times \prod_{\lambda=A,B} (\alpha_{xy} - m_\lambda \beta_{xy})^2, \tag{5}$$

$$g_n(x,y) = \frac{\sinh(x+y) + \Phi(nK)\sinh(x-y)}{\cosh(x+y) + \Phi(nK)\cosh(x-y)}, \tag{6}$$

and

$$\Phi(nK) = \frac{1+\Delta_n(K)}{1-\Delta_n(K)}, \tag{7}$$

where $K=\beta J$, $\alpha_\mu=\cosh(KD_\mu)$, $\beta_\mu=\sinh(KD_\mu)$, $\alpha_{xy}=\cosh[K(D_x+D_y)]$, $\beta_{xy}=\sinh[K(D_x+D_y)]$, $D_\mu=\frac{\partial}{\partial\mu}(\mu=x,y)$, $\Delta_n(K)=I_{n/2}(nK)/I_{n/2-1}(nK)$, and $I_p(x)$ is the modified Bessel function of the first kind of order p. m_B is the magnetization of sublattice B.

In particular, we are interested only in the function $\Delta_n(x)$ for the cases of $n=1,2,3$, and $n\to\infty$, that are given by

$$\Delta_n(K) = \begin{cases} \tanh(K), & n=1 \\ \dfrac{I_1(2K)}{I_0(2K)}, & n=2 \\ \mathcal{L}(3K), & n=3 \\ \dfrac{2K}{1+\sqrt{1+4K^2}}, & n\to\infty, \end{cases} \tag{8}$$

where $\mathcal{L}(x)=\coth(x)-1/x$ is the *Langevin function*.

Applying the boundary condition in Eq. (4) for the AF-I phase $m_A=-m_B=m$, we obtain the equation of state given by

$$m = \Psi_{AF}(m,T,n) = \sum_{p=0}^{8} a_{2p+1}(T,n) m^{2p+1}, \tag{9}$$

with

$$a_k(T,n) = \frac{1}{k!}\left(\frac{\partial^k \Psi_{AF}(m,T,n)}{\partial m^k}\right)_{m=0}, \tag{10}$$

and

$$\Psi_{AF}(m,T,n) = \hat{\Omega}\,(m,-m) g_n(x,y)\big|_{x,y=0}. \tag{11}$$

In the case of the boundary condition for the ferromagnetic (F) phase, we have $m_A=m_B=m$ and the equation of state is given by

$$m = \Psi_F(m,T,n) = \sum_{p=0}^{8} b_{2p+1}(T,n) m^{2p+1}, \tag{12}$$

with

$$b_k(T,n) = \frac{1}{k!}\left(\frac{\partial^k \Psi_F(m,T,n)}{\partial m^k}\right)_{m=0}, \tag{13}$$

and

$$\Psi_F(m,T,n) = \hat{\Omega}_F\,(m,m)\tilde{g}_n(x,y)\big|_{x,y=0}, \tag{14}$$

where $\hat{\Omega}_F(m,m)$ corresponds to the differential operator $\hat{\Omega}(m,m)$ substituting K by $-K$, and similarly $\tilde{g}_n(x,y)$ corresponds to the function $g_n(x,y)$ substituting K by $-K$. The coefficients $\{a_k(T,n), b_k(T,n)\}$ are determined by applying the identity $e^{aD_x+bD_y}f(x,y)=f(x+a,y+b)$. The corresponding expressions for the above quantities are rather lengthy to be reproduced here.

III. RESULTS AND DISCUSSION

In order to study the phase transition of the fcc O(n) model using EFT-2 we analyze the thermal behavior of the order parameter as a function of the temperature. For the AF and F cases we numerically study the equations of state given by Eqs. (9) and (12), respectively. When the transition is of second order, $m(T)$ decreases as the temperature increases and at $T=T_c$ the order parameter is null (continuously). In the F case, we indeed observe a continuous transition $T_c(n)$ as a function of n, which is numerically obtained through the condition

$$b_1(T_c,n) = 1. \tag{15}$$

The above equation corresponds to the equation of state (12) in the limit $m\to 0$.

For first-order transitions we cannot use a similar condition as given by Eq. (15) because in this case one has $m\neq 0$. For a qualitative estimate of the first-order temperature $T_N^*(n)$ we use the criterion of the infinity of the first temperature derivative of the order parameter at $T=T_N^*(n)$ [i.e., $\left(\frac{dm}{dT}\right)_{T=T_N^*}\to\infty$], as depicted in Fig. 2 for the Ising model ($n=1$). Similar behavior as in Fig. 2 is observed for other values of n. In this scheme the first-order temperature $T_c^*(n)$ is overestimated in relation to the value to be obtained using the free energy stability (Maxwell construction method). This method to locate T_N^* has been recently used to study the

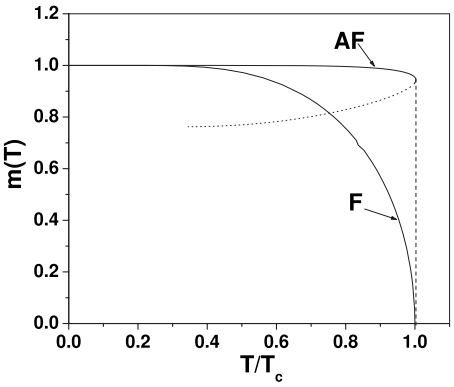

FIG. 2. Magnetization as function of the reduced temperature for the Ising model ($n=1$) in the antiferromagnetic (AF) and ferromagnetic (F) cases. The dotted line is the unphysical solution, and the dashed line represents the discontinuity in the magnetization at the infinite derivative point for the AF model.

quantum phase transition of the frustrated Heisenberg (spin-1/2) on a square lattice.[36] From Eq. (9) we then have

$$\sum_{p=0}^{8} (2p+1) a_{2p+1}(T_N,n) m_c^{2p} = 1. \tag{16}$$

Simultaneously solving Eqs. (9) and (16) we obtain an estimate for T_N and the value of the discontinuity of order parameter $m_c=m(T_N)$. This procedure can also be used to obtain the critical temperature $T_c(n)$ in the F case, but in this limit we have the solution $m_c=0$ (see Fig. 2), and the results are equivalent to those from Eq. (15).

The numerical results for T_c and T_N, and when available, a comparison with exact Monte Carlo simulations, and series expansion, are shown in Table I. One can clearly see that the agreement is quite good, even having in mind the simplicity of the present approximation. Of course, there are other analytical procedures of the same level of the EFT. However, the corresponding results are not as good as the present ones. For instance, the Bragg-Willians[47] and quasichemical approximation[48] are clearly inadequate for the treatment of antiferromagnetism in the fcc lattice. Improved mean-field theories, such as the pair approximation[49] and the Bethe scheme[50] yield no finite temperature AF ordering. Only a more sophisticated approximation, the Kikuchi scheme [the so-called cluster variation method (CVM)] in both tetrahedral[51] and the tetrahedral-octahedral[52] approximations, is capable of yielding first-order transitions. More recently, a mean-field theory in cluster with four spins (MFT-4) has been applied[19] to this model and for the F case it was found $k_BT_c/J=11.719$ and for the AF case (first-order transition) $k_BT_N/J=3.502$. In the present formalism the values $k_BT_c/J=8.910$ (F case) and $k_BT_N/J=1.526$ (AF case) are clearly superior in quality than the values from MFT-4 in comparison with the results from Monte Carlo (MC) simulation[7,23] as can be seen from Table I. In particular, for the fcc Heisenberg antiferromagnet the present results are in good accordance with recent MC simulations.[28]

TABLE I. Transition temperature k_BT_c/J (F case, $J<0$) and k_BT_N/J (AF case, $J>0$) for the O(n) model on an fcc lattice obtained in this work using EFT-2. We compare with exact solution for the spherical ferromagnet, Monte Carlo (MC) simulations for the Ising and Heisenberg models, and series expansion (series) for the XY ferromagnetic model. Except for the EFT-2 approach and the exact solution of the spherical model, here and also in the text, the errors in the temperatures are in the next decimal digit (not shown).

Model	Method	F case	AF case
Ising ($n=1$)	EFT-2	8.910	1.526
	MC[7]	9.794	1.721
XY planar ($n=2$)	EFT-2	8.911	1.493
	Series (Ref. 45)	9.639	
Heisenberg ($n=3$)	EFT-2	8.913	1.476
	MC (Refs. 28 and 30)	8.671	1.329
Spherical ($n\to\infty$)	EFT-2	8.919	1.434
	Exact (Ref. 46)	6.675	

On the other hand, for the fcc XY ($n=2$) and spherical ($n\to\infty$) antiferromagnets there exists (up to our knowledge) no estimate for T_N, only values of T_c (F case). However, preliminary results of MC simulations[28] indicate a possible first-order transition in the XY model, corroborating the previsions of the present work.

IV. CONCLUSIONS

In summary, we have studied, using effective-field theory in finite cluster, the criticality of the fcc O(n) model with F and AF interactions. For the F case the phase transition is of second order and the AF case is of first order. The results for the ferromagnetic system are in good agreement with the exact ones or those coming from Monte Carlo simulations. In addition, a similar treatment applied to the quantum fcc Heisenberg model using EFT-2 (Ref. 53) has given $k_BT_c/J=8.769$ (F case) and $k_BT_N/J=1.289$ (AF case). These values are smaller than the present classical ones, due to the presence of the quantum effects.

To obtain an estimate of T_N (AF case) we used the derivative method of the order parameter, where at $T=T_N$ we impose $(dm/dT)_{T=T_N}\to\infty$. Qualitatively, we have found first-order transition for the fcc O(n) antiferromagnet and all values of n. The quantitative results for T_N in the Ising and Heisenberg models are in good agreement with MC simulations. The present approach does not provide a free energy for the system. For this reason one is not able to completely describe the first-order behavior such as transition point, latent heat, etc. However, more recently, a functional form for the free energy has been proposed in order to get first-order transitions.[43] The method has given good estimates for the phase diagram of the Ising model with nn and nnn competi-

tive interactions on a simple cubic lattice. We have also used this new methodology to the present system but could not find any numerical solution for the Néel temperature. Probably, the series for the present model is still too short to get a reasonable free energy.

Although there are some arguments sustaining no antiferromagnetism in this system[54,55] for $n=3$, MC simulations[25] have indicated a finite Néel temperature. Since our results are close to MC simulations, as can be seen in Table I, we believe that the present approach can actually give a good picture of the criticality of the system, even in the AF case, including the less studied models $n=2$ and $n\to\infty$.

As a final comment, we would like to point out that the recursive lattice technique[42] should be worthy to be applied to the present problem. As this method allows one to calculate the free energy, an unambiguous location of first-order transition lines can be correctly obtained.

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