Reentrant behavior in the nearest-neighbor Ising antiferromagnet in a magnetic field

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Motived by the H-T phase diagram in the bcc Ising antiferromagnetic with nearest-neighbor interactions obtained by Monte Carlo simulation [Landau, Phys. Rev. B **16**, 4164 (1977)] that shows a reentrant behavior at low temperature, with two critical temperatures in magnetic field about 2% greater than the critical value $H_c=8J$, we apply the effective field renormalization group (EFRG) approach in this model on three-dimensional lattices (simple cubic-sc and body centered cubic-bcc). We find that the critical curve $T_N(H)$ exhibits a maximum point around of $H\simeq H_c$ only in the bcc lattice case. We also discuss the critical behavior by the effective field theory in clusters with one (EFT-1) and two (EFT-2) spins, and a reentrant behavior is observed for the sc and bcc lattices. We have compared our results of EFRG in the bcc lattice with Monte Carlo and series expansion, and we observe a good accordance between the methods.

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The antiferromagnetic Ising model, with its simple version of two-state variables, is among the simplest conceivable classes of models in statistical mechanics to describe ordered materials strongly anisotropic with localized magnetic moments (insulating), for example, the $FeCl_2$ and $FeBr_2$ antiferromagnets.[1–4] This class shows an overwhelming richness in phase structure and critical behavior with application of a magnetic field. A field along the easy axis will destroy the magnetic order in the ferromagnetic case, but the antiferromagnetic model has an ordered phase (AF) with decreasing transition temperature $T_N(H)$ as the field intensity increases. The magnetic field (H) versus temperature (T) phase diagram display an AF phase being of first order at low temperatures and of second order at higher temperatures and lower fields. In $FeCl_2$, the two kinds of transitions meet at a tricritical point. For $FeBr_2$, a possible decomposition of the tricritical point into a critical end point and a bicritical end point has been observed.[1] These multicritical points have been attributed to two crucial ingredients: the ferromagnetic intraplanar interaction and antiferromagnetic interplanar interactions,[5] so-called *metamagnet*.

On the other hand, the nearest-neighbor Ising antiferromagnet in a magnetic field presents only second order phase transition for all values of field H in the interval between $H=0$ to the critical value $H=H_c=zJ$ ($T_N=0$-**ground state**, z is the coordination number). Since the nature of the symmetry breaking is not affected by the magnetic field, one expects that the transition at finite field is of second order and belongs to the same universality class as the zero-field Ising model. The phase diagram at low temperatures (around the critical field $H\simeq H_c$) show some qualitative differences between two- and three-dimensional lattices. Exact results of a decorated Ising model on a square lattice ($2d$) (Ref. 6) show that the critical temperature $T_N(H)$ decreases with an increase of H, going to zero at $H=H_c$. The phase diagram of the quasi-two-dimensional Ising antiferromagnetic $CoCs_3Br_5$ (Ref. 7) agree with these theoretical results. Various approximative methods have shown this critical behavior of the curve T_N versus H, such as mean field approximation (MFA),[8] effective-field theory (EFT),[9] mean field renormalization group (MFRG),[10] Monte Carlo simulation (MC),[11] and high-temperature series expansion (SE).[12] For the case of three-dimensional ($3d$) lattice, the theoretical calculations show disagreement between different methods. The results obtained by the MFA, EFT, and MC methods show a *reentrant behavior* in the phase diagram in low-temperature, i.e., if H is just above H_c, then these are two phase transitions as the temperature is increased. In contradiction, SE suggests a phase diagram like the two-dimensional results, i.e., have no re-entrance at low-temperature. The MFRG approach fails at low temperature, where only solution for low fields are found for $T_N(H)$.

Another interesting result in the nearest-neighbor Ising antiferromagnet in a magnetic field is the slope of the phase boundary at $T=0$, i.e., $H\simeq H_c+a_cT$, that for the two-dimensional lattice is negative ($a_c<0$) and the simple cubic lattice ($3d$) is nearly zero ($a_c\simeq 0$). This model at low temperatures is equivalent to hard-core lattice gases, that use the high-density series for the order parameter of the lattice gas up to 24 terms.[14] We can estimate values for the slope of the phase boundary a_c(square lattice-sq)$=-0.67<0$ and $a_c\geqslant 0$ [a_c(simple cubic lattice-sc)$=0$ and a_c(body-centered cubic lattice-bcc)$=0.13$],[15] indicating that the critical curve $T_N(H)$ for the bcc lattice shows a reentrant behavior in accordance with Monte Carlo simulation[11] ($a_c=0.16$). Results of the renormalization-group[16] and high-temperature series[12] do not reproduce this feature of the phase diagram for the bcc lattice (i.e., $a_c>0$). The critical magnetization m_c, which is the limiting value of the magnetization as the $T=0$ and $H=H_c$ point is approached along the critical line $T_N(H)$, is also a quantity of interest. For the sc and bcc lattices, Racz[15] have estimated $m_c=0.57$ and $m_c=0.645$ ($m_c=0.644$ for Monte Carlo[11]), respectively, while the MFA (Ref. 8) and EFT (Ref. 9) methods found $m_c=1.0$. When the number of nearest-neighbors (z) increase, we expected that the values of a_c and m_c tend towards their MFA values $a_c=\infty$ $[H\simeq H_c-T\ln(T)/2]$ and $m_c=1.0$, because MFA becomes exact as the coordination number goes to infinity ($z\rightarrow\infty$). MFA overestimate the or-

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dering tendencies; the results for a_c are always larger than the *exact* SE estimates (or Monte Carlo simulation). This analysis shows that for small values of coordination number ($z<8$) we have $a_c \leqslant 0$ indicating absence of re-entrance in the phase diagram, and an increase of the z slope a_c also increase, with $a_c>0$ for the bcc lattice. We speculate that a given approximation applied in this model will reproduce, qualitatively, the effect of the re-entrance as a function of the coordination number, while the MFA and EFT approaches do not confirm these speculations.

To study the critical properties of spin models, the renormalization group (RG) approaches[17] have shown to be efficient when compared with more accurate methods, such as Monte Carlo simulation. The great advantages of these RG methods are the small CPU time and the possibility of obtaining good critical values using small systems. Due to these successes, we decided to use the effective field RG (EFRG) approach[18] to obtain the phase diagram of the nearest-neighbor Ising antiferromagnet in a magnetic field for the sc ($z=6$) and bcc ($z=8$) lattices. The main objective is to analyze the influence of the re-entrance in the critical curve T_N versus H as a function of the coordination number (z), where results of Monte Carlo[11] show a reentrant behavior for the bcc ($z=8$) lattice. The EFRG approach is based on the comparison of two clusters of different sizes, each of them simulating an infinite system. For constructing effective field equations of states (magnetization) we use the Callen–Suzuki identity[19] as a starting point. The method treats the effects of the surrounding spins of each cluster through a convenient differential operator technique[20] which, in contrast to the usual mean field approximation procedure, all the relevant self-spin correlations are taken exactly into account (see, for example, Ref. 17 for details and applications of the EFRG method, as well as the potentiality). In order to apply the RG idea, we have used small clusters. The interactions within the clusters are exactly treated and the effect of the remaining lattice spins is replaced by a symmetry breaking field (here are used two fields associated to the two sublattice). In the standard effective field theory (EFT) this field is identified with the order parameter of the system. In this scheme, both the magnetization of the clusters and the respective symmetry breaking fields scale in the same way.

The model considered in this work is the nearest-neighbor (nn) Ising antiferromagnet in a field magnetic divided into two equivalent interpenetrating sublattice A and B, that is described by the following Hamiltonian:

$$\mathcal{H} = J\sum_{\langle\langle i,j\rangle\rangle}\sigma_i\sigma_j - H\sum_i \sigma_i, (\sigma_i = \pm 1), \tag{1}$$

where J is the nn exchange coupling, $\langle i,j\rangle$ denoting the sum over all pairs of nn spins (z) on a three-dimensional lattice [here we treat the sc ($z=6$) and bcc ($z=8$) lattices] and H is the strength of the external magnetic field. The competition between the antiferromagnetic exchange interaction and the alignment of the local moments with the external field present interesting properties in the phase diagram. In particular, model (1) has an antiferromagnetic (ordered) phase (AF) in the presence of a field, with the decreasing transition temperature as the field intensity increases, where in $T=0$ (ground state) a second-order transition occurs at critical field $H_c=zJ$.

To treat the model (1) by the EFRG approach, we consider a simple example of renormalization in clusters of sizes $N'=1$ and $N=2$ spins, and the Hamiltonian for these clusters is given by

$$-\beta\mathcal{H}_1' = a_{1B}'\sigma_{1A}, \tag{2}$$

and

$$-\beta\mathcal{H}_{12} = -K\sigma_{1A}\sigma_{2B} + a_{1B}\sigma_{1A} + a_{2A}\sigma_{2B}, \tag{3}$$

where $a_{1B}'=L'-K'\Sigma_\delta^z\sigma_{1B+\delta}$ ($K'=\beta J'$, $L'=\beta H'$) and $a_{i\lambda}=L-K\Sigma_\delta^{z-1}\sigma_{i\lambda+\delta}$ ($K=\beta J$, $L=\beta H$, $i=1$, 2 and $\lambda=A,B$).

By using the Callen–Suzuki relation[19] and following the same strategy of the differential operator technique developed by de Sousa and Araújo[21] to treat the antiferromagnet Heisenberg, the average magnetizations in sublattice A, $m_{1A}'(K',L')=\langle \mathrm{Tr}_1\, \sigma_{1A}e^{-\beta\mathcal{H}_1'}/\mathrm{Tr}_1\, e^{-\beta\mathcal{H}_1'}\rangle$ and $m_{2A}(K,L)=\langle \mathrm{Tr}_{1,2}\, \sigma_{iA}e^{-\beta\mathcal{H}_{1,2}}/\mathrm{Tr}_{1,2}\, e^{-\beta\mathcal{H}_{1,2}}\rangle$ for clusters with $N'=1$ and $N=2$ spins, respectively, are given by

$$m_{1A}'(K',L') = \left\langle \prod_{\delta\neq 1}^{z}(\alpha_x' + \sigma_{\delta B}\beta_x')\right\rangle f(x)|_{x=0}, \tag{4}$$

and

$$m_{2A}(K,L) = \left\langle \prod_{\delta\neq 1,2}^{z-1}(\alpha_x + \sigma_{\delta B}\beta_x)\prod_{\delta\neq 1,2}^{z-1}(\alpha_y + \sigma_{\delta A}\beta_y)\right\rangle \times g(x,y)|_{x,y=0}, \tag{5}$$

with

$$g(x,y) = \frac{\sinh(2L-x-y) + e^{2K}\sinh(x-y)}{\cosh(2L-x-y) + e^{2K}\cosh(x-y)}, \tag{6}$$

where $\alpha_x'=\cosh K'D_x$, $\beta_x'=\sinh K'D_x$, $\alpha_\nu=\cosh KD_\nu$, $\beta_\nu=\sinh KD_\nu(\nu=x,y)$, $D_\nu=\partial/\partial\nu$ is the differential operator, $f(x)=\tanh(L'-x)$ and, z the coordination number.

Equations (4) and (5) are exact, but mathematically intractable. Here we use an approximation which neglects correlations between different spins but takes relations such as $\langle\sigma_{i\lambda}^2\rangle=1$ *exactly* into account, i.e.,

$$\langle\sigma_{iA}\cdots\sigma_{lB}\cdot\sigma_{pB}\cdot\ \cdot\rangle \simeq \langle\sigma_{iA}\rangle\cdot\ \cdot\langle\sigma_{lB}\rangle\cdot\langle\sigma_{pB}\rangle\cdot\ \cdot\ , \tag{7}$$

where $i\neq j\neq\cdots l\neq p\neq\cdots$, and we adopt $b_\lambda'=\langle\sigma_{i\lambda}\rangle$ and $b_\lambda=\langle\sigma_{i\lambda}\rangle$, which correspond to the symmetry-breaking fields in clusters with one ($N'=1$) and two ($N=2$) spins, respectively, for the sublattice $\lambda=A$ and B. Using the approximation (7), Eqs. (4) and (5) are rewritten as

$$m_{1A}'(K',L') = \sum_{p=0}^{z}\binom{z}{p}A_{1p}^z(K',L')b_B'^{p}, \tag{8}$$

and

$$m_{2A}(K,L) = \sum_{p=0}^{z-1}\sum_{q=0}^{z-1}\binom{z-1}{p}\binom{z-1}{q}A_{2pq}^{z}(K,L)b_A^p b_B^q, \quad (9)$$

with $A_{1p}^{z}(K',L')=\alpha_x'^{z-p}\beta_x'^{p} f(x)|_{x=0}$ and $A_{2pq}^{z}(K,L) =\alpha_x^{z-1-q}\beta_x^{q}\alpha_y^{z-1-p}\beta_y^{p}\, g(x,y)|_{x,y=0}$.

This system has two distinct sublattice, which in the ordered phase (AF) have different magnetizations (and symmetry-breaking fields). A natural order parameter is half of the difference in the magnetization of the two sublattice: $m_s=\frac{1}{2}(m_A-m_B)$ (*staggered magnetization*). Is also convenient to define the uniform magnetization by $m=\frac{1}{2}(m_A+m_B)$. The expansion of the right-hand side of Eqs. (8) and (9) in powers of the parameters $b'=\frac{1}{2}(b'_A+b'_B)$, $b'_s=\frac{1}{2}(b'_A-b'_B)$, $b=\frac{1}{2}(b_A+b_B)$, and $b_s=\frac{1}{2}(b_A-b_B)$, in first order in b'_s and b_s are given by

$$m_{1s}(K',L') \simeq A_{1s}(K',L',b')b'_s, \quad (10)$$

$$m_{1}(K',L') \simeq A_{1}(K',L',b'), \quad (11)$$

$$m_{2s}(K,L) \simeq A_{2s}(K,L,b)b_s, \quad (12)$$

and

$$m_{2}(K,L) \simeq A_{2}(K,L,b), \quad (13)$$

with $A_{1s}(K',L',b')=\Sigma_{p=0}^{z}pA_{1p}^{z}(K',L')b'^{p-1}$, $A_1(K',L',b')=\Sigma_{p=0}^{z}A_{1p}^{z}(K',L')b'^{p}$, $A_{2s}(K,L,b)=\Sigma_{p=0}^{z-1}(p-q)A_{2pq}^{z}(K,L)b^{p+q-1}$, and $A_2(K,L,b)=\Sigma_{p=0}^{z-1}\Sigma_{q=0}^{z-1}A_{2pq}^{z}(K,L)b^{p+q}$.

Solving Eqs. (10) and (11) simultaneously, i.e., identifying the symmetry breaking field with the magnetization, $m_{1s}(K,L)=b'_s$, and $m_1(K,L)=b'$, we obtain the critical temperature as a function of H ($K\equiv 1/T_N(H)$) that constitutes the effective field theory in cluster with one spin (EFT-1).[9] For cluster with two spins, the *T*-*H* phase diagram in the EFT-2 scheme is obtained from Eqs. (12) and (13) with $m_{2s}(K,L)=b_s$ and $m_2(K,L)=b$. EFT scheme of this simple type gives, for small clusters, generally poor estimates for the critical temperature. These estimates converge to true values as $N\to\infty$, but this convergence is slow. The critical exponents remain, as for all mean fieldlike theories, classical for all N. The EFRG approach combines EFT ideas with the renormalization group (RG) ideas, and assumes that the staggered magnetizations (order parameter) and symmetry breaking fields they scale in the same way (see Ref. 19), i.e., $m_{N's}=\xi m_{Ns}$ and $b'_s=\xi b_s$. In the EFRG approach for clusters of one and two spins, the fixed critical point $K'=K=K^*=1/T_N(H)$ is obtained from Eqs. (10) and (12), i.e.,

$$A_{1s}(K^*,L',b')=A_{2s}(K^*,L,b), \quad (14)$$

where this critical condition now depends on the *noncritical* variables b' and b, and a reasonable choice for the size dependence of these must be given in order to proceed. A natural choice was proposed by Plascak and Sá Barreto,[22] that postulate an identity between the symmetry breaking field and the uniform magnetization of each cluster, i.e.,

$$m(T)=b'=b, \quad (15)$$

and

$$A_1(K',L',b')=A_2(K,L,b). \quad (16)$$

TABLE I. Values of critical temperature $T_N(0)$, slope of the phase boundary a_c, and critical magnetization $m_c(0)$ for the Ising antiferromagnet on simple cubic (sc) and body-centered cubic (bcc) lattices. Results obtained by the MFRG (Ref. 13), EFRG (present work), series expansion (SE) (Ref. 15), and Monte Carlo (MC) (Ref. 11) methods are presented.

		$m_c(0)$	a_c	$T_N(0)$
MFRG	sc			4.93
	bcc			6.95
EFRG	sc	0.67	−0.44	4.85
	bcc	0.75	0.07	6.88
SE	sc	0.57	−0.04	4.52
	bcc	0.65	0.13	6.35
MC	sc	0.59		4.51
	bcc	0.64	0.16	6.36

We can simultaneously solve the set of three equations (14)–(16) with $L'=L\equiv h/T_N$ ($h=H/J$), and obtain the values of T_N and $b'=b$ for each value of the intensity of the external field H on a simple cubic-sc ($z=6$) and body-centered cubic-bcc ($z=8$) lattices. Results of the numerical values for the slope of the phase boundary $a_c=(dH/dT)_{T=0}$, critical magnetization which is the limiting value of the magnetization as the $T=0$ and $H=H_c$ point is approached along the critical line $m_c=m(T=0)$ and the critical temperature for $H=0$, $T_N(0)$, on the sc and bcc lattices, are displayed in Table I and compared with the series expansion (SE) (Ref. 15) and Monte Carlo (MC) (Ref. 11) values. Our results for the slope $a_c<0$, indicate that the sc cubic lattice does not exhibit the reentrant behavior, while the bcc lattice shown the presence of a small reentrance in the *T*-*H* phase diagram ($a_c>0$). We note here that the EFT method has recently been applied[9] to the simple cubic lattice Ising antiferromagnet in a magnetic field, but in this work the slope values $a_c(\text{EFT-1})=0.29$ and $a_c(\text{EFT-2})=0.24$ are presented indicating a significant decrease in $H_c=6J$ (reentrant behavior). The value $|a_c|=0.44$ obtained by the EFRG approach is systematically larger than the SE results $|a_c|=0.04$, but present the correct qualitative behavior for the critical curve ($a_c<0$).

In Fig. 1, the critical curve T versus H is presented for the sc lattice by using the EFT-1,[9] EFT-2, and EFRG approaches, where we observe a line of continuous phase transitions between the antiferromagnetic (AF) and paramagnetic (P) phases. The data obtained by the EFT-1 and EFT-2 methods clearly show a weak and broad maximum, qualitatively similar to, but much smaller in magnitude, than predicted by mean field approximation (MFA). The effective-field theories (EFT and MFA) ignores correlations in fluctuations away from the ordered state which will tend to destroy the order. An improved approximation which can account for these correlations in fluctuations will show a transition at a lower

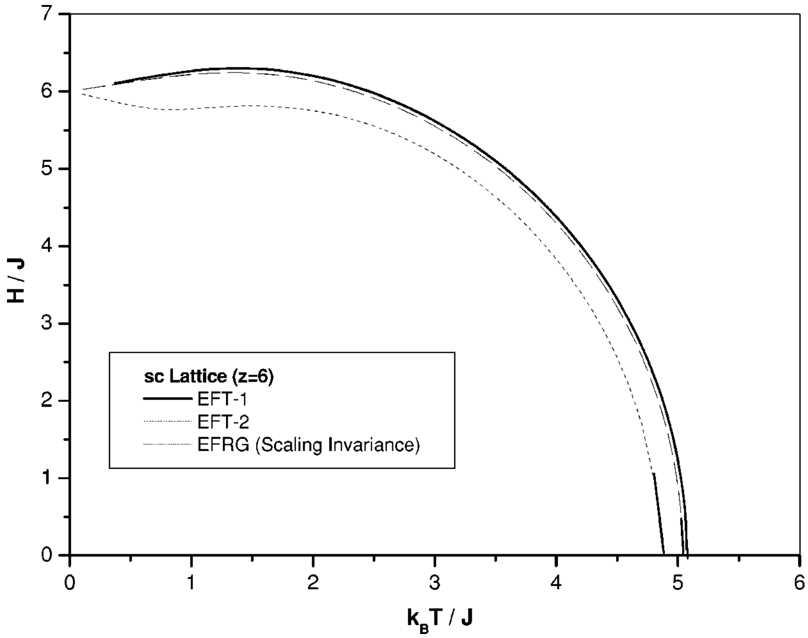

FIG. 1. The dependence of the reduced magnetic field H/J as a function of the reduced critical temperature k_BT/J of the Ising antiferromagnetic model on a simple cubic lattice $(z=6)$. We present the results obtained by the EFT-1 (Ref. 9), EFT-2 (present work), and EFRG (present work) methods.

temperature or at a lower external field than in the EFT case. The RG approaches show this general feature, in accordance with series expansions and Monte Carlo simulations. Of this previous analysis from detailed numerical investigations of finite size scaling (small systems), we found a small tendency for the re-entrance decreasing with an increase of cluster size, and we speculate that for larger values of N these re-entrances disappear in accordance with rigorous results of series expansion.[15] Our results obtained by the EFRG scheme indicate absence of reentrant behavior.

In Fig. 2, we show the phase diagram in the H-T plane for the body-centered cubic (bcc) lattice obtained by the EFRG approach and compared with the results of Monte Carlo simulations.[11] The transition line is of second order for all temperatures and it crosses the H axis at $H_c=8J$. We observe reentrant phenomenon for a certain range of magnetic field around the critical value $H\simeq H_c=8J$. Meanwhile, similar phenomenon can also be seen according to the comparison with MC results. Hence we can infer that the coordination number (z) strongly affects the thermodynamic properties of the present model. Results of Monte Carlo simulation[11] with finite size scaling analysis in bcc lattice show a small increase in H_c with a maximum occurring at $H/zJ\simeq 1.02$ and $H/zJ\simeq 1.04$ obtained by the EFRG scheme. The results obtained may be attributed to the increase of the value of z, that we expected the MFA (or EFT) results become exact as the coordination number goes to infinity $(z\rightarrow\infty)$. We have also applied the MFRG approach,[10,13] but for larger values of H there are no critical temperatures solution in the expected region $(H\simeq H_c$ and $T\simeq 0)$.

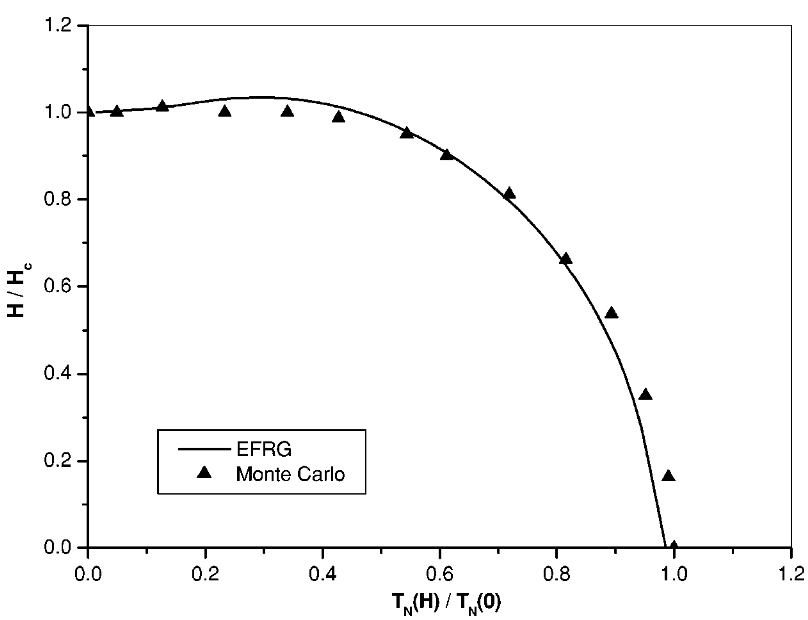

FIG. 2. The dependence of the reduced magnetic field H/J as a function of the reduced critical temperature k_BT/J of the Ising antiferromagnetic model on a body-centered cubic lattice $(z=8)$. We compare our results (EFRG) with Monte Carlo simulations (Ref. 11).

In summary, we have investigated the three-dimensional nearest-neighbor Ising antiferromagnet in a magnetic field by the EFRG approach. Two different types of phase diagram are observed dependent on the value of coordination number (z). First, in the simple cubic lattice $(z=6)$ case we do not observe reentrant phenomenon, in contradiction with spurious results of effective-field theory (EFT) (Ref. 9) and in complete accordance with MC simulations[11] and series expansion.[15] Analyzing finite-size effects (small clusters) with EFT, we found clear evidence of a change in critical behavior, i.e., we observe a tendency of change in the signal of the slope a_c. Second, in the bcc lattice case the reentrant behavior appear with a small increase of critical curve $H(T)$ at low temperature, and our results are in good accordance with Monte Carlo simulation.[11] An interesting extension of this EFRG method is to treat quantum spin models such as the spin $1/2$ Heisenberg and the spin 1 Heisenberg antiferromagnets in the presence of external magnetic field. A solution to this problem (spin $1/2$) has been recently treated by series expansion[23] and variational method.[24] The EFRG approach was developed for the quantum spin $1/2$ Heisenberg antiferromagnet with null field.[21] A further extension, that would increase the size of the clusters, will be welcome in order to give more information of the reentrant behavior in the bcc lattice.

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