Monte Carlo study of the Blume-Emery-Griffiths model at the ferromagnetic-antiquadrupolar-disordered phase interface

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In this paper, we give high precision Monte Carlo (MC) results for the Blume-Emery-Griffiths (BEG) model at the ferromagnetic-antiquadrupolar-disordered phase interface. The data are analyzed by the multiple histogram technique. We show that this point of the phase diagram presents a highly degenerate ground-state with a residual entropy at temperature $T=0$ taking the values $S_\infty=0.7670\pm0.0005$ and 0.7048 ± 0.0008 for the two and the three-dimensional systems, respectively. We prove that the system with dimension $d=2$ does not present any re-entrant behavior, while a re-entrance occurs in the system $d=3$ with a phase transition at $T_c=1.036\pm0.007$. Results for a multilayer system are also presented. They show that the re-entrance begins to appear for $M\geqslant5$, where M is the number of layers. Finally, the staggered quadrupolar phase is shown to be unstable for $d=2$ and $d=3$ as well.

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I. INTRODUCTION

In addition to the bilinear exchange interaction J of the standard Ising model, the spin-1 Ising model possesses a biquadratic exchange interaction K and a single ion crystal field Δ. It is also known as the Blume-Emery-Griffiths (BEG) model and was originally introduced in order to explain the phase separation and superfluidity in He^3–He^4 mixtures[1] and was later developed to describe multicomponent fluids, liquid crytal mixtures, microemulsions and semiconductor alloys (see Ref. 2, and references therein). The model is described by the following Hamiltonian:

$$\mathcal{H}=-J\sum_{\langle ij\rangle}S_iS_j-K\sum_{\langle ij\rangle}S_i^2S_j^2+\Delta\sum_i S_i^2, \qquad (1)$$

where $S_i=0$, $+1$ or -1 is the spin at site i and $\Sigma_{\langle ij\rangle}$ stands for a summation over all nearest-neighbor pairs. The model with vanishing biquadratic interaction ($K=0$) is known as the Blume-Capel model.[3–5] Without loss of generality, we can assume that $J>0$, because the antiferromagnetic case can be obtained from the ferromagnetic one by redefining the spin direction of one of the two sublattices in a bipartite lattice and we can set $J=1$ for what follows.

From a theoretical point of view, the BEG model has attracted considerable interest due to the variety of topologies of its phase diagrams and the multitude of critical behaviors it exhibits for different values of its parameters. In this respect, we mention the mean field extensive study[2] of the phase diagrams. A similar global work was done on a magnetic bilayer[6] using a cluster variational theory within the pair approximation. The latter results apply to the BEG model on a fivefold coordination Bethe lattice as well. The two-dimensional model was also studied by real-space renormalization group theory and by finite size scaling analysis.[7] Monte Carlo simulations have been also applied and revealed interesting features of the BEG model.[8–10]

At temperature $T=0$, we can define three regions of the phase space: the ferromagnetic (F), the disordered (D), and the staggered quadrupolar (SQ) phases (the SQ phase is also known as the antiquadrupolar phase). These phases minimize the Hamiltonian (1) and are represented in the (K,Δ) plane by

$$F=\{(K,\Delta):1+K-2\Delta/z>0;1+K-\Delta/z>0\},$$

$$D=\{(K,\Delta):1+K-2\Delta/z<0;\Delta>0\},$$

$$SQ=\{(K,\Delta):1+K-\Delta/z<0;\Delta<0\},$$

where z is the coordination number. The SQ phase is characterized at $T=0$ by a highly degenerate ground-state with one sublattice (say A) occupied by spins $S_i^A=0$ and the other sublattice (B) is randomly occupied by spins $S_i^B=\pm1$, or equivalently $S_i^B=0$ and $S_i^A=\pm1$. This leads to an exact number of configurations equal to the partition function at $T=0$: $Z_N^0=2\times2^{N/2}=2^{N/2^+1}$, where N is the total number of sites in the lattice. In the thermodynamic limit $N\to\infty$, the reduced free energy per site defined by $f=N^{-1}\ln Z^0$ becomes $f=\ln 2/2$ and represents the ground-state entropy of the system. In addition, at the SQ boundaries SQ-D and SQ-F, the BEG model has also infinitely many ground-state configurations, especially at the F-SQ interface where there appears a kind of a ferromagnetic ordering.[2]

There exists a point in the phase diagram where all the above mentioned three phases meet. It has coordinates $(K=-1,\Delta=0)$ and is very highly degenerate as we will prove. It has been shown,[2] using mean field theory, that the BEG model at this point, exhibits a re-entrant behavior in the continuous F–D phase boundary. Monte carlo studies[9] in one hand, and real space renormalization group investigations and finite size scaling analysis[7] in the other hand, found no evidence of this re-entrant behavior in the two-dimensional system. A slight re-entrance was also found in the bilayer system[6] with the use of the cluster variational theory within the pair approximation. The bilayer system ($z=5$) lies somewhat between the two-dimensional square lattice ($z=4$) and the three-dimensional cubic lattice ($z=6$). On the other hand, it is well established that the mean field picture is valid

only for higher dimensions, and we find it useful to give more insight into the nature of the critical behavior at this special point.

In the present paper, extensive Monte Carlo simulations were performed in order to clarify the situation about the re-entrant behavior of the BEG model at $(K=-1,\Delta=0)$ making use of the Mixed Cluster Algorithm (MCA) (Refs. 11,12) and the multiple-histogram technique.[13,14] It is found that no re-entrance is present in dimension $d=2$ while for $d=3$ a clear re-entrance takes place. In addition, we have studied a system with M layers and found that the bilayer system presents no re-entrance in contrary to what was speculated in Ref. 6. The re-entrance appears only for $M \geqslant 5$. Finally, we find that the staggered quadrupolar phase is unstable at $T=0$ for all system dimensions.

II. SIMULATION ALGORITHMS

For the purpose of this work, we have used the Mixed Cluster Algorithm (MCA) developed by Bouabci and Carneiro[11] and recently generalized by Rachadi and Benyoussef.[12] This algorithm has the advantage that it uses, in each step, mixed clusters of either + and 0 spins or − and 0 spins in addition to the well known Wolff clusters of like spins. This fact makes of it a useful tool to simulate the physics of the BEG model at the region of the parameter space lying at the interface between the ferromagnetic, the staggered quadrupolar and the disordered phases. The algorithm proceeds with the following way. We select randomly two different spin values S^0 and S^1. If $S^1=-S^0$, we build Wolff clusters with probability $p_w=1-\exp[-2\beta]$ for making bonds between sites having spins S^0 and flip them automatically. In the other case, we construct mixed clusters with probability $p_{\mathrm{eq}}=1-\exp[-2\beta/3]$ and $p_{\mathrm{eq}}=1-\exp[-4\beta/3]$ for making bonds between like spins and different spins, respectively. (This corresponds to taking the value $-2/3$ for the parameter λ in Ref. 12.) Then the mixed clusters are flipped with the metropolis rate according to the energy change of the system. The flip of the mixed clusters consists of performing the moves $(+\rightarrow 0$ and $0\rightarrow -)$ or $(-\rightarrow 0$ and $0\rightarrow +)$ for the $(+,0)$ and $(-,0)$ clusters, respectively.

We have also taken advantage of the local nature of the metropolis algorithm. Indeed, for the BEG model at the point $(K=-1,\Delta=0)$, the energies E_{ij} of link $\langle ij\rangle$ are all equal except when $S_i=-S_j$ (and $S_i\neq 0$). This guarantees that the standard Metropolis algorithm does not suffer from the fact that the majority of the flip attempts are unsuccessful. In short, we have adopted an hybrid algorithm which performs an MCA sweep followed by a standard Metropolis sweep. Such hybrid algorithms are shown to be useful in increasing the performance substantially and reducing statistical errors of the simulations especially for the spin-1/2 and the spin-3/2 Ising models.[15] The Monte Carlo time is normalized so to get one MC step per site for one unit time. The simulations performed in this paper are of lengths up to 10^6 MCS/spin.

In order to locate the critical temperature, we have used a slightly modified version of the probability changing cluster (PCC) algorithm.[16] The numerical advantage of this algorithm is that it can find the system critical temperature in its own in a single run. The main idea of the PCC algorithm is to adjust continuously the system temperature so that this latter is always brought back to stay near its critical temperature. This can be achieved by decreasing or increasing the probability p of constructing a bond between neighboring sites having the same spin depending on the observation that the system is percolating or not. The existence of at least one cluster invading the lattice and wrapping around the periodic conditions is a sufficient condition for percolation. After completing a sufficient number of MC steps, we obtain the critical temperature T_c as an output of the simulation by the formula $T_c=-2/\ln(1-p)$.

When applied to the BEG model, the PCC algorithm, in its original form, is not ergodic because it does not change the magnitude of the spins but only their signs. The solution adopted is based on a simple idea. We supplement every PCC updating sweep by a standard Metropolis sweep which we perform at the actual simulation temperature $T=-2/\ln(1-p)$.

Some of the MC results are analyzed with the multiple-histogram technique[13,14] which is particularly useful when determining the ground-state entropy of the system. In the simulations presented here, the multiple-histogram results are obtained using combined data from up to 22 simulations at different temperatures. These simulations are performed at regular intervals for dimension $d=2$ ranging from 0 to 4.5. While for the three-dimensional system, more simulations are performed at the vicinity of the transition temperature where strong statistical fluctuations are present.

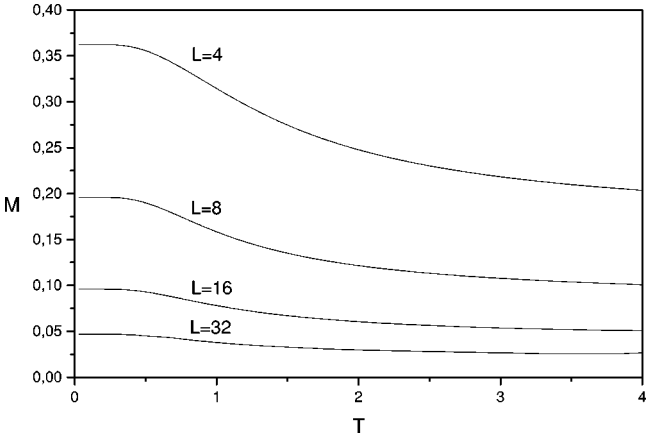

FIG. 1. Magnetization as a function of temperature in two dimensions for system sizes $L=4$, 8, 16, and 32. The results are obtained with 16 histograms for $L=4$ and 8 and 22 histograms for $L=32$, with 10^6 MCS per spin for each run.

III. RESULTS AND DISCUSSIONS

In this section we present the results of our simulations concerning the BEG model at the point $(K=-1,\Delta=0)$. We have plotted in Fig. 1, the magnetization M of the two-dimensional square lattice as a function of temperature T with the use of the multiple-histogram method for system linear sizes $L=4$, 8, 16, and 32. Our Monte Carlo data are consistent with no spontaneous magnetization in the thermo-

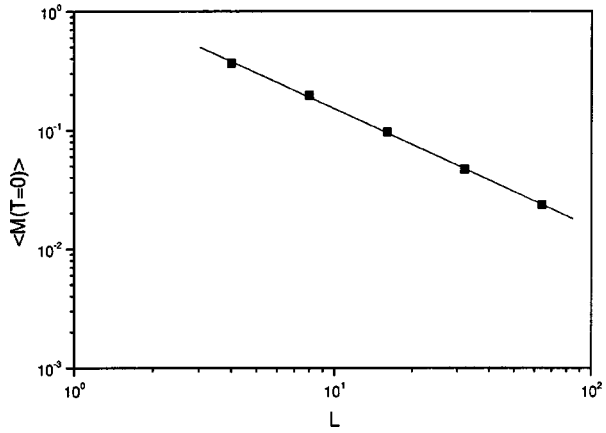

FIG. 2. Log–log plot of the zero-temperature magnetization $M(T=0)$ vs linear size L in a two-dimensional lattice. The straight line is a linear fit with a slope -1.

dynamic limit at all temperatures, including $T=0$. Indeed, if we represent the variation of the magnetization $M(T=0)$ with system size up to $L=64$ as shown in Fig. 2 in a log–log scale, we can see that it decreases as $M(T=0)\propto L^{-d/2}$ within statistical errors as expected for a paramagnetic phase.

Thus, even at $T=0$, there is no temperature driven phase transition. In relation to this point, it was stated in Ref. 9 that the critical temperature approaches zero linearly as $T_c=3.8(1+K)$ when K approaches -1. our results suggest that despite this result, the point $(K=-1,\Delta=0)$ does not belong the universality class of the critical line it terminates and no evidence of a re-entrant behavior is found for a two-dimensional square lattice at this point.

On the other hand, our results for the $d=3$ system are compatible with a nonvanishing zero-temperature magnetization in the thermodynamic limit as can be seen from Fig. 3.

Apart from a slightly higher value for system size $L=4$, the $T=0$ magnetization decreases towards a finite value 0.4260 ± 0.0025 supporting the idea of a finite temperature second order phase transition. We note also that this value of the magnetization is much lower than that of maximal ferro-

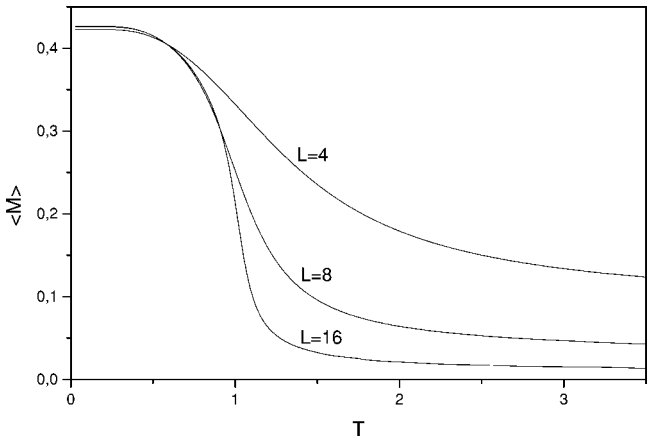

FIG. 3. Magnetization as a function of temperature in three dimensions for system sizes $L=4$, 8, and 16. The results are obtained with 22 histograms with 10^6 MCS per spin for each run.

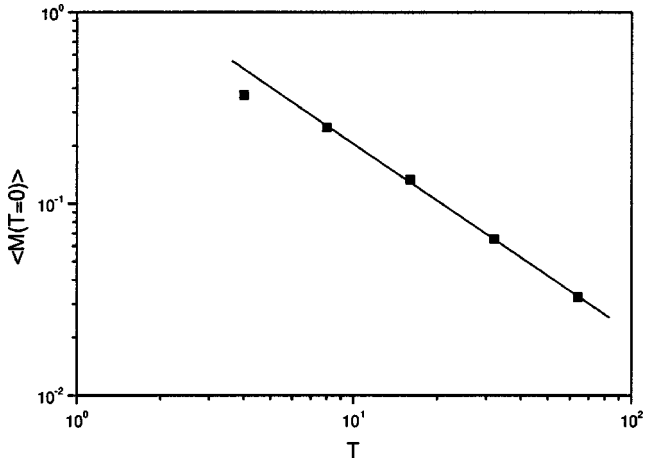

FIG. 4. Log–log plot of the zero-temperature magnetization $M(T=0)$ vs linear size L in a bilayer lattice. The straight line is a linear fit with a slope -1.

magnetic order due to the existence of other phases. In order to determine the critical temperature for $d=3$, we have used the hybrid probability changing cluster (PCC) algorithm described above. Our simulations with this algorithm lead to $T_c=1.036\pm0.007$ which, as can be expected, is much lower than the mean field prediction.[2]

We have demonstrated that the bidimensional square BEG model $(z=4)$ cannot order ferromagnetically at any temperature while the three-dimensional system $(z=6)$ does show a re-entrant behavior. There is a system which lies somewhat between these two ones and which has coordination number $z=5$. This is the magnetic bilayer system. It was studied[6] in the framework of the cluster variational method within the pair approximation and found to possess a slight re-entrant behavior.

We did simulations at $T=0$ for this bilayer system and found (Fig. 4) that the zero-temperature magnetization decreases with the total number of sites N as $M(T=0)\propto N^{-1/2}$ which characterizes a paramagnetic phase excluding the presence of any re-entrant behavior for this system.

Moreover, we did simulations for a system of M layers to see for what value of M, the system becomes to present a re-entrance. For $M=1$ and $M=2$ which correspond to the two-dimensional and the bilayer systems respectively, we have proven the absence of any re-entrance. For $M\to\infty$ which corresponds to the three-dimensional system, there is a clear ferromagnetic re-entrance. So, we expect that for some intermediary value $2<M_c<\infty$, the re-entrance becomes to appear. In fact, our MC simulations for an $L\times L\times M$ system indicate that for $M_c=5$, the system becomes to preserve a nonvanishing zero-temperature magnetization in the thermodynamic limit with $\langle M(T=0)\rangle=0.3541\pm0.0015$. To confirm the existence of a finite temperature transition, we performed a simulation with the hybrid PCC algorithm as described above and found a critical temperature $T_c=0.616\pm0.001$.

Although there is no re-entrance for the multilayer system with $M\leqslant4$, we found a peculiar behavior for $M=4$. Indeed, the decrease of the zero-temperature with system size does

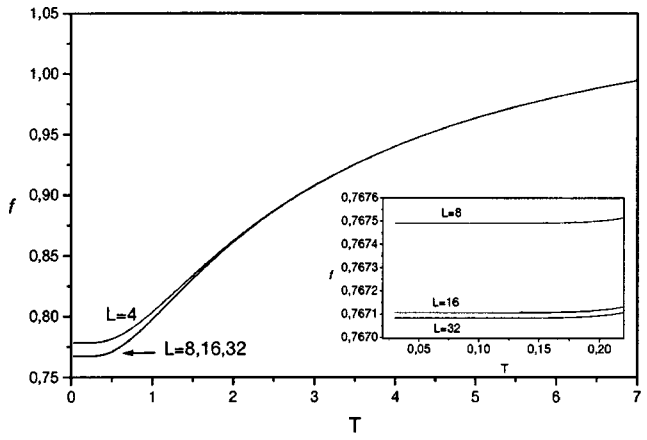

FIG. 5. Reduced free energy per site $f=N^{-1}\ln Z$ as a function of temperature for dimension $d=2$. The histograms used are taken from the same set of data as those of Fig. 1. The inset shows the low temperature part in a greater scale to distinguish the values corresponding to higher values of L.

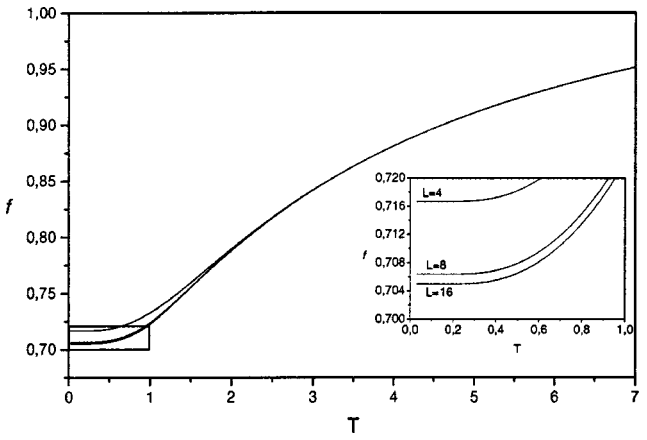

FIG. 6. Reduced free energy per site f as a function of temperature for dimension $d=3$. The histograms used are taken from the same set of data as those of Fig. 3. The inset shows the low temperature part in a greater scale to distinguish the values corresponding to higher values of L.

not follow the paramagnetic scaling, but a scaling law $\langle M(T=0)\rangle \propto L^{-\beta/\nu}$ characterizing a ferromagnetic-paramagnetic transition at $T=0$ with an exponent $\beta/\nu=0.21$. This is a somewhat intermediary behavior between a strong decrease of the magnetization characterizing the absence of a phase transition and a stability of the ferromagnetic phase at $T=0$ characterizing a nonzero phase transition.

Now, we return to the highly degenerate character of the system ground-state at $(K=-1,\Delta=0)$. As it is known, numerous systems present such an infinitely many ground-state configurations. A typical example of these systems is the antiferromagnetic three state Potts model.[17] This model is equivalent to the Blume-Emery-Griffiths model at $(K=-3,\Delta/z=2)$ with the spin direction of one of the two sublattices being redefined and $J>0$. This means that this model lies at the antiquadrupolar-disordered interface. Thus, we expect the zero-temperature entropy of our model to be higher than the values $\frac{3}{2}\ln\frac{4}{3}$ (see Refs. 17,18) and 0.3673 (see Ref. 18) found for the antiferromagnetic three state Potts model with $d=2$ and $d=3$, respectively. This is due to the fact that the space of the ground-states of this model is in fact a subset of the configuration space of the BEG model at $(K=-1,\Delta=0)$ located at the ferromagnetic-antiquadrupolar-disordered interface. Another model which presents a highly degenerate ground-state is the q-state antiferromagnetic $Z(q)$ model recently studied for $q=5$ and $q=7$ (see Ref. 19).

One way to determine the ground-state entropy is to make use of the multiple histogram technique. As we pointed out before, if we perform MC simulations in different temperatures up to a sufficiently high temperature, we can cover the entire range of temperature from $T=\infty$ where the entropy is known to be $\ln 3$ down to $T=0$. Then using the multiple histogram self-consistent relations we can compute the free energy as a function of temperature and shift it by adding a convenient constant such that for higher temperatures the free energy coincides with the limit $\ln 3$.

Figures 5 and 6 presents plots of the variation with temperature of the reduced free energy per site $f=N^{-1}\ln Z$, where Z is the system partition function, for $d=2$ and $d=3$, respectively. The results are obtained using up to 22 histograms each with 10^6 MCS per spin. The zero-temperature entropies extrapolate to the thermodynamic limit $L\to\infty$ as $S(L)=S_\infty+bL^{-d}$, where b is some constant. We found $S_\infty=0.7670\pm0.0005$ and $S_\infty=0.7048\pm0.0008$, respectively, for the two and the three-dimensional systems. As we expected, these values are much higher than those of the three-state antiferromagnetic Potts model.

Concerning the staggered quadrupolar phase, our MC simulations are in favor of the fact that this phase is unstable at $T=0$ for both the $d=2$ and the $d=3$ systems. This can be deduced from the variation with system size of the order parameter $Q=2/N[\Sigma_{i\in A}S_i^2-\Sigma_{i\in B}S_i^2)]$, where A and B stand for the two interpenetrating sublattices in a bipartite lattice such that all sites in sublattice A have their nearest neighbors in sublattice B and vice versa. Figure 7 shows

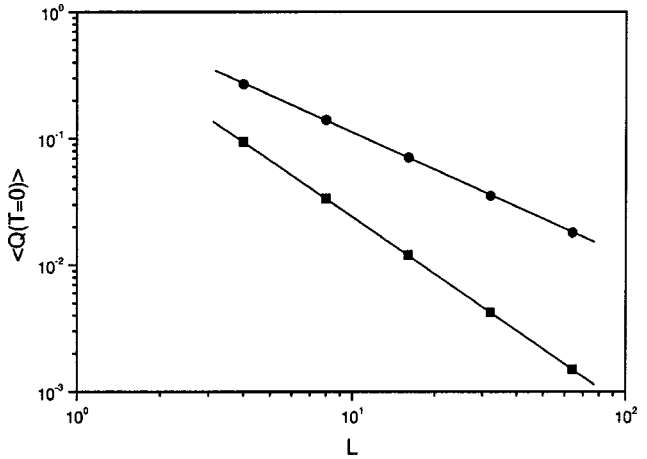

FIG. 7. Plot of the variation with system size of the order parameter $Q=2/N[\Sigma_{i\in A}S_i^2-\Sigma_{i\in B}S_i^2)]$, for both the $d=2$ (circles) and the $d=3$ (squares) systems. The corresponding straight lines have slopes -1 and -1.5, respectively.

these variations which follow clearly the law $\langle Q(T=0)\rangle \propto L^{-d}$ indicating that the SQ phase in indeed unstable in the thermodynamic limit.

In the following, we give an argument which, though not rigorous, can give more insight into the reasons of the unstability of the SQ phase at $T=0$. As we pointed out before, a completely ordered SQ phase has an exact number of configurations equal $N_{\mathrm{SQ}}=2^{N/2+1}$ in a lattice of N sites. Correspondingly, the total number N_T of configurations of our model at $T=0$ can be estimated from the ground-state entropy $S_N=N^{-1}\ln N_T$. Then the ratio N_{SQ}/N_T can be written

$$\frac{N_{\mathrm{SQ}}}{N_T}=\frac{2^{N/2+1}}{\exp[NS_N]}=\exp\left\{N\left[\left(1+\frac{1}{N}\right)\ln 2-S_N\right]\right\}. \quad (2)$$

As $N\to\infty$, this ratio tends to $\exp\{N[\ln 2-S_\infty]\}$. The values S_∞ calculated for the two and the three-dimensional systems (see above), are much greater than $\ln 2$. Then, we conclude that in the thermodynamic limit, the number of configurations characterizing a SQ phase are negligible in comparison to the huge total number of configurations at $T=0$ and the SQ phase becomes unstable. Moreover, even if we consider incompletely ordered SQ configurations and overestimate N_{SQ} to $N_{\mathrm{SQ}}\sim N^{\alpha}\times 2^{N/2+1}$ with $\alpha>0$, the precedent argument still holds and the contribution of these configurations to the total number vanishes in the infinite-size limit. Thus, we conclude that the high values of the zero-temperature entropy are responsible for the unstability of the SQ phase at $T=0$.

Recently, it was shown[20] that the BEG model at the SQ-D phase interface presents a spin–spin correlation function which decays exponentially fast at all nonzero temperatures. The authors argued that this behavior indicate the absence of re-entrance for $\Delta=0$ and $K<K_d$, where K_d depends on the dimension d ($K_d=-6.395$ for $d=2$). These results cannot be applied to the model studied here which is a limiting case where the staggered quadrupolar phase is unstable even at zero temperature.

IV. CONCLUSION

Using both the Monte Carlo mixed cluster algorithm (MCA) and the probability changing cluster (PCC) algorithm, we studied the BEG model at the ferromagnetic-antiquadrupolar-disordered phase interface located at ($K=-1,\Delta=0$) with infinitely many ground-state configurations. We showed that the ferromagnetic phase is unstable at $T=0$ in the thermodynamic limit for dimension $d=2$ and stable for the three-dimensional system giving rise to a re-entrant behavior. This re-entrance is shown to be absent for a multilayer system with less than 5 layers. We computed the values of the zero-temperature entropy for $d=2$ and $d=3$ and found that these values are relatively high which causes the instability of the staggered quadrupolar phase for all dimensions at $T=0$.

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