Phase diagrams of the three-dimensional semi-infinite Blume-Emery-Griffiths model

A. Bakchich
Département de Physique, Faculté des Sciences Dhar Mahraz, B.P. 1796 Atlas, Fès, Morocco

M. El Bouziani
Laboratoire de Physique de la Matière Condensée, Département de Physique, Faculté des Sciences, B.P. 20, El Jadida, Morocco

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Within a real-space renormalization-group framework based on the Migdal-Kadanoff recursion relations, we investigate the three-dimensional semi-infinite Blume-Emery-Griffiths model with nearest-neighbor interactions, both bilinear and biquadratic, and with a crystal-field interaction. According to the values of the interactions on the surface and in the bulk of the system, we determine the various generic types of phase diagrams in the case of repulsive biquadratic interactions. Our analysis has led to a classification scheme with eleven fundamental types of phase diagrams describing a large variety of phase transitions associated with the surface and multicritical topologies. [S0163-1829(97)05837-2]

I. INTRODUCTION

The Blume-Emery-Griffiths (BEG) model[1] is a spin-1 Ising model with bilinear (J) and biquadratic (K) nearest-neighbor pair interactions in which a single-ion anisotropy parameter (Δ) is included. First studied[1] in the context of superfluidity and phase separation in helium mixtures, this model has been extended to describe phase transitions in simple[2] and multicomponent fluids,[3,4] microemulsions,[5] and semiconductor alloys.[6]

The infinite BEG model is described by the following reduced Hamiltonian:

$$-\beta H=J\sum_{\langle ij\rangle} S_iS_j+K\sum_{\langle ij\rangle} S_i^2S_j^2+\Delta\sum_i S_i^2, \tag{1}$$

where the spins ($S_i=-1,0,1$) are located on the sites of a cubic lattice and the first and second summations run over all neighboring pairs of spins.

An extensive analysis of this model was made by means of mean-field approximation (MFA),[1–4] renormalization-group techniques,[7,8] series expansions methods,[9] and by Monte Carlo simulations.[10,11] All those treatments have essentially been confined to the parameter space with positive ($J,K>0$) interactions, and features of the phase transitions in these cases are now well understood. In the case of repulsive ($K<0$) interactions, the phase diagram is expected to be much more complicated by the analogy with the previous case. However, a recent study[12] of the global phase diagram of the BEG model for three-dimensional lattices with $K<0$ was made using MFA, showing a variety of interesting features, including single and double reentrancy regions and ferrimagnetic phases. In a renormalization-group calculation,[13] a qualitatively different sequence of phase diagrams does set in above a threshold spatial dimension around $d\approx 3$, but these diagrams are different from the ones of MFA. The main discrepancy is that no ferrimagnetic phase is seen. Attention has been drawn independently to the negative biquadratic interactions region of the BEG model through a connection to the t-J model of electronic conduction[14] and through the applicability to ordering in semiconductor alloys.[15]

In the last few years some attention has been devoted to the study of the BEG model over semi-infinite lattices, with different couplings at the surface and in the bulk. A special case of this model has been studied[16] by Benyoussef, Boccara, and Saber. They use MFA to discuss the possible phase diagrams of the model for $K=0$ [which corresponds to the semi-infinite Blume-Capel (BC) model[17,18]]. However, they use a single order parameter (the magnetization) to characterize the different phases, and do not allow for the full spatial variation of the magnetization. A few other works have carried out the same investigation by means of a real-space renormalization-group (RSRG) framework,[19] and a cluster variation method (CVM).[20] Some applications of the semi-infinite BEG model to the study of surface superfluidity in ^{3}He-^{4}He mixtures have been also investigated both with RSRG (Refs. 21, 22) and MFA.[23]

For the semi-infinite BEG model no explicit calculations have appeared in the literature with repulsive biquadratic interactions, which is drastically and richly different, as will be seen from the global study reported in this paper. Using a renormalization-group transformation in position space based on the Migdal-Kadanoff[24,25] (MK) recursion relations, first we locate the 16 separate fixed points underlying the structure of the infinite model. Then this method will be used to study the three-dimensional semi-infinite system, and since in this case the recursion relations have a large number of fixed points, the results obtained for the infinite system will help in understanding the meaning of the various fixed points.

According to the values of the interactions on the surface and in the bulk of the system, we observe four different types of phase transitions associated with the surface, which can be designated using the same known terminology,[26] namely, the ordinary transition with simultaneous onset of bulk and surface order, the surface transition where the surface orders first, the subsequent extraordinary transition where the bulk orders in the presence of an already ordered surface, and the special transition with bulk and surface ordering at the same temperature but with a different set of critical exponents. While these results are well established, the literature shows a controversy about the order of these transitions. Indeed it is shown, both by MFA (Ref. 16) and CVM,[20] that the ordinary, extraordinary, and surface transitions can be either second or first order. By contrast, in the research reported here, we shall determine the various phase diagrams given by renormalization-group theory. Our analysis has led to a classification scheme with eleven fundamental types of phase diagrams, some of which we have illustrated in the $(J_s^{-1},\Delta_s J_s^{-1})$ plane, where the subscript s refers to the surface. Taking into account the nature of the fixed points we show that the ordinary transition, which presents the reentrant phenomenon, can be either first order, second order, or tricritical (we used the Nienhuis-Nauenberg criterion[27] to determine which fixed points characterize first-order transitions), while the extraordinary and surface transitions are always of second order. Moreover, it is shown that such a system can exhibit critical and (ordinary and special) tricritical points, critical end points, and multicritical points.

One should note also that the method we have used did not obtain reentrancy, and the ferrimagnetic phase, which was referred to in Refs. 12, 28 and 29, has never appeared in the whole temperature range since there exists only one ferromagnetically ordered fixed point. The phase boundary between the ferromagnetic and staggered quadrupolar phases is controlled by a singly unstable fixed point. Thus the RSRG does not reproduce the mean-field results, and may miss certain features of the phase diagram owing to the restricted flow space in which the renormalization by necessity must be carried out. This has been first speculated by Hoston and Berker,[13] and later proven by Netz and Berker,[30] who showed how to enlarge the flow space and reproduce the main features of the mean-field calculation in a RSRG framework. This assumption was also confirmed[31] by means of Monte Carlo calculations, and the MFA results were assumed to be correct for $d=3$.

II. THE SEMI-INFINITE BEG MODEL

We will be concerned with the three-dimensional semi-infinite BEG model with ferromagnetic nearest-neighbor interactions on a simple cubic lattice. The reduced Hamiltonian is given by

$$-\beta H=J_s\sum_{\langle ij\rangle} S_iS_j+K_s\sum_{\langle ij\rangle} S_i^2S_j^2+\Delta_s\sum_i S_i^2+J_B\sum_{\langle kl\rangle} S_kS_1 +K_B\sum_{\langle kl\rangle} S_k^2S_l^2+\Delta_B\sum_k S_k^2, \tag{2}$$

where i, j, k, and l are site labels, $\Sigma_{\langle ij\rangle}$ denotes a sum over all nearest-neighbors with both sites lying on the surface, $\Sigma_{\langle kl\rangle}$ denotes a sum over the remaining nearest neighbors, and $\beta=(k_BT)^{-1}$ (with k_B the Boltzmann constant and T the absolute temperature). J_S and J_B (both positive, since we study the ferromagnetic case) are reduced exchange interactions, while K_S and K_B are reduced biquadratic exchange interactions and Δ_S and Δ_B are reduced crystal fields, respectively, at the surface and in the bulk.

The resulting phases (on the surface or in the bulk) of the model described by the Hamiltonian (2) are variously distinguished by four order parameters

$$m_A=\langle S_i\rangle_A,\quad m_B=\langle S_i\rangle_B,\quad q_A=\langle S_i^2\rangle_A,\quad q_B=\langle S_i^2\rangle_B,$$

where A and B refer to the two sublattices.

The ferromagnetic (F) phase is characterized by $m_A=m_B\neq 0$. The two paramagnetic phases labeled P_+ and P_- are distinguished by $m_A=m_B=0$ with $q_A=q_B>\frac{1}{2}$, and $q_A=q_B<\frac{1}{2}$, respectively. Those distinct dense and dilute versions of the disordered phase have no different symmetry, and one can continuously pass from one to the other without crossing any transition surfaces. The staggered quadrupolar (SQ) phase has $m_A=m_B=0$ and $q_A\neq q_B$. It is characterized by two interpenetrating sublattices. One sublattice has $S_i=0$ at every site, while the other sublattice has its sites occupied at random by $S_i=\pm 1$. The ferrimagnetic (FR) phase is distinguished by nonzero magnetization and sublattice symmetry breaking ($m_A\neq m_B\neq 0$ and $q_A\neq q_B$).

We apply a RSRG transformation based on the MK bond-moving approximation. This technique is tractable in all space dimensionalities, so we shall give the recursion relations for a d-dimensional hypercubic model. Let us briefly describe the method.

Dictated by the possible sublattice symmetry breaking, we may restrict ourselves to an odd scale factor b. In the present study we choose $b=3$ and consider a one-dimensional chain of spins coupled by nearest-neighbor interactions J, K, and a crystal-field Δ. We perform the trace over all spins on the chain except those at the end. The end spins are then coupled by effective interactions $\tilde{J}$, $\tilde{K}$, and $\tilde{\Delta}$, which are functions of J, K, and Δ. In a semi-infinite d-dimensional cubic lattice, it is straightforward[32,33] to extend Migdal's argument and obtain the renormalized couplings J', K', and Δ' as functions of J, K, and Δ. In the particular case of the semi-infinite BEG model we get

$$\begin{aligned} J_B'&=b^{d-1}\tilde{J}(J_B,K_B,\Delta_B),\\ K_B'&=b^{d-1}\tilde{K}(J_B,K_B,\Delta_B),\\ \Delta_B'&=b^{d-1}\tilde{\Delta}(J_B,K_B,\Delta_B), \end{aligned} \tag{3a}$$

$$\begin{aligned} J_s'&=b^{d-2}\tilde{J}(J_s,K_s,\Delta_s)+\tfrac{1}{2}(b-1)b^{d-2}\tilde{J}(J_B,K_B,\Delta_B),\\ K_s'&=b^{d-2}\tilde{K}(J_s,K_s,\Delta_s)+\tfrac{1}{2}(b-1)b^{d-2}\tilde{K}(J_B,K_B,\Delta_B),\\ \Delta_s'&=b^{d-2}\tilde{\Delta}(J_s,K_s,\Delta_s)+\tfrac{1}{2}(b-1)b^{d-2}\tilde{\Delta}(J_B,K_B,\Delta_B). \end{aligned} \tag{3b}$$

The renormalization-group phase diagrams are derived from the global study of flows in Hamiltonian space, which are governed by fixed points (points invariant under the transformation). The determination of the various fixed points of the recursion relations (3) seems at first sight a rather complicated problem. However, as usual for the semi-infinite systems, the renormalized bulk interactions given by Eq. (3a) depend only on the initial bulk interactions J_B, K_B, and Δ_B. Therefore, in order to determine the six coordinates $(J_B^*,K_B^*,\Delta_B^*,J_s^*,K_s^*,\Delta_s^*)$ of each fixed point, we shall first determine the (J_B^*,K_B^*,Δ_B^*) coordinates from Eq. (3a), and

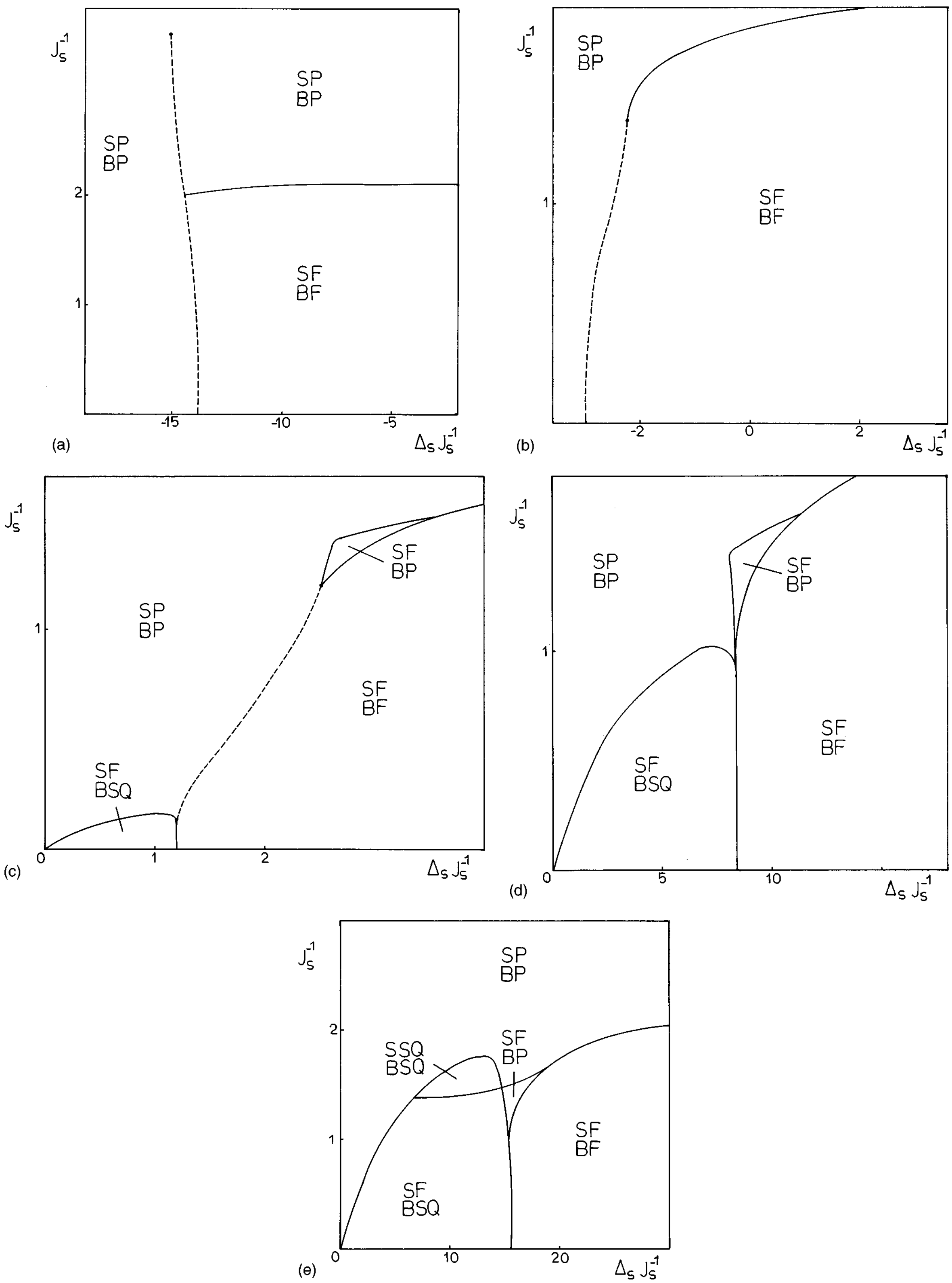

FIG. 1. Typical phase diagram for the three-dimensional semi-infinite BEG model, from global renormalization-group theory, calculated for ($R = 0.75$, $D = 1.25$) and (a) $R_0 = -5$ and $R_1 = -1$, (b) $R_0 = -5$ and $R_1 = -0.1$, (c) $R_0 = -5$ and $R_1 = 0.2$, (d) $R_0 = -5$ and $R_1 = 0.5$, and (e) $R_0 = -5$ and $R_1 = 0.8$. Dashed and solid lines represent, respectively, first- and second-order phase transitions. The symbols SP, BP, SF, BF, SSQ, and BSQ denote, respectively, surface paramagnetic, bulk paramagnetic, surface ferromagnetic, bulk ferromagnetic, surface staggered quadrupolar, and bulk staggered quadrupolar phases.

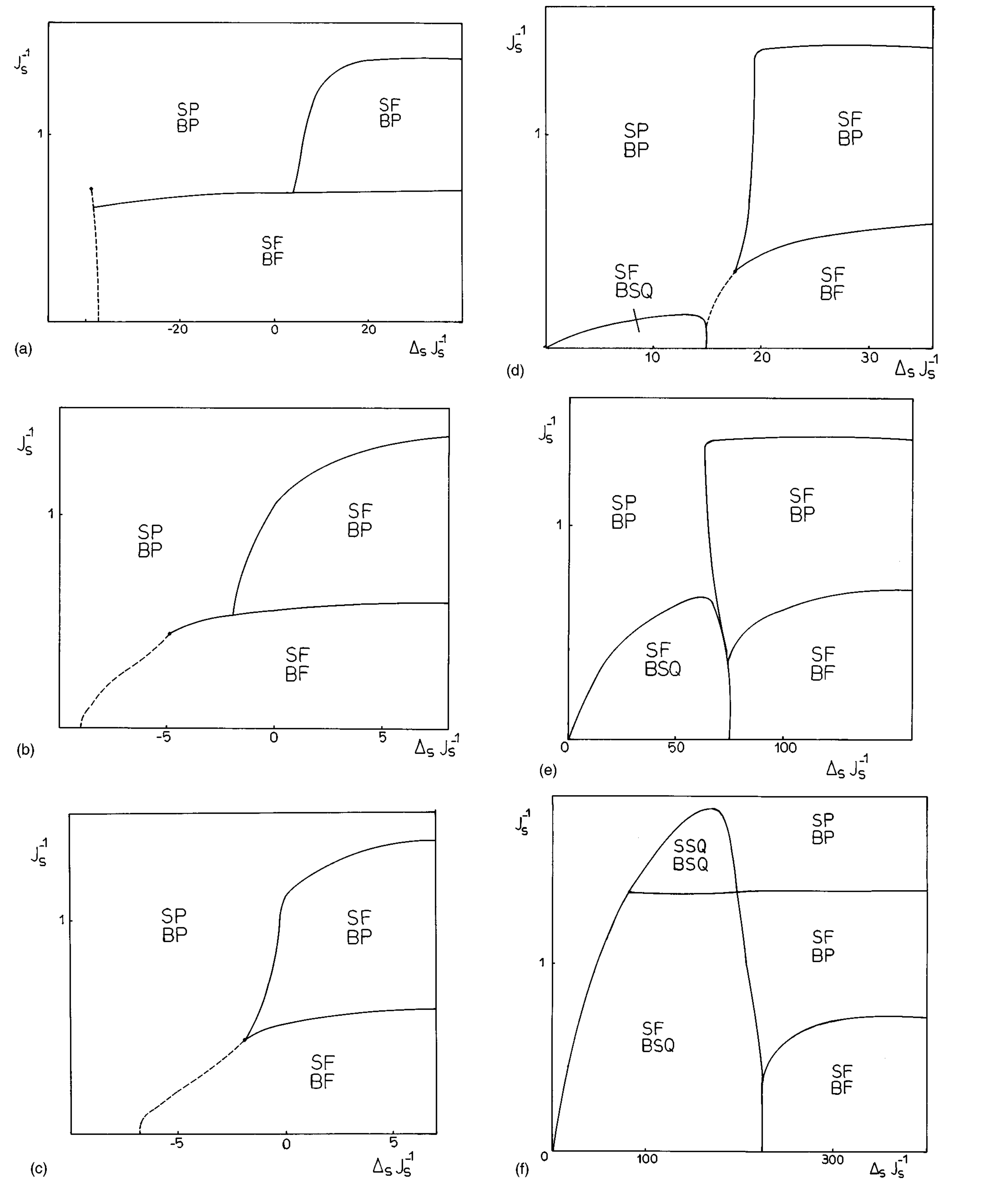

FIG. 2. Typical phase diagram for the three-dimensional semi-infinite BEG model, from global renormalization-group theory, calculated for $R=0.25$ and (a) $R_0=-0.5$ and $R_1=-2$, (b) $R_0=-0.5$ and $R_1=-0.1$, (c) $R_0=-0.5$ and $R_1=0.05$, (d) $R_0=-0.5$ and $R_1=1$, (e) $R_0=-0.5$ and $R_1=3$, and (f) $R_0=-0.5$ and $R_1=8$.

subsequently, we determine the remaining $(J_s^*, K_s^*, \Delta_s^*)$ coordinates from Eq. (3b) after having replaced J_B, K_B, and Δ_B by the fixed point values of J_B^*, K_B^*, and Δ_B^*. This procedure shows that in the six-dimensional parameter space there are 16 three-dimensional invariant subspaces in which the fixed points are determined by recursion relations (3b).

The results obtained from our investigation of the three-dimensional semi-infinite BEG model are rather complicated. Referring to the 16 fixed points of the infinite BEG model, in the six-dimensional parameter space we found 113 fixed points underlying the structure of the semi-infinite system and we study the connectivity of the renormalization-group flows linking them. Taking into account the nature of the fixed points, new properties characterizing a variety of phase transitions associated with the surface are thus obtained, which can be summarized as follows:

(a) If the bulk is ferromagnetic, the surface is also necessarily ferromagnetic.

(b) If the bulk is staggered quadrupolar, the surface can be either ferromagnetic or staggered quadrupolar.

(c) When the bulk is paramagnetic, the surface can be ferromagnetic, paramagnetic, or undergo a critical phase transition between the phases F and P. This phase transition is similar to the surface transition in three-dimensional semi-infinite Ising models.

(d) If the bulk exhibits a smooth continuation between the two paramagnetic phases P_+ and P_-, the surface can be in any of the four phases F, SQ, P_+, and P_-, or it can undergo one of the 12 different phase transitions of an infinite system.

(e) When the bulk undergoes a first-order transition between the two paramagnetic phases, the surface can exhibit a first-order transition between the phases F and P_-, an ordinary first-order transition between the two paramagnetic phases, or a critical end-phase transition.

(f) When the phases ferromagnetic and paramagnetic are coexisting on the surface, the bulk exhibits a critical end-phase transition.

(g) If the surface is ferromagnetic, the bulk is paramagnetic (P_+) or undergoes a critical phase transition of second order between the phases F and P_+. This transition is similar to the extraordinary phase transition in three-dimensional semi-infinite Ising models. Therefore, the bulk cannot undergo a first-order phase transition while the surface is ferromagnetic.

(h) For the bulk undergoing critical or tricritical phase transitions, we found ordinary and special phase transitions associated with the surface. Moreover, the surface cannot undergo a first-order phase transition while the bulk exhibits a second-order phase transition.

These results enable us to exclude the possibility of first-order surface and extraordinary phase transitions, and forbid certain phase diagrams found within other techniques.[16,20] One should note also that the MK renormalization-group scheme we have applied did not obtain ferrimagnetic phases, either in the surface or in the bulk. This picture is irrespective of the space dimensionality d, since the results are qualitatively similar for $d>3$. This confirms, once again, the statement of Hoston and Berker,[13] as a consequence of the restricted flow space in which the renormalization is carried out.

III. DISCUSSIONS AND CONCLUSION

A real-space renormalization-group calculation, in a restricted flow space, is used to analyze the critical behavior of the three-dimensional semi-infinite BEG model with surface interactions which may differ from the bulk interactions. We determine explicitly the effect of any bulk and surface biquadratic interactions on the surface transitions. Our new results have been obtained with repulsive biquadratic interactions K_B and K_S. Referring to the 16 fixed points of the infinite model, the fixed points of the semi-infinite system have been classified. Using renormalization-group theory we have obtained 11 generic types of phase diagrams, some of which we have illustrated in the $(J_s^{-1},\Delta_s J_s^{-1})$ plane. They show a variety of phase transitions associated with the surface and unusual multicritical topologies, including certain types of ordinary, extraordinary, and special phase transitions which do not occur in the Ising-like systems.

The semi-infinite BEG model reduces to the semi-infinite BC model if we set $K_B=K_S=0$. As mentioned in the Introduction, the last model has been studied[19] within MK renormalization-group and three generic types of phase diagrams have been obtained as a function of the ratios $R=J_B/J_S$ and $D=\Delta_B/\Delta_S$. Their domain of existence is classified as follows:

Domain I: For $R>0.59$ the system exhibits only ordinary phase transition.

Domain II: For $R<0.59$ two different types of phase diagram have been found, according to whether $D>1$ or $D\leqslant 1$. In this case the phase diagrams present ordinary, extraordinary, surface, and special phase transitions.

For the semi-infinite BEG model we define the new ratios $R_0=K_B/K_S$ and $R_1=K_S/J_S$ and classify the possible phase diagrams at fixed R and D. According to the values of R_0 and R_1 different types of phase diagrams are *a priori* expected. To classify them we shall proceed as follows:

(1) Type A. If R and D are in domain I, varying R_0 and R_1 we obtain five main types of phase diagrams which we report in Figs. 1(a–e); solid and dashed lines represent, respectively, second- and first-order transitions. B and S stand for bulk and surface, respectively, while P, F, and SQ stand for paramagnetic, ferromagnetic, and staggered quadrupolar phases.

(a) For $R_0=-5$ and $R_1=-1$, the system exhibits only ordinary phase transitions of first-order, second-order, or tricritical. The corresponding phase diagram presents also reentrant phenomenon with a critical end point.

(b) For $R_0=-5$ and $R_1=-0.1$, the surface and the bulk order at the same temperature. This ordinary transition, according to the values of Δ_S/J_S, can be first order, second order, or tricritical.

(c) For $R_0=-5$ and $R_1=0.2$, we have shown ordinary first-order, ordinary second-order, extraordinary second-order, and surface second-order phase transitions. There exists also a point where the surface and the bulk become ordered simultaneously. According to its position, this point is a multicritical point where a first-order transition line meets two second-order transition lines. For another particular value of Δ_S/J_S we can observe also a special phase transition point where a second-order transition line meets two second-order transition lines.

Moreover, in this case the staggered quadrupolar phase occurs in the bulk. Thus, as mentioned above, the model presents a ordinary second-order phase transition where the bulk and the surface of the system exhibit a transition between different phases, namely, from (SP,BP) to (SF,BSQ), where SP, BP, SF, and BSQ denote, respectively, surface paramagnetic, bulk paramagnetic, surface ferromagnetic, and bulk staggered quadrupolar phases. An extraordinary phase transition also occurs, where only the bulk exhibits a transition between the two phases BF and BSQ, the surface being in the ferromagnetic phase SF. This gives rise to a multicritical point appearing at the termination of the phase boundary between these phases.

(d) For $R_0 = -5$ and $R_1 = 0.5$ we can observe a special phase transition point in addition to the ordinary, extraordinary, and surface second-order phase transitions. As in the previous case, we have shown the second-order ordinary and extraordinary phase transitions. Moreover, the two multicritical points occuring in Fig. 1(c) merge into a single multicritical point.

(e) For $R_0 = -5$ and $R_1 = 0.8$ we have shown a phase where the surface and the bulk of the system are in the staggered quadrupolar phases (SSQ,BSQ). Moreover, the unusual feature of this phase diagram is the presence of three phase transitions of second order, with three multicritical points.

(2) Type B. If R and D are in domain II, according to the values of the ratios R_0 and R_1, we obtain six main types of phase diagrams, which we report in Figs. 2(a–f).

(a) For $R_0 = -0.5$ and $R_1 = -2$, the system exhibits reentrant ordinary first-order, ordinary second-order, extraordinary second-order, and surface second-order phase transitions. For three particular values of Δ_S / J_S, we can observe an ordinary tricritical point, a critical end point, and a multicritical point characterizing the special phase transition.

(b) For $R_0 = -0.5$ and $R_1 = -0.1$, according to the values of Δ_S / J_S, we have shown an ordinary tricritical point and a special phase transition point, in addition to an ordinary first-order, ordinary second-order, extraordinary second-order, and surface second-order phase transitions.

(c) For $R_0 = -0.5$ and $R_1 = 0.05$, the corresponding phase diagram is characterized by the presence of an ordinary first-order transition at high temperature, while in the low-temperature region one has extraordinary and surface second-order transitions. The three transition lines meet at a multicritical point.

(d) For $R_0 = -0.5$ and $R_1 = 1$, we have shown ordinary first-order, extraordinary second-order, and surface second-order phase transitions, with two multicritical points. Besides these transitions the SQ phase occurs in the bulk, which gives rise to the ordinary and extraordinary phase transitions described above.

(e) For $R_0 = -0.5$ and $R_1 = 3$ the system exhibits phase transitions between different phases as indicated above, with a single multicritical point. All those transitions are of second order.

(f) For $R_0 = -0.5$ and $R_1 = 8$ the corresponding phase diagram is characterized by the presence of all the second-order phase transitions obtained previously with three multicritical points.

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