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Real-space renormalization-group investigation of the three-dimensional semi-infinite Blume-Emery-Griffiths model

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We investigate the three-dimensional semi-infinite Blume-Emery-Griffiths (BEG) model using the Migdal-Kadanoff renormalization-group method. The parameter space is six dimensional. We find 69 fixed points describing a large variety of critical behaviors and discuss various semi-infinite models which are special cases of the BEG model such as the Blume-Capel model. For this last model we determine the various generic types of phase diagrams according to the values of the interactions on the surface and in the bulk of the system.

I. INTRODUCTION

Semi-infinite systems have been the subject of numerous studies, and a detailed review article containing an extensive list of references has been published by Binder.[1] Most works have been devoted to systems which undergo second-order phase transitions. A relatively small number of papers have considered semi-infinite systems which exhibit first-order and tricritical phase transitions.[2–5]

Recently the three-dimensional semi-infinite spin-1 ferromagnetic Ising model with a crystal field has been studied.[6] The spin-1 ferromagnetic Ising model with a crystal field has been introduced independently by Blume[7] and Capel[8] and is often called the Blume-Capel model.

As a function of the ratio R of bulk and surface interactions and the ratio D of bulk and surface crystal fields all the possible phase diagrams have been determined using mean-field approximation. Eight generic types of phase diagrams have been found. They show a variety of phase transitions and multicritical points.

One aim of this paper is to study the three-dimensional semi-infinite Blume-Capel model using a real-space renormalization-group technique. In order to achieve such an aim, we shall investigate the more general three-dimensional semi-infinite Blume-Emery-Griffiths[9] (BEG) model.

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

$$\beta H = -J\sum_{(i,j)} S_i S_j - K\sum_{(i,j)} S_i^2 S_j^2 + \Delta \sum_i S_i^2 , \qquad (1)$$

where the spins ($S=-1,0,1$) are located on the sites of a cubic lattice and the first and second summations run over all neighboring pairs of spins. J, K, and Δ denote, respectively, the reduced bilinear exchange, biquadratic exchange, and crystal-field interactions. This model is an extension of the Blume-Capel model, which corresponds to $K=0$.

Using a real-space renormalization-group techique, it is not possible to restrict our study to the Blume-Capel model, since in the three-dimensional parameter space (J,K,Δ) the subspace $K=0$ is not invariant.

II. THE INFINITE BEG MODEL

This model was introduced to describe phase separation and superfluid ordering in ^{3}He-^{4}He mixtures and was subsequently reinterpreted to describe phase transitions in simple[10] and multicomponent fluids.[11–13] In this section we shall determine the phase diagram in the (J,K,Δ) space for the two- and three-dimensional infinite BEG models using the Migdal-Kadanoff renormalization-group method.[14,15]

This method will be used in the following section 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 systems will help in understanding the meaning of the various fixed points. The infinite BEG model has been studied by many different methods. Most references can be found in a review article on the theory of tricritical points by Lawrie and Sarbach.[16] In what follows, we shall first briefly describe the results obtained by the mean-field approximation and those of Berker and Wortis,[17] who used a different real-space renormalization-group technique.

The different phases of the BEG model can be characterized by two parameters: the magnetization $m=\langle S_i\rangle$ and the quadrupole parameter $q=\langle S_i^2\rangle$. Since the lattice

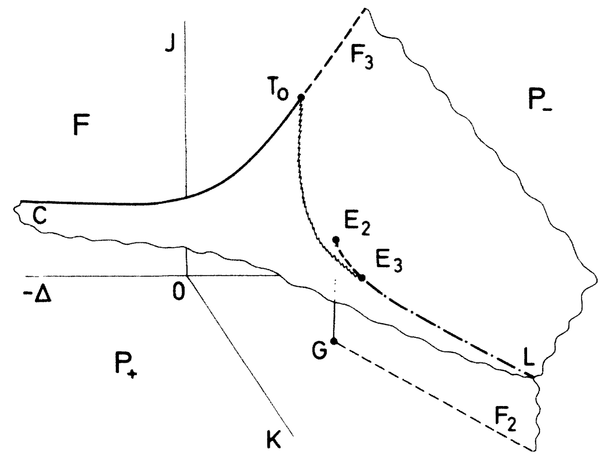

FIG. 1. BEG phase diagram obtained with the mean-field approximation described in Sec. II. Wavy lines denote smooth continuation of surfaces.

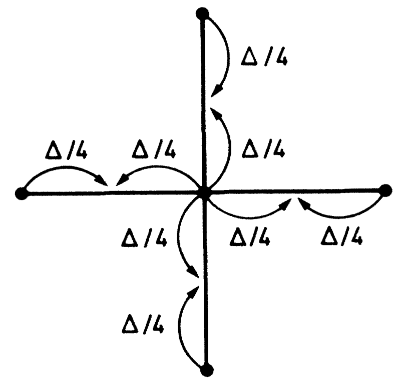

FIG. 2. Distribution of the crystal-field term between the surrounding bonds in the case $d=2$.

is translationally invariant, m and q do not depend upon the site i.

The BEG phase diagram in the (J,K,Δ) space obtained with the mean-field approximation is represented in Fig. 1. The notations are those of Berker and Wortis. According to the values of m and q, three different phases can be distinguished as follows:

Paramagnetic P_-: $m=0, \quad q<\frac{1}{2}$

Paramagnetic P_+: $m=0, \quad q>\frac{1}{2}$

Ferromagnetic F: $m\neq 0, \quad q \lessgtr \frac{1}{2}$.

The ferromagnetic phase F is separated from the paramagnetic phase P_+ by the second-order transition surface CT_0E_3L, and from the paramagnetic phase P_- by the first-order transition surface $F_3T_0E_3L$. On the other hand, the two paramagnetic phases are separated by the first-order transition surface F_2GE_2L. These two phases have no different symmetry, and one can continuously pass from one to the other without crossing the three transition surfaces mentioned above. These three surfaces, which have in common the line E_3L, are bounded by the tricritical line T_0E_3, the critical line GE_2, and the three-phase coexistence line E_2E_3. The E_3L line is the locus of points where a second-order transition line meets a first-order transition line. A point of this kind will be called a critical end point.

Berker and Wortis studied the two-dimensional BEG model using a block transformation. Their phase diagram is qualitatively similar to that obtained with the mean-field approximation, except that the three-phase coexistence line E_2E_3 shrinks into the so-called Potts point [cf. (c), Sec. IV] in renormalization theory. These authors found three trivial fixed points which correspond to the three phases P_-, P_+, and F, and ten nontrivial fixed points characterizing the various phase transitions. These fixed points have been classified according to their relative stability and connectivity.

The Migdal-Kadanoff renormalization-group technique we have used gives very similar results: the same number of fixed points and the same phase diagram. This renormalization technique being tractable in all space dimensionalities, we shall give the recursion relations for a d-dimensional hypercubic model. Let us briefly describe the method. Choose a scale factor $b=2$ and consider a one-dimensional chain of three spins S_1, S_2, and S_3. The reduced Hamiltonian of this three-spin cluster reads

$$\beta H=-J(S_1S_2+S_2S_3)-K(S_1^2S_2^2+S_2^2S_3^2)+\frac{\Delta}{2d}(S_1^2+2S_2^2+S_3^2) . \quad (2)$$

The coefficient in the crystal-field term takes into account the coordination of the sites 1, 2, and 3 in the d-dimensional hypercubic lattice (Fig. 2). Perform the trace over spins S_2 to obtain the transformed reduced Hamiltonian

$$\beta\widetilde{H}=-\widetilde{J}S_1S_3-\widetilde{K}S_1^2S_3^2+\frac{\widetilde{\Delta}}{2d}(S_1^2+S_3^2) . \quad (3)$$

The renormalized one-dimensional interactions $\widetilde{J}$, $\widetilde{K}$, and $\widetilde{\Delta}$ are given as functions of J, K, and Δ by

$$\widetilde{J}=\tfrac{1}{2}\ln\frac{1+2\cosh(2J)\exp(2K-\Delta/d)}{1+2\exp(2K-\Delta/d)} ,$$
$$\widetilde{K}=\tfrac{1}{2}\ln\frac{(1+2\exp-\Delta/d)^2[1+2\exp(2K-\Delta/d)][1+2\cosh(2J)\exp(2K-\Delta/d)]}{[1+2\cosh(J)\exp(K-\Delta/d)]^4} , \quad (4)$$
$$\widetilde{\Delta}=\Delta-6\ln\frac{1+2\cosh(J)\exp(K-\Delta/d)}{1+2\exp(-\Delta/d)} .$$

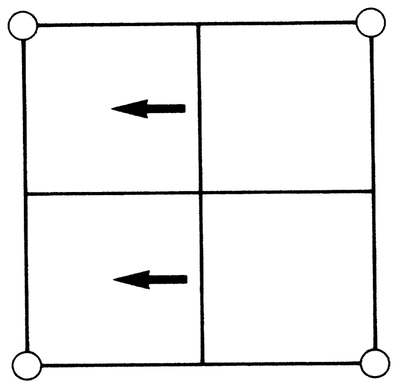

FIG. 3. Bond moving in the case $d=2$. Open circles remain after decimation has been performed.

The Migdal-Kadanoff recursion relations for the d-dimensional hypercubic lattice are obtained using the usual moving procedure, as illustrated in Fig. 3. They are given by

$$\begin{aligned} J' &= 2^{d-1}\widetilde{J}(J,K,\Delta) , \\ K' &= 2^{d-1}\widetilde{K}(J,K,\Delta) , \\ \Delta' &= 2^{d-1}\widetilde{\Delta}(J,K,\Delta) . \end{aligned} \tag{5}$$

These relations have been obtained by first performing the trace and then moving the bonds. We could have first moved the bonds and then performed the trace. This last procedure would have given recursion relations of the following form:

$$\begin{aligned} J' &= \widetilde{J}(2^{d-1}J, 2^{d-1}K, 2^{d-1}\Delta) , \\ K' &= \widetilde{K}(2^{d-1}J, 2^{d-1}K, 2^{d-1}\Delta) , \\ \Delta' &= \widetilde{\Delta}(2^{d-1}J, 2^{d-1}K, 2^{d-1}\Delta) . \end{aligned} \tag{6}$$

where $\widetilde{J}$, $\widetilde{K}$, and $\widetilde{\Delta}$ are the functions defined by (4).

In general, the first procedure underestimates critical temperatures, while the second procedure overestimates them. To obtain more precise values, we used a symmetrized procedure which gives the following recursion relations:

$$\begin{aligned} J' &= \tfrac{1}{2}[2^{d-1}\widetilde{J}(J,K,\Delta)+\widetilde{J}(2^{d-1}J,2^{d-1}K,2^{d-1}\Delta)] , \\ K' &= \tfrac{1}{2}[2^{d-1}\widetilde{K}(J,K,\Delta)+\widetilde{K}(2^{d-1}J,2^{d-1}K,2^{d-1}\Delta)] , \\ \Delta' &= \tfrac{1}{2}[2^{d-1}\widetilde{\Delta}(J,K,\Delta)+\widetilde{\Delta}(2^{d-1}J,2^{d-1}K,2^{d-1}\Delta)] . \end{aligned} \tag{7}$$

The various fixed points of this transformation have been determined for $d=2$ and $d=3$. Their coordinates and the phase transitions they characterize are given in Table I. We used the Nienhuis-Nauenberg criterion[18] to determine which fixed points characterize first-order phase transitions.

The phase diagrams for $d=2$ and $d=3$ are very similar. A typical one, on which the locations of the various fixed points have been indicated, is represented in arbitrary units in Fig. 4. It is qualitatively similar to that obtained by the mean-field approximation, except that like Berker and Wortis, we found that the three-phase coexistence line E_2E_3 shrinks to the Potts point P.

The ferromagnetic phase F is separated from the paramagnetic phase P_+ by the second-order transition surface CT_0PL, and from the paramagnetic phase P_- by the first-order transition surface F_2GPL. These three surfaces, which have in common the line PL, are bound by the tricritical line T_0P and the critical line GP. Like in

TABLE I. Coordinates and classification of the fixed points of transformation (7) for $d=2$ and $d=3$.

Fixed points	Type	(J^*,K^*,Δ^*) coordinates $d=2$	$d=3$	Domain in the (J,K,Δ) space
F	sink for $(m\neq 0,\ q \lessgtr \frac{1}{2})$ phase	$(\infty,-\infty,-\infty)$	$(\infty,-\infty,-\infty)$	volume F
P_-	sink for $(m=0,\ q<\frac{1}{2})$ phase	$(0,0,\infty)$	$(0,0,\infty)$	volume P_-
P_+	sink for $(m=0,\ q>\frac{1}{2})$ phase	$(0,0,-\infty)$	$(0,0,-\infty)$	volume P_+
C	second order	$(0.456,-0.068,-\infty)$	$(0.163,-0.003,-\infty)$	surface CT_0PL
F_J	first order	(∞,∞,∞) $\Delta^*\gg J^*\gg K^*$	(∞,∞,∞) $\Delta^*\gg J^*\gg K^*$	portion of surface F_3T_0PL
A	first order	(∞,∞,∞) $J^*\sim K^*\sim \Delta^*$	(∞,∞,∞) $J^*\sim K^*\sim \Delta^*$	line in surface F_3T_0PL
F_K	first order	(∞,∞,∞) $J^*\ll K^*\ll \Delta^*$	(∞,∞,∞) $J^*\ll K^*\ll \Delta^*$	remainder of surface F_3T_0PL
F_2	first order	$(0,\infty,2K^*+0.462)$	$(0,\infty,3K^*+1.2)$	surface F_2GPL
S	smooth continuation between P_- and P_+	$(0,0,0)$	$(0,0,0)$	surface $SGPT_0$
T	ordinary tricritical	$(1.56,0.053,3.11)$	$(0.259,-0.011,0.214)$	line T_0P
L	critical end	$(0.456,\infty,2K^*+0.665)$	$(0.163,\infty,3K^*+1.3)$	line LP
G	critical	$(0,1.82,4.34)$	$(0,0.68,2.55)$	line GP
P	Potts	$(0.520,1.56,4.16)$	$(0.206,0.618,2.47)$	point P

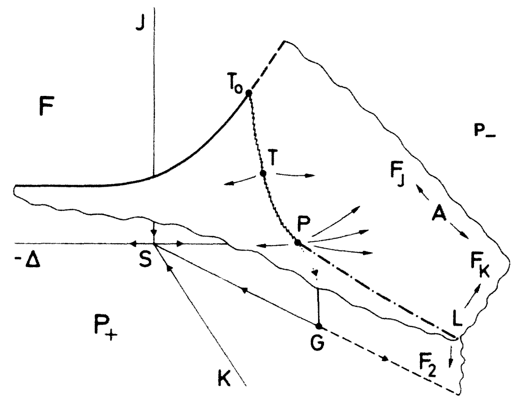

FIG. 4. Phase diagram obtained by the Migdal-Kadanoff renormalization-group treatment. Wavy lines denote smooth continuation of surfaces. Arrows indicate the relative stability and connectivity of fixed points.

the case of the phase diagram obtained by the mean-field approximation the line PL is the locus of points where a second-order transition line meets a first-order transition one.

III. THE SEMI-INFINITE BEG MODEL

The three-dimensional semi-infinite cubic BEG model is described by the following reduced Hamiltonian:

$$\beta H = -J_S \sum_{(i,j)} S_i S_j - K_S \sum_{(i,j)} S_i^2 S_j^2 + \Delta_S \sum_i S_i^2 - J_B \sum_{(k,l)} S_k S_l - K_B \sum_{(k,l)} S_k^2 S_1^2 + \Delta_B \sum_k S_k^2 , \quad (8)$$

where the first and second summations run over all pairs of neighboring spins located on the two-dimensional surface of the system, the fourth and fifth summations run over all pairs of remaining neighboring spins, the third summation runs over all spins located on the surface, and the last summation runs over all spins located in the bulk. The subscripts S and B refer, respectively, to the surface and the bulk.

The extension of the Migdal-Kadanoff renormalization technique to semi-infinite systems is straightforward.[19–21] In the particular case of the semi-infinite BEG model we have

$$\begin{aligned} J_B' &= \tfrac{1}{2}[4\tilde{J}(J_B,K_B,\Delta_B)+\tilde{J}(4J_B,4K_B,4\Delta_B)] , \\ K_B' &= \tfrac{1}{2}[4\tilde{K}(J_B,K_B,\Delta_B)+\tilde{K}(4J_B,4K_B,4\Delta_B)] , \quad (9a) \\ \Delta_B' &= \tfrac{1}{2}[4\tilde{\Delta}(J_B,K_B,\Delta_B)+\tilde{\Delta}(4J_B,4K_B,4\Delta_B)] , \end{aligned}$$

$$\begin{aligned} J_S' &= \tfrac{1}{2}[2\tilde{J}(J_S,K_S,\Delta_S)+\tilde{J}(2J_S,2K_S,2\Delta_S) + 2\tilde{J}(J_B,K_B,\Delta_B)] , \\ K_S' &= \tfrac{1}{2}[2\tilde{K}(J_S,K_S,\Delta_S)+\tilde{K}(2J_S,2K_S,2\Delta_S) + 2\tilde{K}(J_B,K_B,\Delta_B)] , \quad (9b) \\ \Delta_S' &= \tfrac{1}{2}[2\tilde{\Delta}(J_S,K_S,\Delta_S)+\tilde{\Delta}(2J_S,2K_S,2\Delta_S) + 2\tilde{\Delta}(J_B,K_B,\Delta_B)] , \end{aligned}$$

where $\tilde{J}$, $\tilde{K}$, and $\tilde{\Delta}$ are the functions defined by (4). The determination of the various fixed points of these recursion relations seems at first sight a rather complicated problem. However, as usual for semi-infinite systems, the renormalized bulk interactions given by (9a) depend only upon the initial bulk interactions J_B, K_B and Δ_B (see the Appendix).

Therefore, in order to determine the six coordinates of each fixed point, we shall first determine the (J_B^*,K_B^*,Δ_B^*) coordinates from (9a), which is a problem we already solved in Sec. II, and subsequently, determine the remaining (J_S^*,K_S^*,Δ_S^*) coordinates from (9b) after having replaced J_B, K_B, and Δ_B by the different values of J_B^*, K_B^*, and Δ_B^* taken from Table I (for $d=3$). This procedure shows that in the six-dimensional parameter space there are 13 three-dimensional invariant subspaces in which the fixed points are determined by recursion relations (9b).

To denote the various fixed points in the six-dimensional parameter space, we shall use the symbols defined in Table I. More precisely, each fixed point will be denoted by a pair (X,Y) where the symbol X refers to the coordinates (J_B^*,K_B^*,Δ_B^*) and Y to the coordinates (J_S^*,K_S^*,Δ_S^*) of the fixed point (see the Appendix).

The procedure we followed to determine the various fixed points implies, therefore, that the symbol X characterizes the three-dimensional invariant subspace in which the fixed point (X,Y) is located.

In order to classify the different fixed points, we shall distinguish the following cases. The coordinates of fixed points which can be found from Table I will not be given.

(a) In the invariant subspace $X=F$ there is only one fixed point: $Y=F$. This means that if the bulk is ferromagnetic, the surface is also necessarily ferromagnetic.

(b) In the invariant subspace $X=P_-$ there are six fixed points: $Y=P_-,F_J,A,F_K,L,F_2$. The first is trivial and characterizes the paramagnetic phase P_- of the surface. The remaining five are nontrivial but are all located at infinity. In this case the surface cannot exhibit a phase transition at a finite temperature.

(c) In the invariant subspace $X=P_+$ there are three points: $Y=F,P_+,C$. The first two are trivial and characterize, respectively, the ferromagnetic F and the paramagnetic P_+ phase of the surface. The last point is nontrivial. It characterizes the five-dimensional second-order transition hypersurface in the six-dimensional $(J_B, K_B,\Delta_B,J_S,K_S,\Delta_S)$ phase diagram between the phases F and P_+ on the surface, the bulk being in the paramagnetic P_+ phase. This phase transition is similar to the "surface" transition in three-dimensional semi-infinite Ising models. See the Appendix for a description of the terminology of phase transitions in a three-dimensional semi-infinite system.

(d) In the invariant subspace $X=C$ there are three fixed points: $Y=F,C,C_s$. The first point characterizes a five-dimensional hypersurface in the phase diagram which corresponds to the transition in the bulk between phases F and P_+, the surface being in the ferromagnetic phase. This phase transition is similar to the "extraordinary" phase transition in three-dimensional semi-infinite Ising models. The coordinates of the point (C,C) are $((0.163,0.029),(-0.003,-0.819),(-\infty,-\infty))$. The coordinates of a fixed point in the six-dimensional parameter space are denoted $((J_B^*,J_S^*),(K_B^*,K_S^*),(\Delta_B^*,\Delta_S^*))$. It characterizes a five-dimensional transition hypersurface. At a point of this hypersurface, the bulk and the surface of the system exhibit a transition between the phases F and P_+. Such a phase transition is similar to the "ordinary" phase transition in three-dimensional semi-infinite Ising models.

The coordinates of the point (C,C_S) are $((0.163,0.386),(-0.003,-0.566),(-\infty,-\infty))$. It characterizes a four-dimensional transition hypersurface. At a point of this hypersurface the bulk and the surface of the system exhibit a transition between the phases F and P_+. However, in this case the critical exponents are different from the previous case. Such a phase transition is similar to the "special" phase transition.

(e) In the three invariant subspaces $X=F_J$, $X=A$, and $X=F_K$ there is only one fixed point in each of them, namely, (F_J,F_J), (A,A), and (F_K,F_K). At a point of the hypersurface characterized by these fixed points, the bulk and the surface exhibit an ordinary first-order transition between the phases F and P.

(f) In the invariant subspace $X=F_2$, there are three fixed points $Y=A,F_2L$. The point (F_2,A) characterizes a first-order transition on the surface between the phases F and P_-, while the bulk undergoes a first-order transition between the two paramagnetic phases.

The point (F_2,F_2) characterizes a five-dimensional hypersurface on which the bulk and the surface of the system exhibit an ordinary first-order transition between the two paramagnetic phases.

The point (F_2,L) characterizes a four-dimensional hypersurface on which the bulk undergoes a first-order transition between the two paramagnetic phases while the surface exhibits a critical end phase transition.

(g) The determination of the fixed points located in the invariant subspace $X=S$ is very simple. Their (J_B^*,K_B^*,Δ_B^*) coordinates are equal to zero and their (J_S^*,K_S^*,Δ_S^*) coordinates are those of the two-dimensional infinite system given in Table I. In this case, the bulk exhibits a smooth continuation between P_+ and P_-, while the surface can be in any of the three phases F, P_+, and P_- or it can undergo one of the ten different phase transitions of an infinite system.

(h) In the invariant subspace $X=L$ there are three fixed points $Y=A,L,L_s$. The fixed point (L,A) characterizes a three-dimensional hypersurface on which the bulk exhibits a critical end phase transition, while on the surface the phases F and P are coexisting.

The coordinates of the fixed point (L,L) are $((0.163,0.029),(\infty,\infty),(\infty,\infty))$. It characterizes a three-dimensional hypersurface on which the bulk and the surface undergo an ordinary critical end phase transition.

The coordinates of the fixed point (L,L_s) are $((0.163,0.386),(\infty,\infty),(\infty,\infty))$. It characterizes a two-dimensional hypersurface on which the bulk and the surface undergo a special critical end phase transition.

(i) In the subspace $X=T$ there are 12 fixed points. Their classification and J_S^*, K_S^*, and Δ_S^* are indicated in Table II. For the bulk undergoing a tricritical phase transition we shall only give information concerning the surface. The fixed points (T,C) and (T,C_s) characterize similar phase transitions. The first one is said to be ordinary and the second one special. They have different critical exponents and if we denote by $\dim(X,Y)$ the dimensionality of the hyperspace characterized by the fixed point (X,Y), we have $\dim(T,C_s)=\dim(T,C)-1$. This remark is valid for all the following couples of fixed points: (T,T) and (T,T_s), (T,L) and (T,L_s), and (T,P) and (T,P_s). This nomenclature has been adopted in analogy with what occurs for the usual semi-infinite Ising model (see the Appendix).

(j) In the subspace $X=G$ there are 12 fixed points. Their classification and (J_S^*,K_S^*,Δ_S^*) coordinates are indicated in Table III. For the bulk undergoing a critical phase transition, we shall only give information concerning the surface. As in the previous case, we have special phase transitions.

(k) In the subspace $X=P$ there are ten fixed points. Their classification and (J_S^*,K_S^*,Δ_S^*) coordinates are indicated in Table IV. For the bulk undergoing a Potts phase

TABLE II. Classification and coordinates of the fixed points located in subspace $X=T$. Dim. is the dimensionality of the domain in the $(J_B,K_B,\Delta_B,J_S,K_S,\Delta_S)$ space.

Y	Type	(J_S^*,K_S^*,Δ_S^*)	Dim.
F	sink for $(m\neq 0,\ q\gtrless\frac{1}{2})$ phase	$(\infty,-\infty,-\infty)$	4
C	second order	$(0.0865,-0.738,-\infty)$	4
C_s	special second order	$(0.306,-0.580,-\infty)$	3
F_J	first order	(∞,∞,∞) $\Delta^*\gg J^*\gg K^*$	4
A	first order	(∞,∞,∞) $J^*\sim K^*\sim\Delta^*$	3
F_K	first order	(∞,∞,∞) $J^*\ll K^*\ll\Delta^*$	4
T	ordinary tricritical	$(0.047,-0.088,-0.120)$	3
T_s	special tricritical	$(1.23,0.286,3.35)$	2
L	critical end	$(0.086,\infty,\infty)$	3
L_s	special critical end	$(0.306,\infty,\infty)$	2
P	Potts	$(0.049,1.75,4.69)$	2
P_s	special Potts	$(0.429,1.51,4.48)$	1

TABLE III. Coordinates and classification of the fixed points located in subspace $X=G$. Dim. is the dimensionality of the domain in the $(J_B,K_B,\Delta_B,J_S,K_S,\Delta_S)$ space.

Y	Type	(J_S^*,K_S^*,Δ_S^*)	Dim.
F	sink for $(m\neq 0,\ q\lessgtr\frac{1}{2})$ phase	$(\infty,-\infty,-\infty)$	4
C	second order	$(0,-0.8664,-\infty)$	4
C_s	special second order	$(0.4294,-0.5645,-\infty)$	3
F_J	first order	(∞,∞,∞) $\Delta^*\gg J^*\gg K^*$	4
A	first order	(∞,∞,∞), $J^*\sim K^*\sim\Delta^*$	3
F_K	first order	(∞,∞,∞) $J^*\ll K^*\ll\Delta^*$	4
F_2	first order	$(0,\ \infty,\ 2K_S^*+2.86)$	4
L	critical end	$(0.429,\ \infty,\ 2K_S^*+1.1)$	3
G	critical	(0,0.116,0.504)	3
G_s	special critical	(0,1.58,4.32)	2
P	Potts	(1.00,0.443,3.18)	2
P_s	special Potts	(0.561,1.19,3.98)	1

transition, we shall only give information concerning the surface. Here again we find special phase transitions.

IV. DISCUSSIONS, APPLICATIONS, AND CONCLUSION

The results obtained from our investigation of the three-dimensional semi-infinite BEG model are rather complicated. In the six-dimensional parameter space we found 69 fixed points. Referring to the 13 fixed points of the infinite BEG model, the fixed points of the semi-infinite system have been classified and denoted by a symbol (X,Y), where the first symbol refers to the bulk and the second to the surface. This notation is illustrated in the Appendix in the case of the much simpler three-dimensional semi-infinite Ising model. Some models are particular cases of the BEG model and we can deduce their phase diagram from our investigation of the BEG model.

(a) If $\Delta\ll -1$, the configurations in which all spins are nonzero dominate completely the ensemble averages. Therefore[17] the J component of fixed point C for the infinite model should give the critical temperature of the spin-$\frac{1}{2}$ Ising model. For $d=2$ we found 0.456 in good agreement with the exact Onsager value 0.441, and for $d=3$ we found 0.163 in fair agreement with 0.221 obtained by series expansions.

In the region $\Delta=-\infty$, the recursion relations for the infinite BEG model have only three fixed points, namely, F, P_+, and C. In the case of the semi-infinite BEG, the recursion relations have only seven fixed points for $\Delta_S=-\infty$ and $\Delta_B=-\infty$ [see Sec. III, subsections (a), (c), and (d)], namely, (F,F), (P_+,P_+), (P_+,C), (P_+,F), (C,F), (C,C), and (C,C_s), in complete agreement with what has been found for the semi-infinite Ising model (see the Appendix).

(b) Griffiths[22] pointed out that the BEG model reduces

TABLE IV. Coordinates and classification of the fixed points located in subspace $X=P$. Dim. is the dimensionality of the domain in the $(J_B,K_B,\Delta_B,J_S,K_S,\Delta_S)$ space.

Y	Type	(J_S^*,K_S^*,Δ_S^*)	Dim.
F	sink for $(m\neq 0,\ q\gtrless\frac{1}{2})$ phase	$(\infty,-\infty,-\infty)$	3
C	second order	$(0.0483,-0.789,-\infty)$	3
F_J	first order	(∞,∞,∞) $\Delta^*\gg J^*\gg K^*$	3
A	first order	(∞,∞,∞) $J^*\sim K^*\sim\Delta^*$	2
F_K	first order	(∞,∞,∞) $J^*\ll K^*\ll\Delta^*$	3
L	critical end	$(0.083,\infty,2K_S^*)$	2
G	critical	(0.034,0.102,0.382)	2
G_s	special critical	(0.0347,1.60,4.33)	1
P	Potts	(1.014,0.353,2.99)	1
P_s	special Potts	(0.481,1.29,4.04)	0

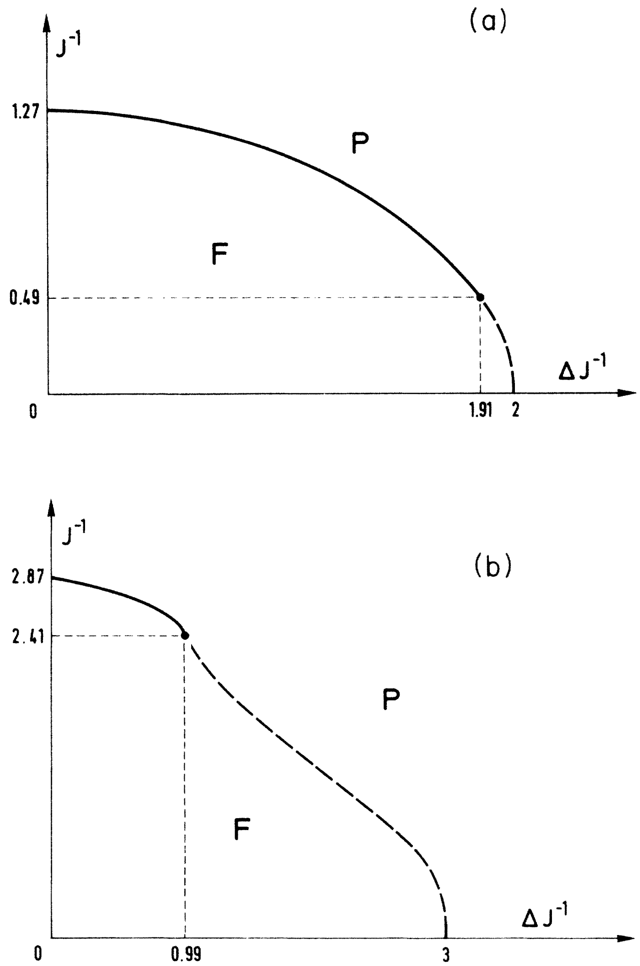

FIG. 5. Phase diagrams of the infinite Blume-Capel model determined by the Migdal-Kadanoff renormalization-group technique for (a) $d=2$ and (b) $d=3$. The symbols P and F refer, respectively, to the paramagnetic and ferromagnetic phases. First- and second-order phase transitions are represented by dashed and solid lines, respectively.

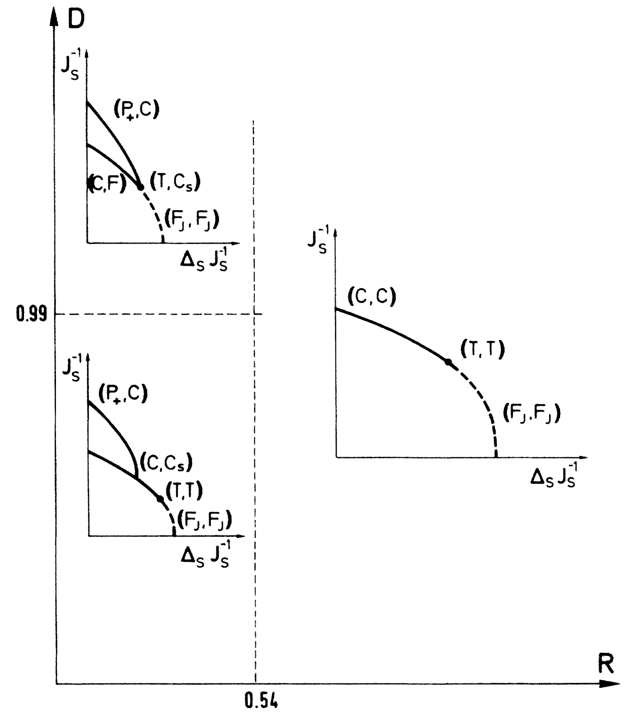

FIG. 6. Domains of existence in the (R,D) plane of the different phase diagrams for the three-dimensional semi-infinite Blume-Capel model. The symbols on the transition lines and multicritical points refer to the fixed points characterizing the transition.

to a spin-$\frac{1}{2}$ Ising model in a zero external field if $J=0$ and $\Delta=dK+\ln 2$. The exchange interaction is then equal to $K/4$, and therefore the coordinates of the fixed point G should be (0,1.763,4.219) for $d=2$, and (0,0.887,1.358) for $d=3$. Here again the agreement with our numerical results is good for $d=2$. For $d=3$, the agreement is fair for the K component but bad for the Δ component. Note also that the fixed point S, which is the intersection of the line $J=0$, $\Delta=dK+\ln 2$, and the Δ axis should be located at (0,0,ln2) instead of (0,0,0) (cf. Table I).

On the line S,G,F_2 we have three fixed points. For the spin-$\frac{1}{2}$ Ising model these points play, respectively, the role of the fixed points P, C, and F.

In the case of the semi-infinite system in the invariant subspaces S, G, and F_2, for $J_B=0$ and $J_S=0$ we only found the fixed points (S,S), (S,G), (S,F_2), (G,F_2), (G,G), (G,G_s), and (F_2,F_2) in agreement with what has been found for the semi-infinite Ising model.

(c) It can be shown[17] that the three-state Potts model is a special case of the BEG model. Therefore, the exact location of the fixed point P which characterizes the phase transition of the Potts model for $d=2$ is (0.503,1.51,4.02), in satisfactory agreement with our result (0.520,1.56,4.16).

(d) The infinite BEG model reduces to the Blume-Capel model if $K=0$. In Figs. 5(a) and 5(b) are represented the phase diagrams in the plane $J^{-1},\Delta J^{-1}$ obtained by the Migdal-Kadanoff renormalization-group technique for $d=2$ and $d=3$. Note that for the Blume-Capel model there is no distinction between paramagnetic phases P_+ and P_-. For the semi-infinite model, according to the ratios $R=J_B/J_S$ and $D=\Delta_B/\Delta_S$, different types of phases diagrams are *a priori* expected. As mentioned in the Introduction, this model has been studied within the mean-field approximation by Benyoussef, Boccara, and Saber[6] (hereafter referred to as BBS), and eight generic types of phase diagrams have been obtained. In this section we shall determine the various phase diagrams in the $J_S^{-1},\Delta_S J_S^{-1}$ plane given by renormalization theory. Taking into account the nature of the fixed points found in the previous section, if the surface of the system is ferromagnetic, the bulk cannot undergo a first-order phase transition, since no fixed point of the following types exist: (F_J,F), (A,F) or (F_K,F).

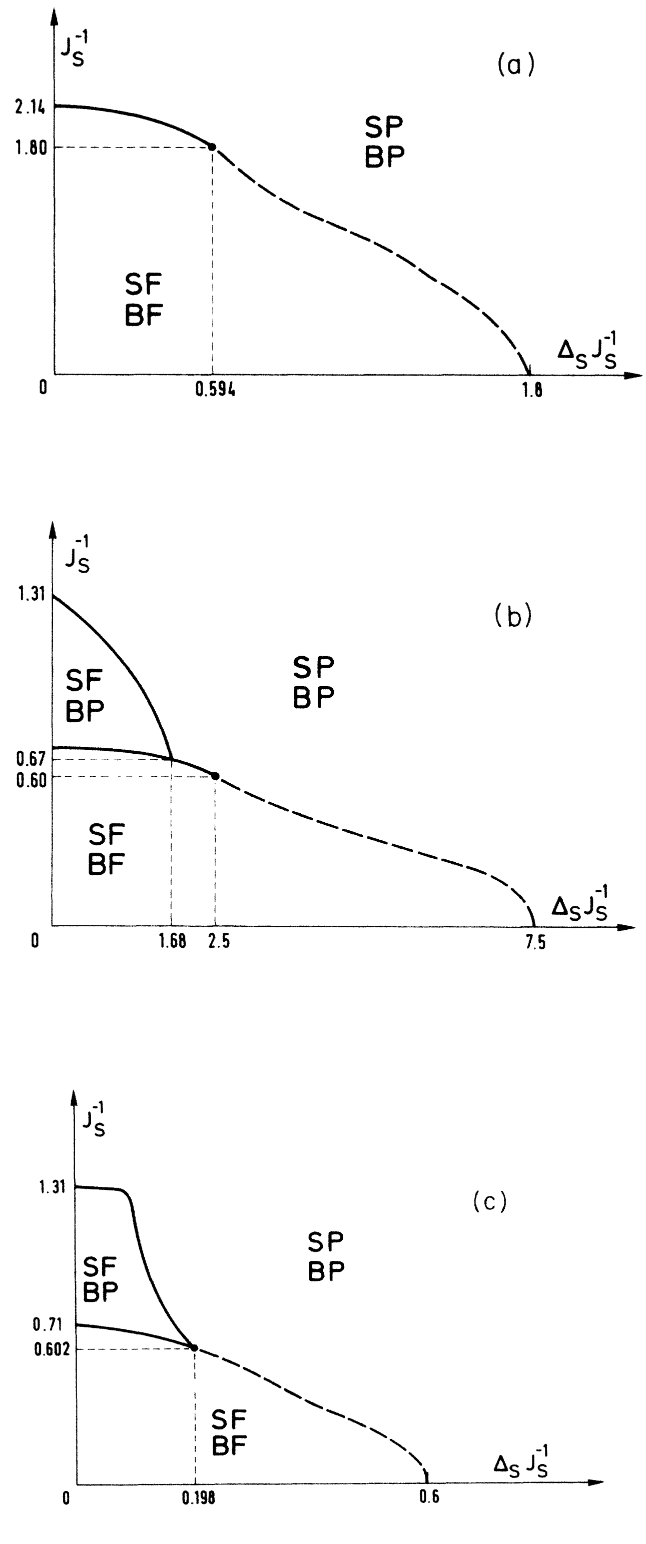

FIG. 7. Typical phase diagram for the three-dimensional semi-infinite Blume-Capel model calculated for (a) $R=0.75$, $D=1.25$, (b) $R=0.25$, $D=0.1$, and (c) $R=0.25$, $D=1.25$. The symbols SP, BP, SF, and BF denote, respectively, surface paramagnetic, bulk paramagnetic, surface ferromagnetic, and bulk paramagnetic phases.

This fact forbids many phase diagrams found in BBS, namely, types 2, 3a, 4a, 4b, and 4c. Moreover, since no fixed points of types (C,F_J), (C,A), (C,F_K), and (C,F_2) have been found, the surface cannot undergo a first-order phase transition while the bulk exhibits a second-order phase transition. This fact forbids the phase diagram of type 3c in BBS.

Therefore, we can observe three types of phase diagrams which are schematically represented, and their domain of existence is indicated in Fig. 6. For $R>0.54$ the surface and the bulk orders at the same temperature. This ordinary phase transition, according to the value of Δ_S/J_S, can be first order, second order, or tricritical (type 1 in BBS).

For $R<0.54$, according to the value of D, two different types of phase diagram have been found. If $D<0.99$, according to the value of Δ_S/J_S, we can observe ordinary first-order, ordinary second-order, extraordinary second-order, and surface second-order phase transitions. For two particular values of Δ_S/J_S (which depends upon D) we can also observe an ordinary tricritical point and a multicritical point described by the fixed point (C,C_s) (type 3b in BBS). If $D>0.99$, according to the value of Δ_S/J_S, we can observe ordinary first-order, extraordinary second-order, and surface second-order phase transitions. For a particular value of Δ_S/J_S (which depends upon D), we can also observe a multicritical point described by the fixed point (T,C_s). Figures 7(a), 7(b), and 7(c) represent three typical phase diagrams calculated, respectively, for $(R=0.25, D=1.25)$, $(R=0.25, D=0.1)$, and $(R=0.75, D=1.25)$.

It is well known that mean-field theory very often predicts phase transitions that do not exist. The results reported in this section confirms this fact once again.

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APPENDIX

The three-dimensional semi-infinite simple-cubic spin-$\frac{1}{2}$ Ising model is described by the reduced Hamiltonian

$$\beta H = -J_S \sum_{(i,j)} \sigma_i \sigma_j - J_B \sum_{(k,l)} \sigma_k \sigma_l ,$$

where J_S is the reduced coupling constant between neighboring spins located on the two-dimensional surface, and J_B the reduced coupling constant between remaining neighboring spins. This system exhibits four types of phase transitions associated with the surface. The accepted terminology[23,24] is the following: If the ratio $R=J_B/J_S$ is greater than a critical value R_c, the system orders at the bulk ferromagnetic transition temperature. This is the *ordinary* phase transition. If R is less than R_c, the system exhibits two successive transitions. The surface orders at a temperature higher than does the bulk, and as the temperature is lowered in the presence of the ordered surface, the bulk orders at the bulk transition temperature. These two phase transitions are, respectively, the *surface* and the *extraordinary* transition. If $R=R_c$ the system orders at the bulk transition temperature but in this case the critical exponents differ from those of the ordinary transition. This is the *special* phase transition.

The Migdal-Kadanoff recursion relations for this model are easy to derive.[21] For a scaling factor $b=2$ we have

$$J_B'=2\ln[\cosh(2J_B)]\ , \tag{A1}$$

$$J_S'=\ln[\cosh(2J_S)]+\tfrac{1}{2}\ln[\cos(2J_B)]\ . \tag{A2}$$

To determine the various fixed points of these recursions relations, we note that the renormalized bulk interaction J_B' given by (A1) depends only upon the initial bulk interaction J_B. Therefore, in order to determine the (J_B^*, J_S^*) coordinates of each fixed point in the two-dimensional parameter space, we first determine J_B^* from (A1) and then determine J_S^* from (A2) after having replaced J_B by J_B^*. Since (A1) has three fixed points, namely, $J_B^*=\infty$, $J_B^*=0$, and $J_S^*=0.261$, respectively denoted F, P, and C in the two-dimensional parameter space there are three invariant subspaces. As explained in Sec. III, each fixed point in the two-dimensional parameter space will be labeled by a symbol (X,Y), where X will refer to J_B^* and Y to J_S^*. In the invariant subspace $X=F$, there is only one fixed point, namely (F,F). It is trivial, and characterizes the ferromagnetic phase.

In the invariant subspace $X=P$, there are three fixed points, namely, (P,F), (P,P), and (P,C). The first two are trivial, and they characterize, respectively, the ferromagnetic and paramagnetic phases of the surface, the bulk being paramagnetic. The third point is nontrivial and characterizes the surface phase transition. Its coordinates are (0,0.610).

In the invariant subspace $X=C$, there are three fixed points, namely, (C,F), (C,C), and (C,C_s). They all are nontrivial. The first characterizes the extraordinary phase transition, the second the ordinary phase transition, and the third the special phase transition. The coordinates of (C,C) and (C,C_s) are, respectively, (0.261,0.077) and (0.261,0.502).

[1] K. Binder, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. Lebowitz (Academic, New York, 1983), Vol. 8, p. 1–444.

[2] K. Binder and D. P. Landau, Surf. Sci. **61**, 577 (1976).

[3] R. Lipowsky, Phys. Rev. Lett. **49**, 1575 (1982).

[4] R. Lipowsky and W. Speth, Phys. Rev. B **28**, 3983 (1983).

[5] W. Speth, Z. Phys. B **51**, 361 (1983).

[6] A. Benyoussef, N. Boccara, and M. Saber, J. Phys. C **19**, 1983 (1986).

[7] M. Blume, Phys. Rev. **141**, 517 (1966).

[8] H. W. Capel, Physica **32**, 966 (1966).

[9] M. Blume, J. V. Emery, and R. B. Griffiths, Phys. Rev. A **4**, 1071 (1971).

[10] J. Lajzerowicz and J. Sivardière, Phys. Rev. A **11**, 2079 (1975).

[11] J. Sivardière and J. Lajzerowicz, Phys. Rev. A **11**, 2090 (1975).

[12] J. Sivardière and J. Lajzerowicz, Phys. Rev. A **11**, 2101 (1975).

[13] D. Mukamel and M. Blume, Phys. Rev. A **10**, 610 (1974).

[14] A. A. Migdal, Zh. Eksp. Teor. Fiz. **69**, 1457 (1975) [Sov. Phys—JETP **42**, 743 (1975)].

[15] L. P. Kadanoff, Ann. Phys. (N.Y.) **100**, 359 (1976).

[16] D. Lawrie and S. Sarbach, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. Lebowitz (Academic, New York, 1984), Vol. 9, p. 1–155.

[17] A. N. Berker and M. Wortis, Phys. Rev. B **14**, 4946 (1976).

[18] B. Nienhuis and M. Nauenberg, Phys. Rev. Lett. **35**, 477 (1975).

[19] R. Lipowsky and H. Wagner, Z. Phys. B **42**, 355 (1981).

[20] O. Nagai and M. Toyonaga, J. Phys. C **14**, L545 (1981).

[21] A. Benyoussef, N. Boccara, and M. Saber, J. Phys. C **18**, 4275 (1985).

[22] R. B. Griffiths, Physica **33**, 689 (1967).

[23] T. C. Lubensky and M. H. Rubin, Phys. Rev. B **12**, 3885 (1975).

[24] A. J. Bray and M. A. Moore, J. Phys. A **10**, 1927 (1977).