Renormalization-group approach to surface critical behavior in the Ising model

Theodore W. Burkhardt
Institut Laue-Langevin, 156X Centre de Tri, 38042 Grenoble Cédex, France

Erich Eisenriegler
Institut Laue-Langevin, 156X Centre de Tri, 38042 Grenoble Cédex, France
and Institut für Festkörperforschung der Kernforschungsanlage, D-5170 Jülich, West Germany

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A modification of Kadanoff's lower-bound renormalization transformation is used to analyze the critical behavior of the semi-infinite Ising model with surface interactions which may differ from the bulk interactions. The $d = 2$ square lattice and the $d = 3$ bcc lattice are considered. Surface critical exponents, various critical couplings, and a phase diagram for $d = 3$ are calculated. The surface critical exponents are compared with the scaling laws relating surface and bulk exponents and the ϵ-expansion results due to Bray and Moore. The eigenvalues determining the surface exponents agree within 10% with the predictions of Bray and Moore except in the case of the eigenvalue determining the surface-bulk crossover exponent, where the discrepancy is much larger.

I. INTRODUCTION

The renormalization-group approach,[1] which has been applied with enormous success to problems in bulk critical phenomena, has also been used to investigate the effects of surfaces[2] on phase transitions. On the basis of mean-field theory Lubensky and Rubin[3] classified the four types of transitions (ordinary, surface, surface-bulk or special,[4] and extraordinary) exhibited by the semi-infinite n-vector model with short-range ferromagnetic interactions. For the ordinary transition they calculated the surface critical exponents to first order in $\epsilon = 4 - d$. In important recent work Bray and Moore[5] have obtained results for all four transitions to first order in ϵ and in the limit $n \to \infty$. In addition they propose scaling relations expressing the surface critical exponents at the ordinary, surface, and extraordinary transitions in terms of bulk critical exponents. Their considerations are largely based on a continuum Hamiltonian similar to that of Ref. 3 except that the system is infinite rather than semi-infinite. The translational invariance is broken by a plane of modified interactions. Bray and Moore argue that this model belongs to the same universality class as the semi-infinite model.

Position-space renormalization-group methods,[6] which are applicable to spin systems on a lattice in integer dimensions, have also been used to investigate surface effects in the Ising model. With these methods one can calculate critical temperatures, phase diagrams, and thermodynamic functions as well as critical exponents. Švrakić and Wortis[7] have given a general discussion of the position-space approach in systems with a free surface and have carried out an approximate calculation for the $d = 2$ Ising model, where there is only the ordinary transition. Burkhardt and Eisenriegler[8] applied a similar approach to the $d = 3$ Ising model. Their renormalization transformations, which only involve nearest-neighbor interactions, exhibit full sets of fixed points for the various transitions but are too crude to yield reliable quantitative information.

In this paper a modification of an approximate position-space renormalization transformation due to Kadanoff[9] is applied to the semi-infinite Ising model with a free surface. Both the $d = 2$ square lattice and the $d = 3$ bcc lattice are considered. For a variety of models Kadanoff's variational method describes the bulk critical behavior with impressive accuracy.[9,10] The new scaling laws of Bray and Moore relating the surface and bulk exponents are not built into the position-space approach in an obvious way. Although they may be satisfied in an exact calculation, they will not be satisfied in general in an approximate real-space calculation. In carrying out the calculations reported here, we hoped to obtain sufficiently accurate numbers to check Bray and Moore's new scaling laws, which were proposed on the basis of a model which superficially at least looks quite different.

II. RENORMALIZATION TRANSFORMATION

The basic renormalization step transforms the Hamiltonian $\mathcal{H}(\sigma)$ for a system of Ising spins σ to an equivalent Hamiltonian $\mathcal{H}'(\mu)$ for a reduced number of Ising spins μ. For the $d = 2$ square-lattice bulk calculation the σ spins (dots) and the μ spins (crosses) are shown in Fig. 1(a). In devising a

lower-bound variational transformation for a bulk system, Kadanoff[9] considers Hamiltonians of the form $\mathcal{H}=-\sum H_b$, where the sum is over all squares of the lattice, and H_b only depends on the four spins making up the square. He introduces a transfer function coupling the μ and σ spins which leaves the partition function invariant and which involves a variational parameter p_b. He then performs the renormalization transformation on the Hamiltonian $\mathcal{H}(\sigma)+V(\sigma)$ rather than $\mathcal{H}(\sigma)$, where $V(\sigma)$ translates all the H_b's and the parts of the weight function which depend on σ but not on μ into the shaded squares in Fig. 1(a) so that the shaded squares are only coupled by the μ spins. Then the renormalization transformation only involves the four σ spins in a single shaded square and the four surrounding μ spins. The transformation has the form

$$\exp[H_b'(\mu_1,\ldots,\mu_4)]=\operatorname{Tr}_{\sigma_1,\ldots,\sigma_4}\frac{\exp[p_b(\mu_1\sigma_1+\cdots+\mu_4\sigma_4)+4H_b(\sigma_1,\ldots,\sigma_4)]}{2\cosh p_b(\sigma_1+\cdots+\sigma_4)}\,. \tag{1}$$

Since V shifts the interactions about without introducing any new interactions, $\langle V\rangle_{\mathcal{H}}=0$ in a translationally invariant system. From this it follows that the approximate free energy calculated with shifted interactions is a lower bound to the exact free energy. The variational parameter p_b may be adjusted to maximize the lower bound.

The first of two renormalization transformations we have considered for the $d=2$ semi-infinite Ising model uses a $V(\sigma)$ which distributes the σ interactions in the shaded squares as shown in Fig. 1(b). First the interactions are shifted parallel to the surface into columns b, d, f, ... Next, half of the interactions in row 3 are shifted into row 2 and half into row 4. Similarly the interactions in rows 5, 7, 9, ... are moved into the upper and lower adjacent rows. We denote by p_1 and p_2 the variational parameters which couple the first layer of μ spins to the first two layers of σ spins. Everywhere else the μ and σ spins are coupled with the bulk variational parameter p_b. The transformation just described generates Hamiltonians with the form $\mathcal{H}=-\sum H_s-\sum H_b$, where the first sum is over all surface squares and the second is over all other squares. H_b transforms according to Eq. (1). H_s obeys the recursion relation

$$\exp[H_s'(\mu_1,\ldots,\mu_4)]$$

$$=\operatorname{Tr}_{\sigma_1,\ldots,\sigma_6}\frac{\exp[p_1(\mu_1\sigma_1+\mu_2\sigma_2)+p_2(\mu_1\sigma_3+\mu_2\sigma_4)+p_b(\mu_3\sigma_5+\mu_4\sigma_6)+2H_s(\sigma_1,\ldots,\sigma_4)+3H_b(\sigma_3,\ldots,\sigma_6)]}{2\cosh[p_1(\sigma_1+\sigma_2)+p_2(\sigma_3+\sigma_4)][2\cosh p_b(\sigma_3+\cdots+\sigma_6)]^{1/2}}\,. \tag{2}$$

As long as V only shifts interactions parallel to the surface, $\langle V\rangle_{\mathcal{H}}=0$ by translational invariance, and the lower-bound principle follows as before. However, in the transformation described above, V shifts interactions perpendicular to the surface as well, and the variational principle does not hold for arbitrary Hamiltonians and variational parameters. From a practical point of view it is desirable to shift the interactions perpendicular to the surface as we have done, even though it constitutes an additional approximation. Then no interactions are produced which involve more than four spins in a square, and one automatically incorporates Kadanoff's successful bulk transformation. However, since the variational principle no longer holds, the criterion for choosing optimal values for p_1, p_2, and p_b is no longer clear.

Figure 1(c) shows the redistribution of interactions in a second transformation we have considered. The interactions are shifted as before except that the shifts perpendicular to the surface begin with row 5 rather than row 3. Variational parameters $p_1,\ldots,p_4$ are associated with the first four layers of σ spins. For the other layers the bulk parameter p_b is used. This transformation generates an H_s which depends on six spins. The second transformation is closer to a lower-bound transformation than the first since the perpendicular shifts begin farther from the surface, where the system is more nearly translationally invariant.

The transformations of Figs. 1(b) and 1(c) are the first two of a sequence of transformations converging to a true lower-bound transformation as the length of the surface cluster is extended indefinitely. We have used both transformations to calculate the critical fixed point and the associated eigenvalue $y_{h_1}^{o}$ which, as discussed in more detail below, determines the surface critical exponents. Even though the transformations are not rigorous lower-bound transformations, the variational parameters were chosen to maximize the approximate free energy, since the sequence of variational parameters so generated converges to the optimal set for a true lower-bound transformation as the length of the surface cluster is increased. The two transformations yield values of $y_{h_1}^{o}$ 10.8% and 9.0% larger than the exact value[11] of

$\frac{1}{2}$. At the fixed point the long-range many-spin interactions present in the second transformation but not in the first (such as the two-, four-, and six-spin interactions involving spins separated by two lattice constants) are very weak, and the interactions common to both calculations change very little. These results suggest that only a limited improvement can be expected in the reasonably accurate values obtained from a small surface cluster by extending the cluster deeper into the system. To obtain a significant improvement it is probably important to change the width of the surface cluster as well as the length. Our calculations for $d=3$ are based on a generalization of the transformation of Fig. 1(b) to a simple cubic lattice. The surface cluster consists of three square layers of four σ spins coupled to a cube of eight adjacent μ spins.

Difficulties associated with an extra relevant variable[12] are encountered if Kadanoff's bulk transformation is used outside the invariant subspace in which $H_b(\sigma_1, \ldots, \sigma_{2d})$ is invariant under interchange of any pair of spin variables. To avoid these problems we begin with a square lattice for $d=2$ and a bcc lattice for $d=3$. We apply an exact decimation[9,12,13] transformation eliminating half

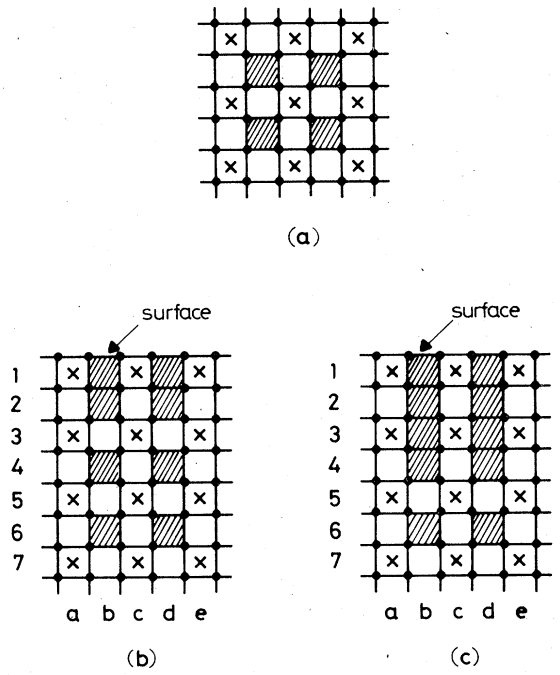

FIG. 1. Dots indicate σ spins and the crosses μ spins. $V(\sigma)$ shifts the σ interactions into the shaded areas, so that they are only coupled by the μ spins. (a) Kadanoff's renormalization transformation for the bulk problem. (b) and (c) two transformations we applied to the semi-infinite problem.

the spins to the initial Hamiltonian to enter the symmetric subspace before repeatedly applying the transformations described above. In the $d=2$ calculation the decimation leaves a square lattice with lattice constant increased by a factor $\sqrt{2}$. The $d=3$ decimation eliminates all the spins on one of the two simple cubic sublattices, leaving a simple cubic sublattice with the same lattice constant as the original bcc lattice.

III. RESULTS

The initial Hamiltonian considered in our $d=3$ bcc calculation only contains nearest-neighbor interactions. The free surface is assumed to be a (100) plane. We denote by $K_s=J_s/k_BT$ the coupling between a surface spin and each of its four nearest neighbors at the centers of bcc cells. All other couplings are assumed equal to the bulk coupling $K_b=J_b/k_BT$. Repeating for the bcc lattice a calculation for the simple cubic lattice found in Ref. 14, one finds the mean-field phase diagram shown in Fig. 2. The bulk transition occurs for $K_b=K_b^c=\frac{1}{8}$. The region $K_b>K_b^c$ marked BF denotes the bulk ferromagnetic phase. For $K_b>K_b^c$ there exist both surface ferromagnetic (SF) and paramagnetic phases (P). The critical line of surface transitions S is given by

$$K_s=(1/4\sqrt{2})\{1+[(1-8K_b)(1+8K_b)]^{1/2}\}^{1/2}. \quad (3)$$

The line of ordinary transitions O separates phases P and BF. The line of extraordinary transitions E separates phases SF and BF. All three critical lines intersect at the multicritical point SB of the surface-bulk or special transition. Mean-field exponents for the four transitions S, O, E, SB are given in Refs. 3, 5, and 14.

The intersection of the critical line S with the K_s axis gives a value for the critical nearest-neighbor coupling $K_c^{d=2}$ of the $d=2$ square-lattice bulk Ising model. $K_c^{d=2}=\frac{1}{4}$ in mean-field theory. The coordinates of point SB $[K_s^{SB}=(1+\Delta_c)K_b^c,\ K_b^{SB}=K_b^c]$ determine the critical surface enhancement Δ_c. For $J_s=(1+\Delta)J_b$ with $\Delta>\Delta_c$, the surface transition precedes the bulk transition as the temperature is lowered. For $\Delta<\Delta_c$ there is no surface transition. Only the bulk transition takes place. It follows from Eq. (3) that $\Delta_c=\sqrt{2}-1$ in mean-field theory.

In our renormalization-group approach each of the four transitions for $d=3$ is associated with a different fixed point.[8] Because of the two-dimensional nature of the surface transition, one expects $d=2$ bulk exponents for the corresponding fixed point. With our transformation the surface fixed point, which occurs for $H_b=0$, $p_2=p_b=0$, is identical with Kadanoff's $d=2$ bulk fixed point[9] and

TABLE I. Optimal variational parameters for fixed points.

Fixed point					
$d=2$					
O, transformation of Fig. 1(b)	$p_1=0.5818$	$p_2=0.6720$	$p_b=0.7660$		
O, transformation of Fig. 1(c)	$p_1=0.5704$	$p_2=0.6716$	$p_3=0.7067$	$p_4=0.6277$	$p_b=0.7660$
$d=3$					
S	$p_1=0.7660$	$p_2=0$	$p_b=0$		
O	$p_1=0.2419$	$p_2=0.3697$	$p_b=0.4034$		
SB	$p_1=0.6250$	$p_2=0.2340$	$p_b=0.4034$		
E	$p_1=\infty$	$p_2=0$	$p_b=0.4034$		

yields the same excellent values for the temperature and magnetic-field eigenvalues $y_t^{d=2}$, $y_h^{d=2}$, which determine the critical exponents.[6] The fixed points for the other three transitions are found in the hyperplane $H_b=H_b^*$, where the bulk couplings have their fixed-point values. In the hyperplane the ordinary and extraordinary fixed points are completely attractive, whereas the surface-bulk fixed point has one repulsive eigenvector with eigenvalue $y_{t_1}^{SB}$, consistent with its multicritical character. In the position-space approach the surface exponents at the ordinary and surface-bulk transitions are determined by the bulk temperature and magnetic field eigenvalues $y_t^{d=3}$ and $y_h^{d=3}$, the eigenvalues $y_{h_1}^O$, $y_{h_1}^{SB}$ corresponding to a magnetic eigenperturbation in the surface cluster H_s, and $y_{t_1}^{SB}$. We refer to Ref. 8 for more details.

TABLE II. Relevant eigenvalues of the renormalization-group (RG) transformation at the various fixed points.

Eigenvalue	RG result	Exact value or best estimate
$d=2$		
$y_t^{d=2}$	1.001	1
$y_h^{d=2}$	1.875	$\frac{15}{8}$
$y_{h_1}^O$	0.5541,[a] 0.5452[b]	$\frac{1}{2}$[c]
$d=3$		
$y_t^{d=3}$	1.590	1.56 ± 0.04
$y_h^{d=3}$	2.465	2.50 ± 0.02
$y_t^{d=2}$	1.001	1
$y_h^{d=2}$	1.875	$\frac{15}{8}$
$y_{h_1}^O$	0.7363	1.0 ± 0.2[d]; $y_{h_1}^O=\frac{1}{2}(d-y_t^{d=3})=0.72\pm0.02$
$y_{t_1}^{SB}$	0.8664	$y_{t_1}^{SB}=y_t^{d=3}-1=0.56\pm0.04$
$y_{h_1}^{SB}$	1.745	$y_{h_1}^{SB}=2-\frac{1}{3}\epsilon+O(\epsilon^2)=1.667$
$y_{h_1}^E$	2	2

[a] Calculated with the transformation of Fig. 1(b).
[b] Calculated with the transformation of Fig. 1(c).
[c] Exact result (see Ref. 11) which is also consistent with the scaling law of Bray and Moore for $y_{h_1}^O$.
[d] Calculated from estimates of β_1^O reviewed in Ref. 14.

The variational parameters which maximize the free energy at the various fixed points are shown in Table I. The corresponding critical exponents are shown in Table II. Since Kadanoff's successful bulk transformation was incorporated in our approach, the bulk y_t's and y_h's are all in impressive agreement with the exact values or best estimates. For $d=2$ the surface only undergoes the ordinary transition. No surface transition takes place since such a transition would be one-dimensional. For the ordinary and surface-bulk transitions Bray and Moore propose the scaling relations $y_{h_1}^O=\frac{1}{2}(d-y_t)$, $y_{t_1}^{SB}=y_t-1$, and $y_{h_1}^{SB}=2-\frac{1}{3}\epsilon+O(\epsilon^2)$, where $\epsilon=4-d$. Our calculated eigenvalues for $d=2$, 3 agree with these predictions to within an accuracy of about 10% except for the case of $y_{t_1}^{SB}$, where the discrepancy is much larger. We discuss this disagreement in more detail in the next section. The eigenvalue $y_{h_1}^E=2$ we find is consistent with the existence of a nonzero surface magnetization[6,8,15] at the extraordinary transition. We have not been able to predict the critical exponents of the leading singularities at the extraordinary transition with our approach.

Results for several critical couplings, computed with the variational parameters in the renormalization transformation equal to the optimum values for the fixed point in question, are given in Table III. The bulk critical nearest-neighbor couplings are within 4% of the accepted values. For the bcc lattice we find Δ_c to be about 2.4 times its mean-field value. The series work of Binder and Hohenberg[14] yields a similar result for the simple cubic lattice.

Since the variational parameters for the various fixed points are quite different, one cannot expect a globally accurate phase diagram for a single choice of the variational parameters. The dashed

TABLE III. Various critical couplings calculated with the renormalization-group (RG) transformation. Δ_c^{MF} denotes the value of Δ_c in mean-field theory.

Coupling	RG result	Exact value or best estimate
	$d=2$, square lattice	
$K_c^{d=2}$	0.458	$\frac{1}{2}\ln(1+\sqrt{2})=0.441$
	$d=3$, bcc lattice	
$K_c^{d=3}$	0.162	0.157
$K_c^{d=2}$	0.458	$\frac{1}{2}\ln(1+\sqrt{2})=0.441$
Δ_c	0.976, $\Delta_c/\Delta_c^{MF}=2.36$	0.6 ± 0.1,[a] $\Delta_c/\Delta_c^{MF}=2.4\pm0.4$ for simple cubic lattice

[a]Series estimate from Ref. 14.

lines in Fig. 2 indicate the phase diagram calculated with p_b adjusted for the bulk fixed point H_b^* and with p_1 and p_2 obtained by averaging the optimal values for fixed points S and SB. The arrows show the accepted values of $K_c^{d=2}$ and $K_c^{d=3}$, where the phase diagram should intersect the K_s and K_b axes. Calculated with the optimal variational parameters for fixed point S, the diagram intersects the K_s axis at the empty point 1, closer to the arrow. Calculated with the optimum variational parameters for fixed point SB, the multicritical point SB drops down to the empty point 2. (The two empty points correspond to the values of $K_c^{d=2}$ and Δ_c in Table III.) To obtain a better global description, one should treat the variational parameters in each application of the renormalization transformation as independent variational parameters and change the p's as the coupling constants change. Kadanoff and co-workers[9] found that this procedure improves the results obtained for the thermodynamic functions of the $d=2$ Ising model.

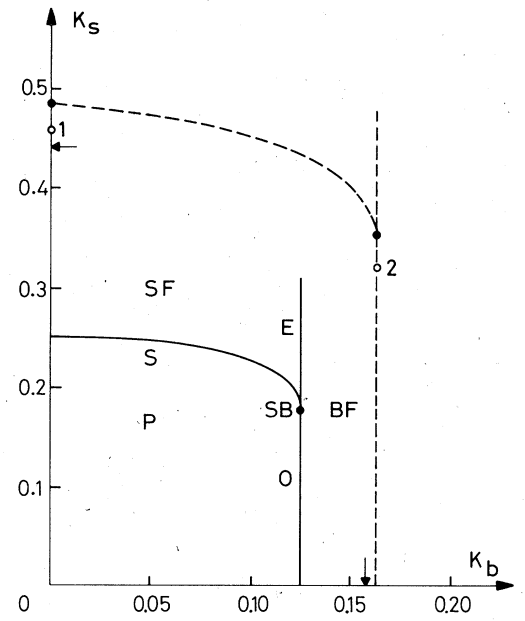

FIG. 2. Phase diagram for the semi-infinite Ising model with nearest-neighbor interactions on the $d=3$ bcc lattice. K_s denotes the surface coupling and K_b the bulk coupling. The solid lines show the results of mean-field theory. BF, SF, and P refer to the bulk ferromagnetic, surface ferromagnetic, and paramagnetic phases. S, O, E label the lines of surface, ordinary, and extraordinary transitions. SB labels the surface-bulk multicritical point. The dashed lines show the results of the renormalization-group calculation with p_b adjusted for the bulk fixed point and with p_1 and p_2 obtained by averaging the optimal values for fixed points S and SB. The arrows show the accepted bulk critical couplings $K_c^{d=2}$ and $K_b^c = K_c^{d=3}$ where the exact phase diagram intersects the K_s and K_b axes. The empty points 1 and 2 show the ends of the line of surface transitions when the variational parameters are optimized for fixed points S and SB, respectively.

IV. CONCLUDING REMARKS

The only scaling law of Bray and Moore which our results appear to contradict is the relation $\phi=1-\nu$ or $y_{t_1}^{SB}=y_t-1$ for the crossover exponent $\phi=y_{t_1}^{SB}/y_t$. This scaling law is certainly correct for an infinite system with the surface simulated by a plane of modified interactions.[5] In this model the ordinary and extraordinary transitions are observed for interactions in the special plane weaker and stronger than the bulk interactions, respectively. The surface-bulk transition corresponds to the pure bulk transition with no special plane at all. All the surface-bulk exponents can be readily worked out in terms of bulk exponents, since the response to the appropriate perturbations is determined by bulk quantities. One finds the above scaling law for $y_{t_1}^{SB}$ and also $y_{h_1}^{SB}=y_h-1$ [which implies $\beta_1^{SB}=\beta$ or $\gamma^{SB}=(1-\eta)\nu$, for example]. At the surface-bulk transition the infinite and semi-infinite models clearly do not belong to the same universality class. For the semi-infinite system Bray and Moore find a different result for $y_{h_1}^{SB}$ to first-order in ϵ. Our results suggest that there is also a difference in $y_{t_1}^{SB}$ for the two models. However, to first order in ϵ Bray and moore find no

difference. Unfortunately it is difficult to judge the accuracy of our approximate transformation. The reasonably good agreement of the calculated values of $y_{h_1}^{O}$ with the exact result for $d=2$ and the scaling law for $d=3$ (for $d=2$ the scaling law is consistent with the exact result) gives us some confidence in our procedure. However, one cannot completely rule out the possibility that the transformation yields a less reliable result for the eigenvalue $y_{t_1}^{SB}$.

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