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The Migdal-Kadanoff Renormalization Group Scheme for the Ising Model with a Free Surface

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The Migdal-Kadanoff scheme is applied to the Ising model with a free surface. The resulting renormalization group transformation and the duality transformation commute in any dimension. Two simple recursion relations are obtained which reproduce the global phase diagram for the semi-infinite Ising model. The surface critical exponents calculated in this way are comparable to those obtained by more complex position-space methods. In dimension $d=2+\varepsilon'$, we find the exponents $y_{t_1}^{(\mathrm{SB})}=\varepsilon'$ and $y_{h_1}^{(\mathrm{SB})}=1+\varepsilon'$ for the multicritical surface-bulk transition. We also derive and discuss approximate differential recursion relations for the bulk and the surface free energies.

1. Introduction

The presence of a free surface strongly affects the phase diagram of an Ising model. There are four different types of phase transitions for dimension $d>2$: the ordinary, the surface, the extraordinary, and the special or surface-bulk transition [1]. In order to discuss the thermodynamics of these transitions one has to consider the surface free energy in addition to the bulk free energy [2, 3]. Near the various phase boundaries the singular part of the surface free energy is described by scaling laws. These scaling laws define a variety of surface critical exponents [2, 3].

Different renormalization group methods have been used to calculate these exponents. In a field theoretic approach one maps the Ising model with a free surface on a continuous ϕ^4-theory with an additional surface term [1, 2, 4-7]. Then, one can calculate the surface exponents in an ε-expansion where $\varepsilon=4-d$ [4, 5]. Recently, this expansion has been accomplished up to $o(\varepsilon^2)$ for the ordinary transition [6, 7]. On the other hand, various position-space renormalization schemes have also been used [8-12]. They are directly applicable to the discrete Ising model defined on a lattice. Comparing the exponents obtained in this way with exact results known in dimension $d=2$ one finds a typical accuracy of the order of 10%. In contrast to the field theoretic approach, one may also use the position-space methods to investigate the global phase diagram as well as thermodynamic functions like the surface free energy in the whole temperature regime (e.g. [11]).

The position-space methods used so far for the semi-infinite Ising model include cell cluster expansions [8, 9, 11], cumulant expansions [9, 12], and Kadanoff's variational method [10]. In this paper we apply the Migdal-Kadanoff (MK) scheme [13, 14] to this problem. This approach has several advantages:

1. It turns out that we can use the same prescription both for the bulk and for the surface. In a cell cluster or cumulant expansion one must use different majority rules for the surface and the bulk spins in order to avoid unphysical features of the resulting renormalization group transformation [9].

2. The recursion relations obtained in the MK scheme are easily continued to arbitrary dimension [13]. Thus, we can explicitly incorporate the presence of two lower critical dimensions $d_1^*=1$ and $d_2^*=2$: for $d\leqq d_1^*$ there is no phase transition at all,

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and for $d \leq d_2^*$ there is only the ordinary transition. This reveals the possibility to calculate the surface critical exponents for the surface and for the surface-bulk transition by an ε'-expansion in dimension $d = d_2^* + \varepsilon'$.

3. The MK renormalization scheme has been applied to a large variety of lattice models with periodic boundary conditions (e.g. [15-18, 25]). For all of these models, the effect of a free surface can be easily investigated by our approach.

The paper is organized as follows. After the definition of the model in Sect. 2 we show in Sect. 3 that the MK scheme may be easily extended to this problem. In Sect. 4 we discuss the MK schemes for the dual models and show that the MK transformation and the duality transformation commute in any dimension. Section 5 contains the global phase diagram and the relevant eigenvalues. Finally, we discuss the free energy in Sect. 6. Although our system is not translationally invariant the infinitesimal MK transformation still yields a lower bound approximation to the free energy. In order to estimate the accuracy of this bound we investigate the MK approximation both for the bulk and for the surface free energy.

2. Model

Consider an Ising model on a d-dimensional hypercubic lattice with free boundary conditions in one Cartesian direction which we denote by z and periodic boundary conditions in the remaining $(d-1)$ directions which we denote by x_β, $\beta = 2, \ldots, d$. The lattice has N sites with N_s sites belonging to the surface. Thus, the free surface consists of two parts: a "front" and a "back" surface. The free energy of this system is given by

$$F(E, E_s, K, K_s, H, H_s) = (N - N_s) E + N_s E_s + \ln \sum_{\{\sigma\}} e^{\mathscr{H}(\sigma)} \tag{2.1}$$

with the Hamiltonian

$$\mathscr{H}(\sigma) = \sum_{\langle ij \rangle} B(\sigma_i, \sigma_j), \tag{2.2}$$

$$B(\sigma_i, \sigma_j) = \begin{cases} K \sigma_i \sigma_j + \dfrac{H}{2d}(\sigma_i + \sigma_j) & i, j \in \Lambda - \Lambda_s \\ K_\perp \sigma_i \sigma_j + \dfrac{H}{2d} \sigma_j & i \in \Lambda_s, j \in \Lambda - \Lambda_s \\ K_s \sigma_i \sigma_j + \dfrac{H_s}{2(d-1)}(\sigma_i + \sigma_j) & i, j \in \Lambda_s \end{cases} \tag{2.3}$$

$\langle ij \rangle$ indicates a sum over nearest neighbours, and Λ_s is the set of all surface sites while $\Lambda - \Lambda_s$ is the set of all sites not at the surface. K, $K_\perp$ and K_s are nearest neighbour couplings (see Fig. 1a) while H and H_s are the bulk and surface magnetic field respectively. The spin independent couplings E and E_s have also been included since we generate such couplings under renormalization.

3. Renormalization Group Method

We apply the Migdal-Kadanoff scheme to the above model. This scheme consists of successive transformations by a scale factor b along each of the d Cartesian directions [14]. For integer $b = 2, 3, \ldots$ one must consider both anisotropic bulk couplings $\mathbf{K} := (K_1, \ldots, K_d)$ with $K_1 = K_z$ and anisotropic surface couplings $\mathbf{K}_s := (K_{s2}, \ldots, K_{sd})$ as indicated in Fig. 1a for $d = 2$ and $H = H_s = 0$. In Fig. 1b and Fig. 1c the successive transformations are depicted for $b = 3$. In the first step, the bonds K_2 are moved in such a way that we may sum over the spins indicated by a cross in Fig. 1b. This results in new couplings $\hat{K}_1$, $\hat{K}_2$, $\hat{K}_\perp$, and $\hat{K}_s$. If one looks at Fig. 1b it may seem that we could move any fraction of the shifted $(b-1)$ couplings K_2 onto the surface bond K_s. However, for finite N, N_s one should require that both "back" and "front" surface are treated in the same way. This

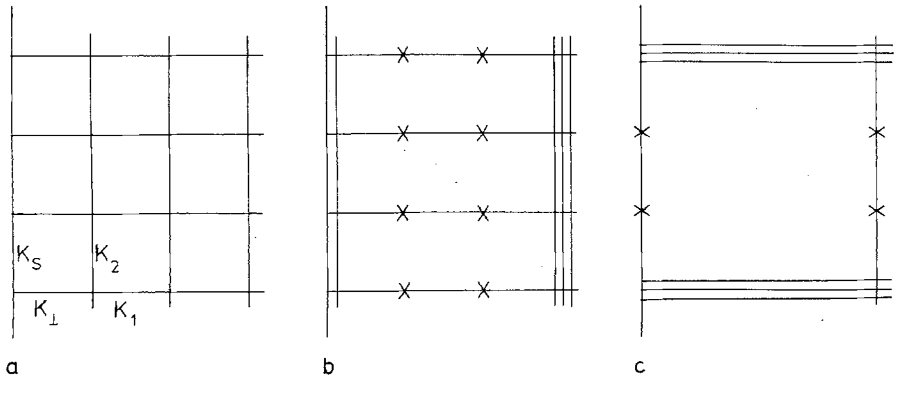

Fig. 1. Successive steps of the MK transformation at the free surface for $b = 3$ as explained in the text

uniquely determines the fraction $\frac{b-1}{2}$. Now we move the bonds $\hat{K}_1$ and $\hat{K}_\perp$ and sum over the crossed spins of Fig. 1c. In this way we arrive at a new Ising model with lattice constant b and renormalized couplings K'_1, K'_2, $K'_\perp$ and K'_s.

The summations performed in each step are called dedecoration transformations [19]. They are discussed in Appendix A. Extending this procedure to arbitrary dimension d we obtain the recursion relations

$$K'_\alpha = b^{d-\alpha}\,\mathscr{D}(b^{\alpha-1}K_\alpha) \qquad \alpha=1,\dots,d, \tag{3.1a}$$

$$K'_{s\beta} = b^{d-1-\beta}\,\mathscr{D}(b^{\beta-2}J_{s\beta}) \qquad \beta=2,\dots,d,$$

$$J_{s\beta} := K_{s\beta} + \tfrac{1}{2}(b-1)K_\beta \tag{3.1b}$$

$$K'_\perp = b^{d-1}\,\mathrm{arth}\{th K_\perp (th K_1)^{b-1}\} \tag{3.1c}$$

with $\mathscr{D}(x) := \mathrm{arth}(th x)^b$. For finite b, the renormalized couplings depend on the order in which the d successive transformations have been performed. However, in the infinitesimal rescaling limit $b \to 1+\delta l$ the transformations in the different directions commute. As a consequence, we may set $K_\alpha = K$ and $K_{s\beta} = K_s$ as in our model defined by (2.3). In this limit we obtain from (3.1) the differential recursion relations

$$\frac{dK}{dl} = (d-1)K + \tfrac{1}{2} sh 2K \ln th K, \tag{3.2a}$$

$$\frac{dK_s}{dl} = \tfrac{1}{2}K + (d-2)K_s + \tfrac{1}{2} sh 2K_s \ln th K_s, \tag{3.2b}$$

$$\frac{dK_\perp}{dl} = (d-1)K_\perp + \tfrac{1}{2} sh 2K_\perp \ln th K. \tag{3.2c}$$

(3.2a) is the well known recursion relation for the bulk i.e. for the isotropic Ising model with periodic boundary conditions (e.g. [16]). Note that the d-dimensional recursion relation (3.2b) for the surface coupling K_s reduces with $K=0$ to the recursion relation (3.2a) for a $(d-1)$-dimensional bulk system. In a cell cluster approach, one has to change the majority rule at the surface in order to obtain this property [9] which must hold in an exact renormalization group transformation.

In order to handle the magnetic fields H, H_s in a similar fashion each bulk field H is divided into $2d$ pieces [20, 21] and each surface field H_s is divided into $2(d-1)$ pieces as indicated in (2.3). The resulting bond interaction terms $\frac{H}{2d}(\sigma_i+\sigma_j)$ and $\frac{H_s}{2(d-1)}(\sigma_i+\sigma_j)$ of the Hamiltonian (2.2) are moved along with the nearest neighbour couplings. For $b \to 1+\delta l$ this procedure yields (to first order in the magnetic fields):

$$\frac{dH}{dl} = (d-1-sh 2K \ln th K)H, \tag{3.3a}$$

$$\frac{dH_s}{dl} = (d-2-sh 2K_s \ln th K_s)H_s + \{\tfrac{1}{2}(d-1) - \tfrac{1}{2} sh 2K_\perp \ln th K\}\frac{H}{d}. \tag{3.3b}$$

Of course, one could use another division of the surface field H_s. The above choice ensures, however, that (3.3b) for $H=0$ reduces to the bulk field recursion relation (3.3a) in $(d-1)$ dimensions. In this respect, our choice is unique.

The infinitesimal MK transformation when applied to the bulk problem has two interesting features: it yields a lower bound to the free energy [14, 15], and it commutes with the duality transformation. We show in Sect. 6 that the lower bound property still holds in our case where translational invariance is broken in the z-direction. The relationship between the Migdal-Kadanoff and the duality transformation is discussed in the next Section.

4. Migdal-Kadanoff Transformation and Duality

From (3.2a, b, c) we may obtain differential recursion relations for the dual couplings K^*, $K^*_\perp$ and K^*_s defined by $K^* = -\frac{1}{2}\ln th K$ etc.:

$$\frac{dK^*}{dl} = \frac{dK}{dl}\,\frac{dK^*}{dK} = K^* + \tfrac{1}{2}(d-1) sh 2K^* \ln th K^*, \tag{4.1a}$$

$$\frac{dK^*_s}{dl} = K^*_s + \tfrac{1}{2} sh 2K^*_s [\tfrac{1}{2}\ln th K^* + (d-2)\ln th K^*_s], \tag{4.1b}$$

$$\frac{dK^*_\perp}{dl} = K^* + \tfrac{1}{2}(d-1) sh 2K^*_\perp \ln th K^*_\perp. \tag{4.1c}$$

On the other hand, we may apply the appropriate Migdal-Kadanoff transformation directly to the dual model obtained from (2.2) with $H=H_s=0$. In dimension $d=2$, the dual model is an Ising model with fixed boundary conditions in the z-direction (the duality transformation is discussed in [22, 23] for periodic, and in [24] for more general boundary conditions). Since we have to treat both the "front" and the "back" surface in the same way and require that every new bond contains b old bonds, we must shift bonds perpendicular to the fixed surface as shown in Fig. 2 for $b=3$. Parallel to the fixed surface the bonds are still shifted as in Fig. 1c. For $b \to 1+\delta l$

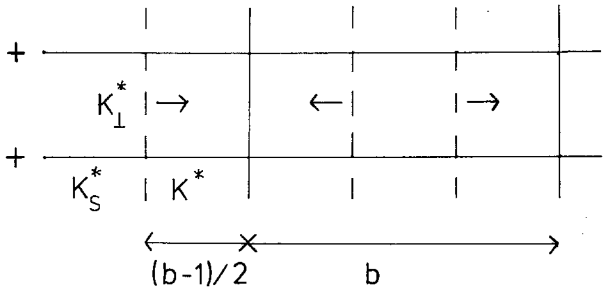

Fig. 2. Bond moving perpendicular to the fixed surface in the 2-dimensional dual model. The (+)-spins are fixed

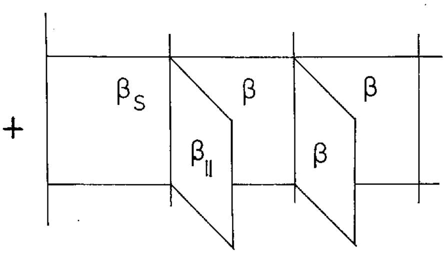

Fig. 3. Coupling constants of the 3-dimensional pure $\mathbb{Z}_2$-gauge model at the fixed surface. The fixed bond variable is indicated by (+)

this procedure results in the recursion relations (4.1) with $d=2$. In this case, $\frac{dK^*}{dl}(K^*)$ has the same functional dependence as $\frac{dK}{dl}(K)$ which reflects the self-duality of the 2-dimensional Ising model in the bulk thermodynamic limit. As a consequence, (3.2a) and (4.1a) give the exact Onsager value for the critical coupling $K^c = K^{*c} = \frac{1}{2}\ln(1+\sqrt{2})$ [13, 16].

In $d=3$, the dual model is a pure $\mathbb{Z}_2$-gauge model with fixed boundary conditions in the z-direction, i.e. fixed bond variables at the surface. This model is schematically depicted in Fig. 3 with $\beta := K^*$, $\beta_s := K_s^*$ and $\beta_{\|} := K_\perp^*$. The plaquette couplings have been renamed since we want to consider this model for arbitrary dimension. For $d=2$, the pure $\mathbb{Z}_2$-gauge model is exactly soluble. For $d>2$ one has to shift plaquette interaction terms as discussed by Kadanoff [14, 15] for the bulk. The generalization to our case is straightforward if we determine the shifts perpendicular to the fixed surface as in the Ising model above. For $b \to 1+\delta l$ we arrive at

$$\frac{d\beta}{dl} = (d-2)\beta + sh\,2\beta \ln th\,\beta, \tag{4.2a}$$

$$\frac{d\beta_s}{dl} = (d-2)\beta_s + sh\,2\beta_s\left(\tfrac{1}{4}\ln th\,\beta + \tfrac{1}{2}\ln th\,\beta_s\right), \tag{4.2b}$$

$$\frac{d\beta_{\|}}{dl} = (d-3)\beta_{\|} + sh\,2\beta_{\|}\ln th\,\beta_{\|} + \beta. \tag{4.2c}$$

For $d=3$, (4.2) and (4.1) are identical since $\beta = K^*$, $\beta_s = K_s^*$ and $\beta_{\|} = K_\perp^*$ in this case. Thus we have shown that the MK transformation and the duality transformation commute for $d=2$ and $d=3$. This argument can be easily extended to all integer dimensions.

5. Global Phase Diagram and Relevant Eigenvalues

We now take the thermodynamic limit in such a way that we end up with a semi-infinite system. This enables us to integrate the recursion relation (3.2) till $l=\infty$ and thus to reach various fixed points.

In contrast to more complex position-space schemes [8–12], the subspace $K_\perp = K$ is invariant under the MK renormalization transformation (3.2). In addition, all fixed points lie in this 2-dimensional coupling constant subspace. Since $\delta K_\perp := K_\perp - K$ is always an irrelevant perturbation we may confine the discussion of the phase diagram to the case $K_\perp = K$. The flow in this subspace is governed by (3.2a, b). These simple recursions reproduce the whole phase diagram for the semi-infinite Ising model [3, 8–10]. In Fig. 4a and 4b we depict the global phase diagrams for $1<d\leqq 2$ and $2<d$ respectively. In the figure caption, we refer to the fixed point terminology of Burkhardt and Eisenriegler [9, 10]. The K_s-coordinates of the various fixed points are: $K_s^{(0)} = 0.092$ in $d=2$, and $K_s^{(0)} = 0.026$, $K_s^{(S)} = \frac{1}{2}\ln(1+\sqrt{2})$, and $K_s^{(SB)}) = 0.346$ in $d=3$.

From the bulk recursion (3.2a) one derives the thermal eigenvalue y_t [13, 16] along the phase boundary $K = K^c$:

$$y_t = d + ch\,2K^c \ln th\,K^c = \begin{cases} \varepsilon & d = 1+\varepsilon \\ 0.754 & d=2 \\ 0.943 & d=3. \end{cases} \tag{5.1}$$

The $O(\varepsilon)$ result for y_t also follows from (3.1) and is therefore independent of b. Thus, one expects that it is exact [25]. This expectation is supported by the field theoretic renormalization of the drumhead model [26]. The perturbation $\delta K_s := K_s - K_s^{(\cdot)}$ is irrelevant at the ordinary critical fixed point (0) and relevant at the surface critical and surface-bulk multicritical fixed points (S) and (SB). The corresponding eigenvalues for $d=3$ are compared in Table 1 with results obtained by other position-space methods [9, 10, 12] and with exact results. The position-space methods referred to in Table 1 include: the two-cell cluster approximation with the usual majority rule (CCL) and with a changed majority rule denoted by $M2$ in [9] (CCL′), the lowest order cumulant approximation with the usual majority

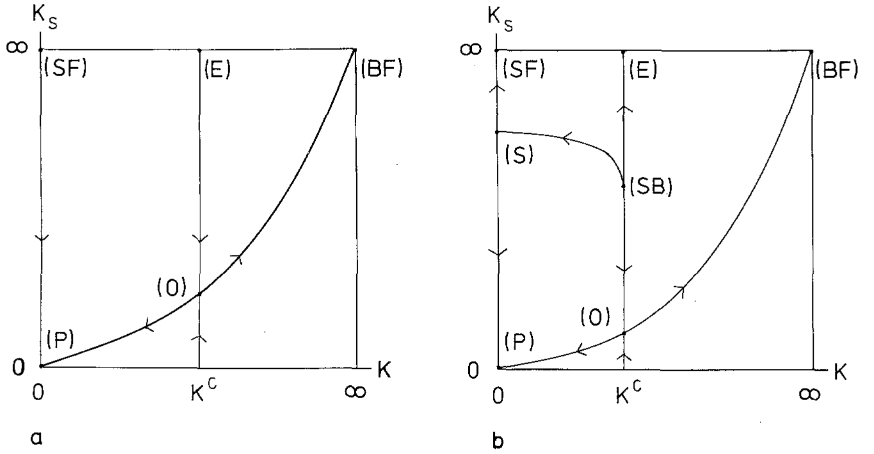

Fig. 4. Global phase diagram for **a** $1<d\leqq 2$ and **b** $2<d$. The various fixed points are: bulk ferromagnetic (BF), extraordinary (E), surface ferromagnetic (SF), ordinary critical (O), surface critical (S), and surface-bulk multicritical (SB). The arrows indicate trajectories of the MK renormalization group

rule (CUM) and with majority rule $M2$ (CUM′), and Kadanoff's variational method (KV) (note that $y_{h_1}^{(S)}$ is denoted by $y_h^{d=2}$ in [9, 10, 12]).

The magnetic eigenvalue along the line $K=K^c$ as obtained from (3.3a) is [13, 27]

$$y_h=d-1-sh2K^c\ln thK^c=\begin{cases}1+\varepsilon & d=1+\varepsilon\\ 1.881 & d=2\\ 2.558 & d=3.\end{cases}\tag{5.2}$$

At the discontinuity fixed point (BF) the bulk field recursion (3.3a) gives the exact result $y_h=d$ [28]. From the surface field recursion (3.3b) one finds that the surface field H_s is relevant at all fixed points. The corresponding eigenvalues are denoted by $y_{h_1}^{(\cdot)}$. At the fixed points (BF), (E), and (SF) where $K_s^{(\cdot)}=\infty$ the MK scheme yields the values $y_{h_1}^{(BF)}=y_{h_1}^{(E)}=y_{h_1}^{(SF)}=d-1$ consistent with the existence of a nonzero surface magnetization at the corresponding transitions [9, 10, 28]. The results for $y_{h_1}^{(\cdot)}$ at the fixed points (0), (S), and (SB) are listed in Table 1 for $d=2, 3$. At the high temperature fixed point (P) both the bulk field recursion (3.3a) and the surface field recursion (3.3b) are spurious since the magnetic perturbations must be marginal for all d while these recursions yield $y_h^{(P)}=d-1$ and $y_{h_1}^{(P)}=d-2$. This is an artifact of the above bond moving scheme where magnetic fields are moved even for $K=K_s=0$ [29, 16].

Of course, we cannot expect to get precise values for the exponents in $d=3$. In $d=2+\varepsilon'$, however, we may obtain the surface critical exponents at (S) and (SB) correct up to $O(\varepsilon')$. Since the surface recursion (3.2b) with $K=0$ reduces to the bulk recursion (3.2a) in $(d-1)$ dimensions the exact scaling relation $y_{t_1}^{(S)}(d)=y_t(d-1)$ holds in our scheme. Thus, from (5.1) we get $y_{t_1}^{(S)}(2+\varepsilon')=\varepsilon'$ at the surface fixed point (S). At the surface-bulk fixed point we find the same value since $y_{t_1}^{(SB)}=d-1+ch\;2K_s^{(SB)}\ln th\;K_s^{(SB)}$ and $K_s^{(SB)}=\frac{1-K^c}{2\varepsilon'}$ with $K^c=\frac{1}{2}\ln(1+\sqrt{2})+O(\varepsilon')$ in $d=2+\varepsilon'$. We argue that this value $y_{t_1}^{(SB)}=\varepsilon'$ is exact in $O(\varepsilon')$ since it also follows from (3.1) and therfore does not depend on the rescaling factor b [25]. For finite b, the coordinates of (SB) in $d=2+\varepsilon'$ are

$$K_{s\beta}^{(SB)}=\frac{1}{2\varepsilon'}b^{-(\beta-2)}\left(1-\frac{b-1}{\ln b}K_1^c\right)$$

with $\beta=2, \ldots, d$. K_1^c is obtained from (3.1a).

We may also calculate $y_{h_1}^{(\cdot)}$ near to the lower critical dimensions $d_1^*=1$ and $d_2^*=2$. Since the fixed points

Table 1

		Exact value	MK	CCL [9]	CCL′ [9, 11]	CUM [12]	CUM′ [9]	KV [10]
$d=2$	$y_{h_1}^{(O)}$	1/2	0.44	0.64	0.61	–	–	0.55
$d=3$	$y_{t_1}^{(S)}$	1	0.75	0.46	0.89	1.12	1.01	1.00
	$y_{t_1}^{(SB)}$	–	0.63	0.08	0.72	0.05	0.79	0.87
	$y_{h_1}^{(O)}$	–	1.19	1.13	0.79	1.54	0.56	0.74
	$y_{h_1}^{(S)}$	15/8	1.88	1.84	1.66	2.65	2.15	1.88
	$y_{h_1}^{(SB)}$	–	1.82	1.21	1.56	1.62	1.97	1.75
	$y_{h_1}^{(E)}$	2	2	1.98	2	∞	2	2

Relevant eigenvalues $y_{t_1}^{(\cdot)}$ and $y_{h_1}^{(\cdot)}$ obtained by different position-space methods. The abbreviations at the head of the table are explained in the text

(0) and (BF) merge un $d_1^* = 1$ one obtains $y_{h_1}^{(0)}(1+\varepsilon) = \varepsilon$. This implies that the scaling relation $y_{h_1}^{(0)} = \frac{1}{2}(d - y_t)$ of Bray and Moore [5] does not hold in $d = 1 + \varepsilon$. Since the fixed points (S) and (SF), and the fixed points (SB) and (E) merge in $d_2^* = 2$ it follows that $y_{h_1}^{(S)}(2+\varepsilon') = y_{h_1}^{(SB)}(2+\varepsilon') = 1 + \varepsilon'$.

6. MK approximation for the Free Energy

Moving bonds as depicted in Fig. 1b and 1c means that we add terms of the form

$$\Delta := (b-1)\, B(\sigma_1, \sigma_1') - \sum_{n=2}^{b} B(\sigma_n, \sigma_n')$$

to the Hamiltonian (2.2). If the expectation value $\langle \Delta \rangle$ vanishes this procedure yields a lower bound approximation for the free energy [14, 15] due to the Peierls inequality $\langle e^{\Delta} \rangle \geqq e^{\langle \Delta \rangle}$. This holds in the Ising model with periodic boundary conditions since all $\langle B(\sigma, \sigma') \rangle$ are equal in this case. However, in the Ising model with a free surface as defined by (2.1) the expectation values $\langle B(\sigma, \sigma') \rangle$ depend on the distance from the surface. Thus, $\langle \Delta \rangle \neq 0$ for the bond shifting performed perpendicular to the surface, and our scheme is not a lower bound approximation for finite b. The same problem arises in Kadanoff's variational method as discussed by Burkhardt and Eisenriegler [10]. There, the authors considered a sequence of RG transformations such that the perpendicular shifts begin farther and farther away from the surface. In our case, it is possible to devise a modified bond moving scheme where all bonds are moved parallel to the surface. This scheme is described in Appendix *B*. For integer b the resulting transformation is quite different from the MK transformation (3.1). However, in the limit $b \to 1 + \delta l$ we recover the differential recursions (3.2a, b) and (3.3a, b). This implies that the MK scheme described in Sect. 3 is a lower bound approximation in the infinitesimal rescaling limit for $K = K_\perp$.

In order to get an estimate for the accuracy of this bound for $H = H_s = 0$ and $K_\perp = K_1$ we introduce an approximate free energy $F_{\mathrm{MK}} := (N - N_s)\, E + N_s E_s + f_{\mathrm{MK}}(\mathbf{K}, \mathbf{K}_s)$ which is not changed under the MK transformation i.e.

$$N E + N_s(E_s - E) + f_{\mathrm{MK}}(\mathbf{K}, \mathbf{K}_s) = N' E' + N_s'(E_s' - E') + f_{\mathrm{MK}}(\mathbf{K}', \mathbf{K}_s') \tag{6.1}$$

where the number of sites and of surface sites transform according to

$$N' = b^{-d} N + (b^{-(d-1)} - b^{-d})\, \tfrac{1}{2} N_s \tag{6.2a}$$

$$N_s' = b^{-(d-1)} N_s \tag{6.2b}$$

and the renormalized spin independent coupling E' is

$$E' = b^d E + \sum_{\alpha=1}^{d} b^{d-\alpha}\, \delta E(b^{\alpha-1} K_\alpha) \tag{6.3a}$$

$$\delta E(x) := (b-1) \ln 2 + \tfrac{1}{2} \ln \{(ch\, x)^{2b} - (sh\, x)^{2b}\}. \tag{6.3b}$$

The δE-terms are generated by the dedecoration transformations as explained in Appendix *A*. There, we also derive the corresponding expression for E_s'. Note that the transformation (6.2a) for the total number of sites N depends on the number of surface sites N_s, and is therefore affected by the presence of the free surface. This should be compared with an Ising model with periodic boundary conditions where N transforms according to $N' = b^{-d} N$.

The quantity of interest in (6.1) is the function f_{MK} which approximates the configuration sum in (2.1). In the next two subsections we will investigate the corresponding bulk and surface free energies.

6.1. *Bulk Free Energy*

We define the approximate bulk free energy f_{B} by $f_{\mathrm{B}}(\mathbf{K}) := \lim_{N \to \infty} \frac{f_{\mathrm{MK}}(\mathbf{K}, \mathbf{K}_s)}{N}$. Deviding (6.1) by N and taking the thermodynamik limit we arrive at

$$f_{\mathrm{B}}(\mathbf{K}') = b^d f_{\mathrm{B}}(\mathbf{K}) + b^d E - E' \tag{6.4}$$

In the infinitesimal rescaling limit we set $K_\alpha = K$, $\alpha = 1, \ldots, d$ and obtain from (6.3)

$$E' = E + \delta l\, d(E + g(k)), \tag{6.5a}$$

$$g(K) := \ln 2 + ch^2 K \ln ch K - sh^2 K \ln sh K. \tag{6.5b}$$

If this is inserted into (6.4) the differential recursion relation

$$\frac{d f_{\mathrm{B}}}{dl} = d f_{\mathrm{B}}(K) - d g(K) \tag{6.6}$$

results. The general solution of this differential equation is

$$f_{\mathrm{B}}(K) = d \int_0^\infty dl\, e^{-dl} g(\tilde{K}(l, K)) + C(K), \tag{6.7a}$$

$$C(K) := \lim_{l \to \infty} e^{-dl} f_{\mathrm{B}}(\tilde{K}(l, K)) \tag{6.7b}$$

where K is the initial value $\tilde{K}(l = 0, K)$. In order to get a unique solution we must specify the boundary condition $C(K)$. In general, this depends on the fixed point reached in the limit $l \to \infty$. We would like to choose these boundary conditions in such a way that the approximate bulk free energy (6.7) has the exact asymptotic behaviour [11]:

$$f_B(K) \sim \begin{cases} dK & K \to \infty \qquad (6.8\text{a}) \\ \ln 2 + \frac{1}{2} dK^2 & K \to 0. \qquad (6.8\text{b}) \end{cases}$$

It is shown in Appendix C that $C(K)=0$ is appropriate for both $K > K_c$ and $K < K_c$. Thus, in contrast to the cell cluster approximation [11], one can easily incorporate the correct asymptotic behaviour (6.8) in the MK scheme.

In $d=1$, (6.7) with $C(K)=0$ gives the exact bulk free energy $f_B(K) = \ln(2chK)$. In $d=2$, we may compare (6.7) with the exact result [30]. This is done in Fig. 5a. The corresponding bulk energies $\varepsilon_B := -\frac{\partial f_B}{\partial K}$ are compared in Fig. 5b. As expected, the approximate f_B is always bigger than the exact one. (Note, that we have absorbed a factor (-1) in the definition of F and f_B. Thus, a lower bound approximation gives an upper bound for these quantities.) The relative error of the approximation is less than 5% for f_B over the whole temperature regime.

6.2. Surface Free Energy

We define the approximate surface free energy f_s by

$$f_s(\mathbf{K}, \mathbf{K}_s) = \lim_{\substack{N \to \infty \\ N_s \to \infty}} \frac{f_{MK}(\mathbf{K}, \mathbf{K}_s) - N f_B(\mathbf{K})}{N_s} \qquad (6.9)$$

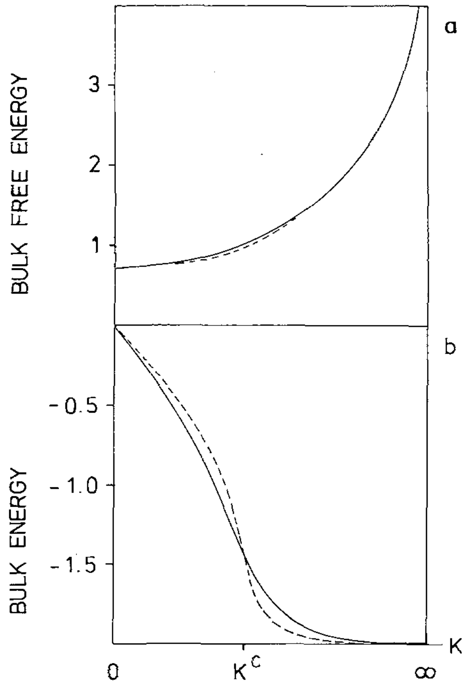

Fig. 5. MK approximations (full curves) and exact results (dashed curves) for the bulk free energy and the bulk energy of the 2-dimensional Ising model. The scale for the K-axis is proportional to $th(K)$

If we use the transformation laws (6.2a, b) and (6.4) for N, N_s and f_B in (6.1) and take the thermodynamic limit we obtain

$$\begin{aligned} f_s(\mathbf{K}', \mathbf{K}_s') &= b^{d-1} f_s(\mathbf{K}, \mathbf{K}_s) \\ &+ b^{d-1}(E_s - E) - (E_s' - E') \\ &- \tfrac{1}{2}(b^d - b^{d-1})(E + f_B). \end{aligned} \qquad (6.10)$$

Note that the bulk free energy f_B is present in the recursion relation for the surface free energy f_s. In the limit $b \to 1 + \delta l$ the spin independent coupling E' is given by (6.5) and the spin independent surface coupling E_s' given by (A.8) for finite b reduces to

$$E_s' = E_s + \delta l \{(d-1) E_s + (d-1) g(K_s) + \tfrac{1}{2} E + \tfrac{1}{2} g(K)\} \qquad (6.11)$$

where $g(x)$ is defined by (6.5b). If we use these expressions in (6.10) we arrive at the differential recursion relation

$$\frac{df_s(K, K_s)}{dl} = (d-1) f_s + G(K, K_s), \qquad (6.12\text{a})$$

$$G(K, K_s) := (d-1)\{g(K) - g(K_s)\} + \tfrac{1}{2}\{g(K) - f_B(K)\}. \qquad (6.12b)$$

Direct integration of the differential equation (6.12a) yields

$$f_s(K, K_s) = \int_0^\infty dl\, e^{-(d-1)l} G(l) + C_s(K, K_s), \qquad (6.13\text{a})$$

$$C_s(K, K_s) := \lim_{l \to \infty} e^{-(d-1)l} f_s(\tilde{K}(l, K), \tilde{K}_s(l, K, K_s)) \qquad (6.13\text{b})$$

with $G(l) := G(\tilde{K}(l, K), \tilde{K}_s(l, K, K_s))$ and the initial values $K = \tilde{K}(0, K)$ and $K_s = \tilde{K}_s(0, K, K_s)$. It is again possible to choose the boundary conditions $C_s(K, K_s)$ such that the approximate surface free energy (6.13) has the exact asymptotic behaviour given by [11]

$$f_s(K, K_s) \sim \begin{cases} -\frac{1}{2} dK + (d-1)(K_s - \frac{1}{2} K) & K, K_s \to \infty \qquad (6.14\text{a}) \\ (d-1)\frac{1}{2}(K_s^2 - K^2) - \frac{1}{4} K^2 & K, K_s \to 0. \qquad (6.14\text{b}) \end{cases}$$

It is shown in Appendix C that the appropriate boundary conditions are $C_s(K, K_s) = 0$ for $K < K_c$ and

$$\begin{aligned} C_s(K, K_s) &= \lim_{l \to \infty} e^{-(d-1)l}(-\tfrac{1}{2}) d\tilde{K}(l, K) \\ &= -\tfrac{1}{2} dK + \tfrac{1}{4} \frac{d}{d-1} \end{aligned} \qquad (6.15)$$

for $K>K_c$. For the bulk free energy (6.7) we found $C(K)=0$ both at the high and at the low temperature fixed point since the factor e^{-dl} in (6.7b) dominates in both cases. In contrast, the term (6.15) survives for the surface free energy at the low temperature fixed point (BF) since $\tilde{K}(l,K)$ is proportional to $e^{(d-1)l}$ for $K>K_c$ and large l which cancels the factor $e^{-(d-1)l}$ in (6.13b) and (6.15).

In dimension $d=1$ the recursion relation (6.12a) reduces to

$$\frac{df_s}{dl}=\frac{dK}{dl}\frac{df_s(K,K_s(K))}{dK}=\tfrac{1}{2}\{g(K)-f_B(K)\}. \tag{6.16}$$

The solution to this equation yields the exact surface free energy $f_s(K,K_s)=-\frac{1}{2}\ln chK$ which does not depend on K_s. In $d=2$, the exact surface free energy is known only along the physical line $K=K_s\propto$ (temperature)$^{-1}$ [30]. In order to calculate the approximate f_s from (6.12) for this special case we have to integrate along the renormalization group trajectories shown in Fig. 6. The result of these integrations is compared in Fig. 7a with the exact result. In Fig. 7b we compare the corresponding surface energies $\varepsilon_s:=-\dfrac{\partial f_s(K,K_s=K)}{\partial K}$. For $K>K_c$ the approximation is quite good, the relative error being less than 15%. For $K<K_c$, the approximation is less reliable with a maximum relative error of 36%. In contrast to the approximate bulk free energy (see Fig. 5a), the approximate surface free energy is always smaller than the exact one. This is consistent since a bound on the total free energy does not imply any bound on the surface free energy. The singular part of the surface free energy which is a solution of the homogeneous part of the recursion relation (6.12) is proportional to $|K-K^c|^{(d-1)\nu}$ near K^c. In $d=2$, the MK scheme gives $\nu=1.33$ which follows from (5.1) while the exact value is $\nu=1$. As a consequence, the exact surface energy ε_s has a logarithmic divergence [30] while the MK scheme gives a cusp. The same misrepresentation of the singularity is encountered in a cell cluster approximation [11].

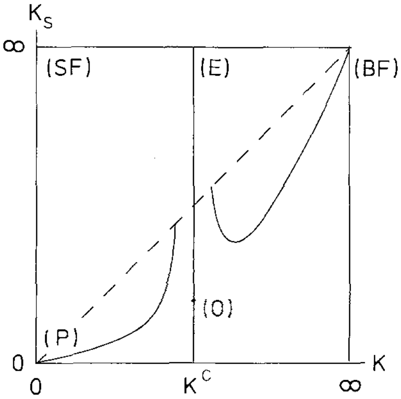

Fig. 6. Typical renormalization group trajectories (full curves) along which the surface free energy is integrated. The initial values of these trajectories lie on the physical line $K=K_c\propto$ (temperature)$^{-1}$ (dashed curve)

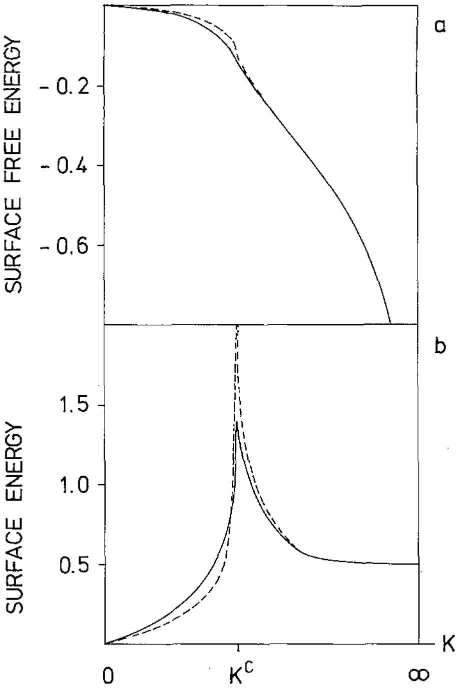

Fig. 7. MK approximations (full curves) and exact results (dashed curves) for the surface free energy and the surface energy of the 2-dimensional Ising model with $K_s=K$. The apparent increase of the slope of the surface free energy for large K is due to the scale for the K-axis which is proportional to $th(K)$

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Appendix A

The effect of a dedecoration transformation in $d=1$ for arbitrary rescaling factor b is most easily derived by the transfer matrix method. If we sum over $(b-1)$ out of b spins of a one-dimensional Ising chain we get the renormalized couplings from the matrix equation

$$T(E',K',H')=T^b(E,K,H) \tag{A.1}$$

for the transfer matrix

$$T(E,K,H)=e^{E/2}\begin{pmatrix} e^{K+H} & e^{-K} \\ e^{-K} & e^{K-H}\end{pmatrix}e^{E/2}. \tag{A.2}$$

It is easy to analytically continue (A.1) to non-integer b since

$$T^b=\sum_n \omega_n^b |\omega_n\rangle\langle\omega_n| \tag{A.3}$$

for any matrix T where ω_n and $|\omega_n\rangle$ are the eigenvalues and eigenvectors of T respectively.
For $H=0$ one finds

$$T^b=e^{bE/2}\,2^{b-1}\begin{pmatrix} t_+ & t_- \\ t_- & t_+ \end{pmatrix} e^{bE/2} \tag{A.4}$$

with $t_\pm := (chK)^b \pm (shK)^b$. If we insert (A.4) in (A.1) it follows that

$$\begin{aligned} &E'=bE+\delta E(K)\\ &\delta E(K):=(b-1)\ln 2+\tfrac{1}{2}\ln\{(chK)^{2b}-(shK)^{2b}\} \end{aligned} \tag{A.5}$$

which is the recursion for the spin independent bulk coupling E in $d=1$. For $d>1$ each of the d successive MK transformations described in Section 3 generates such a term:

$$\begin{aligned} &E^{(1)}=bE+\delta E(K_1)\\ &E^{(2)}=bE^{(1)}+\delta E(bK_2)\\ &\vdots\\ &E^{(d)}=bE^{(d-1)}+\delta E(b^{d-1}K_d). \end{aligned} \tag{A.6}$$

If we denote $E':=E^{(d)}$ we arrive at

$$E'=b^d E+\sum_{\alpha=1}^{d} b^{d-\alpha}\,\delta E(b^{\alpha-1}K_\alpha). \tag{6.3a}$$

At the free surface the corresponding transformations for the spin independent surface coupling E_s are

$$\begin{aligned} &E_s^{(1)}=E_s+\tfrac{1}{2}(b-1)E+\tfrac{1}{2}\,\delta E(K_1)\\ &E_s^{(2)}=bE_s^{(1)}+\delta E(J_{s2})\\ &\vdots\\ &E_s^{(d)}=bE_s^{(d-1)}+\delta E(b^{d-2}J_{sd}) \end{aligned} \tag{A.7}$$

where $J_{s\beta}=K_{s\beta}+\frac{1}{2}(b-1)K_\beta$ as defined in (3.1b). As compared to the transformation (A.6) the only change occurs in the first step where we shift bonds perpendicular to the surface. If we denote $E_s':=E_s^{(d)}$ we obtain from (A.7)

$$\begin{aligned} &E_s'=b^{d-1}\{E_s+\tfrac{1}{2}(b-1)E\}+\tfrac{1}{2}b^{d-1}\,\delta E(K_1)\\ &+\sum_{\beta=2}^{d} b^{d-\beta}\,\delta E(b^{\beta-2}J_{s\beta}). \end{aligned} \tag{A.8}$$

Appendix B

In this appendix we describe a modified MK scheme where bonds are shifted only parallel to the free surface. This scheme may be applied in arbitrary dimension. For simplicity, we confine the description to the 2-dimensional case. In Fig. 8 the successive steps of this modified bond moving procedure are depicted for $b=5$ and $H=0$. In the first step, we generate "ladders" of length $\frac{1}{2}(b-1)$ as shown in Fig. 8a. We rearrange bonds by parallel shifts in such a way that each "ladder" bond in Fig. 8a becomes proportional to $\dfrac{1}{b-1}$.

All spins of the "ladders" indicated by a cross in Fig. 8a are summed over. This gives an effective coupling $\tilde{J}$ between the two spins at the end of the "ladder" as indicated in Fig. 8b. Since we want to take the infinitesimal rescaling limit $b\to 1+\delta l$ we have to evaluate $\tilde{T}^{\frac{1}{2}(b-1)}$ where

$$\tilde{T}=\begin{pmatrix} e^{J_x+2J_z} & e^{J_x-2J_z} & 1 & 1\\ e^{J_x-2J_z} & e^{J_x+2J_z} & 1 & 1\\ 1 & 1 & e^{-J_x+2J_z} & e^{-J_x-2J_z}\\ 1 & 1 & e^{-J_x-2J_z} & e^{-J_x+2J_z} \end{pmatrix}$$

is the transfer matrix of one square of the "ladder" shown in Fig. 9 for zero magnetic field. The eigenvalues of this matrix are

$$\begin{aligned} &\omega_{1/2}=e^{\pm J_x}\,2sh2J_z\\ &\omega_{3/4}=2\{chJ_x ch2J_z \pm\sqrt{1+sh^2J_x ch^2 2J_z}\}. \end{aligned} \tag{B.2}$$

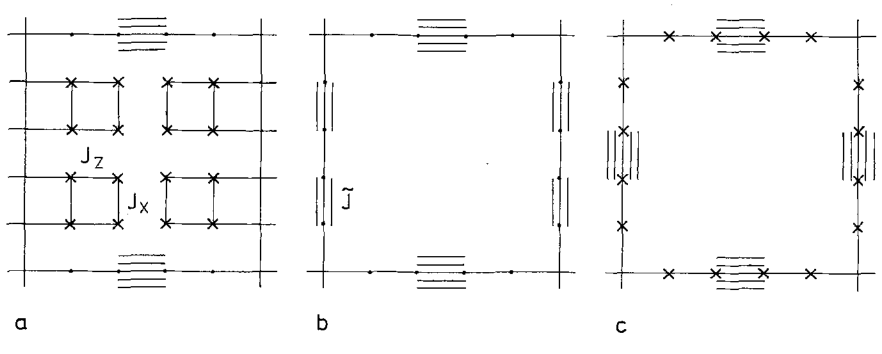

Fig. 8. Successive steps in the modified bond moving scheme. The horizontal direction is perpendicular to the free surface

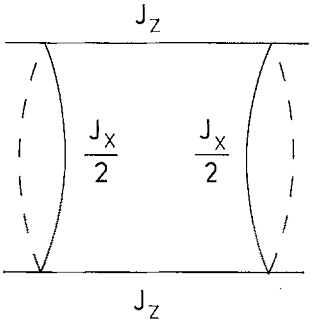

Fig. 9. Generic "ladder" square which yields the transfermatrix $\tilde{T}$. The interaction term J_x is equally divided between adjacent squares

For finite b we obtain from $\tilde{T}^{\frac{1}{2}(b-1)}$ the effective coupling $\tilde{J}$ by

$$th\tilde{J}=2\,shJ_x sh^2 J_z \frac{1-\Omega^{\frac{1}{2}(b-1)}}{A_+ +\Omega^{\frac{1}{2}(b-1)}A_-} \tag{B.3}$$

with $\Omega:=\frac{\omega_4}{\omega_3}$ and $A_\pm:=\pm chJ_x+\sqrt{1+sh^2J_x ch^2 2J_z}$.
In the infinitesimal rescaling limit $b\to 1+\delta l$ we obtain from (B.3)

$$\tilde{J}=K+\delta l\, sh2K(\coth K - thK)+O(e^{-1/\delta l}) \tag{B.4}$$

since $J_x=J_z=\frac{2}{\delta l}K$ in this limit. For $H\neq 0$ we have evaluated the eigenvectors of $\tilde{T}(H)$ to first order in the magnetic field while the eigenvalues are not changed in this order.
Finally, we move all effective couplings $\tilde{J}$ onto one bond as indicated in Fig. 8c. This ensures that the renormalized couplings K'_α, $\alpha=1,2$ which are effected by summing over the crossed spins in Fig. 8c are identical for both Cartesian directions. Since we have moved bonds only parallel to the surface the scheme just described is a lower bound approximation for all b. For $b\to 1+\delta l$ this procedure yields the differential recursion relations (3.2a, b) and (3.3a, b).

Appendix C

First, we discuss the behaviour of the bulk and surface free energies near to the low temperature fixed point (BF). Near to this fixed point, the recursion relations (3.2a, b) reduce to

$$\frac{d\tilde{K}}{dl}=(d-1)\tilde{K}-\tfrac{1}{2}, \tag{C.1}$$

$$\frac{d\tilde{K}_s}{dl}=\tfrac{1}{2}\tilde{K}+(d-2)\tilde{K}_s-\tfrac{1}{2}. \tag{C.2}$$

If we integrate these recursion relations we obtain

$$\tilde{K}(l,K)=Ke^{(d-1)l}+\frac{1}{2(d-1)}(1-e^{(d-1)l}), \tag{C.3}$$

$$\tilde{K}_s(l,K,K_s)=K_s e^{(d-2)l}+b_1(e^{(d-1)l}-e^{(d-2)l}) +b_2(e^{(d-2)l}-1) \tag{C.4}$$

with $b_1:=\frac{1}{2}\left(K-\frac{1}{2(d-1)}\right)$ and $b_2:=\frac{1}{2(d-2)}\left(\frac{1}{2(d-1)}-1\right)$. In order to obtain the large K behaviour of the bulk free energy f_B we use the asymptotic behaviour $g(\tilde{K})\underset{\tilde{K}\to\infty}{\simeq}\tilde{K}+\frac{1}{2}$. This, together with (C.3) and (6.7a) yields

$$\begin{aligned} f_B(K)\underset{K\to\infty}{\simeq} d\int_0^\infty dl\Big\{&Ke^{(d-1)l} \\ &+\frac{1}{2(d-1)}(1-e^{(d-1)l})+\tfrac{1}{2}\Big\}+C(K) \\ =dK+C(K).& \end{aligned} \tag{C.5}$$

Thus $C(K)=0$ is appropriate for $K>K_c$.
The corresponding asymptotic expression for the surface free energy f_s is

$$f_s(K,K_s)\underset{K,K_s\to\infty}{\simeq}(d-1)(K_s-\tfrac{1}{2}K)-\tfrac{1}{4}\frac{d}{d-1}+C_s(K,K_s). \tag{C.6}$$

This is obtained when the asymptotic form

$$G(\tilde{K},\tilde{K}_s)\underset{\tilde{K},\tilde{K}_s\to\infty}{\simeq}(d-1)(\tilde{K}_s-\tilde{K})+\tfrac{1}{2}\{(d-1)\tilde{K}-\tfrac{1}{2}\} \tag{C.7}$$

is inserted in (6.13a).
Comparing (C.6) with the exact asymptotic limit (6.14a) we conclude that $C_s(K,K_s)=-\frac{1}{2}dK+\frac{1}{4}\frac{d}{d-1}$ is the correct choice. This is self-consistent since this value for C_s also follows if we insert the exact asymptotics for f_s into the definition (6.13b) of $C_s(K,K_s)$:

$$\begin{aligned} &\lim_{l\to\infty} e^{-(d-1)l} f_s(\tilde{K}(K,l),\tilde{K}_s(l,K,K_s)) \\ &=\lim_{l\to\infty} e^{-(d-1)l}\{-\tfrac{1}{2}d\tilde{K}+(d-1)(\tilde{K}_s-\tfrac{1}{2}\tilde{K})\} \\ &=-\tfrac{1}{2}dK+\tfrac{1}{4}\frac{d}{d-1} \end{aligned} \tag{C.8}$$

where we used (C.3) and (C.4).
Next, consider the behaviour near to the high temperature fixed point (P). In this case, the recursions (3.2a, b) reduce to

$$\frac{d\tilde{K}}{dl}=\tilde{K}\ln\tilde{K}, \tag{C.9}$$

$$\frac{d\tilde{K}_s}{dl}=\tilde{K}_s\ln\tilde{K}_s. \tag{C.10}$$

Integrating (C.9) and (C.10) we obtain

$$\tilde{K}(l,K)=\exp(e^{l}\ln K), \tag{C.11}$$

$$\tilde{K}_s(\tilde{K},K,K_s)=\tilde{K}^{x} \tag{C.12}$$

with $x:=\dfrac{\ln K_s}{\ln K}$. In order to obtain the small K behaviour of the bulk free energy f_{B} we need the asymptotic form $g(\tilde{K})\rightsquigarrow\ln 2+\tilde{K}^2(\frac{1}{2}-\ln\tilde{K})$ valid for small $\tilde{K}$. If we insert this in (6.7a) with $C(K)=0$ we arrive at

$$f_{\mathrm{B}}(K)\underset{K\to 0}{\simeq}\ln 2+\tfrac{1}{2}K^2+(d-1)\,|\ln K|\,E_d(2|\ln K|) \tag{C.13}$$

where

$$E_d(z):=\int_1^{\infty} dt\,\frac{e^{-zt}}{t^d}$$

is an exponential integral. If we use its asymptotic form [31]

$$E_d(z)\underset{z\to\infty}{\simeq}\frac{e^{-z}}{z} \tag{C.14}$$

we obtain the high temperature limit (6.8b) of the bulk free energy. In order to derive the same limit for the surface free energy we use the small $\tilde{K}$, $\tilde{K}_s$ form of the kernel $G(\tilde{K},\tilde{K}_s)$ in (6.13a)

$$G(\tilde{K},\tilde{K}_s)\rightsquigarrow(d-1)\,\{\tilde{K}_s^2(\tfrac{1}{2}-\ln\tilde{K}_s)-\tilde{K}^2(\tfrac{1}{2}-\ln\tilde{K})\}$$
$$+\tfrac{1}{2}\{\tfrac{1}{2}d\tilde{K}^2-\tilde{K}^2(\tfrac{1}{2}-\ln\tilde{K})\} \tag{C.15}$$

together with (C.11) and (C.12). This leads to

$$f_s(K,K_s)=|\ln K|^{d-1}\sum_{n=1}^{3} I_n(K,K_s)+C_s(K,K_s) \tag{C.16}$$

with

$$I_1:=(d-1)\int_0^K d\tilde{K}\,\frac{\tilde{K}^{2x}(\frac{1}{2}-x\ln\tilde{K})}{\tilde{K}|\ln\tilde{K}|^d},$$

$$I_2:=-(d-1)\int_0^K d\tilde{K}\,\frac{\tilde{K}^2(\frac{1}{2}-\ln\tilde{K})}{\tilde{K}|\ln\tilde{K}|^d},$$

$$I_3:=\tfrac{1}{2}\int_0^K d\tilde{K}\,\frac{\frac{1}{2}d\tilde{K}^2-\tilde{K}^2(\frac{1}{2}-\ln\tilde{K})}{\tilde{K}|\ln\tilde{K}|^d}.$$

In the above integrals we have changed variables from l to $\tilde{K}=\exp(e^{l}\ln K)$. The three integrals may be expressed by exponential integrals. Using the asymptotic expression (C.14) one arrives at

$$|\ln K|^{d-1}I_1\rightsquigarrow(d-1)\tfrac{1}{2}K^{2x}=(d-1)\tfrac{1}{2}K_s^2$$
$$|\ln K|^{d-1}I_2\rightsquigarrow-(d-1)\tfrac{1}{2}K^2$$
$$|\ln K|^{d-1}I_3\rightsquigarrow-\tfrac{1}{4}K^2 \tag{C.17}$$

for K, $K_s\to 0$. The sum of these terms gives the correct high temperature limit (6.14b) of the surface free energy.

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