

## Migdal–Kadanoff Renormalization Group for the $O(n)$ Model

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We perform a Migdal–Kadanoff renormalization group calculation on an  $O(n)$  symmetric model on a  $d$ -dimensional hypercubic lattice,  $d=2, 3$ . We find that in two dimensions the critical fixed point disappears as  $n = n_{KT} \approx 1.96$ , which is in good agreement with the exact value  $n_{KT}=2$ . In three dimensions the fixed point persists much longer, albeit not all the way up to infinity. Surface critical phenomena in a semiinfinite  $O(n)$  model are also considered.

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**KEY WORDS:** Migdal-Kadanoff renormalization group;  $O(n)$  model; surface critical phenomena.

### 1. INTRODUCTION

The Migdal–Kadanoff renormalization group (MKRG)<sup>(1,2)</sup> is, because of its simplicity, one of the most widely used renormalization group (RG) schemes. However, it is not straightforward to apply it to the  $n$ -component Heisenberg model, although special cases (Ising and  $XY$  models) have received considerable attention. In his original paper, Migdal<sup>(1)</sup> considered models with  $n \geq 2$  in  $2 + \varepsilon$  dimensions, but to our knowledge the general  $n$ -component model has not been investigated with the MKRG, and, in particular, the interesting case of  $n < 2$  in two dimensions, where a critical phase transition occurs, has not. The reason for this is easy to understand. Even the simplest case, with a rescaling factor of 2, requires highly non-trivial integrals of exponentials of dot products over the  $(n-1)$ -sphere, i.e., the unit sphere in  $n$  dimensions. Although these integrals in principle can be evaluated numerically, the approximate nature of the MKRG would not motivate such an effort.

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In a previous publication (ref. 4, henceforth to be referred to as I), a formal expression for the high-temperature series of a modified  $O(n)$  symmetric model was given, introduced by Domany *et al.*<sup>(5)</sup> This model was used by Nienhuis to obtain exact results for the critical exponents on a honeycomb lattice.<sup>(6,7)</sup> Because the symmetry of this model is the same as that of the  $n$ -component Heisenberg model, it is widely believed that these results carry over to the latter model as well. Even if this not is the case, the Nienhuis results should be applicable to the modified  $O(n)$  model on different two-dimensional lattices. The purpose of the article is to show how to construct a Migdal–Kadanoff-like RG for the modified model, for arbitrary  $n$ .

The paper is organized as follows: In Section 2 the MKRG for the modified  $O(n)$  model is constructed. We will still have to integrate over the  $(n-1)$ -sphere, but the integrands are now so simple that this may be done in closed form. Unfortunately, the form of the Hamiltonian is not conserved by the MKRG. This feature is not particular to the modified model, but was already encountered in the  $XY$  model by José *et al.*<sup>(8)</sup> In order to obtain a working RG transformation, we truncate the recursion relations. Section 3 contains our results for the two- and three-dimensional  $O(n)$  models. Finally, in Section 4 we apply the formalism developed in this paper to the problem of an  $O(n)$  model with a free surface.

## 2. MODEL AND MIGDAL–KADANOFF RENORMALIZATION GROUP

We consider the following  $O(n)$ -symmetric Hamiltonian, expressed in units of  $k_B T$ .

$$\begin{aligned} \mathcal{H} &= - \sum_{\langle ij \rangle} \ln [1 + J \mathbf{S}_i \cdot \mathbf{S}_j + \mathbf{h} \cdot (\mathbf{S}_i + \mathbf{S}_j)] \\ &\equiv - \sum_{\langle ij \rangle} V(\mathbf{S}_i, \mathbf{S}_j) \end{aligned} \quad (2.1)$$

$\mathbf{S}_i = (S_i^a)$  is an  $n$ -component, classical spin of unit length, located at site  $i$ , and the sum runs over all pairs of nearest neighbors  $\langle ij \rangle$ . In the Ising ( $n=1$ ) model,  $J = \tanh K$ , where  $K$  is the usual coupling constant. When  $n \neq 1$ , (2.1) is not completely equivalent to an  $n$ -component classical Heisenberg model, but because the symmetry is the same, critical exponents should agree with the usual ones, by universality. We have also included a symmetry-breaking magnetic field  $z\mathbf{h}$ , where  $z$  is the coordination number of the lattice. To facilitate future bond-moving, we have split the magnetic interaction at site  $i$  on the  $z$  nearest-neighbor bonds

emerging from that site. There are other ways to handle single-spin interaction terms within the MKRG,<sup>(3)</sup> but these will not be considered here. The partition function defined by (2.1) takes on the following simple form

$$Z = \text{Tr} \prod_{\{S_i\}} \prod_{\langle ij \rangle} (1 + JS_i \cdot S_j) \equiv \text{Tr} \prod_{\{S_i\}} \prod_{\langle ij \rangle} Z(S_i, S_j) \quad (2.2)$$

Note that we use  $Z$  for two different quantities in (2.2). This should not create any confusion, however, since one quantity has two arguments while the other has none.

We now proceed to do the MKRG on the model (2.2). On a  $d$ -dimensional hypercubic lattice, we move interaction terms perpendicular to themselves, which leaves us with enhanced interactions on a decorated, more sparse lattice. The lattice spacing on the new lattice is  $b$  times that of the original one, while the bond-moved interaction is

$$\tilde{V}(S_i, S_j) = b^{d-1} V(S_i, S_j) \quad (2.3)$$

This corresponds to a bond-moved partition function

$$\tilde{Z}(S_i, S_j) = Z(S_i, S_j)^{b^{d-1}} \quad (2.4)$$

We can now perform an exact dedecoration transformation by tracing over the intermediate spins on a decorated link. This constitutes the second and final step in the MKRG. The renormalized partition function is

$$Z'(S_0, S_b) = C^{-1} \text{Tr}_{S_1, \dots, S_{b-1}} \prod_{k=0}^{b-1} \tilde{Z}(S_k, S_{k+1}) \quad (2.5)$$

If this procedure is to yield any information,  $Z'$  should be of the same form as the original partition function, with  $J$  and  $h$  replaced by their renormalized values  $J'$  and  $h'$ . The constant  $C$  is the exponential of the free energy due to fluctuations on length scales up to  $b$  lattice constants. Equation (2.5) defines the renormalization transformation of  $J$  and  $h$ .

$$J' = R_J(J, h) \quad h' = R_h(J, h) \quad (2.6)$$

If we are only interested in fixed points with  $h=0$ , it suffices to calculate  $R_J$  to zero and  $R_h$  to first order in  $h$ . The RG eigenvalues follow as usual from (2.6).

$$y_t = \ln(\partial R_J / \partial J) / \ln(b) \quad y_h = \ln(\partial R_h / \partial h) / \ln(b) \quad (2.7)$$

evaluated at the fixed point  $J=J^*$ ,  $h=0$ . The critical exponents may be expressed in terms of  $y_t$  and  $y_h$ , as is well-known.

From now on, we limit ourselves to a rescaling factor  $b = 2$ . In two dimensions, (2.5) becomes

$$CZ'(\mathbf{S}_0, \mathbf{S}_2) = \text{Tr}_{S_1} Z^2(\mathbf{S}_0, \mathbf{S}_1) \cdot Z^2(\mathbf{S}_1, \mathbf{S}_2) \tag{2.8}$$

In order to evaluate the trace above, we must learn how to calculate expressions like

$$\text{Tr}_{S_1} (\mathbf{S}_0 \cdot \mathbf{S}_1)^A (\mathbf{S}_1 \cdot \mathbf{S}_2)^B = S_0^a \dots S_0^b S_2^c \dots S_2^d \text{Tr}_{S_1} S_1^a \dots S_1^b S_1^c \dots S_1^d \tag{2.9}$$

The trace on the RHS was evaluated in I, where we found

$$\text{Tr}_{S_1} S_1^a \dots S_1^{2m} = c_{2m} A^{a, \dots, 2m} \tag{2.10a}$$

$$c_{2m} = \frac{1}{n(n+2) \cdots (n+2m-2)} \tag{2.10b}$$

$$A^{a, \dots, 2m} = \delta^{ab} \dots \delta^{(2m-1), 2m} + \text{permutations} \tag{2.10c}$$

The symmetrized product of Kronecker symbols,  $A^{a, \dots, 2m}$ , contains a total of  $(2m - 1)!!$  terms. Note that we have included a factor  $n^m$  in the definition of  $c_{2m}$  compared to I. We can now devise a graphical method to calculate (2.9) in a simple way, according to the following rules.

1. If  $A + B$  is odd, (2.9) vanishes.
2. Otherwise, write  $A$  0s and  $B$  2s on a piece of paper and combine them pairwise with a line.
3. For each pair 0–2, we get a factor  $(\mathbf{S}_0 \cdot \mathbf{S}_2)$ . Each pair, 0–0 or 2–2, contributes unity, because the spins are of unit length.
4. Calculate the number of ways the 0s and 2s can be combined to produce this number of unequal pairs.
5. Repeat steps 2 to 4 above until all different terms have been calculated. The total number of combinations should sum to  $(2m - 1)!!$ .
6. Finally, multiply the result with the factor  $c_{2m}$ , from (2.10).

A sample trace is evaluated according to these rules in Fig. 2.

We now return to the calculation of (2.8). When  $h = 0$ , we have

$$C[1 + J'(\mathbf{S}_0 \cdot \mathbf{S}_2)] = 1 + \frac{2}{n} J^2 + c_4 J^4 + \frac{4}{n} J^2 (\mathbf{S}_0 \cdot \mathbf{S}_2) + 2c_4 J^4 (\mathbf{S}_0 \cdot \mathbf{S}_2)^2 \tag{2.11}$$

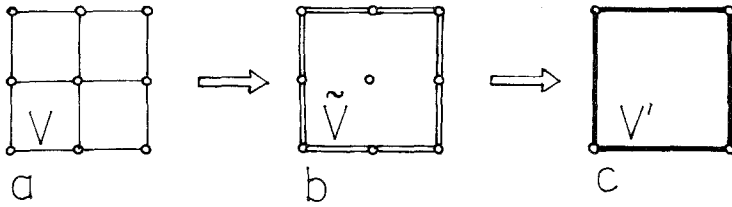


Fig. 1. The Migdal-Kadanoff renormalization transformation consists of two steps: (1)  $a \rightarrow b$ : bond-moving; (2)  $b \rightarrow c$ : decimation.

Unfortunately, the Hamiltonian does not retain the same form after renormalization because of the last term in (2.11). Therefore, we should really have considered a more general form of  $Z$  from the outset, so that the RG transformation acts in some infinite-dimensional parameter space. Of course, in practice we have to truncate somewhere. To this end, we replace  $(\mathbf{S}_0 \cdot \mathbf{S}_2)^2$  by its average over the  $(n-1)$ -sphere, which is  $1/n$ . This truncation is exact when  $n=1$ , as are all subsequent truncations in this paper. Thus the RG transformation becomes

$$C = 1 + \frac{2}{n} J^2 + \frac{1}{n^2} J^4 \tag{2.12a}$$

$$CJ' = \frac{4}{n} J^2 \tag{2.12b}$$

The magnetic field is treated along the same lines. If we make the replacement

$$\mathbf{S}_0(\mathbf{S}_0 \cdot \mathbf{S}_2) \rightarrow \text{Tr}_{\mathbf{S}_0} \mathbf{S}_0(\mathbf{S}_0 \cdot \mathbf{S}_2) = \frac{1}{n} \mathbf{S}_2 \tag{2.13}$$

the recursion relation for the magnetic field becomes, to first order in  $h$

$$Ch' = 2h \left[ 1 + \frac{3}{n} J + \frac{n+2}{n^2} J^2 + \frac{1}{n^2} J^3 \right] \tag{2.14}$$

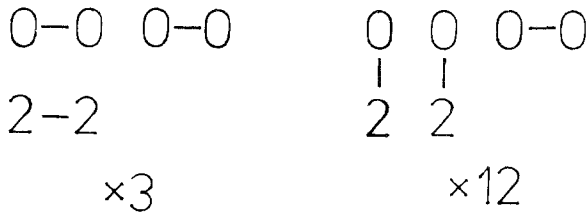


Fig. 2. Evaluation of  $\text{Tr}_{\mathbf{S}_1}(\mathbf{S}_0 \cdot \mathbf{S}_1)^4(\mathbf{S}_1 \cdot \mathbf{S}_2)^2$  according to the rules described in the text. The trace equals  $c_6[3 + 12(\mathbf{S}_0 \cdot \mathbf{S}_2)^2]$ .

The fixed points of (2.12) and the corresponding RG eigenvalues are presented in Section 3. However, it is clear that we should be able to improve our results by incorporating more interaction terms in the Hamiltonian. We therefore expand the pair interaction term in (2.1) to

$$V(\mathbf{S}_i, \mathbf{S}_j) = \ln[1 + J\mathbf{S}_i \cdot \mathbf{S}_j + K(\mathbf{S}_i \cdot \mathbf{S}_j)^2 + \mathbf{h} \cdot (\mathbf{S}_i + \mathbf{S}_j) + \mathbf{L} \cdot (\mathbf{S}_i + \mathbf{S}_j)(\mathbf{S}_i \cdot \mathbf{S}_j)] \quad (2.15)$$

This is henceforth referred to as the improved Hamiltonian.

The calculations follow the same path as before, although the algebra becomes considerably more cumbersome. The only new feature is that we have to truncate somewhat differently. Consider, for example, a term  $(\mathbf{S}_0 \cdot \mathbf{S}_2)^4$ , which should be approximated by a polynomial in  $x \equiv (\mathbf{S}_0 \cdot \mathbf{S}_2)$  of degree 2 or less. One well-defined way of doing this is to require that the error in this approximation be orthogonal to all second-order polynomials on the  $(n-1)$ -sphere. We are then lead to consider ultraspherical, or Gegenbauer, polynomials, which have precisely this property. Hence, they are the proper generalization of the Legendre polynomials to  $n$  dimensions.<sup>(9)</sup> In particular we have

$$C_4^{(\alpha)}(x) = \frac{1}{\Gamma(\alpha)} \left[ \frac{\Gamma(\alpha+4)}{4!} (2x)^4 - \frac{\Gamma(\alpha+3)}{2!} (2x)^2 + \frac{\Gamma(\alpha+2)}{2!} \right] \quad (2.16)$$

where  $\alpha = (n-2)/2$ . We then get the approximation by setting  $C_4^{(\alpha)} \approx 0$  and solving for  $x^4$ . With this prescription, we obtain the following truncation scheme

$$(\mathbf{S}_0 \cdot \mathbf{S}_2)^4 \approx \frac{6}{n+4} (\mathbf{S}_0 \cdot \mathbf{S}_2)^2 - \frac{3}{(n+4)(n+2)} \quad (2.17a)$$

$$(\mathbf{S}_0 \cdot \mathbf{S}_2)^3 \approx \frac{3}{n+2} (\mathbf{S}_0 \cdot \mathbf{S}_2) \quad (2.17b)$$

New interaction terms also arise from the renormalization of the symmetry-breaking interactions. We extend (2.17) in the following, rather ad hoc, way.

$$(\mathbf{S}_0 \cdot \mathbf{S}_2)^2 \mathbf{S}_0 \approx \frac{1}{n} \mathbf{S}_0 \quad (2.18a)$$

$$(\mathbf{S}_0 \cdot \mathbf{S}_2)^3 \mathbf{S}_0 \approx \frac{3}{n+2} (\mathbf{S}_0 \cdot \mathbf{S}_2) \mathbf{S}_0 \quad (2.18b)$$

These manipulations give rise to a closed set of rather lengthy recursion relations, which we choose not to reproduce here. The thermal and magnetic eigenvalues now follow from the matrices of derivatives at the fixed point. Only the largest eigenvalues give rise to positive exponents; from the smaller ones one can deduce the correction-to-scaling exponents.

We then turn to the three-dimensional case, which is analyzed analogously. For simplicity, we only considered the Hamiltonian (2.1) and not the improved version (2.15). After grinding through the algebra we find the following recursion relations.

$$C = 1 + \frac{12}{n} J^2 + \frac{6(7+12n)}{n^2(n+2)} J^4 + \frac{36}{n^2(n+2)} J^6 + \frac{9(n^2+26n+8)}{n^2(n+2)^2(n+4)(n+6)} J^8 \quad (2.19a)$$

$$CJ' = \frac{16}{n} J^2 + \frac{96}{n(n+2)} J^4 + \frac{144}{n(n+2)^2} J^6 \quad (2.19b)$$

$$Ch' = 4h \left[ 1 + \frac{7}{n} J + \frac{3(3n+4)}{n^2} J^2 + \frac{15(3n+4)}{n^2(n+2)} J^3 + \frac{21(n+4)}{n^2(n+2)} J^4 + \frac{63}{n^2(n+2)} J^5 + \frac{9n+96}{n^2(n+2)(n+4)} J^6 + \frac{9}{n^2(n+2)^2} J^7 \right] \quad (2.19c)$$

### 3. FIXED POINTS AND EXPONENTS

We first consider the two-dimensional recursion relation (2.12). For all values of  $n$  there is a high-temperature fixed point, having its basin of attraction in the disordered phase, at  $J=0$ . For small  $n$ , there are also two other fixed points, which we identify with the critical and low-temperature fixed points, respectively. They are plotted in Fig. 3. The critical and low-temperature fixed points collide and annihilate at  $n=n_{KT} \approx 1.67$ . We interpret this as the symptom of the Kosterlitz–Thouless transition<sup>(10)</sup> (hence the index!) within the MKRG. It is interesting to compare this description of the Kosterlitz–Thouless transition with the mechanism that causes the transition in the two-dimensional Potts model to become first order as the number of Potts states equals four.<sup>(11)</sup> In that case the critical fixed point collides with the tricritical branch of the Potts lattice gas. Since in two dimensions both the  $O(n)$  and Potts models may be expressed in terms of a Coulomb gas<sup>(7)</sup>, this similarity is probably more than coincidental.

The form of the renormalization function  $R_J(J)$  for different values of  $n$ , together with the corresponding RG flows, is sketched in Fig. 4. We see

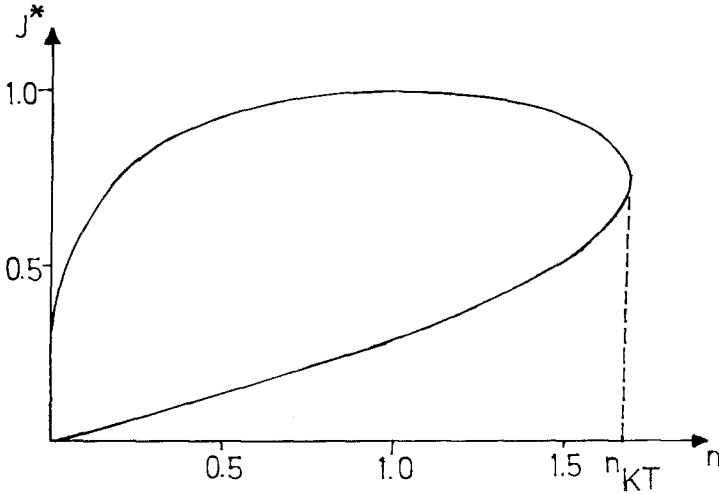


Fig. 3. Critical fixed point (lower branch) and low-temperature fixed point (upper branch) from the two-dimensional recursion relation (2.12).

that the function  $R_J$  undergoes a reversed tangent bifurcation when  $n = n_{KT}$ . Couplings stronger than the bifurcation value  $J_{KT}$  flow into this fixed point under the RG. However, we know that there should be a whole fixed line, terminating at  $J_{KT}$ , in the  $XY$  model. This fixed line is not correctly reproduced by the MKRG,<sup>(8)</sup> and probably not by any approximate position-space RG. For  $n > n_{KT}$ , all RG trajectories flow into the high-temperature fixed point, irrespective of the initial value of  $J$ , so the  $O(n)$  model is in the disordered phase at all temperatures.

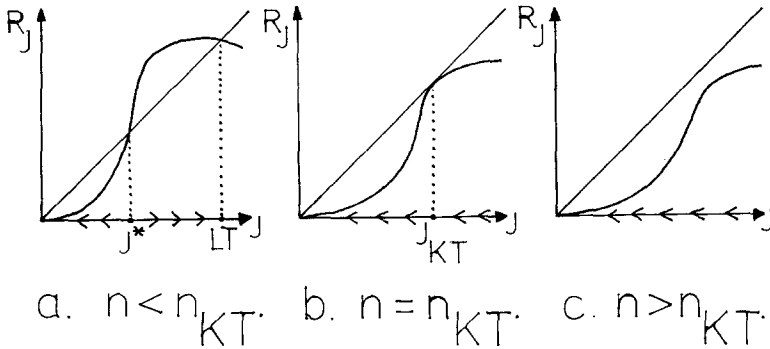


Fig. 4. Schematic behavior of the function  $R_J(J)$  for different values of  $n$ . RG flows are indicated on the  $J$  axis.



The improved model (2.15) shows very similar behavior, except that the Kosterlitz–Thouless transition is moved to  $n_{\text{KT}} \approx 1.96$ . This is clearly much closer to the exact value from the Nienhuis solution,<sup>(6)</sup>  $n_{\text{KT}} = 2$ . The question then arises whether the MKRG without any truncations would reproduce the correct  $n_{\text{KT}}$ . Even if we are not in the position to give a definite answer to this question, there are arguments in favor of such a conclusion. Although a fixed line was not found in Ref. 8, the corrections are exponentially small at low temperatures. Moreover, Migdal found that the critical temperature diverges proportionally to  $(n-2)/(d-2)$  close to  $n = d = 2$ <sup>(1)</sup>, which indicates that something special happens for  $n = 2$ , also within the MKRG. However, these results were obtained for the conventional Heisenberg model. Universality implies that the modified  $O(n)$  model should behave in the same way, but it is not certain that universality survives the MKRG approximation.

Barber<sup>(12)</sup> considered the MKRG for the modified  $O(2)$  model (he calls it the truncated model, but we use the word “truncate” in a different context). His result qualitatively agrees with those of José *et al.*,<sup>(8)</sup> which further corroborates the conclusion that  $n_{\text{KT}} = 2$  within the MKRG. Remarkably, he finds an unphysical value for the beginning of the fixed line,  $J^* \approx 1.5$  (the Hamiltonian is not always real if  $J > 1$ ). This is clearly different from the fixed point at  $n_{\text{KT}}$  found by us. We cannot offer any explanation for this discrepancy.

The eigenvalue exponents  $y_t$  and  $y_h$ , obtained from the improved model, are shown in Figs. 5 and 6, respectively. They are also compared to the exact values derived by Nienhuis,<sup>(6)</sup> namely

$$\begin{aligned} n &= -2 \cos(2\pi/t) \\ y_t &= 4 - 2t \quad y_h = 1 + \frac{3}{4}t + t/4 \end{aligned} \quad (3.1)$$

and  $1 \leq t \leq 2$ .

Consider first the thermal exponent in Fig. 5. Since the MKRG effectively is a decimation, it always yields  $y_t \leq 1$ , while from the exact treatment,  $y_t > 1$  for  $n < 1$ . We see that the improved Hamiltonian produces a substantially more accurate estimate for  $y_t$  when  $n$  is large, while for  $n \lesssim 1.2$  this prediction is indistinguishable, on the scale of the diagram, from that of (2.1). Consequently, we believe that the truncations do not seriously affect the thermal eigenvalue for  $n \lesssim 1.2$ , and that incorporation of more interaction terms in the Hamiltonian probably will not improve the estimate of  $y_t$ , except close to  $n_{\text{KT}}$ . The serious limitation in obtaining a good  $y_t$  estimate is inherent in the MKRG itself, rather than being an artifact of truncation.

The estimates for  $y_h$  are remarkably accurate already from (2.1). Note

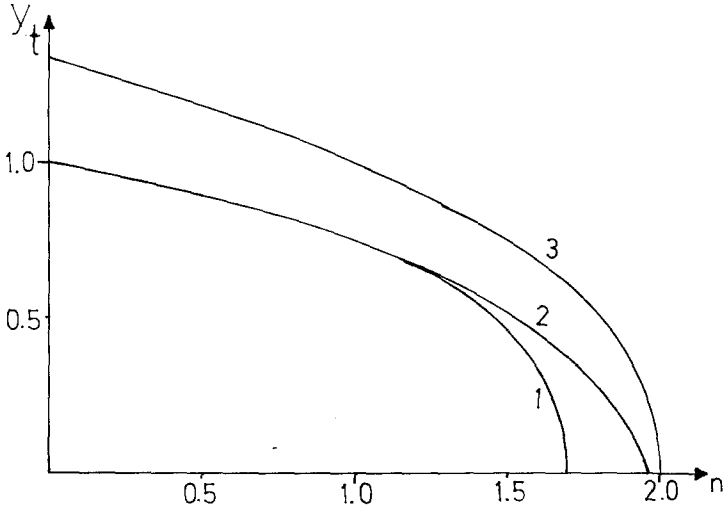


Fig. 5. Thermal eigenvalue exponent  $y_t$  in two dimensions, (1) MKRG on the Hamiltonian (2.1), (2) MKRG on the improved Hamiltonian (2.15), (3) exact result.

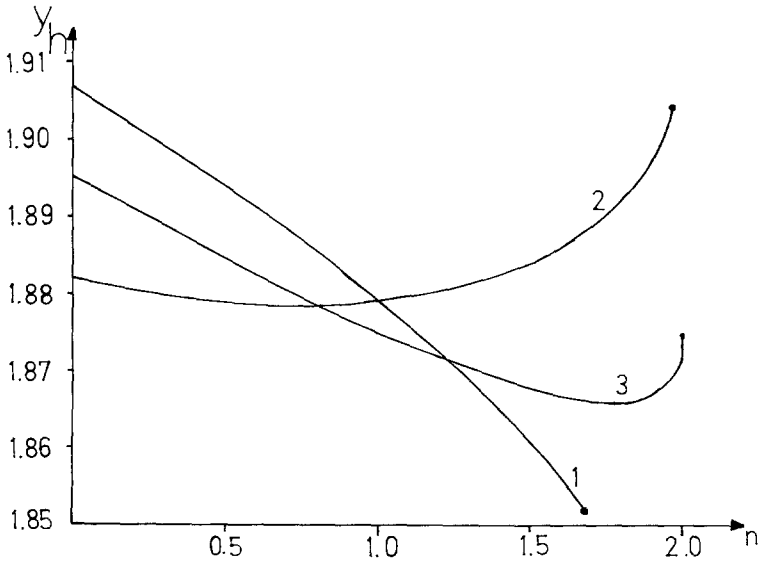


Fig. 6. Magnetic eigenvalue exponent  $y_h$  in two dimensions. The curves are labeled as in Fig. 5.

that the whole scale in Fig. 6 only spans a region of  $y_h$  of width 0.06. Curiously, the improved Hamiltonian does not result in a more accurate  $y_h$ . Perhaps the error introduced by truncation cancels some error due to the Migdal-Kadanoff approximation.

There are a number of internal consistency checks in the above calculations that provide great help in preventing algebraic mistakes. We know that (2.1) reduces to the ordinary Ising model when  $n=1$ , to first order in the magnetic field. Since all truncations in Section 2 in fact were exact in this case, we must recover the  $b=2$  MKRG values for  $J^*$ ,  $y_t$ , and  $y_h$  obtained for the Ising model. Furthermore, at the low-temperature fixed point we must get  $J^*=1$ ,  $y_t = -\infty$  and  $y_h=2$  for this value of  $n$ . Also, the improved Hamiltonian reduces to the Ising model, because for one-component spins,  $(\mathbf{S}_i \cdot \mathbf{S}_j)^2 = 1$ . Note that the constant term in (2.15) has been arbitrarily split up into two pieces, 1 and  $K$ . The values of  $J$  and  $K$  separately do not carry any information, but the combination  $J/(1+K)$  is interesting.

In Fig. 7, we finally present the MKRG exponents in three dimensions. We see that  $y_t$  vanishes at  $n = n_{KT} \approx 7.4$ , due to the same mechanism as occurs in two dimensions. This is clearly unphysical, since we know that the Heisenberg model possesses a critical point for all  $n$ . The question is then if this vanishing fixed point is an artifact of the model, of the MKRG,

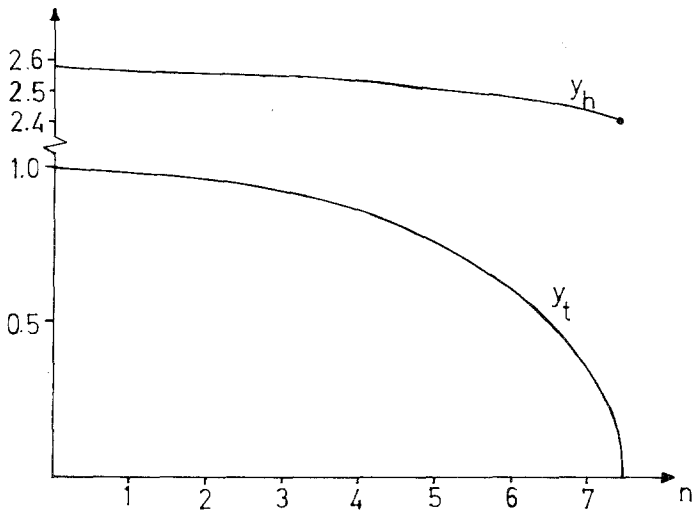


Fig. 7. Magnetic (upper curve) and thermal eigenvalue exponents in three dimensions from the MKRG.

or of truncating. The first alternative is ruled out if one believes in universality. We think that truncations are solely responsible for the same reasons that lead us to suspect that the MKRG without the truncation approximation would give  $n_{\text{KT}} = 2$  in two dimensions. However, it is not clear to us if  $n_{\text{KT}}$  will move to infinity if one truncates after a large but finite number of interaction terms, or if infinitely many are needed to reproduce the correct value of  $n_{\text{KT}}$ .

#### 4. $O(n)$ MODEL WITH FREE SURFACE

We now apply the formalism developed in Section 2 to another problem, namely, finding the surface critical exponents for a semi-infinite  $O(n)$  model. This problem has been attacked using field-theoretic methods,<sup>(13,14)</sup> and special cases, like the semi-infinite Ising model, have been investigated with the MKRG<sup>(15)</sup>. A comprehensive review of this subject can be found in Ref. 16.

Consider the following modification of the  $O(n)$  Hamiltonian

$$\mathcal{H} = - \sum_{\langle \vec{ij} \rangle} \ln[1 + J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \mathbf{h}_{ij} \cdot (\mathbf{S}_i + \mathbf{S}_j)] \quad (4.1)$$

where all sites are now restricted to lie in the positive half-space, where some coordinate, say  $z$ , is non-negative. The coupling constants are all equal,  $J_{ij} \equiv J$  unless both  $i$  and  $j$  lie on the boundary  $z=0$ , in which case  $J_{ij} = J_s$ . Similarly,  $\mathbf{h}_{ij} = \mathbf{h}_s$  if both  $i$  and  $j$  are surface sites, and  $\mathbf{h}_{ij} = \mathbf{h}$  otherwise. This form of the Hamiltonian is clearly not the most general semi-infinite  $O(n)$  model conceivable. For example, the interactions may differ from the bulk value also some distance away from the surface, as long as  $J$  is reached asymptotically. However, the form of (4.1) is preserved by the MKRG.

Now consider the bond-moving step in  $d$  dimensions. There is some ambiguity as to how to shift the bonds close to the surface. We choose the following symmetric prescription, which has the virtue of simplicity. All bonds to be moved are divided into  $2^{d-1}$  equally large pieces, and then each fraction is moved perpendicular to itself, to one of the surrounding interactions, which are to be strengthened. No two fractions of the same bond are to be moved to the same place. It is easy to verify that this recipe reduces to the usual MKRG for the bulk couplings. The bond-moved surface term, on the other hand, becomes

$$\tilde{V}_s(\mathbf{S}_i, \mathbf{S}_j) = 2^{d-2} V_s(\mathbf{S}_i, \mathbf{S}_j) + 2^{d-3} V(\mathbf{S}_i, \mathbf{S}_j) \quad (4.2)$$

The dedecoration transformation is done in the same way as before. We get, with  $Z_s = \exp(-V_s)$

$$C_s Z'_s(\mathbf{S}_0, \mathbf{S}_2) = \text{Tr}_{\mathbf{S}_1} Z_s^{2^{d-2}}(\mathbf{S}_0, \mathbf{S}_1) \cdot Z_s^{2^{d-3}}(\mathbf{S}_0, \mathbf{S}_1) \cdot Z_s^{2^{d-2}}(\mathbf{S}_1, \mathbf{S}_2) \cdot Z_s^{2^{d-3}}(\mathbf{S}_1, \mathbf{S}_2) \quad (4.3)$$

In two dimensions this equation is very hard to evaluate. This is because there is a factor

$$Z^{1/2}(\mathbf{S}_0, \mathbf{S}_1) = [1 + J\mathbf{S}_0 \cdot \mathbf{S}_1 + \mathbf{h} \cdot (\mathbf{S}_0 + \mathbf{S}_1)]^{1/2} \quad (4.4)$$

present in (4.3). It is not difficult to write a formal expression for  $Z'_s$ , but this involves an  $(n-1)$ -dimensional integral of a nonpolynomial function of  $(\mathbf{S}_0 \cdot \mathbf{S}_1)$ . Because of this difficulty, and also because a semi-infinite two-dimensional model is not terribly interesting (the boundary is one-dimensional!), we limit ourselves to the three-dimensional case. The recursion relation for the bulk coupling  $J$  is still (2.20), while we obtain for the surface interaction and magnetic field

$$C_s = 1 + \frac{2}{n} (J_s^2 + 2JJ_s) + \frac{1}{n^2} (J_s^2 + 2JJ_s)^2 \quad (4.5a)$$

$$C_s J'_s = \frac{1}{n} (J + 2J_s)^2 + \frac{6}{n(n+2)} (2J_s + J) J_s^2 J + \frac{9}{n(n+2)^2} J_s^4 J^2 \quad (4.5b)$$

$$\begin{aligned} C_s h'_s = 2h_s \left[ 1 + \frac{1}{n} (3J_s + 2J) + \frac{1}{n} (J_s^2 + 3J_s J) \right. \\ \left. + \frac{1}{n^2} (J_s + J)(2J_s + J) + \frac{3}{n(n+2)} J_s^2 J + \frac{1}{n^2} \right. \\ \left. \times (J_s^3 + 5J_s^2 J + 3J_s J^2) + \frac{3}{n^2(n+2)} (J_s + J) J_s^2 J \right. \\ \left. + \frac{1}{n^2} J_s J (J_s^2 + 2J_s J) + \frac{3}{n^2(n+2)} J_s^3 J^2 \right] \quad (4.5c) \end{aligned}$$

In particular, if  $J=0$ , (4.5) reduces to the formulas (2.12) and (2.14) for the two-dimensional bulk model. This is quite natural. If we turn off the bulk interactions, the surface becomes a two-dimensional system, decoupled from its substrate. The corresponding critical point, located at  $J=0$ ,  $J_s = J_s^*$ , is known as the surface transition.

In the Ising model, there are two different surface phases at bulk criticality, separated by the multicritical special (or surface-bulk) critical

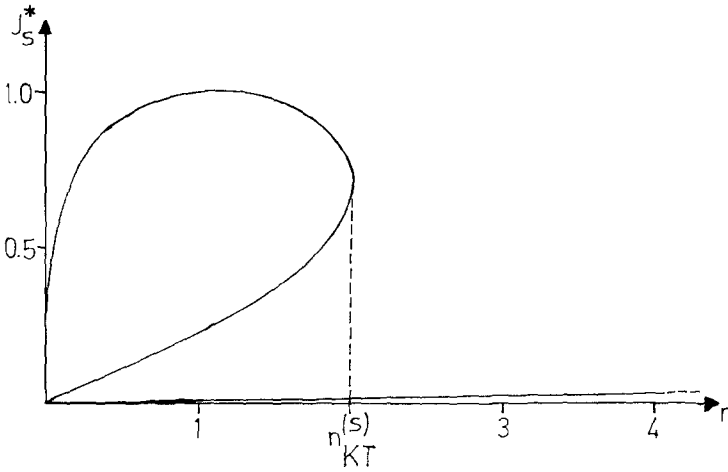


Fig. 8. Fixed points  $J_s^*$  at bulk criticality. Ordinary transition (lower curve). Special transition (upper curve, lower branch). Extraordinary transition (upper curve, upper branch).

point. The two phases are the basins of attraction for the ordinary and extraordinary fixed points. The ordinary, special, and extraordinary fixed points are graphed for different  $n$  in Fig. 8. For the surface fixed point, we refer to Fig. 3. In Fig. 9, we show the surface eigenvalue exponents that are relevant (positive) at the various transitions. These exponents were obtained from the recursion relations (4.5), just as the bulk exponents were calculated in Section 2. The RG flows for different  $n$  are sketched in Fig. 10. For  $n < n_{KT}$ , the general features are the same as in the Ising

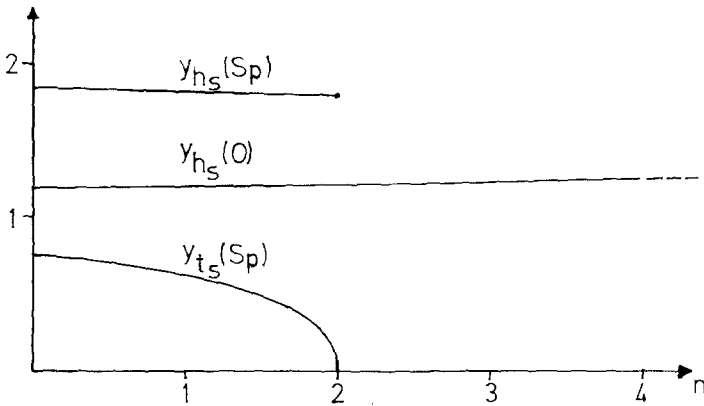


Fig. 9. Relevant and nontrivial surface critical exponents. Upper curve:  $y_{h_s}$ , special transition. Middle curve:  $y_{h_s}$ , ordinary transition. Lower curve:  $y_{t_s}$ , special transition.

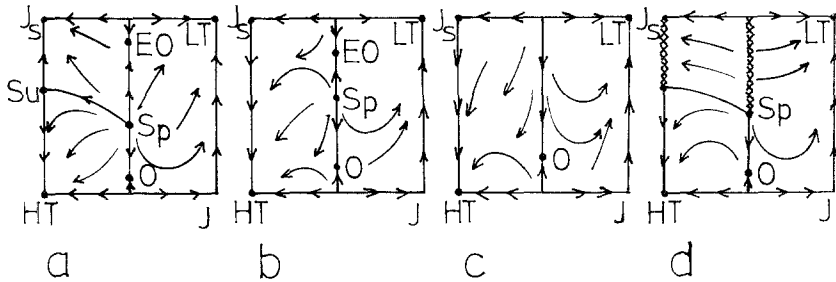


Fig. 10. RG flows in the  $J$ - $J_s$  plane, according to the MKRG: (a)  $n < n_{KT}$ , (b)  $n_{KT} < n < n_{KT}^{(s)}$ , (c)  $n > n_{KT}^{(s)}$ , (d) Speculation on exact RG flows if  $n_{KT} = n_{KT}^{(s)} = 2$ . The various fixed points are: (HT) high-temperature, (LT) low-temperature, (O) ordinary, (Su) surface, (Sp) special, (EO) extraordinary.

model. At  $n = n_{KT}$ , a free surface undergoes a Kosterlitz–Thouless transition, while for  $n > n_{KT}$  the surface fixed point has vanished and the situation is that depicted in Fig. 10b. When  $n$  increases further, the special and extraordinary fixed points will collide and annihilate, which happens when  $n = n_{KT}^{(s)} \approx 2.00$ . This phenomenon is completely analogous to the appearance of the Kosterlitz–Thouless phase in two bulk dimensions, and hence we expect an algebraic phase to emerge on the surface at bulk criticality. When  $n$  increases beyond  $n_{KT}^{(s)}$ , we are left with the situation in Fig. 10c. Here the surface is never ordered at bulk criticality, irrespective of the surface coupling constant.

We know that  $n_{KT} = 2$ , exactly. The exact value of  $n_{KT}^{(s)}$  is not known, but by analogy we expect it to be larger than the MKRG prediction. On the other hand, it is not inconceivable that  $n_{KT}^{(s)}$  in fact is also exactly equal to 2, in which case the phase diagram would be that of Fig. 10d. The rows of crosses indicate fixed lines. Whether the three-dimensional  $XY$  model shows an algebraic surface phase at bulk criticality, or if the presence of the bulk is sufficient to stabilize an ordered surface phase, is something we believe is worthwhile to explore with more sophisticated methods.

## 5. CONCLUSIONS

We have applied the MKRG to the modified  $O(n)$  model introduced by Domany *et al.*,<sup>(5)</sup> in two and three dimensions. In two dimensions, the accuracy of the thermal eigenvalue exponent is rather poor, while the magnetic exponent comes out quite accurately. This is not surprising if we compare this to MKRG results for the Ising model. The MKRG also reproduces the disappearance of the fixed point when  $n$  increases, although the Kosterlitz–Thouless fixed line is not found. Finally, the semi-infinite  $O(n)$  model was investigated.

One of the main objectives here has been to demonstrate the usefulness of modifying the Hamiltonian. As long as the modified Hamiltonian retains the correct symmetry, we expect it to yield the same universal quantities as the original model. Such a modification was accomplished in reference 5 in order to calculate the high-temperature series, which we extended in I to  $O(n)$  models on arbitrary lattices, and in this paper we have shown it to perform the MKRG. We believe that other methods may also be applied to the  $O(n)$  model with advantage, e.g., Monte Carlo renormalization. More importantly, by modifying the Hamiltonian to make the partition function simpler, one might be able to solve previously intractable problems exactly, just as Nienhuis found the exact  $O(n)$  critical exponents.

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