

Preserving the free energy in a Migdal-Kadanoff approximation for the q -state Potts model

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(Received 29 June 1982)

We study a new modification of the Migdal-Kadanoff (MK) approximation, in which the bond-shifting step is generalized so that the resulting transformation preserves the free energy. This method is then utilized to study the q -state Potts model in two and three dimensions. While this method is just as easy to implement as the standard MK approximation, significant quantitative improvement is achieved by preserving the free energy even to very low order in a series expansion. We also discuss the limitations inherent in employing a single-parameter renormalization-group transformation.

I. INTRODUCTION

The Migdal-Kadanoff (MK) approximation¹ is by far the easiest position-space renormalization-group (RG) method available today. In fact, for most cases it is simpler to do an MK calculation than the corresponding mean-field treatment. While the MK method is clearly an improvement over the latter, it is still not as quantitatively accurate as more elaborate renormalization-group techniques. What one would like, then, is a straightforward way to improve the basic MK transformation, while at the same time retaining its simplicity and ease of calculation. Many modifications have been studied in recent years,² often involving schemes to exploit the fact that the standard MK calculation is a lower bound to the exact free energy. However, in the process of improving on MK the resulting methods generally lose simplicity and become almost as involved as the more difficult calculations one seeks to replace. In this paper we study a recently introduced method³ which retains the basic simplicity of the MK approximation, while achieving significantly better results, and we apply it to the q -state Potts model in two and three dimensions.

This method involves modifying the basic MK approach so that, instead of producing a lower bound to the exact free energy of the system, the resulting calculation preserves the true free energy to a given order in a series expansion. This is achieved by generalizing the *ad hoc* bond-shifting step of the MK transformation. In practice, we find that even by preserving the free energy to low order, significant quantitative improvement is achieved over the MK results. Finally, it is straightforward to improve systematically the calculated free energy by simply working to higher order.

In the calculations presented here we consider only a single interaction parameter. The consequence of this is that, even if the free energy is, in principle, preserved exactly through all orders, the resulting recursion relations become singular. This is demonstrated in Sec. II, where the general features of our method are presented. The method is found to be a useful approximation technique, as shown in Sec. III, where the quantitative results are discussed.

II. METHOD

We now develop in detail the ideas outlined in the Introduction, and we illustrate the method by applying it to the Potts model.^{4,5} First, we consider the standard q -state Potts model, defined by

$$-\beta H_p(K; \{s_i\}) = K \sum_{\langle ij \rangle} \delta_{s_i s_j}, \quad (1)$$

where $s_i = 1, 2, 3, \dots, q$, and $\delta_{s_i s_j}$ is the Kronecker δ function. The reduced free energy per site associated with this Hamiltonian, on a lattice with N sites, is

$$f_p(K) = \lim_{N \rightarrow \infty} \frac{1}{N} \ln \left[\text{Tr}_{\{s_i\}} e^{-\beta H_p(K; \{s_i\})} \right]. \quad (2)$$

For convenience in developing a diagrammatic expansion of the free energy, it is also useful to study a "traceless" version of the Potts model, which can be written as

$$-\beta H_t(K; \{s_i\}) = K \sum_{\langle ij \rangle} (\delta_{s_i s_j} - q^{-1}), \quad (3)$$

from which it follows that

$$f_t(K) = \lim_{N \rightarrow \infty} \frac{1}{N} \ln \left[\text{Tr}_{\{s_i\}} e^{-\beta H_t(K; \{s_i\})} \right] \\ = -\frac{1}{2} z q^{-1} K + f_p(K), \quad (4)$$

$$f_t(K) = \ln q - \frac{1}{2} z q^{-1} K + \frac{1}{2} z \ln [1 + q^{-1} (e^K - 1)] + \lim_{N \rightarrow \infty} \frac{1}{N} \ln \left[q^{-N} \text{Tr}_{\{s_i\}} \prod_{\langle ij \rangle} [1 + v(\delta_{s_i s_j} - q^{-1})] \right], \quad (5)$$

where

$$v = \frac{e^K - 1}{1 + q^{-1} (e^K - 1)}. \quad (6)$$

With the model defined in this way, only closed diagrams contribute in the expansion. One can develop a similar expansion for low temperature (large K), or make use of duality in two dimensions.

Before developing our method we review the usual MK transformation. Figure 1 illustrates the basic steps involved in carrying out the MK procedure for the square and triangular⁶ lattices. The first step is to shift some bonds away from their original positions, and to place them in other locations on the lattice. Thus in Fig. 1 the bonds in the interior of each basic unit are moved onto the perimeter. It is clear that by following this procedure we will have $\tilde{K} = 2K$ for this case. In general, $\tilde{K} = b^{d-1}K$ on a d -dimensional hypercubic lattice with lengths rescaled by a factor b . Also, it is solely in this bond-shifting step that the MK method is approximate. The second step is an exact transformation in which those degrees of freedom labeled by crosses are traced out, leaving a lattice with lengths rescaled by

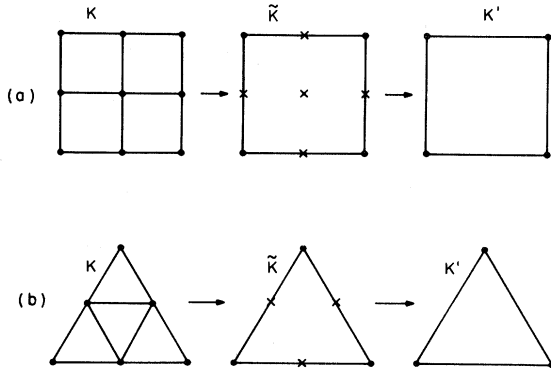


FIG. 1. MK transformation is illustrated for the square (a) and triangular (b) lattices. The sequence shows the original lattice with interaction K , the restructured lattice with interaction \tilde{K} , and the lattice with renormalized interaction K' . The degrees of freedom labeled by crosses are decimated. In this example all lengths are rescaled by a factor of 2 ($b=2$).

where z is the coordination number of the lattice. In what follows the subscripts t and p are suppressed when the results apply equally to both cases. The high-temperature (small- K) expansion of $f_t(K)$ has the form,

a factor of 2 ($b=2$) and renormalized couplings K' . An expression for K' with arbitrary b is easily derived and can be expressed as

$$K' = \ln \left[\frac{\lambda_+^b + (q-1)\lambda_-^b}{\lambda_+^b - \lambda_-^b} \right], \quad (7)$$

where

$$\lambda_+ = e^{\tilde{K}} + (q-1) \quad (8)$$

and

$$\lambda_- = e^{\tilde{K}} - 1. \quad (9)$$

Clearly, this result is equally valid for both the square and triangular lattices, since the same decimation is performed in each case, and thus the MK procedure does not distinguish between these two systems. Finally, the decimation also generates a constant term K'_0 which contributes to the free energy, where

$$K'_0 = q^{-1} K' - b q^{-1} \tilde{K} + \ln \left[\frac{\lambda_+^b - \lambda_-^b}{q} \right]. \quad (10)$$

The free energy is then calculated as follows:

$$f(K) = \sum_{n=0}^{\infty} b^{-nd} G[K^{(n)}], \quad (11)$$

with

$$G[K^{(n)}] = a \ln q + d b^{-d} K'_0 [K^{(n)}]. \quad (12)$$

$K^{(n)}$ denotes the n th iteration of K , so that $K^{(0)} = K$, $K^{(1)} = K'$, etc. The term $a \ln q$ takes into account the disconnected spins that result from the bond shifting, and for hypercubic lattices

$$a = 1 - b^{-d} [1 + d(b-1)]. \quad (13)$$

The basic difference in our approach is that the first step—the bond shifting or lattice restructuring—is generalized so that instead of $\tilde{K} = b^{d-1}K$ we allow $\tilde{K}(K)$ to be a general function of K . The form of this function is then determined such that the free energy of the calculation matches the series expansion for the exact free energy. The

second step of the transformation, the decimation, is exact and is retained unchanged. Recall that for the original lattice we denote the free energy by $f(K)$; similarly, we write $\tilde{f}(\tilde{K})$ for the free energy associated with the restructured lattice. Clearly, $f(K)$ and $\tilde{f}(\tilde{K})$ are not greatly different; both systems belong to the same universality class, and thus have the same type of singularities; only the detailed dependence on the couplings has changed. Therefore, one might expect that a simple function $\tilde{K}(K)$ will describe the mapping from one lattice to the other. We shall now study this function in detail.

To show how this can be carried out, we first consider various limits where the form taken by $\tilde{K}(K)$ is particularly straightforward. All results given below refer to the d -dimensional hypercubic lattice, where $z=2d$, unless specifically stated to apply to the triangular lattice. First, we consider the limit $K \rightarrow \infty$, where f_t and \tilde{f}_t reduce to

$$\lim_{K \rightarrow \infty} f_t(K) = d(1-q^{-1})K, \quad (14)$$

and

$$\lim_{\tilde{K} \rightarrow \infty} \tilde{f}_t(\tilde{K}) = db^{-(d-1)}(1-q^{-1})\tilde{K} + a \ln q. \quad (15)$$

From these results we find that setting $\tilde{f}_t(\tilde{K}) = f_t(K)$ implies

$$\lim_{\tilde{K} \rightarrow 0} \tilde{f}_t(\tilde{K}) = \ln q + b^{-(d-1)} \left[\frac{d}{2} q^{-1} (1-q^{-1}) \tilde{K}^2 + \frac{d}{6} q^{-2} (1-q^{-1})(q-2) \tilde{K}^3 \right] + O(K^4). \quad (19)$$

Thus, equating \tilde{f}_t and f_t yields

$$\lim_{K \rightarrow 0} \frac{\tilde{K}(K)}{K} = b^{(d-1)/2} \left\{ 1 + \frac{1}{6} q^{-1} (q-2) [1 - b^{(d-1)/2}] K \right\} + O(K^2), \quad (20)$$

and in this limit we obtain the square root of the usual MK value. We can see that this resulted from the fact that $f_t(K)$ starts off with order K^2 rather than linearly in K .

For the standard Potts model the limit $K \rightarrow 0$ is the same as in the MK procedure, simply because now the lowest-order term is linear, namely, $dq^{-1}K$. Thus

$$\lim_{K \rightarrow 0} f_p(K) = \ln q + dq^{-1}K + \frac{d}{2} q^{-1} (1-q^{-1}) K^2 + O(K^3) \quad (21)$$

and

$$\lim_{\tilde{K} \rightarrow 0} \tilde{f}_p(\tilde{K}) = \ln q + b^{-(d-1)} \left[dq^{-1} \tilde{K} + \frac{d}{2} q^{-1} (1-q^{-1}) \tilde{K}^2 \right] + O(\tilde{K}^3), \quad (22)$$

from which it follows that

$$\lim_{K \rightarrow 0} \frac{\tilde{K}(K)}{K} = b^{(d-1)} \left[1 + \frac{1}{2} (1-q^{-1})(1-b^{(d-1)})K \right] + O(K^2). \quad (23)$$

In this case the MK result is approached for both high and low temperatures, though again there is in general a deviation for finite K .

Now that various limits have been explored we consider preserving the free energy for arbitrary K .

$$\lim_{K \rightarrow \infty} \frac{\tilde{K}(K)}{K} = b^{(d-1)} \left[1 - \frac{a \ln q}{d(1-q^{-1})K} \right]. \quad (16)$$

When we do this calculation for f_p and \tilde{f}_p we find the same expressions as above, except that the factor $(1-q^{-1})$ is absent. Thus for this case

$$\lim_{K \rightarrow \infty} \frac{\tilde{K}(K)}{K} = b^{(d-1)} \left[1 - \frac{a \ln q}{dK} \right]. \quad (17)$$

In each case we see that the MK result of $\tilde{K}/K = b^{d-1}$ is recovered in the limit, but only asymptotically; for finite K the results will deviate from the MK results. Finally, the square and triangular lattices are distinguished in this method since the quantity a is different for these two systems.

The limit $K \rightarrow 0$ is more interesting in that the MK prescription is not always the asymptotic value of \tilde{K}/K . To see this we expand $f_t(K)$ for small K , with the result

$$\lim_{K \rightarrow 0} f_t(K) = \ln q + \frac{d}{2} q^{-1} (1-q^{-1}) K^2 + \frac{d}{6} q^{-2} (1-q^{-1})(q-2) K^3 + O(K^4). \quad (18)$$

Similarly,

By performing the exact decimation we can write $\tilde{f}(\tilde{K})$ in terms of $f(K')$ as

$$\tilde{f}(\tilde{K}) = a \ln q + db^{-d} K'_0(K) + b^{-d} f(K'). \quad (24)$$

Setting $f(K) = \tilde{f}(\tilde{K})$ then defines an implicit rela-

tionship for $K'(K)$. Solving for the fixed points, $K'(K^*)=K^*$, yields

$$K'_0(K^*)=d^{-1}b^d[(1-b^{-d})f(K^*)-a \ln q]. \quad (25)$$

Clearly, $K^*=0, \infty$ are both stable fixed points, as expected. There is also one critical fixed point for finite K^* . Similarly, we can determine the thermal exponent by taking the derivative with respect to K of Eq. (24), with the result

$$b^{y_T} = \frac{\partial K'}{\partial K} \Big|_{K=K^*} = \frac{b^d \frac{\partial f}{\partial K}}{d \frac{\partial K'_0}{\partial K} + \frac{\partial f}{\partial K}} \Big|_{K=K^*}. \quad (26)$$

These are the basic results of this method, where in practice $f(K)$ and $\partial f/\partial K$ are determined by a series expansion.

It is also useful to consider the limit $b \rightarrow 1$, that is, the limit of an infinitesimal rescaling, since these results are generally better than for finite b . In this limit the fixed point is defined by the condition

$$\frac{\partial K'(K^*, b)}{\partial b} \Big|_{b=1} = 0.$$

In terms of preserving the free energy this condition is

$$f(K^*) = \frac{\partial K'_0(K^*, b)}{\partial b} \Big|_{b=1}. \quad (27)$$

For the thermal exponent we find

$$y_T = \frac{d \left[\frac{\partial f}{\partial K} - \frac{\partial}{\partial K} \left[\frac{\partial K'_0}{\partial b} \Big|_{b=1} \right] \right]}{\frac{\partial f}{\partial K}} \Big|_{K=K^*}. \quad (28)$$

These equations are simple to solve and the results are given in the next section.

Before turning to the quantitative results, we first point out the implications of preserving the free energy exactly. Consider again the condition for the fixed point Eq. (25). In general, one cannot expect $f(K_c)$ and $K'_0(K_c)$ to satisfy such a simple relationship, and as a result one will find that $K^* \neq K_c$. In the same light, consider again the implicit expression for the recursion relation $K'(K)$,

$$f(K) = a \ln q + db^{-d}K'_0(K) + b^{-d}f(K'). \quad (29)$$

If $K=K_c$, but $K'(K_c) \neq K_c$, then the left-hand side of this equation is singular while the right-hand side is not. In order for the equality to be enforced as $K \rightarrow K_c$, it is necessary for $K'(K)$ and $\tilde{K}(K)$ to be singular. Thus working with only a single interac-

tion parameter forces the recursion relations to be nonanalytic.

III. RESULTS

The results in this section are primarily for two dimensions except where d appears explicitly. For the actual calculation we must develop an approximate form for the free energy which is to be used in Eqs. (25) and (26). We choose to approximate the free energy using series-expansion methods. Thus for high temperature (high T) we use Eq. (5), up to order v^6 . Therefore, the quantity we preserve is

$$f_t(K) = \ln q - 2q^{-1}K + 2 \ln[1 + q^{-1}(e^K - 1)] + q^{-3}(1 - q^{-1})v^4 + 2q^{-5}(1 - q^{-1})v^6 \quad (30)$$

for high temperature and the corresponding low-temperature (low- T) expansion to the same order for low temperature. One can easily work to higher order, but based on previous work³ we expect little change in the results. Thus in order to keep the calculation simple, we do not include higher-order terms.

In Fig. 2, \tilde{K}/K is plotted as function of $K/2$ for different values of q . The traceless free energy f_t is

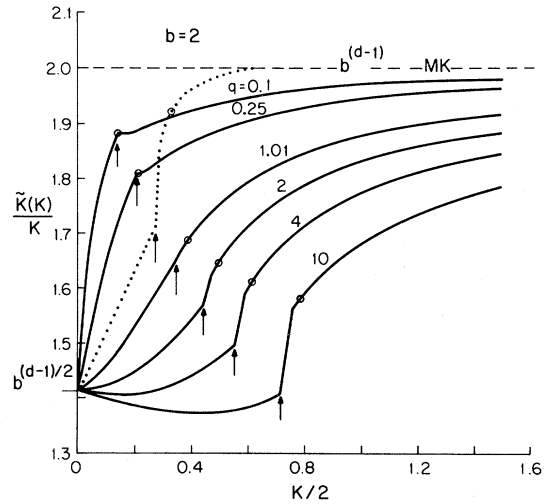


FIG. 2. $\tilde{K}(K)/K$ as a function of $K/2$ for $b=2$ and $q=0.1, 0.25, 1.01, 2, 4$, and 10 on the square lattice (solid line), and on the triangular lattice, for $q=2$ (dotted line). The results are obtained using the traceless free energy $f_t(K)$ preserved to order v^6 . The arrows indicate the exact K_c , and the circles show the fixed points obtained from our method. All lines asymptote to the MK result, b^{d-1} (dashed line) for $K \rightarrow \infty$, and to $b^{(d-1)/2}$ for $K \rightarrow 0$.

used and it can be seen that the MK result b^{d-1} is an upper bound for \tilde{K}/K . The MK value is recovered only in the limit $K \rightarrow \infty$, as shown in Eq. (16). For all q , $\tilde{K}/K \rightarrow b^{(d-1)/2}$, as $K \rightarrow 0$, and the slope at $K=0$ is positive (negative) for $q < 2$ ($q > 2$) as derived in Eq. (20). The deviation from the MK value is greatest for large q . For $q \ll 1$, the MK result is recovered for almost the entire range of K , and thus this method demonstrates why the standard MK method gives good results for small q .

In order to minimize the error in the approximate free energy for all temperatures, we use high- and low- T expansions for temperatures which are above or below the self-dual temperature, respectively. For a given q the fixed point, indicated in Fig. 2 by an open circle, occurs on one of the two branches, and the exponent is calculated there. For almost all cases the fixed point is found to lie below the self-dual temperature, and thus the low- T expansion is used.

For general values of q , there are two points of singularity for \tilde{K}/K , and these are more evident for large q . Recall that we obtain the relation $\tilde{K}(K)$ by equating $\tilde{f}(\tilde{K})$ with $f(K)$. Since the two free energies each have a singular point, this will introduce two singularities into $\tilde{K}(K)$ and hence into the recursion relation $K'(K)$. One of these, denoted by an arrow, is the exact critical point for the original lattice, and the other occurs at the critical point of the restructured lattice. As we add more terms into the free-energy expansion, the singularities will be somewhat less apparent for $q < 4$, since the transition is second order and $\partial f/\partial K$ is continuous for all K . But for $q > 4$, since the transition is first order and $\partial f/\partial K$ is discontinuous at the transition, the singularities will still be evident, reflecting the first-order nature of the transition.

\tilde{K}/K is also obtained for $f_p(K)$ defined in Eq. (2). The corresponding results are shown in Fig. 3, for different values of q . The MK results b^{d-1} is exactly recovered only for $q=1$, in which case the free energy is trivial and nonsingular.⁷ For $q > 1$ ($q < 1$), $\tilde{K}/K < b^{d-1}$ ($\tilde{K}/K > b^{d-1}$) and the equality is obtained only in the limits $K \rightarrow 0, \infty$ independent of q , in agreement with Eqs. (17) and (23). The same general features of the singularities can be seen here, as in the previous case.

\tilde{K}/K for the Ising model ($q=2$) on a triangular lattice is plotted with a dotted line in Figs. 2 and 3. There is a clear difference between $\tilde{K}(K)$ for this case and the Ising model on a square lattice; hence the fixed points of the two models are different, though the exponents are roughly the same (see Table I). Notice that for the triangular lattice \tilde{K}/K converges more quickly to the MK value, which reflects the fact that, in the restructured lattice, there

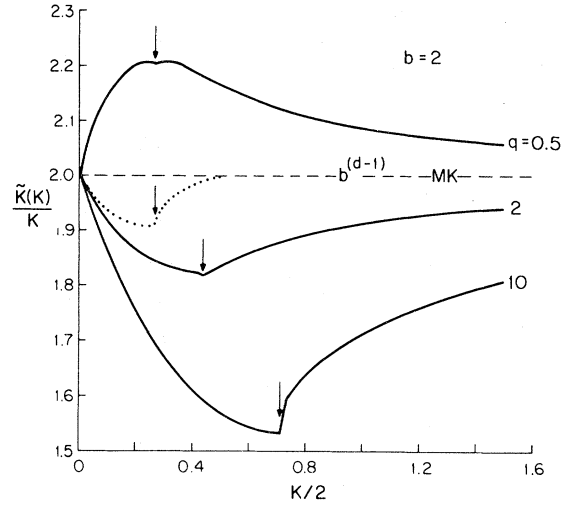


FIG. 3. $\tilde{K}(K)/K$ as a function of $K/2$ for $b=2$ and $q=0.5, 2$, and 10 on the square lattice (solid line), and on the triangular lattice, for $q=2$ (dotted line). The results are obtained using the Potts free energy $f_p(K)$ preserved to order v^6 . The arrows indicate the exact K_c . All the lines asymptote to the MK result b^{d-1} (dashed line) for $K \rightarrow 0, \infty$.

are no decoupled spins left (for $b=2$). Thus one can conclude that the standard MK approximation is more appropriate for the triangular lattice than for the square lattice.

We have determined the fixed points and the exponents for both versions of the Potts model. The results for the traceless case, which are somewhat better, are shown in Fig. 4, where we compare our calculation using a rescaling factor $b=2$ with the MK method and the exact results.^{4,8} Our method clearly gives a much better approximation than MK. Also, in the limit of large q we obtain the correct asymptotic value for the critical point, because in this limit the free energy is $f(K)=dK$, so that the fixed-point equation is

$$K'_0(K^*) = (b^d - 1)K^* - d^{-1}[b^d - 1 - d(b-1)]\ln q, \quad (31)$$

leading to a fixed point $K^* = (1/d)\ln q$. Note that this result is in agreement with the exact critical point⁴ in two dimensions, and also with mean field⁵ for any d and $q \gg 1$. These results are also independent of the rescaling factor b . Similarly, for the triangular lattice we get the correct critical point $K^* = \frac{1}{3}\ln q$. The MK method, which is not b independent, gives $K^* = \frac{1}{3}\ln q$ for the square and triangular lattices for $b=2$.

The results we obtain are especially good for small q . This is in accord with other calculations,⁹

TABLE I. Results for square, triangular, and simple cubic (sc) lattices for various values of q . Shown are the exact values (or best estimates) for the critical points K_c and the thermal exponents y_T . These are compared with our method ($N=6$) and the MK method for $b=2$. For $q=3,4$ on the sc lattice, we do not list the exponents since the transition is believed to be first order (fo).

		$K_c/2$			y_T		
		Exact	Calc. ($N=6$)	MK	Exact	Calc. ($N=6$)	MK
Square	$q=2$	0.441 ^a	0.503	0.305	1.000 ^a	0.922	0.747
Triangular	$q=2$	0.275 ^b	0.336	0.305	1.000 ^b	0.926	0.747
Simple cubic	$q=1$	0.142 ^c	0.169	0.041	1.21 ^d	1.477	0.813
	$q=2$	0.217 ^e	0.237	0.065	1.56 ^f	1.569	0.939
	$q=3$	0.277 ^g	0.287	0.082	fo		
	$q=4$	0.324 ^h	0.326	0.096	fo		

^aReference 12.

^bReference 13.

^cReference 14.

^dReference 15.

^eReference 16.

^fReference 17.

^gReference 18.

^hReference 19.

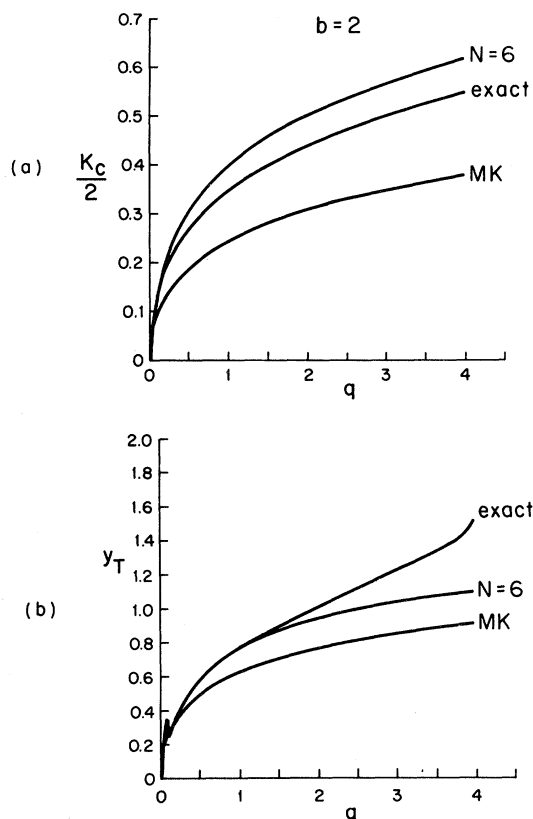


FIG. 4. $K_c/2$ (a) and the thermal exponent y_T (b) as a function of q for the square lattice. The three curves show the exact, the standard MK, and our method with $b=2$. In our calculation, the free energy is preserved to order v^6 ($N=6$).

where the RG flows remain within a one-dimensional parameter space, indicating that for small q a single parameter is sufficient. On the other hand, for $q > 4$ the transition is known to be first order.¹⁰ However, we do not expect to see this changeover from second- to first-order behavior, because the only way to obtain this, with the use of the RG method, is to enlarge the parameter space.^{11,9} Again, we use our method with only a single interaction parameter.

Even though a low-order expansion is used, our approximate free energy differs significantly from the exact free energy only near the critical point³ K_c . When K^* deviates from K_c , the error in the free energy is negligible, and adding more terms has small effect. As a function of q we find that K^* crosses K_c at $q=q_0 \simeq 0.1$; therefore, only near q_0 will the low order of the expansion manifest itself. This is the reason for the discontinuity in the calculated exponent y_T , shown in Fig. 4(b). Adding more terms to the expansion will eventually reduce this gap to zero.

The use of an infinitesimal rescaling factor ($b \rightarrow 1$) produces only a small change in the critical points; however, there is a significant improvement in the exponent as can be seen in Fig. 5. The discontinuity occurs now at $q=q_0 \simeq 0.25$, and as in the $b=2$ case, adding more terms to the expansion will reduce the discontinuity. Since the MK procedure commutes with duality in two dimensions, it gives the exact K_c for $b \rightarrow 1$. However, in the usual MK procedure, one finds essentially no change in the exponents compared with $b=2$.

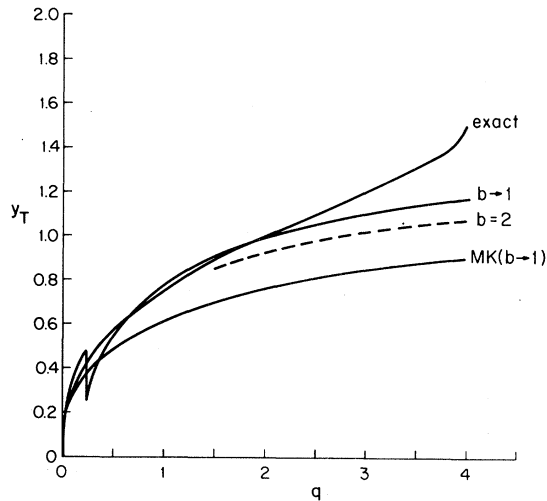


FIG. 5. y_T as a function of q for the square lattice. The solid lines show the exact result, as well as the $b \rightarrow 1$ limit of our method and the MK method. For comparison, the dashed line shows our result for $b=2$, only for $q \geq 1.5$.

We summarize the results for square, triangular, and simple cubic (sc) lattices in Table I for different values of q . For the sc lattice we get good agreement with previous calculations for the critical points, and also with the Ising exponent ($q=2$). For $q=1$ the exponent is not as good, but recall that we use only two terms in the series expansion, whereas the quoted values are obtained with much longer expansions.

Finally, though useful as an approximation technique, clearly the limitation of this method is that we employ only a single interaction parameter. It will be of interest to explore this method for larger parameter spaces, opening the way for the study of many other models of interest as well.

ACKNOWLEDGMENTS

The authors wish to thank A. N. Berker for many useful comments. We also benefited from discussions with M. Kardar. This work was supported by the joint Services Electronics Program, Contract No. DAAG29-80-C0104.

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⁷It is of interest to note that for $q=1$ the existence of a nontrivial fixed point does not imply a singularity in the free energy. Using Eq. (11), for $q \rightarrow 1$, we calculate the free energy for which $G[K^{(n)}] = d[K^{(n)} - b^{-d}K^{(n+1)}]$; therefore, $f_{MK}(K; q=1) = f_p(K; q=1) = dK$. Only the first term in the sum,

Eq. (11), will contribute and all the other terms cancel each other, resulting in a trival nonsingular free energy. This is in contrast to the case $q \neq 1$, where the infinite sum is nontrivial and is the cause of the singularity.

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