Modified Migdal-Kadanoff renormalization for the Potts model

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A modification of the Migdal-Kadanoff (MK) real-space renormalization technique is studied and applied to the q-state Potts model on the square and the simple cubic lattices. A parameter x which describes the boundary condition is introduced to the cluster-decimation (CD) approximation. When $x=2$, the present method is the same as the CD approximation, and in the limit $x\to\infty$ this method reduces to the MK technique. Critical temperatures and exponents of the Potts model are calculated for $0<q\leq 4$ by using various boundary conditions. Very good estimates of critical properties are obtained. The choice of the boundary condition is discussed.

I. INTRODUCTION

The Migdal-Kadanoff (MK) renormalization-group method[1,2] has been widely applied to many spin systems in recent years.[3] This method is simple in procedure as well as in numerical calculations when compared to other real-space renormalization methods. Results obtained by the MK method, however, are less accurate. Many modifications of the MK approximation have been studied.[3–6] The most useful modification considered so far is probably the cluster-decimation (CD) approximation recently introduced by Goldstein and Walker.[6]

Walker[4] first introduced a method in which the bond-moving step in the MK technique is modified such that the free energy of the whole system is preserved exactly through a given number of terms (N terms) in the high- and low-temperature series expansions. As series expansions are known for most spin systems,[7] little increase in calculational effort is involved in the method of Walker, while significant improvement over the standard MK method is obtained. Walker's series-expansion method, however, is not applicable to systems for which the high- or low-temperature series expansions are not available.

Recently, Goldstein and Walker have proposed an alternative modification of the MK method, called the cluster-decimation approximation.[6] The preservation of the free energy by matching series expansions of the infinite lattice is replaced by preserving the free energy (or internal energy) for a finite cluster of spins with periodic boundary conditions. When the cluster size approaches infinity, the CD method will give the same results as those obtained by using an infinite number of terms ($N\to\infty$) in the method of Walker.[4]

The CD method approximates the free energy per spin of the infinite lattice by those of clusters having different sizes but with the same periodic boundary condition. From the work of Goldstein and Walker[6] we see the following: (i) By using the simplest 2×2 and $2\times 2\times 2$ clusters, significant improvements over the standard MK approximation are obtained. (ii) Using a larger cluster in the CD method does not necessarily give better estimates of the critical properties than using a smaller cluster.

In this article we consider a variation of the CD method. We approximate the free energy of the system by those of the simplest cluster (of 2^d spins) having different boundary conditions described by a parameter x.[8] When $x=2$, our method is exactly the same as that of Goldstein and Walker; and for $x\to\infty$, our results reduce to those of the standard MK method with the rescaling factor $b=2$. In Sec. II we describe the method for the Ising model on the square lattice. Application of the present method to the Potts model on the square and the simple-cubic lattices are presented in Sec. III. Summary and discussions are given in Sec. IV.

II. MODIFICATION OF THE MK METHOD

The standard MK method contains two operations: bond moving and site decimation. Figure 1(a) displays a two-dimensional ($d=2$) square lattice with nearest-neighbor interactions. Each bond in the figure represents the coupling K (including the factor $-1/k_BT$) between a pair of nearest-neighbor spins. The first step in the MK method is to restructure the lattice by moving away some of the bonds. Each bond that remains is then given a strengthened coupling $\tilde{K}$ [see Fig. 1(b)]. The second step is to sum over the degrees of freedom of the spins indicated by crosses in Fig. 1(b). We then obtain a lattice with lengths rescaled by a factor of 2 ($b=2$), and renormalized coupling K' [see Fig. 1(c)].

The site-decimation operation is a simple exact transformation; no improvement can be made. But the bond-moving operation is an approximation. In the standard MK scheme, $\tilde{K}$ is set equal to $b^{d-1}K$ for a d-dimensional hypercubic lattice with a rescaling factor b, such that the total bond strength is preserved. This causes the free energy of the restructured lattice to be a lower bound to the exact free energy of the system.[2] In Walker's series-expansion method[4] and the CD approximation,[6] the relationship $\tilde{K}/K=b^{d-1}$ is replaced by temperature-dependent functions such that the difference between the free energies of the original and the restructured lattices be as small as possible.

In the present method, the free energy of the system is required to be preserved only approximately. To illustrate

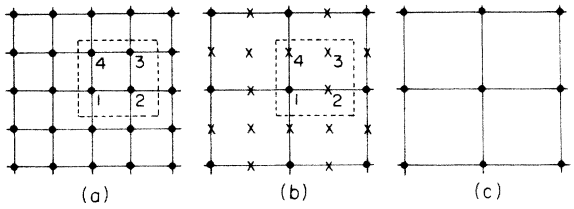

FIG. 1. Bond moving and site decimation of the MK method with $b=d=2$. The original system (a) has coupling K, the restructured lattice (b) has coupling $\tilde{K}$, and the rescaled lattice (c) has coupling K'. In the present method the block of spins enclosed by the dashed line (with a boundary condition) is required to preserve the free energy in the bond-moving operation.

our method (and the CD method using the simplest cluster), consider the Ising model on the square lattice. In a magnetic field H the reduced Hamiltonian is given by

$$-\mathcal{H}/k_BT=K\sum_{\langle i,j\rangle}s_is_j+h\sum_i s_i\ , \tag{1}$$

where $s_i=\pm1$, $K=J/k_BT$, and $h=H/k_BT$.

Consider a block of 4 $(=2^d)$ spins enclosed by the dashed line shown in Fig. 1(a). If the interactions within the block are treated exactly, while interaction between this block and other spins are replaced by a boundary condition, then the partition function for the block of spins is

$$\begin{aligned}Z&=\sum_{s_1,s_2,s_3,s_4}\exp[xK(s_1s_2+s_2s_3+s_3s_4+s_4s_1)\\&\qquad+h(s_1+s_2+s_3+s_4)]\\&=Z_0+h^2Z_2+O(h^4)\ ,\end{aligned}\tag{2}$$

where

$$Z_0=8+8\cosh^2(2xK)\ , \tag{3}$$

$$Z_2=16+16\exp(4xK)\ . \tag{4}$$

The parameter x depends on the boundary condition used. For the free boundary condition (interactions between the block and other spins are ignored), $x=1$; and for the conventional periodic boundary condition, $x=2$. When we use the periodic boundary and consider all bonds connected to the block as energy of the block, we have $x=3$. In general, we can treat x as an adjustable parameter, and extend it to positive numbers.

For the restructured lattice, Fig. 1(b), each bond carries a coupling $\tilde{K}$, and at a lattice site connected by n bonds there is a magnetic field $n\tilde{h}/2$ (including the factor $1/k_BT$). We have used the scheme in which the single-spin interactions are moved together with two-spin interactions in the bond-moving step.[1] The functions $\tilde{K}$ and $\tilde{h}$ are to be determined. We note that Goldstein and Walker[6] treated the magnetic field term in a different way. We will discuss this point later.

In the restructured lattice, the partition function for the block of spins s_1,s_2,s_3,s_4 with the same boundary condition as in the original lattice is given by

$$\begin{aligned}\tilde{Z}&=\sum_{s_1,s_2,s_3,s_4}\exp[x\tilde{K}(s_1s_2+s_1s_4)+\tilde{h}(2s_1+s_2+s_4)]\\&=\tilde{Z}_0+\tilde{h}^2\tilde{Z}_2+O(\tilde{h}^4)\ ,\end{aligned}\tag{5}$$

with

$$\tilde{Z}_0=8+8\cosh(2x\tilde{K})\ , \tag{6}$$

$$\tilde{Z}_2=16+32\exp(2x\tilde{K})\ . \tag{7}$$

By requiring that $Z=\tilde{Z}$ in the low-field limit, i.e., $Z_0=\tilde{Z}_0$ and $h^2Z_2=\tilde{h}^2\tilde{Z}_2$, we obtain the transformations

$$\tilde{K}=(2x)^{-1}\cosh^{-1}[\cosh^2(2xK)]\ , \tag{8}$$

$$\tilde{h}=h[1+\exp(4xK)]^{1/2}[1+2\exp(2x\tilde{K})]^{-1/2}\ . \tag{9}$$

The ratios $\tilde{K}/K$ and $\tilde{h}/h$ as functions of K for several values of x are shown in Fig. 2. The ratio $\tilde{K}/K$ in Walker's method (40 terms in the series expansions are used) is also given for comparison. When $x=2$ our resulting $\tilde{K}/K$ is nothing but that of the 2×2 CD approximation of Goldstein and Walker, but our ratio $\tilde{h}/h$ is different from that of Goldstein and Walker[6] because the magnetic-field term is treated differently.

It is important to note that Eqs. (8) and (9) give correct results in the high- and low-temperature limits for any finite positive value of x. We also see that in the extreme case $x\to\infty$, our results reduce to those of the standard

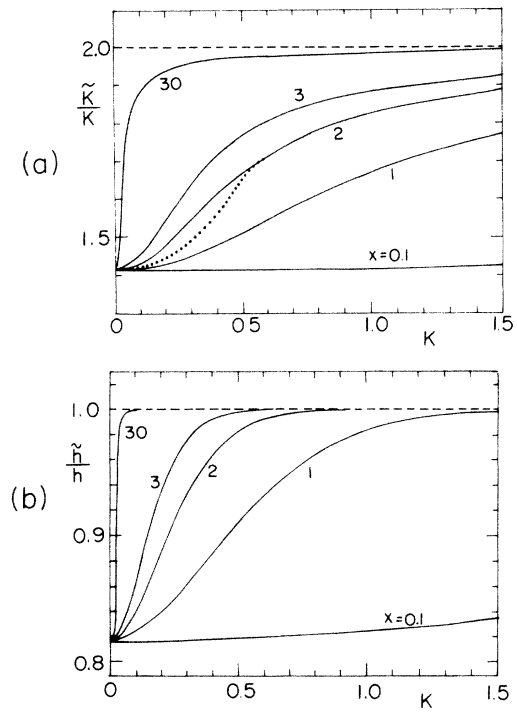

FIG. 2. (a) $\tilde{K}/K$ and (b) $\tilde{h}/h$ as functions of K for the Ising model on the square lattice. The parameter x describes the boundary condition used. Dashed lines represent the MK results and the dotted line is the result of Walker calculated by using 40 terms in the series expansions. The rescaling factor $b=2$.

MK method which gives the correct free energy only at zero temperature. In the limit $x \to \infty$, only the ground state contributes to Z and $\tilde{Z}$. Therefore, our method reduces to the MK method for all modes with nearest-neighbor interactions on general d-dimensional hypercubic lattices. If we consider a cluster larger than 2^d spins, the present method will not reduce to the MK method in the limit $x \to \infty$.

The site-decimation step is straightforward and well known. For $b=d=2$ the transformations are

$$K' = \tanh^{-1}(\tanh^2 \tilde{K}) , \tag{10}$$

$$h' = 2\tilde{h}[1+\tanh(2\tilde{K})] . \tag{11}$$

Equations (8) and (10) define the renormalization-group transformation of the coupling; Eqs. (9) and (11) describe the transformation of the field. By setting $K=K'=K^*$ in Eqs. (8) and (10), the fixed point K^* can be determined. The thermal exponent y_t and the field exponent y_h are then given by $\ln(dK'/dK)/\ln 2$ and $\ln(h'/h)/\ln 2$ (evaluated at K^*), respectively.

III. APPLICATION TO THE POTTS MODEL

The modified MK method described in detail in Sec. II for the Ising model on the square lattice can be extended to other models. We now apply this method to the q-state Potts model[7,8] defined by

$$-\mathcal{H}/k_B T = K \sum_{\langle i,j \rangle} (\delta_{s_i s_j} - q^{-1}) + h \sum_i (\delta_{s_i 1} - q^{-1}) , \tag{12}$$

where $s_i = 1,2,3,\ldots q$, and $\delta_{\alpha\beta}$ is the Kronecker δ function.

Following the procedure described in the preceding section, and defining $V=\exp(xK)$, $\tilde{V}=\exp(x\tilde{K})$, it is easy to show that for the square lattice,

$$Z_0 = q(V)^{-4/q}\{V^4+(q-1)[6V^2+4(q-2)V+q^2-3q+3]\} , \tag{13}$$

$$Z_2 = 2(1-q^{-1})(V)^{-4/q} \times \{4V^4+2(7q-12)V^2+(q-2)[2(3q-8)V+q^2-4q+6]\} , \tag{14}$$

and

$$\tilde{Z}_0 = q^2(\tilde{V})^{-2/q}(\tilde{V}+q-1)^2 , \tag{15}$$

$$\tilde{Z}_2 = (q-1)(\tilde{V})^{-2/q}(2\tilde{V}+q-2)(4\tilde{V}+3q-4) . \tag{16}$$

The corresponding functions for the simple cubic lattice are also straightforward to derive, but they are more lengthy and will not be presented here.

The decimation transformation for the Potts model with the rescaling factor $b=2$ are

$$\exp(K') = [\exp(2\tilde{K})+q-1][2\exp(\tilde{K})+q-2]^{-1} , \tag{17}$$

$$h' = d\tilde{h}[2\exp(2\tilde{K})+q-2][\exp(2\tilde{K})+q-1]^{-1} . \tag{18}$$

The relations $Z_0=\tilde{Z}_0$, $h^2Z^2=\tilde{h}^2\tilde{Z}_2$, and Eqs. (17) and (18) describe the renormalization-group transformations for the Potts model. We note that when the interactions K and h are replaced by $2K$ and $2h$, respectively, the transformations for the Potts model with $q=2$ reduce to those for the Ising model given in Sec. II.

Various values of x are used to calculate critical properties of the Potts model on the square and the simple cubic lattices. Inverse critical temperature K_C calculated by using $x=2$ and 3, respectively, are shown in Fig. 3. Exact values[9,10] (or best estimates) and results obtained by the standard MK method ($b=2$) and by Walker's method[5] ($N=6$) are also given for comparison. For the square lattice, our results using $x=2$ are exactly the same as those of the 2×2 CD method. It is important to note that K_C calculated for the square lattice using $x=3$ are much better than those obtained by Andelman and Walker[5] and by Goldstein and Walker.[6] The reason that $x=3$ gives better estimates of critical properties for the square lattice than $x=2$ will be discussed in Sec. IV. For the simple cubic lattice, Goldstein and Walker[6] have not applied the CD approximation to the Potts model. Our calculations of K_C using $x=2$ show that this method yields better results than Walker's series-expansion method ($N=6$) for $q<3$.

Thermal exponent y_t and field exponent y_h calculated by the present method using $x=2$ for the simple cubic lattice and $x=3$ for the square lattice are shown in Table I for some values of q. Our results for thermal exponents

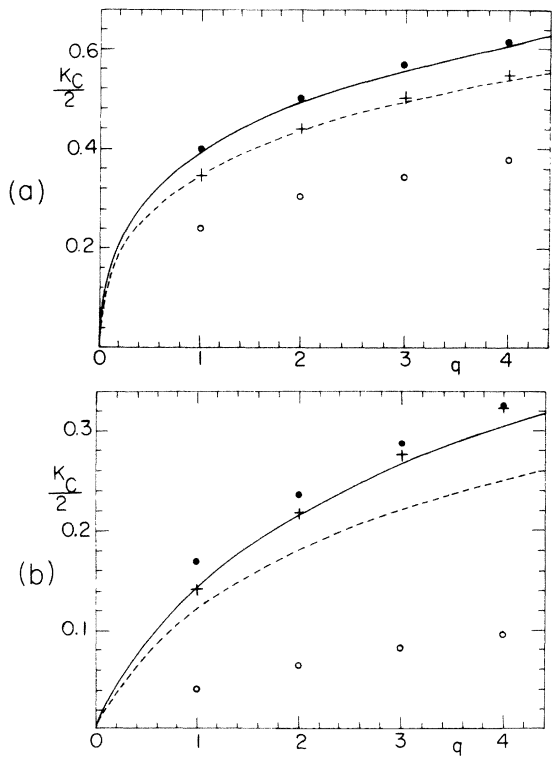

FIG. 3. $K_C/2$ of the Potts model on (a) the square lattice and (b) the simple-cubic lattice. The solid lines are calculated with $x=2$, and the dashed lines with $x=3$. Exact values (denoted by $+$), Walker's results using six terms (●) and the MK results with $b=2$ (○) are given for $q=1,2,3,4$.

TABLE I. Critical points K_C, thermal exponents y_t, and field exponents y_h of the Potts model on the square ($d=2$) and the simple cubic ($d=3$) lattices for some values of q. For $d=2$, $x=3$; and $x=2$ for $d=3$. Unless specified, the exact values (or best estimates) are from Ref. 10. We take the average when several values are listed in Ref. 10. The MK results are calculated for $b=2$. Exponents for $q=3,4$ on the simple cubic lattice are not listed since the transition is first order.

			$K_C/2$			y_t			y_h	
d	q	Exact	$x=3$	MK	Exact	$x=3$	MK	Exact	$x=3$	MK
2	1	0.347	0.348	0.241	0.75	0.716	0.612	1.896	1.926	1.891
2	2	0.441	0.437	0.305	1.00	0.847	0.747	1.875	1.925	1.879
2	3	0.503	0.494	0.347	1.20	0.930	0.830	1.867	1.926	1.875
2	4	0.549	0.537	0.378	1.50	0.989	0.890	1.875	1.927	1.872
d	q	Exact	$x=2$	MK	Exact	$x=2$	MK	Exact	$x=2$	MK
3	1	0.142	0.142	0.041	1.21[a]	0.977	0.815	2.52[a]	2.529	2.570
3	2	0.216	0.215	0.065	1.57[b]	1.165	0.939	2.48[b]	2.542	2.565
3	3	0.276	0.266	0.083						
3	4	0.321	0.304	0.096						

[a]Reference 11.
[b]Reference 12.

are much better than those of the MK method, but are somewhat poorer than those obtained by Walker's series-expansion method.[5] For the field exponent, the MK method yields very good estimates. Therefore, our calculations of y_h for the square lattice are not as good as the MK results. The errors of our estimates, however, are within 3%.

IV. SUMMARY AND DISCUSSION

We have proposed a simple modification of the MK method. Our idea is motivated by the modification schemes of Walker and co-workers.[4–6] In our method, the coupling constant $\tilde{K}$ of the restructured lattice is determined by requiring that the free energy for a block of 2^d spins, with a boundary condition described by a parameter x, is preserved. When $x=2$, the present method in zero field is nothing but the CD method of Goldstein and Walker.[6] We have applied the method to the q-state Potts model on the square and the simple cubic lattices, and obtained very good results.

It is known that the MK method ($x\to\infty$) is exact for $d=1$ (and correct to first order in ϵ for $d=1+\epsilon$).[1] But it gives poor results in high dimensions. On the other hand, finite-cluster calculations with conventional periodic boundary condition ($x=2$) give good results for lattices of high dimensions (or large coordination numbers). Therefore it is expected that $x\geq 2$ should be used in our method. The smaller the value of d is, the larger the value of x should be. This is why $x=2$ gives very good estimates of K_C for the simple cubic lattice, while $x=3$ predicts nearly exact values of K_C for the square lattice. We suggest that for general systems, the best value of x to be used is $x=2$ for $d=3$ or 4, and $x=3$ for $d=2$.

There are two different ways to calculate the magnetic exponent y_h in the MK method. In our method described in Sec. II, the single-spin interactions are moved together with the two-spin term in the bond-moving step. The magnetic-field energy for the block of spins is $h(2s_1+s_2+s_4)$ [see Eq. (5)]. If the single-spin interactions are not moved at all, the magnetic-field term in Eq. (5) becomes $h(s_1+s_2+s_3+s_4)$. In this case, the calculated values of y_h are poorer than what we obtained.

Goldstein and Walker[6] have used an alternative formula. In their method, the magnetic-field term in Eq. (5) is $h(s_1+s_2+s_4)$, which corresponds to neither approach of the MK method. Their method, however, gives a little better estimate of y_h than our method. We find that if we further reduce the field at s_1, and write the magnetic-field term as $h(0.5s_1+s_2+s_4)$, we obtain even better estimate of y_h. But it seems unphysical.

The present method retains the mathematical simplicity of the MK method and is easy to implement even when the high- or low-temperature series expansions are not available. This method employs only a single interaction parameter K (and the field), and is restricted to $b=2$ for the d-dimensional hypercubic lattice. Of course, we can extend the method to other lattices and for larger values of b, but for $b>2$ our method will not reduce to the MK method in the limit $x\to\infty$. Furthermore, $b>2$ does not give better results than $b=2$. It will be of interest to extend the method to larger parameter spaces, and if possible to $b\to 1$, and to nonintegral values of d.

ACKNOWLEDGMENT

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