Modified Migdal-Kadanoff renormalization for the spin-$\frac{1}{2}$ anisotropic Heisenberg model

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The spin-$\frac{1}{2}$ anisotropic Heisenberg model is studied by a modified Migdal-Kadanoff method, called the cluster-decimation approximation. The free energy for a small cluster of spins with an appropriate boundary condition is assumed to be preserved in the bond-moving step and the approximate decimation of Suzuki and Takano is adopted in the site-decimation step. Critical temperatures obtained by the present method are in general much better than those determined by preserving the high-temperature series expansion of the free energy. In particular the XY fixed point and the isotropic Heisenberg fixed point for the square lattice are not found in the present calculation.

I. INTRODUCTION

The determination of critical temperatures and critical properties has been one of the central problems in statistical mechanics. In recent years the renormalization-group approach has been extensively applied to study critical behaviors of spin systems. Among the renormalization-group schemes,[1,2] the Migdal-Kadanoff[3] (MK) approximation is most widely used because of its simplicity. The MK method contains two operations: bond moving and site decimation. The bond-moving operation is no more than an *ad hoc* approximation. Many improvements have been made to obtain more accurate results.[2,4–6] The site-decimation step is exact for Ising-like systems. The decimation transformation, however, cannot be performed exactly for quantum spin systems due to the noncommutativity of spin operators. An approximate decimation has been proposed by Suzuki and Takano[7] to circumvent the difficulty of the noncommutativity.

In previous papers, we have studied the exchange-interaction model[8] and the anisotropic Heisenberg model[9] by using Suzuki's approximate decimation[7] in conjunction with Walker's idea[4] of matching high-temperature series expansions of the free energy. Critical temperatures determined are significantly improved over the standard MK approximation. However, results of this modification are sensitive to the length of the series expansion used. An alternative modification of the MK method called the cluster-decimation (CD) approximation was proposed by Goldstein and Walker,[5] and further extended by the present authors.[10] In the CD approximation, the free energy for a small cluster of spins is preserved exactly instead of matching series expansions of the free energy for an infinite lattice. Even by using the smallest cluster, the CD approximation with an appropriate boundary condition can locate critical temperatures accurately.

For this motivation, this paper is intended to apply the CD approximation to the spin-$\frac{1}{2}$ anisotropic Heisenberg model. A brief description of this method is found in Sec. II. Fixed points and critical lines are presented in Sec. III. Discussions of our results are also given in Sec. III.

II. CLUSTER-DECIMATION APPROXIMATION

The reduced Hamiltonian of the spin-$\frac{1}{2}$ anisotropic Heisenberg model is given by

$$-\beta H=\sum_{\langle ij\rangle} H_{ij}(K_z,K_{xy}) , \tag{1}$$

with

$$H_{ij}(K_z,K_{xy})=K_z\sigma_i^z\sigma_j^z+K_{xy}(\sigma_i^x\sigma_j^x+\sigma_i^y\sigma_j^y) . \tag{2}$$

Here $\boldsymbol{\sigma}_i=(\sigma_i^x,\sigma_i^y,\sigma_i^z)$ is the Pauli spin located at the lattice site i, K_z and K_{xy} are coupling constants, and the summation is over all nearest-neighbor pairs of sites. In the MK approximation, $\mathbf{K}=(K_z,K_{xy})$ is first transformed into $\tilde{\mathbf{K}}=(\tilde{K}_z,\tilde{K}_{xy})$ for the restructured lattice, and then into $\mathbf{K}'=(K_z',K_{xy}')$ for the rescaled lattice. In the bond-moving step of the standard MK method, the bond strength (or the ground-state energy) is preserved. That is

$$\tilde{K}_z=b^{d-1}K_z \tag{3a}$$

and

$$\tilde{K}_{xy}=b^{d-1}K_{xy} , \tag{3b}$$

for a d-dimensional lattice with the rescaling length b. Suzuki's approximate decimation for $b=2$ gives

$$K_{xy}'=\tfrac{1}{4}\ln e^{-\tilde{K}_z}C_+(\tilde{K}_z,\tilde{K}_{xy}) , \tag{4a}$$

$$K_z'=\tfrac{1}{2}\ln\tfrac{1}{2}[e^{2\tilde{K}_z}+e^{-\tilde{K}_z}C_-(\tilde{K}_z,\tilde{K}_{xy})]-K_{xy}' , \tag{4b}$$

with

$$C_\pm(\tilde{K}_z,\tilde{K}_{xy})=\cosh\tilde{L}\pm(\tilde{K}_z/\tilde{L})\sinh\tilde{L} \tag{5a}$$

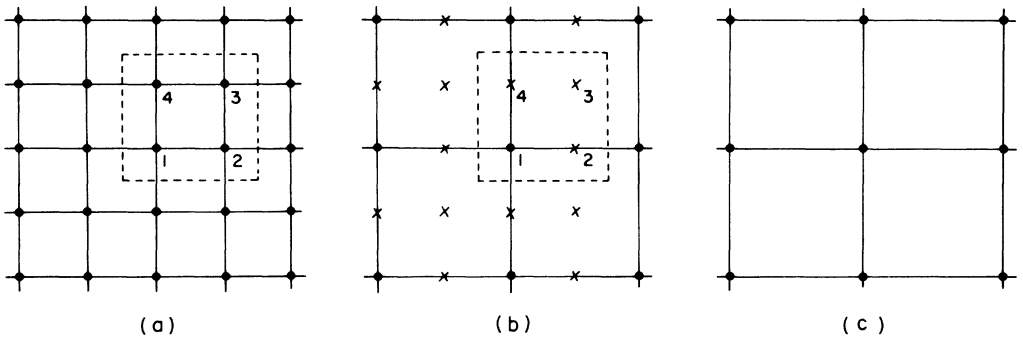

FIG. 1. Bond moving and site decimation of the MK method with $b=2$ for the square lattice. The original lattice (a) has coupling $\mathbf{K}$, the restructured lattice (b) has coupling $\tilde{\mathbf{K}}$, and the rescaled lattice (c) has coupling $\mathbf{K}'$. Free energies of the clusters of four spins enclosed by the dashed lines (with a boundary condition) in (a) and in (b) are assumed to be equal.

and

$$\tilde{L}=(\tilde{K}_z^2+8\tilde{K}_{xy}^2)^{1/2} . \tag{5b}$$

As mentioned in the Introduction, Eqs. (3) are approximate. Various improvements can be made. We consider the CD approximation for the square and the simple cubic (sc) lattices. We use 2×2 and $2\times2\times2$ clusters to match Suzuki's approximation for $b=2$. For the square lattice, consider a cluster of four ($=b^d$) spins enclosed by dashed lines as shown in Fig. 1(a). The partition function for this cluster (with a boundary condition) is

$$Z=\operatorname*{Tr}_{\sigma_1,\sigma_2,\sigma_3,\sigma_4}\exp\{x[H_{12}(K_z,K_{xy})+H_{23}(K_z,K_{xy})+H_{34}(K_z,K_{xy})+H_{41}(K_z,K_{xy})]\} , \tag{6}$$

where $H_{ij}(K_z,K_{xy})$ are defined by Eq. (2). The parameter x depends on the boundary condition used. For the free boundary condition, $x=1$, and for the periodic boundary condition, $x=2$. In general, one can treat x as an adjustable parameter. It is suggested[10] that for general models, the best value of x to be used is $x=2$ for $d=3$, and $x=3$ for $d=2$.

The partition function for the cluster of four spins in the restructured lattice [shown in Fig. 1(b)] is

$$\tilde{Z}=\operatorname*{Tr}_{\sigma_1,\sigma_2,\sigma_3,\sigma_4}\exp\{x[H_{12}(\tilde{K}_z,\tilde{K}_{xy})+H_{14}(\tilde{K}_z,\tilde{K}_{xy})]\} . \tag{7}$$

The equality of the free energies, $\ln Z=\ln\tilde{Z}$, gives the CD transformation for $\tilde{\mathbf{K}}$, i.e.,

$$2e^{4xK_z}+4\cosh(4xK_{xy})+2e^{-2xK_z}\cosh(2xL)+e^{-4xK_z}+7=4e^{2x\tilde{K}_z}+8e^{-x\tilde{K}_z}\cosh(x\tilde{L})+4 , \tag{8}$$

with

$$\tilde{L}=(\tilde{K}_z^2+8\tilde{K}_{xy}^2)^{1/2} . \tag{9}$$

Equation (8) is by no means complete. It cannot determine $\tilde{\mathbf{K}}=(\tilde{K}_z,\tilde{K}_{xy})$ uniquely. We then make a simple assumption[9] which is consistent with Eq. (3),

$$\tilde{K}_{xy}/\tilde{K}_z=K_{xy}/K_z . \tag{10}$$

Equations (8) and (10) reduce to the correct one-parameter cluster-decimation formulas for the Ising and the isotropic Heisenberg models, respectively, in appropriate limits. Equations (4), (8), and (10) constitute the modified MK renormalization transformation for the anisotropic Heisenberg model on the square lattice.

The preceding process can be extended straightforwardly to the sc lattice. Now there are eight spins ($b=2$, $d=3$) in a chosen cluster. The dimension of the matrix H is 256×256. In the $\{\sigma_i^z\}$ representation (the basis states are simultaneous eigenfunctions of the operators σ_i^z) the Hamiltonian of the cluster does not have matrix elements between states having different values of $S_z=\sum_i\sigma_i^z$. Thus, the Hamiltonian is reduced into a direct sum of nine submatrices associated with different values of S_z. For $S_z=\pm8$, ±6, ±4, ±2, and 0, the orders of the submatrices are 1, 8, 28, 56, and 70, respectively. After diagonalization of the submatrices, the partition function Z can be evaluated numerically by computer. For the restructured lattice, the corresponding partition function is easy to show as

$$\tilde{Z}=32e^{3x\tilde{K}_z}+64e^{x\tilde{K}_z}+32e^{-x\tilde{K}_z}\{\cosh(4x\tilde{K}_{xy})+2\cosh(2x\tilde{K}_{xy})+2\cosh[2x(\tilde{K}_z^2+3\tilde{K}_{xy}^2)^{1/2}]\} . \tag{11}$$

III. RESULTS AND DISCUSSIONS

The CD approximation described earlier is used to determine fixed points and critical lines for the anisotrop-

TABLE I. Ising fixed points K_z^*, isotropic Heisenberg fixed points K^*, and XY fixed points (K_z^*, K_{xy}^*) obtained by the CD method with $x=1$, 2, and 3. Fixed points obtained by preserving the free energy to orders $n=6$ and 7 in the high-temperature series expansion are from Ref. 9. Exact (or best known) values are from Refs. 12 and 13. $\times$ indicates that the fixed point is not found.

	Square lattice			Simple cubic lattice		
	K_z^*	K^*	(K_z^*, K_{xy}^*)	K_z^*	K^*	(K_z^*, K_{xy}^*)
$x=1$	0.609	$\times$	$\times$	0.266	0.361	(0.080,0.316)
$x=2$	0.492	$\times$	$\times$	0.215	0.252	(0.046,0.236)
$x=3$	0.437	$\times$	$\times$	0.181	0.207	(0.032,0.196)
MK	0.305	$\times$	(0.289,0.653)	0.065	0.086	(0.004,0.069)
$n=6$	0.521	0.605	(0.332,0.710)	0.247	0.320	(0.076,0.307)
$n=7$	0.516	$\times$	$\times$	0.245	$\times$	(0.079,0.313)
Exact	0.441	$\times$	$\times$	0.221	0.298	(not available)

ic Heisenberg model on the square and the sc lattices. In Table I we show fixed points obtained by different modifications of the MK method. Exact values (or best estimates) are also given for comparison. In the Ising limit, the present calculations reduce to results of Refs. 5 and 10. The XY fixed point and the isotropic Heisenberg fixed point for the square lattice are not found for any finite value of x. This is consistent with the fact that the two-dimensional Heisenberg model and the two-dimensional XY model cannot have a spontaneous magnetization at finite temperatures.[11] The standard MK method predicts an XY fixed point for the square lattice. In Walker's method of preserving the free energy to K^n, XY fixed points are found for $n=5$ and 6, but are not found for $n=4$ and 7. From this point of view, the CD method is superior to the standard MK method and Walker's series-expansion method.

Critical lines for the anisotropic Heisenberg model are shown in Fig. 2 for the square lattice, and in Fig. 3 for the sc lattice. From Fig. 2 we see that the present results using $x=3$ are in extremely good agreement with the best known critical temperatures[12] for the square lattice. For the sc lattice, critical temperatures obtained by the CD method with $x=2$ are, in general, superior to those obtained by preserving the free energy to K^6, and much better than results of preserving the free energy to K^7. Near the isotropic region, critical temperatures obtained by the present method ($x=2$) for the sc lattice are still less accurate (although they are much better than the standard MK results). This is probably due to the approximation introduced in the decimation scheme of Suzuki and Takano.

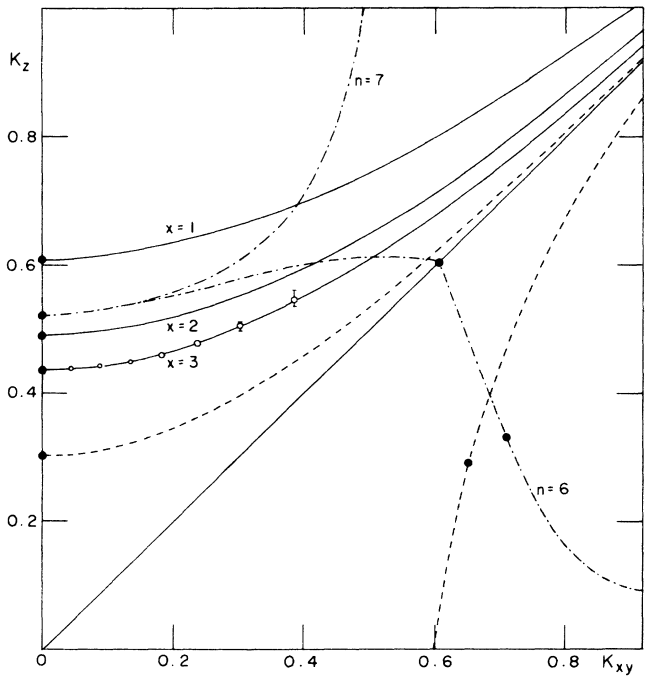

FIG. 2. Fixed points (denoted ●) and critical lines of the anisotropic Heisenberg model on the square lattice. Dashed lines are obtained by the pure MK method. Solid lines are determined by the CD approximation with $x=1$, 2, and 3. Dashed-dotted lines are results of preserving series expansions of the free energies to K^n for $n=6$ and 7. The best known values are shown by open circles with error bars. The XY fixed point and its critical line do not exist for all positive values of x and for $n=7$.

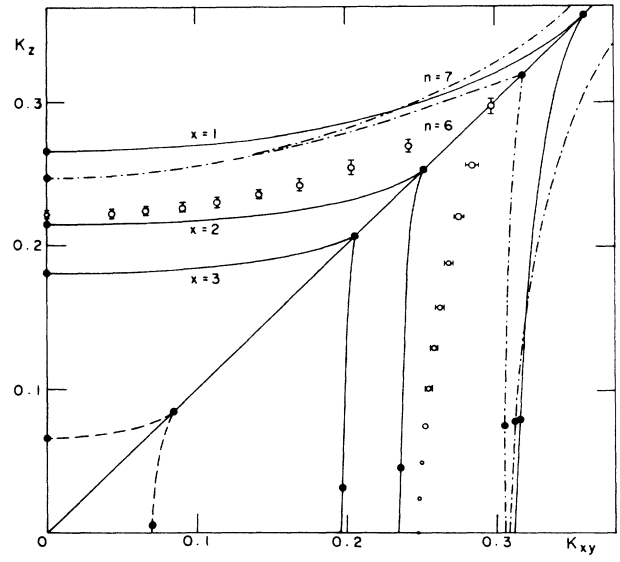

FIG. 3. Fixed points and critical lines of the anisotropic Heisenberg model on the simple cubic lattice. Notations are the same as used in Fig. 2.

In conclusion, the CD approximation with an appropriate boundary condition is superior to the method of preserving the high-temperature series expansion of the free energy, especially for quantum systems of which the series expansions are irregular.

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