Preservation of the free energy in a Migdal-Kadanoff approximation for the spin-1/2 anisotropic Heisenberg model

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A modification of the Migdal-Kadanoff approximation is applied to study the spin-$\frac{1}{2}$ anisotropic Heisenberg model. The approximate decimation introduced by Suzuki and Takano, and the method of preserving the free energy developed by Walker are adopted. Fixed points and critical lines are determined for cubic lattices. The dependence of fixed points on the number of terms used in the series expansion of the free energy is analyzed and discussed.

I. INTRODUCTION

The field of phase transitions and critical phenomena has been an area of great interest and has been extensively studied for a long time. Fluctuation and nonlinearity play essential roles in cooperative phenomena near phase transitions. Various powerful methods have been developed to study critical behavior microscopically. Although the existence of fixed points is still questioned,[1] the real-space renormalization-group technique[2] is widely used to investigate critical properties of spin systems. In particular the Migdal-Kadanoff[3] (MK) approximation is easy to implement, and is usually applied as a preliminary study.

Basically the MK method composes of two steps: bond moving and site decimation. The first step is an *ad hoc* approximation. Several improvements of this approximation have been investigated. The decimation step is exact for Ising-like systems. The exact decimation, however, is formidably difficult for quantum systems because of the noncommutativity of spin operators.

In a recent study,[4] critical temperatures of a quantum exchange interaction model for general spin have been analyzed by using a modified MK method. Walker's idea[5] of preserving the free energy in the renormalization transformation is used to define the bond-moving operation, and Suzuki's approximation[6] to circumvent the difficulty of noncommutativity of spins is adopted in the site-decimation step. Results obtained by the modified MK method are much better than those determined by the simple MK approximation.

In this paper we extend this scheme and apply it to the spin-$\frac{1}{2}$ anisotropic Heisenberg model. Since there are two coupling constants K_z and K_{xy} in this model, an additional assumption is needed in the bond-moving step when Walker's method of preserving the free energy is used. A brief description of the modified MK method is given in Sec. II. Fixed points and critical lines obtained by preserving the free energy to the sixth order in the high-temperature series expansions are presented in Sec. III for cubic lattices. Dependence of fixed points on the number of terms used in the series expansions of the free energy is studied. Discussion of the results is also given in this section.

II. PRESERVING FREE ENERGY IN THE MIGDAL-KADANOFF APPROXIMATION

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

$$-\beta H=\sum_{\langle i,j\rangle}[K_z\sigma_i^z\sigma_j^z+K_{xy}(\sigma_i^x\sigma_j^x+\sigma_i^y\sigma_j^y)]\ , \tag{1}$$

where σ_i^x, σ_i^y, and σ_i^z are components of the Pauli spin σ_i located at the lattice site i. K_z and K_{xy} are coupling con-

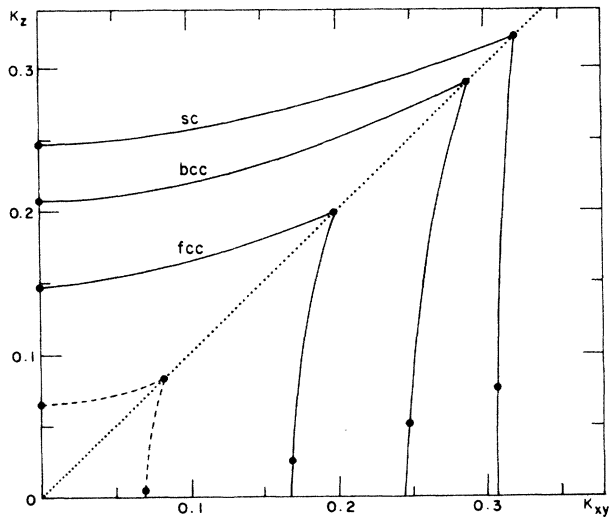

FIG. 1. Fixed points (denoted ●) and critical lines of the anisotropic Heisenberg model on cubic lattices. Dashed lines are obtained by the simple MK method. Solid lines are determined by preserving the free energy in the modified MK method to the 6th order term in the high-temperature series expansion. The dotted line is $K_z=K_{xy}$.

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TABLE I. Ising fixed points K_z^* determined by preserving the free energy to various orders n in the high-temperature series expansions. Exact values (or best estimates) are from Refs. 11 and 12.

Lattice	Modified MK $n=6$	8	10	12	14	16	18	20	40	Simple MK	Best values
Square	0.521	0.513	0.508	0.506	0.504	0.502	0.500	0.499	0.499	0.305	0.441
Triangular	0.353	0.344	0.339	0.335	0.333	0.330	0.329	0.327		0.305	0.275
sc	0.247	0.244	0.242	0.241	0.240	0.240	0.239			0.065	0.221
bcc	0.208	0.201	0.198	0.195	0.193	0.191				0.065	0.157
fcc	0.147	0.140	0.136	0.134	0.131					0.065	0.102

stants, and the summation is over all nearest-neighbor pairs of sites. In the simple MK method the coupling constants K_z and K_{xy} are first transformed into $\tilde{K}_z$ and $\tilde{K}_{xy}$ for the restructured lattice, and then into K_z' and K_{xy}' for the rescaled lattice. A constant K_0 is also created in the site-decimation step.

With the rescaling length $b=2$, the approximation decimation of Suzuki and Takano[6] is given by

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

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

$$K_0=2K_{xy}'+K_z'+\ln 2 , \tag{2c}$$

with

$$C_\pm(\tilde{K}_z,\tilde{K}_{xy})=\cosh\tilde{L}\pm(\tilde{K}_z/\tilde{L})\sinh\tilde{L} , \tag{3}$$

and

$$\tilde{L}=(\tilde{K}_z^{\,2}+8\tilde{K}_{xy}^{\,2})^{1/2} . \tag{4}$$

For a d-dimensional lattice, Eqs. (2) together with

$$\tilde{K}_z=b^{d-1}K_z \tag{5a}$$

and

$$\tilde{K}_{xy}=b^{d-1}K_{xy} \tag{5b}$$

define the simple MK renormalization transformation for the anisotropic Heisenberg model.

As mentioned in Sec. I, Eqs. (5) are approximate. They only ensure that the ground-state energy of the restructured lattice is preserved. The simple MK method predicts critical temperatures much higher than exact (or best) values. An improvement of the MK method considered by Takano and Suzuki[7] is to introduce a lattice anisotropy, such that the coupling constants are different in different lattice dimensions. They assumed that coupling constant along the ith direction of the hypercubic lattice is $K_i=b^{i-1}K_1$. They also assumed that $\sum_i K_i=dK$, $[\mathbf{K}=(K_z,K_{xy})]$. With these assumptions, and using an anisotropic bond moving, better estimates of the critical temperatures are obtained as compared to the simple MK results.

In this paper we follow Walker's method of preserving the free energy in the renormalization transformation. For a system of N sites, the free energy per site is given by

$$f(K_z,K_{xy})=N^{-1}\mathrm{Tr}\exp(-\beta H) . \tag{6}$$

The preservation of the free energy requires that

$$f(K_z,K_{xy})=a\ln 2+qb^{-d}K_0(\tilde{K}_z,\tilde{K}_{xy})/2 + b^{-d}f(K_x',K_{xy}') , \tag{7}$$

where q is the coordination number, and a is the fraction of disconnected sites in the restructured lattice. For a d-dimensional lattice a is given by

$$a=1-b^{-d}[1+q(b-1)/2] . \tag{8}$$

We set $b=2$ in calculations because Eqs. (2) are derived for $b=2$.

The free energy of the system will be preserved exactly in the renormalization transformation if exact functions of $f(K_z,K_{xy})$ and $K_0(K_z,K_{xy})$ are used in Eq. (7). These functions, however, are not known exactly. The free energy $f(K_z,K_{xy})$ will be given approximately by the corresponding high-temperature series expansions derived by Wood and Dalton,[8] and Eq. (2c) will be used for K_0. Equation (7) alone cannot define the bond-moving operation (i.e., define the coupling constants $\tilde{K}_z$ and $\tilde{K}_{xy}$) uniquely. An additional assumption should be made. We make the simplest assumption that

TABLE II. Isotropic Heisenberg fixed points K^* obtained by the modified MK method in which the free energy is preserved to the nth order in K. A cross ($\times$) indicates that the fixed point does not exist.

Lattice	Modified MK $n=4$	5	6	7	8	9	10	Simple MK	Best values
Square	$\times$	0.660	0.605	$\times$	$\times$	0.503	$\times$	$\times$	
Triangular	$\times$	$\times$	0.610	0.415	0.463	$\times$	$\times$	$\times$	
sc	$\times$	0.345	0.320	$\times$	$\times$	0.331	0.326	0.086	0.298
bcc	0.315	0.298	0.288	0.293	0.280	0.287	0.274	0.086	0.199
fcc	0.199	0.204	0.199	0.191	0.186	0.183	0.182	0.086	0.125

TABLE III. XY fixed points (K_z^*, K_{xy}^*) determined by the modified MK method in which n terms are used in the high-temperature series expansions. A cross ($\times$) indicates that the fixed point is not found.

Lattice	$n=4$	5	6	7	Simple MK
Square	$\times$	(0.346,0.729)	(0.332,0.710)	$\times$	(0.289,0.653)
Triangular	$\times$	$\times$	(0.404,0.803)	(0.182,0.497)	(0.289,0.653)
sc	(0.096,0.349)	(0.086,0.327)	(0.076,0.307)	(0.079,0.313)	(0.004,0.069)
bcc	(0.057,0.265)	(0.057,0.263)	(0.051,0.248)	(0.051,0.249)	(0.004,0.069)
fcc	(0.028,0.183)	(0.026,0.173)	(0.024,0.168)	(0.023,0.164)	(0.004,0.069)

$$\tilde{K}_{xy}/\tilde{K}_z = K_{xy}/K_z \ . \tag{9}$$

Equation (9) is consistent with Eq. (5). Therefore, when $K_{xy}=0$ and $K_{xy}=K_z$, the present formulism reduces to those for the Ising and the isotropic Heisenberg models, respectively. Equations (2), (7), and (9) describe the modified MK renormalization transformation for the anisotropic Heisenberg model.

III. RESULTS AND DISCUSSION

The modified MK method described above is used to determine fixed points and critical lines of the anisotropic Heisenberg model for several lattices. Figure 1 shows results for the cubic lattices obtained by using six terms ($n=6$) in the high-temperature series expansions for the free energy. Results obtained by using the simple MK method for three-dimensional lattices are also shown in the figure. We find that: (i) The simple MK method predicts T_c higher than the best known values, while the modified MK method (using $n=6$) gives T_c lower than the best known values.[9,10] (ii) It is well known that T_c determined by the simple MK method depends only on the lattice dimensionality d. The modified MK method also clearly shows the correct dependence of T_c on the coordination number q. (iii) The simple MK method gives poor results for the cubic lattices, especially for the simple cubic (sc) lattice. Results obtained by the modified MK method ($n=6$) are better than those determined by the simple MK method. In particular the modified MK method gives a significant improvement for the sc lattice. But we point out that for the face-centered cubic (fcc) lattice, the modified MK method (using $n=6$) is nearly as poor as the simple MK method.

It is worth noting that the simple MK method and the modified MK method can be applied to all Bravais lattices (lattices having one lattice site in each primitive cell), but they cannot be applied to the diamond and the honeycomb lattices because the restructured lattices cannot be defined for these lattices.

It is interesting to see how the fixed points change when different numbers of terms are included in the series expansions of the free energy. For the Ising case very long series are available from Domb.[11] Table I shows Ising fixed points K_z^* of several lattices obtained by preserving the free energy to various orders n of the inverse temperature K. It is clear that the Ising fixed points converge rapidly for all lattices considered, and better values are obtained when longer series are used.

The isotropic Heisenberg fixed points K^* ($K_z=K_{xy}=K$) for various lattices obtained by using various n are given in Table II. It is surprising that the fixed point disappears for the sc lattice when $n=7$ and 8. This result disagrees with our belief that the Heisenberg model on the sc lattice has a phase transition. We also note that nontrivial fixed points appear for the two-dimensional lattices for some values of n. This is also inconsistent with the fact that two-dimensional Heisenberg model cannot have a spontaneous magnetization at finite temperatures. We believe that these erroneous results arise from the fact that high-temperature series coefficients for the spin-$\frac{1}{2}$ Heisenberg model are irregular for these lattices. We have applied the Pade analyses to determine the isotropic Heisenberg fixed points, but the improvement is not significant. Therefore, the modified MK results must be taken with caution when the series expansions are irregular. We expect that when long enough series are used, the modified MK method should predict rather good results, and we see from Table II that results for $n=10$ are qualitatively correct and quantitatively much better than the simple MK results.

The XY fixed points (K_z^*, K_{xy}^*) for various lattices are shown in Table III. High-temperature series expansions for the anisotropic Heisenberg model are available only to the 7th order. In the XY region ($K_z < K_{xy}$) these series are more regular than the corresponding series for the isotropic case, but are less smooth than those for the Ising model. We find that fixed points for the cubic lattices are moving toward correct values when n increases. From Table III we are not sure whether XY fixed points exist or not for two-dimensional lattices when longer series are used.

Similar to the Potts model, the limiting fixed points of the anisotropic Heisenberg model do not converge to exact values even if the free energy is preserved exactly ($n \to \infty$). This is a general drawback of the renormalization-group scheme when the system is restricted to a small number of interaction parameters. We have also calculated thermal exponents of the model by the modified MK method ($n=6$), but results for cubic lattices are as poor as the simple MK method.

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