Real-space renormalization-group study of the exchange-interaction model

H. H. Chen and Felix Lee

Department of Physics, National Tsing Hua University, Hsinchu, Taiwan 30043, Republic of China

(Received 30 January 1990)

Through use of an approximation introduced by Suzuki and Takano, the Migdal-Kadanoff (MK) renormalization-group transformation with the rescaling length $b=2$ is derived for the exchange-interaction (EI) model. Both the standard MK method and its modification, which preserves the free energy in the renormalization transformation, are used to determine critical temperatures and thermal exponents of the EI model on cubic lattices for various spins.

I. INTRODUCTION

The exchange-interaction (EI) model[1] is a quantum spin model in which the interaction between a nearest-neighbor pair of spins $\mathbf{S}_i$ and $\mathbf{S}_j$ has the form $-JP_{ij}$, where J is the interaction constant and P_{ij} is the exchange operator. The operator P_{ij} has the property that it permutes the spin coordinates of $\mathbf{S}_i$ and $\mathbf{S}_j$. That is,

$$P_{ij}Q(\mathbf{S}_i,\mathbf{S}_j)=Q(\mathbf{S}_j,\mathbf{S}_i)P_{ij} \ , \tag{1}$$

where $Q(\mathbf{S}_i,\mathbf{S}_j)$ is any function of two spins $\mathbf{S}_i$ and $\mathbf{S}_j$, which have the same spin multiplicity.

For $S=\frac{1}{2}$ the EI model is identical to the spin-$\frac{1}{2}$ Heisenberg model. When $S\geq 1$, the exchange operator P_{ij} is a polynomial of degree $2S$ in $\mathbf{S}_i\cdot\mathbf{S}_j$. The expression of P_{ij} in terms of $\mathbf{S}_i\cdot\mathbf{S}_j$ was derived by Schrödinger in 1941.[2] The thermodynamic properties of the EI model were first investigated two decades ago.[3,4] As the calculation of nonlinear terms is very difficult, previous work on the EI model is sparse. Even the mean-field approximation is not yet available. Our understanding of the thermodynamic properties of the EI model is mainly from the study of high-temperature series expansions.[1,5]

In this article we study the critical properties of the EI model by the real-space renormalization-group method. The Migdal-Kadanoff (MK) renormalization[6] for quantum spin models proposed by Suzuki and Takano[7] is described in Sec. II. The decimation transformation of the coupling constant with the rescaling length $b=2$ is derived in Sec. III. In Sec. IV the standard MK scheme and its modification,[8] which preserves the free energy in the renormalization transformation, are used to determine ferromagnetic fixed points and thermal exponents of the EI model on cubic lattices for various spin values. Summary and discussion on the antiferromagnetic fixed points and on the renormalization transformation of the magnetic field are given in Sec. V.

II. MIDGAL-KADANOFF APPROXIMATION FOR QUANTUM SPIN MODELS

The Midgal-Kadanoff renormalization[6] contains two main steps: a bond-moving operation and a site-decimation transformation. In the first step the original lattice is divided into blocks of length b in each direction. All interactions [represented by bonds graphically in Fig. 1(a)] inside a block and those on the surface of a block are moved to the edges of the block to form a decorated lattice [also called restructured lattice; see Fig. 1(b)]. In the decorated lattice, spins connected by two bonds are called decorated spins, those not connected by any bond are called isolated spins, and the others are called block spins.

The interaction between a connected pair of spins $\mathbf{S}_i$ and $\mathbf{S}_j$ in the decorated lattice, denoted $\tilde{H}_{ij}$, is assumed to be proportional to that of the original lattice [Fig. 1(a)]. In the standard MK method,

$$\tilde{H}_{ij}=b^{d-1}H_{ij} \ , \tag{2}$$

for d-dimensional lattices, while in the modified MK methods[8,9] the proportional constant b^{d-1} is replaced by some temperature-dependent functions. This step is an *ad hoc* approximation. It applies to quantum spin models as well as to classical spin systems.

In the second step all decorated spins are then decimated to obtain a rescaled lattice [Fig. 1(c)]. Consider a linear chain of length b, having $b+1$ spins $\mathbf{S}_\alpha,\mathbf{S}_1,\mathbf{S}_2,\ldots,\mathbf{S}_{b-1}$ and $\mathbf{S}_\beta$, where $\mathbf{S}_\alpha$ and $\mathbf{S}_\beta$ are block spins and the others are decorated spins. Let

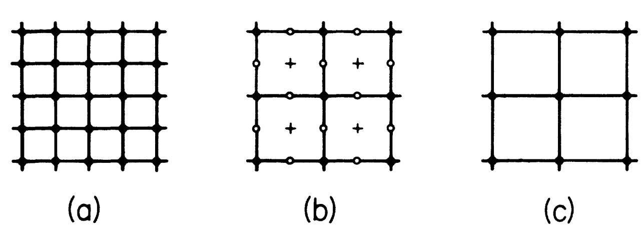

FIG. 1. Bond moving and site decimation of the MK method with $b=2$ and $d=2$. Bonds (interactions) inside blocks of length b in (a) the original lattice are moved to the edges of the blocks to form (b) a decorated lattice. The decorated spins ○ and the isolated spins + are then decimated to obtain (c) the rescaled lattice. The interaction between a connected pair of spins $\mathbf{S}_i$ and $\mathbf{S}_j$ is H_{ij} in the original lattice, is $\tilde{H}_{ij}$ in the decorated lattice, and H'_{ij} in the rescaled lattice.

$$\tilde{H}_{\alpha\cdots\beta}=\tilde{H}_{\alpha 1}+\tilde{H}_{12}+\cdots+\tilde{H}_{b-1,\beta}\,. \quad (3)$$

When the decorated spins in Fig. 1(b) are decimated, we have

$$\operatorname*{Tr}_{\substack{\text{decorated}\\ \text{spins}}}\exp\left[-\sum_{\langle\alpha\beta\rangle}\frac{\tilde{H}_{\alpha\ldots\beta}}{kT}\right]=\exp\left[-\sum_{\langle\alpha\beta\rangle}\frac{H'_{\alpha\beta}}{kT}\right]. \quad (4)$$

Here $H'_{\alpha\beta}$ is the interaction between a pair of block spins $\mathbf{S}_\alpha$ and $\mathbf{S}_\beta$ in the rescaled lattice [Fig. 1(c)].

For classical spin systems, all spins commute, and Eq. (4) is identical to

$$\prod_{\langle\alpha\beta\rangle}\left[\operatorname*{Tr}_{\substack{\text{decorated}\\ \text{spins}}}\exp\left[\frac{-\tilde{H}_{\alpha\ldots\beta}}{kT}\right]\right]=\prod_{\langle\alpha\beta\rangle}\exp\left[\frac{-H'_{\alpha\beta}}{kT}\right]. \quad (5)$$

The determination of $H'_{\alpha\beta}$ in Eq. (4) is reduced to the one-dimensional decimation

$$\exp(-H'_{\alpha\beta}/kT)=\operatorname*{Tr}_{S_1,S_2,\ldots,S_{b-1}}\exp(-\tilde{H}_{\alpha\cdots\beta}/kT)\,. \quad (6)$$

For quantum spin models, Eq. (5) is not valid because the spins do not commute. In the approximate scheme proposed by Suzuki and Takano,[7] Eq. (5) is accepted as an approximation. Then $H'_{\alpha\beta}$ is determined approximately by a one-dimensional decimation transformation [Eq. (6)].

III. ONE-DIMENSIONAL DECIMATION WITH $b=2$ FOR THE EI MODEL

Consider a system of three spins $\mathbf{S}_1$, $\mathbf{S}_2$, and $\mathbf{S}_3$. The reduced Hamiltonian of the EI model is given by

$$-\tilde{H}(\mathbf{S}_1,\mathbf{S}_2,\mathbf{S}_3)/kT=\tilde{K}(P_{12}+P_{23})\,, \quad (7)$$

where P_{ij} are exchange operators and $\tilde{K}=\tilde{J}/kT$ is the reduced coupling constant. For this Hamiltonian, Eq. (6) becomes

$$\operatorname*{Tr}_{S_2}\exp[\tilde{K}(P_{12}+P_{23})]=\exp(K'P_{13}+G)\,, \quad (8)$$

where K' and G are functions of $\tilde{K}$ and S.

To determine K' and G, expand $\exp[\tilde{K}(P_{12}+P_{23})]$ in power series in $\tilde{K}$:

$$\exp[\tilde{K}(P_{12}+P_{23})]=\mathbb{1}+\sum_n\frac{\tilde{K}^n}{n!}(P_{12}+P_{23})^n\,, \quad (9)$$

where $\mathbb{1}$ is the unit matrix. For a system of three spins the operators P_{ij} and their products form elements of the symmetric group of degree 3. There are six different permutations. It can be shown that

$$(P_{12}+P_{23})^{2n-1}=\tfrac{2}{3}(\tfrac{1}{2}+4^{n-1})(P_{12}+P_{23})+\tfrac{2}{3}(-1+4^{n-1})P_{13}\,, \quad (10a)$$

$$(P_{12}+P_{23})^{2n}=\tfrac{4}{3}(\tfrac{1}{2}+4^{n-1})+\tfrac{4}{3}(-\tfrac{1}{4}+4^{n-1})\times(P_{12}P_{23}+P_{23}P_{12})\,. \quad (10b)$$

Summing over the even- and odd-power terms, respectively, Eq. (9) reduces to

$$\exp[\tilde{K}(P_{12}+P_{23})]=f_0(\tilde{K})+f_1(\tilde{K})(P_{12}+P_{23})+f_2(\tilde{K})P_{13}+f_3(\tilde{K})\times(P_{12}P_{23}+P_{23}P_{12})\,, \quad (11)$$

where

$$\begin{aligned}f_0(\tilde{K})&=(\cosh 2\tilde{K}+2\cosh\tilde{K})/3\,,\\ f_1(\tilde{K})&=(\sinh 2\tilde{K}+\sinh\tilde{K})/3\,,\\ f_2(\tilde{K})&=(\sinh 2\tilde{K}-2\sinh\tilde{K})/3\,,\\ f_3(\tilde{K})&=(\cosh 2\tilde{K}-\cosh\tilde{K})/3\,.\end{aligned} \quad (12)$$

Taking trace of S_2, we obtain

$$\operatorname*{Tr}_{S_2}\exp[\tilde{K}(P_{12}+P_{23})]=(2S+1)f_0(\tilde{K})+2f_1(\tilde{K})+[(2S+1)f_2(\tilde{K})+2f_3(\tilde{K})]P_{13}\,. \quad (13)$$

Similarly, the left-hand side of Eq. (8) is

$$\exp(K'P_{13}+G)=e^G\cosh K'+(e^G\sinh K')P_{13}\,. \quad (14)$$

Comparing Eqs. (13) and (14), we have

$$K'=\tfrac{1}{2}\ln[f_+(\tilde{K})/f_-(\tilde{K})] \quad (15)$$

and

$$G=\tfrac{1}{2}\ln[f_+(\tilde{K})f_-(\tilde{K})]\,, \quad (16)$$

where

$$f_\pm(\tilde{K})=(2S+1)[f_0(\tilde{K})\pm f_2(\tilde{K})]+2[f_1(\tilde{K})\pm f_3(\tilde{K})]\,. \quad (17)$$

Usually, a constant $(2S+1)^{-1}$ is subtracted from P_{ij} to make the Hamiltonian traceless.[1] For the traceless EI model, the decimation transformation is

$$\operatorname*{Tr}_{S_2}\exp\{\tilde{K}[P_{12}+P_{23}-2(2S+1)^{-1}]\}=\exp\{K_0+K'[p_{13}-(2S+1)^{-1}]\}\,, \quad (18)$$

where K' is the same as Eq. (15) and K_0 is given by

$$K_0=G+(K'-2\tilde{K})/(2S+1)\,. \quad (19)$$

When $S=\frac{1}{2}$ Eqs. (15) and (19) reduce to those for the spin-$\frac{1}{2}$ Heisenberg model.[7]

IV. CRITICAL PROPERTIES OF THE EI MODEL ON CUBIC LATTICES

In the standard MK method the renormalization transformation of the coupling constant of the EI model on a d-dimensional lattice is given by Eq. (15), in which $\tilde{K}=2^{d-1}K$. We let $b=2$ in Eq. (2) as Eq. (15) is valid only for $b=2$. By setting $K=K'=K^*$ in Eqs. (2) and (15), the fixed points K^* $(=J/kT_c)$ can be determined. The thermal exponents y_t are then given by

TABLE I. Critical temperatures kT_c/J and thermal exponents y_t of the EI model on three-dimensional lattices obtained by the MK method. kT_c/J determined from the high-temperature susceptibility series (Ref. 1) are shown for comparison.

Spin	MK method three-dimensional lattices		kT_c/J from series analyses		
S	kT_c/J	y_t	sc lattice	bcc lattice	fcc lattice
$\frac{1}{2}$	5.82	0.72	1.68	2.52	4.02
1	4.80	0.76	1.27	1.93	3.10
$\frac{3}{2}$	4.32	0.78	1.07	1.64	2.64
2	4.04	0.80	0.99	1.45	2.35
$\frac{5}{2}$	3.86	0.81	0.91	1.32	2.14
3	3.73	0.82	0.85	1.24	1.97
∞	3.00	0.88	0.51	0.74	1.19

$\ln(dK'/dK)/\ln 2$, evaluated at K^*.

When $d \le 2$, nontrivial fixed points are not found. This is in agreement with the rigorous result that two-dimensional spin systems with any form of isotropic interaction cannot have a phase transition.[10] For $d=3$, ferromagnetic critical temperatures and thermal exponents of the EI model for several values of S are shown in Table I. Critical temperatures of the cubic lattices determined from the high-temperature susceptibility series[1] are included in Table I for comparison. Thermal exponents of the EI model have not been studied before. Similar to other models,[9,11] the T_c of the EI model determined by the standard MK method are too high as compared to those determined from the high-temperature susceptibility series.

To improve the MK scheme, in which one assumed $\tilde{K}/K=b^{d-1}$, two different approaches have been proposed. In Walker's series-expansion method,[8] $\tilde{K}(K)$ is determined by the requirement that in the renormalization transformation the free energy of the whole system is preserved exactly through a given number of terms in the high-temperature series expansions. In the cluster-decimation (CD) method,[9] $\tilde{K}(K)$ is determined by preserving the free energy of a finite cluster of spins (with certain boundary conditions) in the bond-moving step.

For a three-dimensional lattice, the smallest cluster involved in the CD method contains eight spins. It is too difficult to calculate the free energy of the EI model of eight spins, as the dimensionality of matrices involved in the calculation is $(2S+1)^8\times(2S+1)^8$. We therefore use Walker's series-expansion method.

For a system of N sites, the free energy per site of the EI model is given by

$$f(K)=N^{-1}\ln\left[\mathrm{Tr}\exp\left[K\sum_{\langle ij\rangle}P_{ij}\right]\right] . \tag{20}$$

The preservation of the free energy requires that

$$f(K)=a\ln(2S+1)+b^{-d}[(q/2)K_0(\tilde{K})+f(K')] , \tag{21}$$

where q is the coordination number of the lattice, Na is the number of isolated spins in the decorated lattice [Fig. 1(b)]. For a d-dimensional lattice, a is given by[8]

$$a=1-b^{-d}[1+q(b-1)/2] . \tag{22}$$

The right-hand side of Eq. (21) is the free energy of the rescaled lattice. Its first term is contributed by isolated spins, and the second term is contributed from connected sites. There are Nb^{-d} connected sites with $Nb^{-d}q/2$ bonds in the rescaled lattice. Besides the energy $f(K')$, each bond of the rescaled lattice carries a constant energy $K_0(\tilde{K})$ given by Eq. (19).

The exact expression of $f(K)$ is not known for general models. It will be replaced by its high-temperature series expansions to order n. High-temperature series expansions of the free energy for the EI model are known to order $n=7$ for general spin values on cubic lattices.[1] We have determined fixed points K^* and thermal exponents y_t from Eqs. (15), (19), and (21) for cubic lattices by using six terms ($n=6$) and seven terms ($n=7$), respectively, in the free-energy series. Critical temperatures $KT_c/J=(K^*)^{-1}$ obtained are given in Table II. The corresponding thermal exponents are shown in Table III.

TABLE II. Critical temperatures kT_c/J of the EI model on cubic lattices determined by the modified MK method using n terms in the free-energy series.

Spin S	sc lattice $n=6$	bcc lattice $n=6$	fcc lattice $n=6$	fcc lattice $n=7$
$\frac{1}{2}$	1.56	1.74	2.51	2.62
1	1.48	1.59	1.96	2.10
$\frac{3}{2}$	1.45	1.59	1.70	1.85
2	1.43	1.58	1.56	1.70
$\frac{5}{2}$	1.42	1.57	1.47	1.61
3	1.40	1.56	1.41	1.54
∞	1.29	1.43	1.20	1.20

TABLE III. Thermal exponents y_t of the EI model on cubic lattices determined by the modified MK method using n terms in the free-energy series.

Spin s	sc lattice $n=6$	bcc lattice $n=6$	fcc lattice $n=6$	fcc lattice $n=7$
$\frac{1}{2}$	1.04	0.99	1.01	1.11
1	1.22	1.21	1.03	1.19
$\frac{3}{2}$	1.32	1.36	1.07	1.23
2	1.38	1.44	1.10	1.27
$\frac{5}{2}$	1.42	1.48	1.14	1.30
3	1.44	1.51	1.18	1.32
∞	1.58	1.67	1.47	1.47

When $n=7$ fixed points are not found for the EI model on the simple cubic (sc) lattice for $\frac{1}{2} \le S \le \frac{13}{2}$, and on the body-centered-cubic (bcc) lattice for $1 \le S \le 6$. Fixed points are not found in these cases because the seventh term of the free-energy series contributes a large negative amount to $f(K)$. The seventh coefficient of the free-energy series is positive for the face-centered-cubic (fcc) lattice. We expect that if longer series expansions are available, the modified MK method will give more accurate estimates of T_c. When $S \gg 1$, $n=6$ and 7 yield the same result for all lattices since the seventh coefficients (and all odd terms) of the free-energy series vanish in the limit $S \to \infty$.

V. SUMMARY AND DISCUSSION

We have derived the MK renormalization of the EI model with the rescaling length $b=2$. Both the simple MK method and a modified MK method are used to determine ferromagnetic critical temperatures and thermal exponents of the EI model on cubic lattices for several spins. Besides those determined by analyzing high-temperature susceptibility series, the T_c obtained by the present method are the only estimates of critical temperatures of the EI model. The present results are higher than the findings of the series-expansion method for large S and small q (coordination number), and are lower than the series-expansion results for small S and large q.

The thermal exponents y_t or the correlation exponents ν $(=1/y_t)$ of the EI model have not been studied before. From Table III we see that y_t is an increasing function of the spin.

In Sec. III we have derived the MK transformation of the EI model at zero field. When there is a magnetic field h (including the factor $-1/kT$) along the z axis, the one-dimensional decimation [Eq. (6)] becomes

$$\operatorname*{Tr}_{S_2} \exp[\tilde{K}(P_{12}+P_{23})+(\tilde{h}/q)(S_{1z}+yS_{2z}+S_{3z})] = \exp[G+K'p_{13}+(h'/q)(S_{1z}+S_{3z})] , \quad (23)$$

where S_{iz} is the z component of the spin $\mathbf{S}_i$, and y is a parameter used to describe the method which we adopted in handling the magnetic field terms[12] in the bond-moving step. In the standard MK method, if the magnetic field terms $(h/q)(S_{iz}+S_{jz})$ are moved together with the exchange interactions KP_{ij}, we have $\tilde{h}=b^{d-1}h$ and $y=2$; if the field terms are not moved at all, $\tilde{h}=h$ and $y=2d$.

In the small field limit we express Eq. (23) in power series in $\tilde{h}$ and h'. The zeroth-order equation is the same as Eq. (8) or (13). The first-order equation which describes the decimation transformation of the magnetic field has the form

$$\tilde{h}[g_0(\tilde{K})(S_{1z}+S_{3z})+g_1(\tilde{K})(S_{1z}+S_{3z})P_{13}] = h'[(e^{G}\cosh K')(S_{1z}+S_{3z}) + (e^{G}\sinh K')(S_{1z}+S_{3z})P_{13}] , \quad (24)$$

where g_0 and g_1 as functions of $\tilde{K}$ are too lengthy to be presented here.

Equation (24) contains two different sets of spin operators, $(S_{1z}+S_{3z})$ and $(S_{1z}+S_{3z})P_{13}$, but there is only one unknown function h'. When $S=\frac{1}{2}$, $(s_{1z}+S_{3z}) \equiv (S_{1z}+S_{3z})P_{13}$, h' can be determined. That is,

$$h'=\tilde{h}(g_0+g_1)e^{-G}/(\cosh K'+\sinh K') , \quad (25)$$

where K' and G are given by Eqs. (15) and (16) [with $S=\frac{1}{2}$]. For $S \ge 1$, the renormalized magnetic field $h'=h'(\tilde{K},\tilde{h})$, which satisfies Eq. (24), does not exist. To obtain the renormalization transformation, high-order fields (multipolar fields) should be included in the renormalization transformation.

In Sec. IV we have only determined ferromagnetic critical temperatures. We do not expect that $b=2$ will give correct antiferromagnetic critical temperatures T_N because the staggered ordering of spins at low temperatures is not preserved when the lattice is rescaled by a factor of 2. But we point out one interesting result that by using the simple MK method with $b=2$, we obtain $|kT_N/J|=kT_c/J=3.002\,03$ for $S \to \infty$. This is in agreement with the fact that $T_c=T_N$ for classical spin models on open lattices.

ACKNOWLEDGMENTS

This work was supported by the National Science Council of the Republic of China under Contract No. NSC79-0208-007-48.

[1]H. H. Chen and R. I. Joseph, J. Math. Phys. **13**, 725 (1972); Phys. Lett. A **30**, 449 (1969); **31**, 251 (1970).
[2]E. Schrödinger, Proc. R. Irish Adad. A **47**, 39 (1941).
[3]R. I. Joseph, Phys. Rev. **163**, 523 (1967).
[4]G. A. T. Allen and D. D. Bett, Proc. Phys. Soc. **91**, 341 (1967).
[5]H. K. Charles, Jr. and R. I. Joseph, Phys. Rev. B **12**, 3918 (1975).
[6]A. A. Midgal, Zh. Eksp. Theor. Fiz. **69**, 1457 (1975) [Sov. Phys.—JETP **42**, 743 (1976)]; L. P. Kadanoff, Ann. Phys. (N.Y.) **100**, 359 (1976).
[7]M. Suzuki and H. Takano, Phys. lett. A **69**, 426 (1979); H. Takano and M. Suzuki, J. Stat. Phys. **26**, 635 (1981).
[8]J. S. Walker, Phys. Rev. B **26**, 3792 (1982); D. Andelman and J. S. Walker, *ibid.* **27**, 241 (1983).
[9]H. H. Chen, F. Lee, and H. C. Tseng, Phys. Rev. B **34**, 6448 (1986); R. E. Goldstein and J. S. Walker, J. Phys. A **18**, 1275 (1985).
[10]M. F. Thorpe, J. Appl. Phys. **42**, 1410 (1971).
[11]F. Lee, H. H. Chen, and H. C. Tseng, Phys. Rev. B **37**, 5371 (1988).
[12]T. W. Burkhardt, in *Real-Space Renormalization,* edited by T. W. Burkhardt and J. M. J. van Leeuwan (Springer-Verlag, Berlin, 1982), p. 41.