

Exact duality-decimation transformations and real-space renormalization for the Ising model on a square lattice

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Critical properties of the Ising model with nearest-neighbor, next-nearest-neighbor, and four-spin interactions on the square lattice are studied by a real-space renormalization-group method. The recurrence relations of the couplings are obtained by a bond-moving operation followed by an exact duality-decimation transformation. Both the ferromagnetic and the superantiferromagnetic phase transitions are considered.

I. INTRODUCTION

The Migdal-Kadanoff¹ (MK) approximation is the simplest real-space renormalization-group² (RG) method for spin systems. It contains two operations: bond-moving and one-dimensional decimation. This method is applicable to models on lattices with only nearest-neighbor (NN) interactions for which the one-dimensional decimation can be performed. The MK method, however, cannot be applied to lattices which contain next-nearest-neighbor (NNN) interactions or multispin interactions. The Ising model with NN and NNN interactions has been well studied.³ This model has the same critical exponents as the Ising model with only NN interactions. For the Ising model with NNN and four-spin interactions, Baxter⁴ has shown that critical exponents of the square lattice vary continuously with the ratio of the NNN coupling constant and the four-spin interaction constant. The nonuniversal critical behavior^{5,6} of the Baxter model is of great theoretical interest.

When the Hamiltonian contains NN, NNN, and four-spin interactions, critical properties of the Ising model are not well studied. We will investigate this model on the square lattice by a real-space renormalization scheme which utilizes a duality-decimation transformation instead of the one-dimensional decimation transformation. The duality-decimation transformation was derived by Burkhardt⁷ for a large class of spin systems on the square lattice. He also combined this transformation with a bond-moving approximation to obtain a real-space renormalization scheme. The duality-decimation transformation has also been applied by Wu⁸ to solve exactly the two-dimensional Ising model with NN, NNN, and four-spin interactions in a pure imaginary magnetic field.

In this paper Burkhardt's method of renormalization and its modifications will be used to study critical properties of the Ising model on the square lattice with NN, NNN, and four-spin interactions. In Sec. II Burkhardt's method which combines a bond-moving and the duality-decimation transformation is discussed briefly and applied to obtain the critical surface of the model in the ferromagnetic region. In Sec. III the idea of preserving the free energy⁹ in the renormalization transformation is ap-

plied to modify Burkhardt's method. In order to study the superantiferromagnetic^{10,11} (SAF) phase transition, a different way of bond-moving and duality-decimation transformation is presented and discussed in Sec. IV. A summary is made in Sec. V.

II. DUALITY-DECIMATION TRANSFORMATION AND REAL-SPACE RENORMALIZATION

Consider an Ising model of N spins arranged on the square lattice [Fig. 1(a)]. Each square surrounded by four spins, say, σ_1 , σ_2 , σ_3 , and σ_4 has the energies (with the factor $-1/k_B T$)

$$E(\sigma_1, \sigma_2, \sigma_3, \sigma_4) = \frac{K_1}{2}(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_4 + \sigma_4\sigma_1) + K_2(\sigma_1\sigma_3 + \sigma_2\sigma_4) + K_4\sigma_1\sigma_2\sigma_3\sigma_4. \quad (1)$$

The coupling constant between an NN pair of spins is K_1 , that between an NNN pair of spins is K_2 , and the four-spin interaction constant is K_4 . The partition function of the square lattice is

$$Z_N = \sum_{(\sigma_i = \pm 1)} \prod_{\text{all squares}} B(\sigma_1, \sigma_2, \sigma_3, \sigma_4), \quad (2)$$

where $B = \exp(E)$ are the Boltzmann weights of a square.

The bond moving of Burkhardt⁷ is to redistribute the interactions of the system in a checkerboard pattern by shifting the interactions from the white squares to the shaded squares [Fig. 1(b)]. Each shaded square has the Boltzmann weights

$$\tilde{B}(\sigma_1, \sigma_2, \sigma_3, \sigma_4) = \exp[\tilde{K}_1(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_4 + \sigma_4\sigma_1) + \tilde{K}_2(\sigma_1\sigma_3 + \sigma_2\sigma_4) + \tilde{K}_4\sigma_1\sigma_2\sigma_3\sigma_4], \quad (3)$$

and the partition function of the checkerboard lattice is

$$\tilde{Z}_N = \sum_{(\sigma_i = \pm 1)} \prod_{\text{shaded squares}} \tilde{B}(\sigma_1, \sigma_2, \sigma_3, \sigma_4). \quad (4)$$

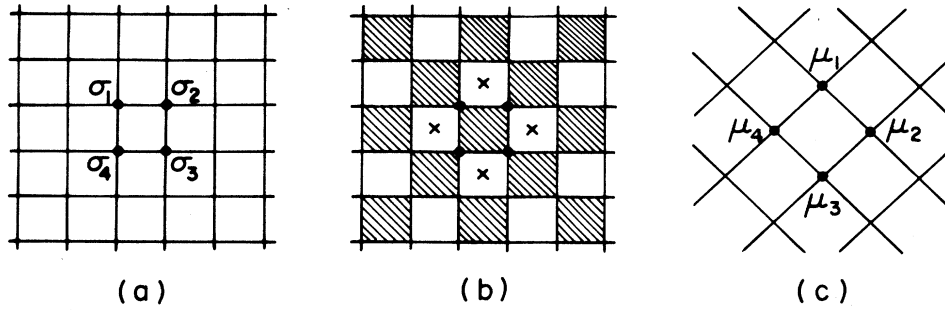


FIG. 1. Real-space renormalization with the rescaling factor $b = \sqrt{2}$. Each square of the original lattice (a) has the interaction $E(\sigma_1, \sigma_2, \sigma_3, \sigma_4)$ given by Eq. (1). The bond-moving operation redistributes the interactions in a checkerboard pattern (b), and a duality-decimation transformation maps the checkerboard lattice onto a dual lattice (c) of lattice constant $\sqrt{2}$. The dual lattice has the Boltzmann weights $W(\mu_1, \mu_2, \mu_3, \mu_4)$ for each square.

Since shifting the interactions out of the white squares doubles the interactions in the shaded squares, Burkhardt assumes that

$$\tilde{K}_1 = K_1, \quad \tilde{K}_2 = 2K_2, \quad \tilde{K}_4 = 2K_4. \quad (5)$$

In order to obtain an approximate renormalization transformation, one then maps the checkerboard lattice onto a square lattice by the duality-decimation transformation. The dual spins μ_i are placed in the white squares of the checkerboard lattice. The dual lattice [Fig. 1(c)] has $N/2$ spins and is oriented at a $\pi/4$ rotation. Each square has the Boltzmann weights $W(\mu_1, \mu_2, \mu_3, \mu_4)$ and the partition function of the dual lattice is

$$Z' = \sum_{(\mu_i = \pm 1)} \prod_{\text{all squares}} W(\mu_1, \mu_2, \mu_3, \mu_4). \quad (6)$$

The Boltzmann weights $\tilde{B}(\sigma_1, \sigma_2, \sigma_3, \sigma_4)$ are spin-reversal invariant, as are the weights $W(\mu_1, \mu_2, \mu_3, \mu_4)$ for the dual lattice. Any function F of four spins (of values ± 1) which has the spin-reversal symmetry takes only eight values. They will be labeled as

$$\begin{aligned} F_1 &= F(1, 1, 1, 1), & F_2 &= F(1, -1, 1, -1), \\ F_3 &= F(1, -1, -1, 1), & F_4 &= F(1, 1, -1, -1), \\ F_5 &= F(-1, -1, 1, -1), & F_6 &= F(1, -1, -1, -1), \\ F_7 &= F(-1, 1, -1, -1), & F_8 &= F(-1, -1, -1, 1). \end{aligned}$$

Following Wu⁸ the components W_i of the dual lattice can be written explicitly as

$$W_i = \sum_j x_{ij} \tilde{B}_j, \quad (7)$$

where W_i and \tilde{B}_i are labeled as F_i described above, and x_{ij} are elements of the 8×8 matrix

$$x = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \end{bmatrix}. \quad (8)$$

For \tilde{B} given by Eq. (3) \tilde{B}_i satisfy $\tilde{B}_3 = \tilde{B}_4$ and $\tilde{B}_5 = \tilde{B}_6 = \tilde{B}_7 = \tilde{B}_8$. Then, W_i also have the similar properties that $W_3 = W_4$ and $W_5 = W_6 = W_7 = W_8$. The Boltzmann weights of the dual lattice can then be expressed as

$$\begin{aligned} W(\mu_1, \mu_2, \mu_3, \mu_4) &= \exp[K_0 + (K'_1/2)(\mu_1\mu_2 + \mu_2\mu_3 \\ &\quad + \mu_3\mu_4 + \mu_4\mu_1) \\ &\quad + K'_2(\mu_1\mu_3 + \mu_2\mu_4) \\ &\quad + K'_4\mu_1\mu_2\mu_3\mu_4], \end{aligned} \quad (9)$$

and the renormalized-coupling constants are

$$K_0 = \frac{1}{8} \ln(W_1 W_2 W_3^2 W_4^4), \quad (10a)$$

$$K'_1 = \frac{1}{4} \ln(W_1/W_2), \quad (10b)$$

$$K'_2 = \frac{1}{8} \ln(W_1 W_2/W_3^2), \quad (10c)$$

$$K'_4 = \frac{1}{8} \ln(W_1 W_2 W_3^2/W_4^4). \quad (10d)$$

Equations (5) and (10) define the RG transformation $K' = R(K)$ which has the length-rescaling factor $b = \sqrt{2}$. Under the transformation R , a point in the parameter space $K = \max\{K_1/2, K_2, K_4\}$, is transformed into a point in the space $K = \min\{K_1/2, K_2, K_4\}$, and vice versa. The flow of the transformation oscillates back and forth between these two regions. To avoid this difficulty, we repeat the transformation twice and consider $L = R^2$ as a renormalization transformation with the rescaling factor $b = 2$.

TABLE I. Fixed points $K=(K_1, K_2, K_4)$, thermal exponents y_i , and correlation exponents $\nu (=1/y_i)$ of the RG transformation L.

Fixed point	K_1	K_2	K_4	y_i	ν
A	0.292	0.095	0.039	1.01	0.989
B	0.230	0.115	0.115	1.03	0.969
C	0.260	0.130	0.032	1.01	0.988
D	0.301	0.071	0.071	1.01	0.988
E	0	0.305	0	0.747	1.34
F	0	0.189	0.189	0.890	1.12
G	0	0	0.305	0.747	1.34

It is easy to show that the three planes: $K_1=0$, $K_2=K_4$, and $K_1=2K_2$ are three invariant subspaces for the double transformation L. We have studied the transformation L numerically in the ferromagnetic region. Seven nontrivial fixed points are obtained and tabulated in Table I. Thermal exponents y_i associated with the fixed points are also given in the table. Figure 2 shows the critical surface and RG flow on the surface. Critical lines at constant K_4 are shown in Fig. 3. Estimates of critical points obtained by analyzing high-temperature susceptibility series¹⁰ for $K_4=0$ are also shown in the figure. The critical surface intersects the K_1 axis at 0.427 which is in good agreement with the exact value 0.441. When $K_1=K_4=0$ the system is decoupled into two independent Ising models with NN interactions K_2 , which also have the critical value 0.441. However, the critical value along the K_2 axis, $K_2=0.305$ is too small as compared to the exact value 0.441.

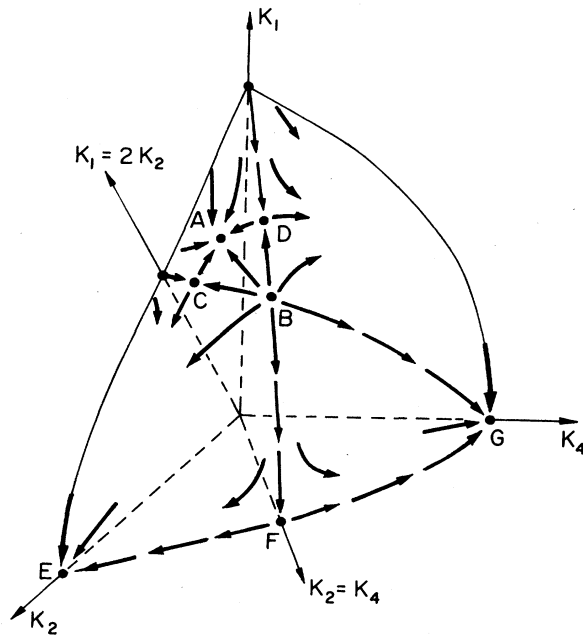


FIG. 2. Fixed points A, B, C, ..., G, and the critical surface in the ferromagnetic region. Arrows show the RG flow on the critical surface. The three planes: $K_1=0$, $K_2=K_4$, and $K_1=2K_2$ are invariant subspaces for the RG transformation L.

III. PRESERVATION OF THE FREE ENERGY IN THE RG TRANSFORMATION

Bond-moving operation in the real-space renormalization method is an *ad hoc* approximation. Bond-moving in the MK method which preserves the bond strengths causes the free energy of the system to be a lower bound² to the exact free energy. Walker⁹ has proposed an improvement to the MK method by requiring that the free energy be preserved in the RG transformation. Significant improvements over the MK method have been obtained. In this section the preservation of the free energy will be implanted in the RG scheme described in the preceding section.

We require that the free energies per spin $f = -(k_B T/N) \ln Z_N$ and $\tilde{f} = -(k_B T/N) \ln \tilde{Z}_N$ satisfy

$$f(K_1, K_2, K_4) = \tilde{f}(\tilde{K}_1, \tilde{K}_2, \tilde{K}_4). \quad (11)$$

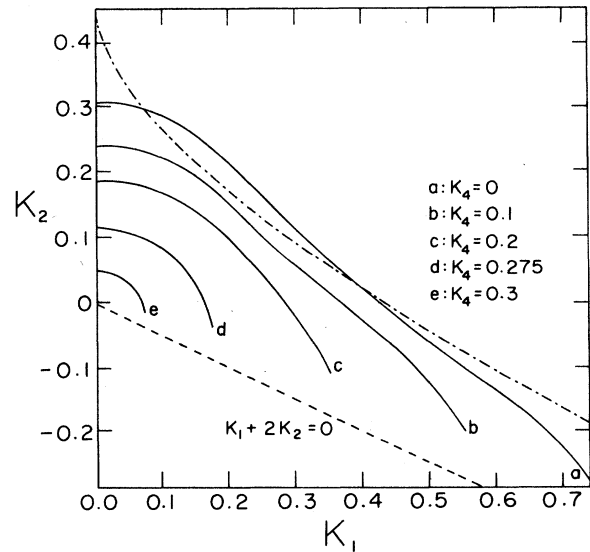


FIG. 3. Critical lines for several values of K_4 obtained by Burkhardt's method. The dash-dotted line is the critical line obtained by analyzing high-temperature series expansions (Ref. 10) for $K_4=0$.

Equation (11) alone cannot determine \bar{K}_1 , \bar{K}_2 , and \bar{K}_4 . Two additional equations are needed. We made use of the simplest assumption,

$$\frac{\bar{K}_1}{K_1} = \frac{\bar{K}_2}{K_2} = \frac{\bar{K}_4}{K_4}. \quad (12)$$

That is, Eqs. (11) and (12) will replace Eqs. (5) for the bond-moving operation. The duality-decimation transformation is the same as before. The dual lattice which is isomorphic to the original lattice has $N/2$ spins and each spin has a constant energy K_0 . Therefore, the total free energy of the dual lattice is

$$[K_0 + f(K'_1, K'_2, K'_4)]N/2.$$

As the free energy is preserved it follows that

$$f(K_1, K_2, K_4) = [K_0 + f(K'_1, K'_2, K'_4)]/2, \quad (13)$$

where K_0 , K'_1 , K'_2 , and K'_4 are given by Eqs. (10). The free energy f is not known, in general, unless the problem is solved. Following Walker,⁹ we will use the high-temperature series expansions of the free energy for f in Eq. (13). For the present model high-temperature series expansions of thermodynamic functions are not available. We have derived high-temperature series expansions for the free energy. To the sixth order this series is given by

$$f(K_1, K_2, K_4) = \ln 2 + \sum_{n=2} A_n(K_1, K_2, K_4), \quad (14)$$

where

$$A_2 = K_1^2 + K_2^2 + \frac{1}{2}K_4^2, \quad (15a)$$

$$A_3 = 4K_1^2K_2 + 2K_1^2K_4 + K_2^2K_4, \quad (15b)$$

$$A_4 = \frac{5}{6}(K_1^4 + K_2^4) - \frac{1}{12}K_4^4 + 10K_1^2K_2^2 + 2K_1^2K_4^2 + 12K_1^2K_2K_4, \quad (15c)$$

$$A_5 = \frac{16}{3}K_1^4K_2 + \frac{80}{3}K_1^2K_2^3 + \frac{4}{3}K_1^2K_4^3 - \frac{1}{3}K_2^2K_4^3 + 20K_1^2K_2K_4^2 + \frac{8}{3}K_1^4K_4 + 44K_1^2K_2^2K_4 + \frac{10}{3}K_2^4K_4, \quad (15d)$$

$$A_6 = \frac{32}{45}(K_1^6 + K_2^6) + \frac{1}{45}K_4^6 + \frac{82}{3}K_1^4K_2^2 + \frac{196}{3}K_1^2K_2^4 + \frac{2}{3}K_1^2K_4^4 + 24K_1^2K_2^2K_4^3 + \frac{14}{3}K_1^4K_4^2 + \frac{15}{2}K_2^4K_4^2 + 108K_1^2K_2^2K_4^2 + 24K_1^4K_2K_4 + 156K_1^2K_2^3K_4. \quad (15e)$$

The RG transformation which preserves the free energy is defined by Eqs. (10), (12), and (13). Similar to the method described in Sec. II, we have determined critical surface for the double transformation \mathbf{L} numerically. Critical lines at constant K_4 are shown in Fig. 4. It is seen that results obtained by the preservation of the free energy are not as good as those determined by preserving

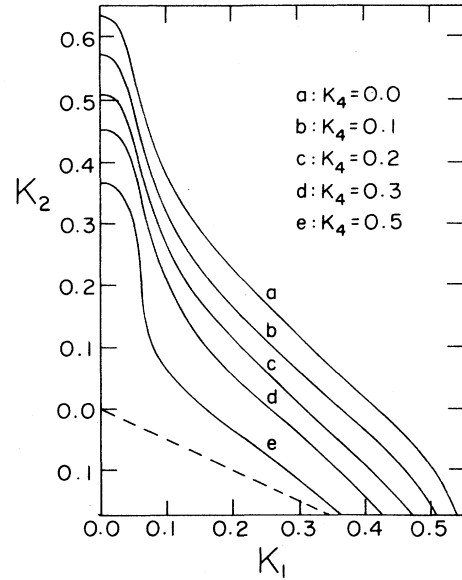


FIG. 4. Critical lines for several values of K_4 obtained by preserving the free energy is the RG transformation. The dashed line is $K_1 + 2K_2 = 0$.

the bond strengths. This is very different from the MK renormalization. In the MK method, the preservation of the free energy to the sixth order in the high-temperature series expansions improves the results significantly for all models^{9,12} studied.

IV. SUPERANTIFERROMAGNETIC PHASE TRANSITIONS

In the preceding two sections, critical temperatures are determined by using real-space renormalization schemes with the rescaling factor $b=2$. Only ferromagnetic phase transitions are observed. The antiferromagnetic phase transition cannot be determined by using $b=2$, because the renormalization transformation with an even number of b does not preserve the antiferromagnetic sublattice structure. To study antiferromagnetic phase transitions the rescaling factor b should be an odd number.

For the Ising model with only NN interactions, the MK transformation can be obtained for any value of b . When there are NNN and four-spin interactions, it is rather complicated to extend the RG transformation from $b=2$ to $b=3$. A renormalization transformation with $b=3$ can be accomplished by the following procedure.

(i) Move interactions away from white squares and redistribute them to shaded squares as shown in Fig. 5(a). Each pair of shaded squares which share an edge [e.g., square $\sigma_1, \sigma_2, \sigma_a, \sigma_b$, and square $\sigma_b, \sigma_a, \sigma_3, \sigma_4$ in Fig. 5(a)] has the interaction

$$E(\sigma_1, \sigma_2, \sigma_3, \sigma_4, \sigma_a, \sigma_b) = K_1(\sigma_1\sigma_2 + \sigma_2\sigma_a + \sigma_a\sigma_3 + \sigma_3\sigma_4 + \sigma_4\sigma_b + \sigma_b\sigma_1 + 3\sigma_a\sigma_b) + (9K_2/4)(\sigma_1\sigma_a + \sigma_2\sigma_b + \sigma_3\sigma_b + \sigma_4\sigma_a) + (9K_4/4)(\sigma_1\sigma_2\sigma_a\sigma_b + \sigma_b\sigma_a\sigma_3\sigma_4). \quad (16)$$

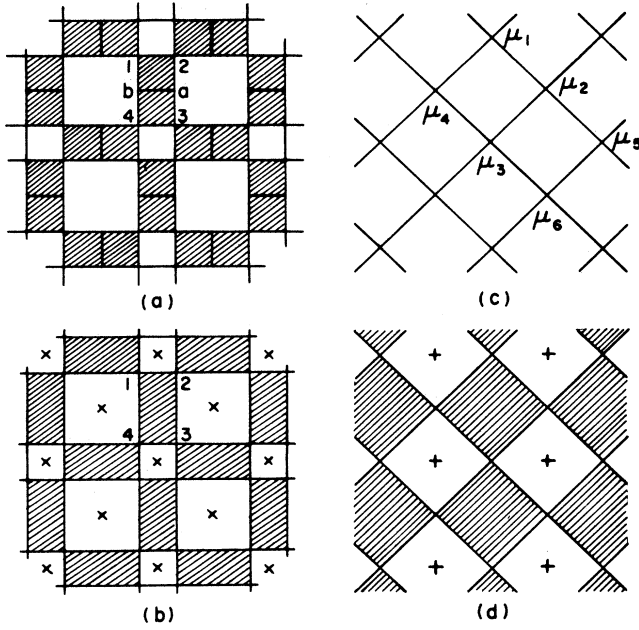


FIG. 5. Real-space renormalization with the rescaling factor $b=3$. Interactions of the original system [Fig. 1(a)] are first redistributed in a pattern shown by (a), where each pair of shaded squares has the interaction $E(\sigma_1, \sigma_2, \sigma_3, \sigma_4, \sigma_a, \sigma_b)$ given by Eq. (16). The pairs of spins shared by two shaded squares (spins σ_a and σ_b) are decimated to obtain figure (b). A duality-decimation transformation then maps the system onto a square lattice (c). A second bond-moving operation redistributes the interactions in a checkerboard pattern (d), and a second duality-decimation transformation maps the checkerboard lattice (d) onto a square lattice of lattice constant 3. The dual spins are located at positions indicated by “+.”

(ii) Decimate all spins connected by the edges shared by two shaded squares [i.e., σ_a and σ_b in Fig. 5(a)]. The lattice shown by Fig. 5(a) is transformed into the one represented by Fig. 5(b). Each shaded rectangular then has the Boltzmann weights

$$\begin{aligned} \bar{B}(\sigma_1, \sigma_2, \sigma_3, \sigma_4) = & 4(\cosh\alpha \cosh\beta \cosh\gamma \\ & + \sinh\alpha \sinh\beta \sinh\gamma) \\ & \times \exp K_1(\sigma_1\sigma_2 + \sigma_3\sigma_4), \end{aligned} \quad (17)$$

where

$$\alpha = 3K_1 + 9K_4(\sigma_1\sigma_2 + \sigma_3\sigma_4)/4, \quad (18a)$$

$$\beta = K_1(\sigma_1 + \sigma_4) + 9K_2(\sigma_2 + \sigma_3)/4, \quad (18b)$$

$$\gamma = K_1(\sigma_2 + \sigma_3) + 9K_2(\sigma_1 + \sigma_4)/4. \quad (18c)$$

(iii) Apply the exact duality-decimation transformation to the lattice given by Fig. 5(b) and obtain a dual lattice shown in Fig. 5(c). The dual lattice has the lattice constant $b=3/\sqrt{2}$ with the dual spins located at the positions indicated by “x” in Fig. 5(b). As the Boltzmann weights given by Eq. (17) have the spin-reversal symme-

try, the weights $W_i = W(\mu_1, \mu_2, \mu_3, \mu_4)$ of Fig. 5(c) are again given by Eq. (7). But for the present case $\bar{B}_3 \neq \bar{B}_4$, $\bar{B}_5 = \bar{B}_6 = \bar{B}_7 = \bar{B}_8$; and $W_3 = W_4$, $W_5 = W_6 \neq W_7 = W_8$. The Boltzmann weights for each square in Fig. 5(c) can be expressed as

$$\begin{aligned} W(\mu_1, \mu_2, \mu_3, \mu_4) = & \exp[K_0 + (K'_1/2)(\mu_1\mu_2 + \mu_2\mu_3 \\ & + \mu_3\mu_4 + \mu_4\mu_1) \\ & + K'_0\mu_1\mu_3 + k'_e\mu_2\mu_4 \\ & + K'_4\mu_1\mu_2\mu_3\mu_4], \end{aligned} \quad (19)$$

where the coupling constants are

$$K_0 = \frac{1}{8} \ln W_1 W_2 (W_3 W_5 W_7)^2, \quad (20a)$$

$$K'_1 = \frac{1}{4} \ln (W_1 / W_2), \quad (20b)$$

$$K'_0 = \frac{1}{8} \ln W_1 W_2 (W_5 / W_3 W_7)^2, \quad (20c)$$

$$K'_e = \frac{1}{8} \ln W_1 W_2 (W_7 / W_3 W_5)^2, \quad (20d)$$

$$K'_4 = \frac{1}{8} \ln W_1 W_2 (W_3 / W_5 W_7)^2. \quad (20e)$$

The two NNN couplings (a horizontal bond and a vertical bond) are different. But the strength of a horizontal NNN bond of a given square is equal to the strength of a vertical NNN bond of its neighboring squares and vice versa. For example, the coupling between μ_1 and μ_3 in Fig. 5(c) is the same as that between μ_3 and μ_5 ($=K'_0$); and the coupling between μ_2 and μ_4 is the same as that between μ_2 and μ_6 ($=K'_e$).

(iv) Redistribute the interactions of Fig. 5(c) in a checkerboard pattern again as shown in Fig. 5(d). In this figure all NNN bonds in shaded squares have the same strength $K'_e + K'_0$. Each shaded square also has NN couplings K'_1 , four-spin couplings $2K'_4$, and the constant energy $2K_0$. Here K_0 , K'_1 , K'_0 , K'_e , and K'_4 are given by Eqs. (20).

(v) Map the checkerboard lattice, Fig. 5(d), onto a square lattice by a second duality-decimation transformation. The dual lattice with spins located at positions indicated by “+” in Fig. 5(d) then has the lattice constant $b=3$. This step is exactly the same as that described in Sec. II.

In this procedure steps (i) and (iv) are approximate, the other steps are exact. The explicit expressions of the renormalization transformation for $b=3$ are too lengthy to be presented here. We have analyzed the transformation to determine the critical surface, especially for $K_2 < 0$. Superantiferromagnetic phase transitions, which cannot be observed for $b=2$, are found in this calculation. Critical lines for several values of K_4 are shown in Fig. 6. The accuracy of the present calculation, however, is poor as compared to estimates of the series expansion¹⁰ method, and Monte Carlo simulations.⁶

When $K_1 + 2K_2 = 0$ the system does not have a phase transition for any value of K_4 . Our numerical analysis near this line is very difficult because overflow always arises in our computer calculation. Different ways of bond movings for $b=3$ have also been studied. However, no significant improvement over the method described above has been obtained.

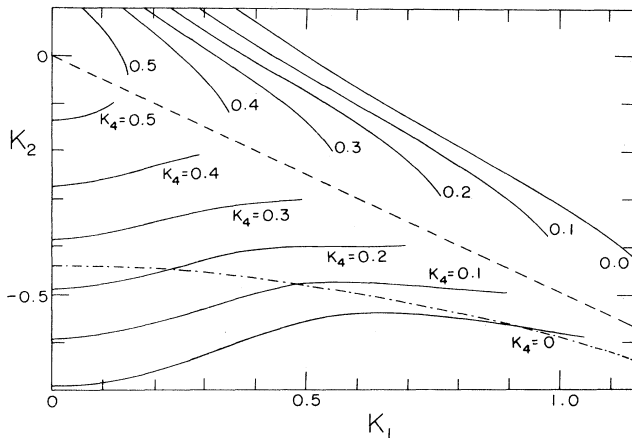


FIG. 6. Critical lines for several values of K_4 obtained by the RG transformation with $b=3$. The dashed line $K_1+2K_2=0$ separated the ferromagnetic and superantiferromagnetic phase transitions. The dash-dotted line represents the critical line obtained by Monte Carlo simulations (Ref. 6) for $K_4=0$.

V. SUMMARY

Exact duality-decimation transformation and bond-moving (energy shifting) operation are combined to construct RG transformation for the Ising model with NN, NNN, and four-spin interactions. In the ferromagnetic

case, two different methods are considered. The first method makes the assumption that bond strengths are preserved in the bond-moving operation. Fixed points, thermal exponents and the critical surface are determined. The present result is in good agreement with the exact value in the pure Ising limit. The nonuniversality of the exponents, however, cannot be found.

The second method uses the assumption that the free energy of the system is preserved in the bond-moving step. Previous studies for systems with only NN interactions have shown that the preservation of the free energy is superior to the preservation of bond strengths in the RG transformation. But for the present case the preservation of the free energy does not yield results better than those obtained from the preservation of the bond strengths.

In order to determine the superantiferromagnetic phase transition, a renormalization transformation with the rescaling length $b=3$ is proposed. The procedure is complicated and the results are less satisfactory. Investigation of simpler and more accurate methods is desired.

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