

## Ising Model with Second-Neighbor Interaction. I. Some Exact Results and an Approximate Solution

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The square Ising lattice with unequal first- and second-neighbor interactions has been considered. Among the exact results discussed, we show that the lowest energy state can be ferromagnetic, antiferromagnetic, or superantiferromagnetic, and the transition temperature should vanish in some cases. It is also shown that this problem is a special case of a more general problem arising in the statistical consideration of the hydrogen-bonded crystals. A well-defined approximation procedure is then introduced to solve the latter problem and to derive the (approximate) critical condition and expressions for the thermodynamic functions. The critical temperature thus determined is exact for the regular Ising lattice and for the lattices with  $T_c=0$ , while for the equivalent neighbor model the error is less than 2%. The specific heat possesses the usual logarithmic singularity in all cases.

### I. INTRODUCTION

IN the last forty years, a considerable amount of interest has been centered on the subject of the Ising model<sup>1</sup> of magnetism. While numerous papers have been written on this subject, the progress toward the understanding of the different aspects of the model has been surprisingly slow. For example, Onsager's classic 1944 paper<sup>2</sup> on the exact solution of the two-dimensional model was published some twenty years after the introduction of the model by Ising. In recent years, a number of new approaches have provided alternate and simpler derivations of the Onsager's solution.<sup>3-6</sup> However, despite the significant amount of effort made in these years, a number of related problems still remains essentially untouched.<sup>7</sup> One of them is the so-called "crossed bond" problem.

For a better description of real magnetic systems, it is desirable to remove the restrictions attached to the original Ising magnets. The most innocent modification seems to be the extension of the interaction into a certain range. However, once the interactions are allowed to "cross" each other thus forming crossed bonds, the conventional methods of treatment invariably fail and the model is no longer soluble. The only progress made in connection with this crossed-bond problem is the Padé study made by Domb and Dalton.<sup>8</sup> Through the

analysis of high-temperature expansion series, they determined some critical indices and estimated the location of the critical point for some models with extended range of interactions. As their discussion was restricted to the equivalent neighbor model (same interaction with all neighbors), it does not answer some pertinent questions of interest. For example, it may be of interest to know the dependence of the critical temperature on the lattice constants.<sup>9</sup> In the present paper, we consider the square Ising lattice with *unequal* first- and second-neighbor interactions and with no external field. We shall discuss some exact results and obtain an approximate solution which gives (approximate) answers to these questions. The approximation involved is a straightforward generalization of a method used earlier by one of us in the study of the ferroelectric phase transitions.<sup>10</sup> It has also been noted by Gibberd<sup>11</sup> that this procedure should be useful in the study of the unsolved Ising problems. However, through the use of a dual transformation, we are able to essentially eliminate the crossed bonds and cast the problem into a form suitable for a straightforward application of the approximation.

Our method of approach also constitutes the basis for obtaining the exact low-temperature series expansions which are usually more difficult to derive. The results on the Padé approximant studies on these series will be reported subsequently.<sup>12</sup> Later on, we hope to study the effect on the inclusion of corrections and eventually discuss some exactly soluble Ising models with crossed interactions.

In Sec. II we discuss some exact results and, by means of the introduction of the dual lattice, transform the

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<sup>1</sup> E. Ising, *Z. Phys.* **31**, 253 (1925).

<sup>2</sup> L. Onsager, *Phys. Rev.* **65**, 117 (1944).

<sup>3</sup> C. A. Hurst and H. S. Green, *J. Chem. Phys.* **33**, 1059 (1960).

<sup>4</sup> P. W. Kasteleyn, *J. Math. Phys.* **4**, 287 (1963).

<sup>5</sup> L. Schultz, D. Mattis, and E. Lieb, *Rev. Mod. Phys.* **36**, 856 (1964).

<sup>6</sup> C. A. Hurst, *J. Math. Phys.* **7**, 305 (1966).

<sup>7</sup> For a description of the outstanding unsolved Ising problems, see, for example, H. S. Green and C. A. Hurst, in *Order-disorder Phenomena* (Wiley-Interscience, Inc., New York, 1964), Chap. 7.

<sup>8</sup> C. Domb and N. W. Dalton, *Proc. Roy. Soc.* **89**, 859 (1966). See also note added in manuscript.

<sup>9</sup> For a study of this problem for the regular Ising lattices, see, for example, C. Y. Weng, R. B. Griffiths, and M. E. Fisher, *Phys. Rev.* **162**, 475 (1967).

<sup>10</sup> F. Y. Wu, *Phys. Rev. Letters* **18**, 605 (1967); *Phys. Rev.* **168**, 539 (1968).

<sup>11</sup> R. W. Gibberd, *Phys. Rev.* **171**, 563 (1968).

<sup>12</sup> This is now under study by C. Fan, W. W. Yeh, and F. Y. Wu. See also note added in manuscript.

problem is considered in some detail and solved under a well-defined approximation in Sec. III. In Sec. IV, we apply this approximation procedure to the Ising model to derive the critical condition and expressions for the thermodynamic functions.

II. SOME EXACT RESULTS

We consider an array of  $\sqrt{N} \times \sqrt{N}$  spins ( $s = \frac{1}{2}$ ) arranged at the vertices of a square lattice. The interaction Hamiltonian is taken to be<sup>13</sup>

$$\mathcal{H} = -J \sum_{ij}^{(1)} \sigma_i \sigma_j - J' \sum_{mn}^{(2)} \sigma_m \sigma_n, \quad (1)$$

where the superscript  $i$  ( $i = 1, 2$ ) restricts the sum to all  $i$ th neighbors of the lattice. The lattice is illustrated in Fig. 1. Here, in agreement with the usual convention, a positive  $J$  or  $J'$  tends to align the spins. Because of the competing effect between the first- and the second-neighbor interactions, the lowest energy state could be any of the following: (i) ferromagnetic, (ii) antiferromagnetic, and (iii) superantiferromagnetic. These situations are illustrated in Fig. 2. The superantiferromagnetic state is so named because the lattice can be viewed as a superposition of two antiferromagnetic sublattices. Since there are altogether  $2N$  first-neighbor and  $2N$  second-neighbor interactions, the total energy for the three cases are, respectively, (i)  $-2N(J+J')$ , (ii)  $2N(J-J')$ , and (iii)  $2NJ'$ . It is then easy to see that the lowest energy state is ferromagnetic if  $J > 2|J'|$  (region I), antiferromagnetic if  $J < -2|J'|$  (region II) and superantiferromagnetic if  $2J' < -|J|$  (region III). These three regions are shown in Fig. 3.

The problem is to evaluate the partition function

$$Z = \sum_{\sigma_i = \pm 1} \exp(-\beta \mathcal{H}), \quad (2)$$

where  $\beta \equiv 1/kT$ . An immediate observation is that the replacement of  $J$  by  $-J$ , while holding  $J'$  fixed, leaves  $Z$  unchanged. That is, we have

$$Z(J, J') = Z(-J, J'). \quad (3)$$

Equation (3) is well known for the simple square lattice ( $J' = 0$ ). To see that this is also true for lattices with nonvanishing second-neighbor interactions, we divide the lattice into two interlacing sublattices. Due to the

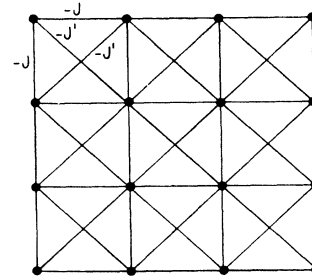


FIG. 1. The square Ising lattice with first- and second-neighbor interactions.

fact that the two sublattices interact with the first-neighbor interactions only, the replacement of  $J$  by  $-J$  has the same effect as reversing all the spins on one of the two sublattices. Therefore, the partition sum (2) is unchanged.

For  $J' = 0$ , the lattice reduces to the usual simple square one with an interaction  $-J$  which is ferromagnetic for  $J > 0$  and antiferromagnetic for  $J < 0$ . For  $J = 0$  (the  $J'$  axis), the lattice is decomposed into two independent simple square lattices. Each of these simple square lattices is ferromagnetic for  $J' > 0$  and antiferromagnetic for  $J' < 0$ , while the over-all lattice is either ferromagnetic or antiferromagnetic for  $J' > 0$  and superantiferromagnetic for  $J' < 0$ . It is also to be noted that the transition temperature vanishes on the boundary  $2J' = -|J|$ . As will be more clearly seen later in Sec. IV, this result is due to the fact that on this boundary the lowest energy state is no longer unique, a phenomenon that is also responsible to the vanishing of the transition temperature for the antiferromagnetic triangular Ising lattice.<sup>14</sup>

We now introduce the dual lattice  $D$  which is formed by drawing the perpendicular bisectors to all the lattice edges of the original lattice  $L$ .<sup>15</sup> It is immediately evident that the simple square lattice is self-dual in that the dual lattice is topologically identical with the original one. For any spin configuration on  $L$ , the positive spins cluster together forming isolated islands in the sea of negative spins. If we enclose these "islands" by drawing polygons on the dual lattice, each spin configuration on  $L$  is then mapped into a polygon configuration on  $D$ . Therefore, instead of considering the spin configurations on  $L$ , we may consider the polygon con-

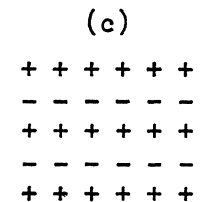
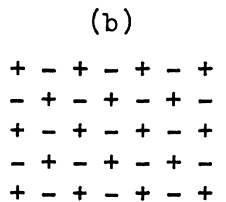
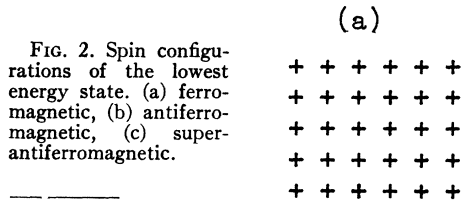


FIG. 2. Spin configurations of the lowest energy state. (a) ferromagnetic, (b) antiferromagnetic, (c) superantiferromagnetic.

<sup>13</sup> Our discussions can be easily extended to the case of unequal horizontal, vertical and diagonal interactions.  
<sup>14</sup> G. H. Wannier, Phys. Rev. **79**, 357 (1950).  
<sup>15</sup> For a more detailed discussion on the duality transformation for two-dimensional lattices, see, for example, Sec. 3.4.2 of C. Domb, Adv. Phys. **9**, 149 (1960).

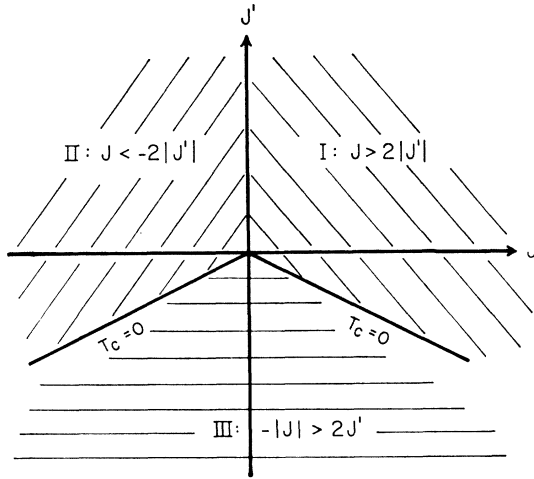


FIG. 3. The three regions in the  $J$ - $J'$  plane. The ground state is ferromagnetic in region I, antiferromagnetic in region II, and superantiferromagnetic in region III. The transition temperature vanishes on the boundary  $-|J| = 2J'$ .

figurations on  $D$ . For the simple square lattice with nearest-neighbor interactions only, the correct Boltzmann factor can also be accounted for by assigning appropriate bond weights to the dual lattice. This fact, together with the self-dual property of the simple square lattice, has essentially been used by Kramers and Wannier to determine the transition temperature<sup>16</sup> before the exact solution was known. When the second-neighbor interactions are included, however, the situation is somewhat complicated. But the correct Boltzmann factor can still be generated by assigning vertex weights to the polygon configurations on the dual lattice.<sup>17</sup> The Ising problem involving crossed bonds is then transformed into a well-defined statistical problem related to the dual lattice.

To see the details of this transformation, it is convenient to break each horizontal and vertical interaction into two equal parts of strength  $-\frac{1}{2}J$  each and focus our attention to a typical lattice point on the dual lattice as shown in Fig. 4. There are now eight possible vertex configurations for a typical lattice point on  $D$  as shown in Fig. 5. From the associated spin configurations on  $L$ , which are also given in Fig. 5, it is not difficult to derive the appropriate vertex weights needed for each kind of vertex. For example, for the vertex (2) the interaction energy is  $4(-\frac{1}{2}J)(-1) + 2(-J') = 2(J - J')$  and the appropriate weight factor is the corresponding Boltzmann factor  $\exp[-2\beta(J - J')]$ . The partition function of the Ising model under consideration therefore becomes

$$Z = 2 \sum_{\text{all polygon configurations on } D} \prod (\text{vertex weights}). \quad (4)$$

<sup>16</sup> H. A. Kramers and G. H. Wannier, Phys. Rev. **60**, 252 (1941); *ibid.* **60**, 263 (1941).

<sup>17</sup> This observation is due to E. H. Lieb (private communication).

The factor 2 comes from the fact that the reversing of all spins leaves the polygon configurations unchanged. The vertex weights are listed in Fig. 5.

The Ising problem under consideration now appears as a special case of a more general problem involving the counting of weighted polygons on  $D$  for which the vertex weights are arbitrary. Now it is known that this general problem is identical to the statistical problem arising in the consideration of hydrogen-bonded crystals.<sup>10</sup> However, it is unfortunate that the technique developed for the solution of the latter problem<sup>18,19</sup> is inapplicable here because of the violation of the so-called "ice condition" in the present case. If we number the eight different kinds of vertices from 1 to 8 as shown in Fig. 5, the technique which proves useful in treating the hydrogen-bonded statistical problems<sup>18,19</sup> explicitly uses the fact that *only* the vertices 1 through 6 are considered (the ice condition). Undoubtedly the inclusion of vertices 7 and 8 makes the problem more difficult and the exact solution is not known at the present except for a few special cases.<sup>20</sup>

It is useful to point out at this point some symmetry relations of the partition function (4). If we write ( $\omega_i$  = the weight of the  $i$ th kind of vertex)

$$Z \equiv Z(\omega_1, \omega_2, \omega_3, \omega_4; \omega_5, \omega_6, \omega_7, \omega_8)$$

and consider each empty lattice edge without bond as a hole, then we have the following bond-hole symmetry relations:

$$\begin{aligned} Z(\omega_1, \omega_2, \omega_3, \omega_4; \omega_5, \omega_6, \omega_7, \omega_8) &= Z(\omega_2, \omega_1, \omega_4, \omega_3; \omega_6, \omega_5, \omega_8, \omega_7) \\ &= Z(\omega_4, \omega_3, \omega_2, \omega_1; \omega_7, \omega_8, \omega_5, \omega_6) \\ &= Z(\omega_3, \omega_4, \omega_1, \omega_2; \omega_8, \omega_7, \omega_6, \omega_5). \end{aligned} \quad (5)$$

The first equality is obtained by interchanging all bonds into holes and all holes into bonds. In particular it reduces to Eq. (3) upon substituting the weights  $\omega_i$  from Fig. 5. The second equality is the result of the interchanging of all bonds and holes in the horizontal direction and the third equality for the same changes in the vertical direction. These relations will be useful in later discussions.

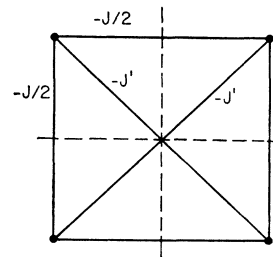


FIG. 4. A typical lattice point on the dual lattice  $D$  (denoted by the dotted lines). Only half of the horizontal and vertical interactions on the Ising lattice  $L$  are associated with this lattice point.

<sup>18</sup> E. H. Lieb, Phys. Rev. Letters **18**, 692 (1967); **18**, 1046 (1967); **19**, 108 (1967); Phys. Rev. **162**, 162 (1967).

<sup>19</sup> B. Sutherland, Phys. Rev. Letters **19**, 103 (1967); C. P. Yang, Phys. Rev. Letters **19**, 586 (1967); B. Sutherland, C. N. Yang, and C. P. Yang, Phys. Rev. Letters **19**, 588 (1967).

<sup>20</sup> F. Y. Wu and C. Fan (unpublished).

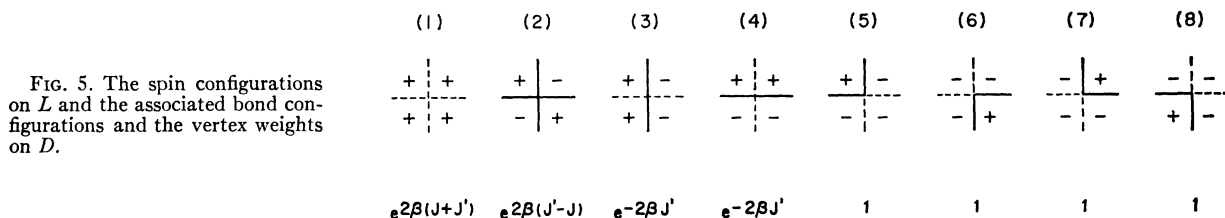


FIG. 5. The spin configurations on  $L$  and the associated bond configurations and the vertex weights on  $D$ .

III. FREE-FERMION APPROXIMATION

In this section we consider the problem of the evaluation of the partition function (4) with arbitrary vertex weights. This problem has been considered by Hurst and Green from a somewhat different point of view. In their consideration of the most general (planar) Ising lattice,<sup>21</sup> they introduce a sublattice at each vertex of a simple square lattice. Various Ising lattices are then generated by making special choices for the sublattice. Clearly, if the internal structure of these sublattices are complicated enough to include crossed bonds, it is possible to generate arbitrary vertex weights and the problem is then identical with ours.

In order to attach a well-defined meaning to the approximation procedure that we shall introduce, we follow Hurst and Green<sup>3</sup> in rewriting the partition function (4) as the vacuum expectation value of a linear combination of products of fermion operators ( $m \equiv \sqrt{N}$ )

$$Z = \langle o | \prod_{j=1}^N (\omega_1 + \omega_2 a_j^{(2)\dagger} a_j^{(1)\dagger} a_{j-m}^{(2)} a_{j-1}^{(1)} + \omega_3 a_j^{(2)\dagger} a_{j-m}^{(2)} + \omega_4 a_j^{(1)\dagger} a_{j-1}^{(1)} + \omega_5 a_j^{(2)\dagger} a_{j-1}^{(1)} + \omega_6 a_j^{(1)\dagger} a_{j-m}^{(2)} + \omega_7 a_j^{(2)\dagger} a_j^{(1)\dagger} + \omega_8 a_{j-m}^{(2)} a_{j-1}^{(1)}) | o \rangle, \quad (6)$$

where  $a_j^\dagger$  and  $a_j$  are the bond creation and annihilation (fermion) operators at the  $j$ th vertex. The superscript 1 refers to bonds in the horizontal direction, 2 refers to bonds in the vertical direction, and  $|o\rangle$  is the vacuum state defined by  $a_j |o\rangle = 0$ . Using the anticommutation relation of the fermion operators, it is easy to reduce (6) into the following expression:

$$Z = \omega_1^N \langle o | T \exp \sum_{j=1}^N [H_0(j) + H_1(j)] | o \rangle, \quad (7)$$

where

$$H_0(j) = \frac{\omega_3}{\omega_1} a_j^{(2)\dagger} a_{j-m}^{(2)} + \frac{\omega_4}{\omega_1} a_j^{(1)\dagger} a_{j-1}^{(1)} + \frac{\omega_5}{\omega_1} a_j^{(2)\dagger} a_{j-1}^{(1)} + \frac{\omega_6}{\omega_1} a_j^{(1)\dagger} a_{j-m}^{(2)} + \frac{\omega_7}{\omega_1} a_j^{(2)\dagger} a_j^{(1)\dagger} + \frac{\omega_8}{\omega_1} a_{j-m}^{(2)} a_{j-1}^{(1)},$$

$$H_1(j) = \frac{\Delta}{\omega_1^2} a_j^{(2)\dagger} a_j^{(1)\dagger} a_{j-m}^{(2)} a_{j-1}^{(1)},$$

$$\Delta = \omega_1 \omega_2 + \omega_3 \omega_4 - \omega_5 \omega_6 - \omega_7 \omega_8,$$

<sup>21</sup> See Sec. 5.3 of the monograph cited in Ref. 7.

and  $T$  is the operator that orders the indices from  $j=1$  to  $j=N$ .

The problem is now reduced to the evaluation of the  $S$ -matrix in the form of (7) with an interaction Hamiltonian which includes terms quadratic and quartic in the field operators. It is the presence of the quartic terms that makes the problem insoluble by the existing techniques.

If  $\Delta=0$ , the exponential contains only the quadratic terms and the evaluation of the partition function  $Z$  can be carried out in a variety of ways.<sup>21</sup> In Appendix A it is evaluated by the standard  $S$ -matrix technique.<sup>6</sup> The partition function  $Z_0$  is found to be given by

$$\lim_{N \rightarrow \infty} \frac{1}{N} \ln Z_0 = \frac{1}{8\pi^2} \int_0^{2\pi} d\theta \int_0^{2\pi} d\phi \ln [\alpha + 2\beta \cos \theta + 2\gamma \cos \phi + 2\delta \cos(\theta - \phi) + 2\epsilon \cos(\theta + \phi)], \quad (8)$$

where the subscript of  $Z_0$  refers to the case  $\Delta=0$  and

$$\alpha = \omega_1^2 + \omega_2^2 + \omega_3^2 + \omega_4^2,$$

$$\beta = \omega_1 \omega_3 - \omega_2 \omega_4,$$

$$\gamma = \omega_1 \omega_4 - \omega_2 \omega_3,$$

$$\delta = \omega_3 \omega_4 - \omega_7 \omega_8,$$

$$\epsilon = \omega_3 \omega_4 - \omega_5 \omega_6.$$

As one easily checks, the symmetry relation (5) holds for this solution. The critical point for the expression (8) has also been investigated by Hurst and Green and is given by<sup>21</sup>

$$\omega_1 + \omega_2 + \omega_3 + \omega_4 = 2 \max\{\omega_1, \omega_2, \omega_3, \omega_4\}. \quad (9)$$

If  $\Delta \neq 0$ , this problem corresponds to the consideration of an interacting many-fermion system and the exact evaluation of (7) cannot be carried out. However, as pointed out by Gibberd,<sup>11</sup> a meaningful approximation as suggested by the structure of Eq. (7) is to ignore the interaction Hamiltonian  $H_1$ . We shall refer to this procedure as the free-fermion approximation. For the potassium dihydrogen phosphate (KDP) model<sup>18</sup> of ferroelectrics, this corresponds to the consideration of the modified model<sup>10</sup> and one obtains the correct critical temperature and the correct critical behavior of the specific heat. For the  $F$  model<sup>18</sup> of antiferroelectrics, this approximation also gives the correct critical temperature as well as the correct (continuous) behavior of the specific heat at the critical point. It is then hoped that for other unsolved problems this procedure is per-

haps comparably useful in furnishing some of the vital informations. Since  $H_0$  does not contain  $\omega_2$ , the free-fermion approximation is essentially to adopt the expression (8) for  $Z$  but to replace  $\omega_2$  by

$$\bar{\omega}_2 = (\omega_5\omega_6 + \omega_7\omega_8 - \omega_3\omega_4)/\omega_1, \quad (10)$$

in order to make  $\Delta=0$  an identity for the set of weights  $\{\omega_1, \bar{\omega}_2, \omega_3, \omega_4, \omega_5, \omega_6, \omega_7, \omega_8\}$ . As discussed in Appendix B, corrections to this approximation can be written in a power series in  $\Delta/\omega_1^2$ . Due to the symmetry relation (5), the approximation can also be made in a variety of ways. For example, from the first equality of (5) we may also make the replacement of  $\omega_1$  by  $\bar{\omega}_1 = (\omega_5\omega_6 + \omega_7\omega_8 - \omega_3\omega_4)/\omega_2$  in (8) and expand the corrections in a power series in  $\Delta/\omega_2^2$ . Among these alternatives, we shall choose as the best approximation the one whose correction expansion parameter is the smallest. Therefore, we have the following working prescription for the free-fermion approximation: Pick the largest among the weights  $\omega_1, \omega_2, \omega_3,$  and  $\omega_4$  and modify the weight of its conjugate<sup>22</sup> to make  $\Delta=0$  an identity. The approximate partition function is then given by  $Z_0$  as a function of these weights, including the modified one. For example, if we find  $\omega_1 \geq \omega_2, \omega_3, \omega_4$ , then use  $\bar{\omega}_2$  defined by (10) and write

$$Z_{\text{approx}} = Z_0(\omega_1, \bar{\omega}_2, \omega_3, \omega_4, \omega_5, \omega_6, \omega_7). \quad (11)$$

The critical condition is given by

$$\omega_1 = \bar{\omega}_2 + \omega_3 + \omega_4, \quad \text{if } \omega_1 > \bar{\omega}_2 \quad (12a)$$

$$\bar{\omega}_2 = \omega_1 + \omega_3 + \omega_4, \quad \text{if } \omega_1 < \bar{\omega}_2. \quad (12b)$$

We also have a graphical interpretation for this approximation. For  $\omega_1 \geq \omega_2, \omega_3, \omega_4$ , the leading terms in the expansion of the partition function (4) consists of polygon configurations with small number of vertices. After drawing out all polygon configurations with a given length of circumference, one is easily convinced that, among the eight different vertex configurations, it is the cross-over type [vertex (2)] that occurs the least number of times. For example, it does not appear in graphs containing less than eight bonds. Among the seven topologically distinct connected polygon graphs with a total of ten bonds, only one graph contains a cross-over type vertex. Similarly among the 34 different graphs with a total of 12 bonds, only nine contain the cross-over type vertices. Therefore it is reasonable to expect that the error introduced will be minimized by modifying the weight of this particular type of vertex.

#### IV. APPLICATION TO ISING MODEL

We shall now apply the free-fermion approximation to the Ising model considered in Sec. II. The vertex

<sup>22</sup> We define the conjugate of a vertex configuration as the configuration obtained by changing all the bonds into holes and holes into bonds. For example, vertices (1) and (2) are conjugate to each other.

weights associated with the dual lattice have been tabulated in Fig. 5

$$\begin{aligned} \omega_1 &= 1/yz, \\ \omega_2 &= z/y, \\ \omega_3 &= \omega_4 = y, \\ \omega_5 &= \omega_6 = \omega_7 = \omega_8 = 1, \end{aligned} \quad (13)$$

where

$$y \equiv e^{-2K'}, \quad z \equiv e^{-2K}, \quad K \equiv \beta J, \quad K' \equiv \beta J'.$$

It is convenient to discuss the different regions in the  $J$ - $J'$  plane separately.

#### A. Region I. $J > 2|J'|$

This is the ferromagnetic region for which  $\omega_1 \geq \omega_2, \omega_3, \omega_4$ . Hence by our prescription we replace  $\omega_2$  by  $\bar{\omega}_2$  given by (10) which now reads

$$\bar{\omega}_2 = yz(2 - y^2).$$

The free energy per spin  $f_{\text{approx}}$  is given by (8)

$$\begin{aligned} -\beta f_{\text{approx}} &= 4(K + K') + \frac{1}{8\pi^2} \int_0^{2\pi} d\theta \int_0^{2\pi} d\phi \\ &\times \ln[1 + 2z^2y^4 + (2z^2y^2 - z^2y^4)^2 \\ &+ 2zy^2(2z^2y^2 - z^2y^4 - 1)(\cos\theta + \cos\phi) \\ &+ 4(z^2y^4 - z^2y^2)\cos\theta\cos\phi]. \end{aligned} \quad (14)$$

The critical condition (12a) now reduces to

$$(1 - zy^2)^2 = 2z^2y^2$$

or

$$e^{2K} = \sqrt{2}e^{-2K'} + e^{-4K'}. \quad (15)$$

This relation is exact for  $K' = 0$  which yields the well-known result<sup>2,16</sup>

$$e^{-2K} = \sqrt{2} - 1 = 0.41421 \dots$$

for the simple square lattice. It is also exact for  $K = -2K'$  in producing  $T_c = 0$ . The vanishing of the critical temperature is a common situation in the consideration of the hydrogen-bonded crystals. For example, it happens for the KDP and the  $F$ -model with the inclusion of an external field.<sup>23</sup> In general, if the ground-state of a system is degenerate with a macroscopic degree of degeneracy, the transition temperature then vanishes because there would be no preferred state at low temperatures. In the present case, the vertices (1), (3), and (4) have the same energy and, as a result, the lowest energy state is no longer unique. Therefore, the vanishing of the transition temperature is an exact result. For  $K = K'$ , the equivalent neighbor model, Eq. (15) gives

$$e^{-2K} = \left\{ \left[ \frac{1}{2} + \left( \frac{1}{4} - 2\sqrt{2}/27 \right)^{1/2} \right]^{1/3} + \left[ \frac{1}{2} - \left( \frac{1}{4} - 2\sqrt{2}/27 \right)^{1/2} \right]^{1/3} \right\}^{-1} = 0.68946 \dots,$$

<sup>23</sup> E. H. Lieb and F. Y. Wu (unpublished).

whereas the Padé value is  $e^{-2K}=0.6837$ .<sup>8</sup> The agreement is surprisingly good. However, for  $K=0$ , our approximation gives

$$e^{-2K'} = (\sqrt{3}-1)/\sqrt{2} = 0.517638 \dots \quad (16)$$

while the exact number should be  $e^{-2K'}=0.41421 \dots$ . This disagreement is somewhat expected because the expansion parameter in connection with this approximation is now  $z^2(1-y^2)^2$  and is largest for  $K=0$ . Because the deviations from the exact results are in the same direction in these cases, it is conceivable that our approximation gives an upper bound to the true transition temperature. In fact, we expect our approximation to be accurate within a few percent in determining the critical temperatures, at least in the region  $|J| > |J'|$ .

The other thermodynamic functions can be computed from (14). We include the details in Appendix C. As in the case of the regular Ising lattices, the specific heat has the same logarithmic singularity both above and below the critical temperature.

**B. Region II.  $J < -2|J'|$**

This is the antiferromagnetic region for which  $\omega_2 \geq \omega_1, \omega_3, \omega_4$ . We may proceed in the discussions according to our prescription by modifying  $\omega_1$ . However, it is more convenient to use the identity (3) to conclude that the thermodynamic properties in this region are identical with those in region I, except with the replacement of  $J$  by  $-J$ . Therefore, in combining the two cases together, the critical condition in both regions I and II ( $2J' > -|J|$ ) is

$$e^{2|K|} = \sqrt{2}e^{-2K'} + e^{-4K'}. \quad (17)$$

The conclusion on the singularity of the specific heat is unchanged.

**C. Region III.  $-|J| > 2J'$**

This is the superantiferromagnetic region with  $\omega_3 = \omega_4 > \omega_1, \omega_2$ . According to our prescription, we replace  $\omega_3$  by  $\tilde{\omega}_3 = (\omega_5\omega_6 + \omega_7\omega_8 - \omega_1\omega_2)/\omega_4 = 2/y - 1/y^3$  and the free energy per spin is then given by

$$\begin{aligned} -\beta f_{\text{approx}} = & -2K' + \frac{1}{8\pi^2} \int_0^{2\pi} d\theta \int_0^{2\pi} d\phi \\ & \times \ln \left\{ 1 + z^2 y^{-4} + \frac{y^{-4}}{z^2} + (2y^{-2} - y^{-4})^2 \right. \\ & + 2y^{-2} \cos\phi \left[ z(2y^{-2} - y^{-4}) - \frac{1}{z} \right] \\ & + 2y^{-2} \cos\theta \left[ \frac{1}{z}(2y^{-2} - y^{-4}) - z \right] \\ & \left. + 4(y^{-4} - y^{-2}) \cos\theta \cos\phi \right\}. \quad (18) \end{aligned}$$

The critical condition is now given by

$$\omega_4 = \tilde{\omega}_3 + \omega_1 + \omega_2$$

or, equivalently,

$$\cosh 2K = 2 \sinh^2 2K'. \quad (19)$$

For  $K=0$ , the lattice decomposes into two independent sublattices and the critical condition (19) reduces to (16). The deviation of other thermodynamic functions is also given in Appendix C. Here, as in the previous cases, the specific heat again possesses a logarithmic singularity in the critical region.

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**APPENDIX A**

The evaluation of the partition function (7) for the special case  $\Delta=0$  will now be given. For convenience, we define a set of four operators for each lattice site  $j$

$$\begin{aligned} A^1(j) &= a_{j-1}^{(1)}, & A^2(j) &= a_{j-m}^{(2)}, \\ A^3(j) &= a_j^{(1)\dagger}, & A^4(j) &= a_j^{(2)\dagger}. \end{aligned} \quad (A1)$$

With the help of Eq. (A1), (7) can be rewritten as, after setting  $H_1=0$ ,

$$Z_0 = \omega_1^N \langle o | T \left[ \exp \frac{1}{2} \sum_{j=1}^N \sum_p \sum_q K_{pq} A^p(j) A^q(j) \right] | o \rangle, \quad (A2)$$

where the summations over  $p$  and  $q$  extend from 1 to 4 and  $[K_{pq}]$  is a skew-symmetric matrix given by

$$[K_{pq}] = \begin{bmatrix} 0 & -\omega_8/\omega_1 & -\omega_4/\omega_1 & -\omega_5/\omega_1 \\ \omega_8/\omega_1 & 0 & -\omega_6/\omega_1 & -\omega_3/\omega_1 \\ \omega_4/\omega_1 & \omega_6/\omega_1 & 0 & -\omega_7/\omega_1 \\ \omega_5/\omega_1 & \omega_3/\omega_1 & \omega_7/\omega_1 & 0 \end{bmatrix}. \quad (A3)$$

Equation (A2) can be evaluated by the standard technique. After expanding the exponential and using the Wick's theorem to evaluate the vacuum expectation values, the following expression is obtained<sup>6</sup>:

$$N^{-1} \ln Z_0 = \frac{1}{2} \sum_{r=1}^N \ln \{ \det [\mathbf{I} - \mathbf{KA}] \} + \ln \omega_1. \quad (A4)$$

In Eq. (A4),  $\mathbf{I}$  is the identity matrix and  $\mathbf{A}$  is the Fourier transform of the lattice-ordered contraction matrix.

That is,

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & \omega^{-r} & 0 \\ 0 & 0 & 0 & \omega^{-mr} \\ -\omega^r & 0 & 0 & 0 \\ 0 & -\omega^{mr} & 0 & 0 \end{pmatrix},$$

where

$$\omega \equiv \exp(2\pi i/N). \quad (\text{A5})$$

Substitution of (A3) and (A5) into (A4) now leads to Eq. (8).

### APPENDIX B

In this Appendix we evaluate the partition function (7) by the perturbation technique. The method is essentially an extension of that given by Gibberd and Hurst.<sup>24</sup> First the expression (7) can be rewritten as

$$Z = \omega_1^N \langle o | T \sum_{n=0}^{\infty} \frac{1}{n!} [\sum_j H_1(j)]^n S(N) | o \rangle, \quad (\text{B1})$$

where

$$S(N) = \exp\left(\sum_{j=1}^N H_0(j)\right).$$

If we keep only the first term in (B1), then we have exactly (A2) which is the free-fermion approximation. The other terms in (B1) provide corrections to the free-fermion approximation in a power series in  $\Delta/\omega_1^2$ . For example, the first-order correction is

$$Z_1 = \omega_1^N \frac{\Delta}{\omega_1^2} \langle o | T \left( \sum_j A^4(j) A^3(j) A^2(j) A^1(j) S(N) \right) | o \rangle. \quad (\text{B2})$$

It is convenient to introduce the free one-particle Green's functions

$$G_0^{st}(u, v) \equiv \langle o | T A^s(u) A^t(v) S(N) | o \rangle / \langle o | T S(N) | o \rangle. \quad (\text{B3})$$

Following Gibberd and Hurst,<sup>24</sup> we can evaluate (B3) by making use of the linked-cluster theorem and thus obtain the  $4 \times 4$  matrix

$$\begin{aligned} [G_0^{st}(u, v)] &= N^{-1} \sum_{r=1}^N \omega^{r(u-v)} \mathbf{A} [\mathbf{I} - \mathbf{K}\mathbf{A}]^{-1} \\ &= N^{-1} \sum_{r=1}^N \omega^{r(u-v)} [G_0^{st}(r, \omega)], \end{aligned} \quad (\text{B4})$$

where  $G_0^{st}(r, \omega)$  is essentially the Fourier transform of  $G_0^{st}(u, v)$ . For completeness we now list all matrix elements

$G_0^{st}(r, \omega)$

$$\omega_1^3 D(r) G_0^{11}(r, \omega) = -\omega_1 \omega_6 \omega_7 (\omega^{-mr} - \omega^{mr}),$$

$$\begin{aligned} \omega_1^3 D(r) G_0^{12}(r, \omega) &= \omega_1^2 \omega_7 \omega^{(m-1)r} - \omega_1 \omega_3 \omega_7 \omega^{-r} - \omega_1 \omega_4 \omega_8 \omega^{mr} \\ &\quad + \omega_8 (\omega_3 \omega_4 - \omega_5 \omega_6 - \omega_7 \omega_8), \end{aligned}$$

$$\begin{aligned} \omega_1^3 D(r) G_0^{13}(r, \omega) &= (\omega_1^3 + \omega_1 \omega_2^2) \omega^{-r} - \omega_1^2 \omega_2 \omega^{-r} (\omega^{mr} + \omega^{-mr}) \\ &\quad + \omega_1^2 \omega_4 + \omega^{mr} \omega_1 (\omega_3 \omega_4 - \omega_5 \omega_6) \\ &\quad + \omega^{-mr} \omega_1 (\omega_3 \omega_4 - \omega_7 \omega_8), \end{aligned}$$

$$\begin{aligned} \omega_1^3 D(r) G_0^{14}(r, \omega) &= \omega_1^2 \omega_6 \omega^{-(1+m)r} - \omega_1 \omega_4 \omega_6 \omega^{-mr} \\ &\quad - \omega_1 \omega_3 \omega_6 \omega^{-r} + \omega_6 (\omega_3 \omega_4 - \omega_5 \omega_6 - \omega_7 \omega_8), \end{aligned}$$

$$\begin{aligned} \omega_1^3 D(r) G_0^{21}(r, \omega) &= \omega_7 (\omega_5 \omega_6 - \omega_3 \omega_4 + \omega_7 \omega_8) - \omega_1^2 \omega_7 \omega^{(1-m)r} \\ &\quad + \omega_1 \omega_4 \omega_7 \omega^{-mr} + \omega_1 \omega_2 \omega_7 \omega^r, \end{aligned}$$

$$\omega_1^3 D(r) G_0^{22}(r, \omega) = \omega_1 \omega_5 \omega_7 (\omega^{-r} - \omega^r),$$

$$\begin{aligned} \omega_1^3 D(r) G_0^{23}(r, \omega) &= \omega_1^2 \omega_5 \omega^{-(1+m)r} - \omega_1 \omega_2 \omega_5 \omega^{-r} \\ &\quad - \omega_1 \omega_4 \omega_5 \omega^{-mr} + \omega_5 (\omega_3 \omega_4 - \omega_5 \omega_6 - \omega_7 \omega_8), \end{aligned}$$

$$\begin{aligned} \omega_1^3 D(r) G_0^{24}(r, \omega) &= (\omega_1^3 + \omega_1 \omega_4^2) \omega^{-mr} - \omega_1^2 \omega_2 \\ &\quad + \omega_4 (\omega_5 \omega_6 + \omega_7 \omega_8 - \omega_3 \omega_4) \\ &\quad + \omega_1 (\omega_3 \omega_4 - \omega_5 \omega_6) \omega^r + \omega_1 (\omega_3 \omega_4 - \omega_7 \omega_8) \\ &\quad + \omega^{-r} - \omega_1^2 \omega_4 \omega^{-mr} (\omega^r + \omega^{-r}), \end{aligned} \quad (\text{B5})$$

$$\begin{aligned} \omega_1^3 D(r) G_0^{31}(r, \omega) &= -(\omega_1^3 + \omega_1 \omega_2^2) \omega^r + \omega_1^2 \omega_2 (\omega^{mr} + \omega^{-mr}) \\ &\quad - \omega^{-mr} \omega_1 (\omega_3 \omega_4 - \omega_5 \omega_6) \\ &\quad - \omega^{mr} \omega_1 (\omega_3 \omega_4 - \omega_7 \omega_8) \\ &\quad - \omega_3 (\omega_7 \omega_8 - \omega_3 \omega_4 + \omega_5 \omega_6) + \omega_1^2 \omega_4, \end{aligned}$$

$$\begin{aligned} \omega_1^3 D(r) G_0^{32}(r, \omega) &= -\omega_1^2 \omega_5 \omega^{(m+1)r} + \omega_1 \omega_4 \omega_5 \omega^{mr} \\ &\quad + \omega_1 \omega_2 \omega_5 \omega^r - \omega_5 (\omega_3 \omega_4 - \omega_5 \omega_6 - \omega_7 \omega_8), \end{aligned}$$

$$\omega_1^3 D(r) G_0^{33}(r, \omega) = -\omega_1 \omega_5 \omega_8 (\omega^{mr} - \omega^{-mr}),$$

$$\begin{aligned} \omega_1^3 D(r) G_0^{34}(r, \omega) &= -\omega_7 (\omega_5 \omega_6 - \omega_3 \omega_4 + \omega_7 \omega_8) - \omega_1 \omega_2 \omega_8 \omega^r \\ &\quad + \omega_1^2 \omega_8 \omega^{-(m-1)r} - \omega_1 \omega_4 \omega_8 \omega^{-mr}, \end{aligned}$$

$$\begin{aligned} \omega_1^3 D(r) G_0^{41}(r, \omega) &= -\omega_1^2 \omega_6 \omega^{(1+m)r} + \omega_1 \omega_4 \omega_6 \omega^{mr} \\ &\quad + \omega_1 \omega_2 \omega_6 \omega^r - \omega_6 (\omega_3 \omega_4 - \omega_5 \omega_6 - \omega_7 \omega_8), \end{aligned}$$

$$\begin{aligned} \omega_1^3 D(r) G_0^{42}(r, \omega) &= -\omega^{mr} (\omega_1^3 + \omega_1 \omega_4^2) + \omega_1^2 \omega_4 \omega^{mr} (\omega^r + \omega^{-r}) \\ &\quad + \omega_1^2 \omega_2 - \omega^r \omega_1 (\omega_3 \omega_4 - \omega_7 \omega_8) \\ &\quad - \omega_4 (\omega_5 \omega_6 + \omega_7 \omega_8 - \omega_3 \omega_4) \\ &\quad - \omega_1 (\omega_3 \omega_4 - \omega_5 \omega_6) \omega^{-r}, \end{aligned}$$

$$\begin{aligned} \omega_1^3 D(r) G_0^{43}(r, \omega) &= -\omega_1^2 \omega_8 \omega^{(m-1)r} + \omega_1 \omega_4 \omega_8 \omega^{mr} \\ &\quad + \omega_1 \omega_2 \omega_8 \omega^{-r} + \omega_8 (\omega_5 \omega_6 + \omega_7 \omega_8 - \omega_3 \omega_4), \end{aligned}$$

$$\omega_1^3 D(r) G_0^{44}(r, \omega) = -\omega_1 \omega_5 \omega_8 (\omega^{-r} - \omega^r),$$

where

$$D(r) \equiv \det(\mathbf{I} - \mathbf{K}\mathbf{A}).$$

From Eq. (B4) we observe the translational invariance of  $G_0^{st}(u, v)$  and write

$$G_0^{st}(u-v) \equiv G_0^{st}(u, v). \quad (\text{B6})$$

<sup>24</sup>R. W. Gibberd and C. A. Hurst, J. Math. Phys. 8, 1427 (1967).

With these notations and the general relation

$$\begin{aligned} & \langle o|TA^4(j)A^3(j)A^2(j)A^1(j)S(\infty)|o\rangle \\ &= \langle o|TA^4(j)A^3(j)S(\infty)|o\rangle\langle o|TA^2(j)A^1(j)S(\infty)|o\rangle \\ & \quad - \langle o|TA^4(j)A^2(j)S(\infty)|o\rangle\langle o|TA^3(j)A^1(j)S(\infty)|o\rangle \\ & \quad + \langle o|TA^3(j)A^2(j)S(\infty)|o\rangle\langle o|TA^4(j)A^1(j)S(\infty)|o\rangle, \end{aligned} \quad (\text{B7})$$

the first order correction (B2) can be written as (in the limit  $N \rightarrow \infty$ )

$$Z_1 = NZ_0^2(\Delta/\omega_1^2)[G_0^{43}(0)G_0^{21}(0) - G_0^{42}(0)G_0^{31}(0) + G_0^{32}(0)G_0^{41}(0)]. \quad (\text{B8})$$

Similar expressions can be written for higher-order corrections. Therefore, the partition function (7) is now given by a power series in  $\Delta/\omega_1^2$  with the coefficients expressed in terms of the one-particle Green's functions.

In the thermodynamic limit, all the one-particle Green's functions are expressible in terms of double integrals with  $D(r)$  appearing in the denominator of the integrands. As in the consideration of  $Z_0$ , the singularity of these integrals is determined by the zero of the expression  $D(r)$ . Therefore, a collection of finite terms in the perturbation expansion will not modify in any way the singularity of the partition function  $Z_0$ . Any significant modification would have to come from the summation or a partial summation of the expansion series, which is a subject still remaining to be investigated.

### APPENDIX C

This Appendix is devoted to the evaluation of the thermodynamic functions for the Ising model under the free-fermion approximation. The free energy per spin  $f_{\text{approx}}$  has been computed and was given by (14) and (18). The evaluation of the energy  $E$  from these expressions is then straightforward, although tedious, and upon which we shall now proceed.

The expression for the energy per spin is

$$E = -\frac{\partial}{\partial \beta}(\beta f_{\text{approx}}) = C + \frac{1}{8\pi^2} \int_0^{2\pi} d\theta \int_0^{2\pi} d\phi \frac{a+b \cos\theta}{d+e \cos\theta}, \quad (\text{C1})$$

where for the ferromagnetic and antiferromagnetic cases ( $-|J| < 2J'$ )

$$C = -4(|J| + J'),$$

$$\begin{aligned} a = 4|J| \{ & 2(2z^2y^2 - z^2y^4)^2 + 2z^2y^4 \\ & + \cos\phi(6z^3y^4 - 3z^3y^6 - zy^2) \} + 8J' \{ (2z^2y^2 - z^2y^4)^2 \\ & - z^2y^4(2z^2y^2 - z^2y^4 - 2) + \cos\phi(4z^3y^4 - 3z^3y^6 - z^2y^2) \}, \end{aligned}$$

$$\begin{aligned} b = 4|J| \{ & 6z^3y^4 - zy^2 - 3z^3y^6 - \cos\phi(4z^2y^2 - 4z^2y^4) \\ & + 8J' \{ 4z^3y^4 - 2zy^2 - 3z^3y^6 - \cos\phi(2z^2y^2 - 4z^2y^4) \}, \end{aligned}$$

$$d = 1 + 2z^2y^4 + (2z^2y^2 - z^2y^4)^2 + 2z^2y^2(2z^2y^2 - z^2y^4 - 1) \cos\phi,$$

$$e = 2zy^2(2z^2y^2 - z^2y^4 - 1) - 4z^2y^2(1 - y^2) \cos\phi,$$

and for the superantiferromagnetic case ( $-|J| > 2J'$ )

$$C = 2J',$$

$$\begin{aligned} a = 4|J| \left\{ \left( z^2y^4 - \frac{y^{-4}}{z^2} \right) + \cos\phi y^{-2} \left[ z(2y^2 - y^{-4}) + \frac{1}{z} \right] \right\} \\ - 8J' \left\{ \left( z^2y^4 + \frac{y^{-4}}{z^2} + 4y^{-4} + 2y^{-8} - 6y^{-6} \right) \right. \\ \left. + \cos\phi y^{-2} \left[ z(4y^2 - 3y^{-4}) - \frac{1}{z} \right] \right\}, \end{aligned}$$

$$\begin{aligned} b = 4|J| \left\{ -y^{-2} \left( \frac{1}{z} [2y^2 - y^{-4}] + z \right) \right\} \\ + 8J' \left\{ y^{-2} \left( z - \frac{1}{z}(4y^2 - 3y^{-4}) \right) + 2y^{-2} \cos\phi(1 - 2y^2) \right\}, \end{aligned}$$

$$\begin{aligned} d = 1 + z^2y^4 + \frac{y^{-4}}{z^2} + (2y^2 - y^{-4})^2 \\ + 2y^{-2} \cos\phi \left[ z(2y^2 - y^{-4}) - \frac{1}{z} \right], \end{aligned}$$

$$e = 2y^{-2} \left[ \frac{1}{z}(2y^2 - y^{-4}) - z \right] - 4y^{-2}(1 - y^2) \cos\phi.$$

In these expressions we have  $z = e^{-2|K|}$ .

The  $\theta$  integration can be performed by the use of the following integration formula:

$$\int_0^{2\pi} d\theta \frac{a+b \cos\theta}{d+e \cos\theta} = 2\pi \frac{b}{e} + 2\pi \left( a - \frac{bd}{e} \right) \frac{\theta(d^2 - e^2)}{(d^2 - e^2)^{1/2}}, \quad (\text{C2})$$

where

$$\begin{aligned} \theta(x) &= 1, \quad x > 0 \\ &= 0, \quad x < 0. \end{aligned}$$

A phase transition occurs at  $d^2 - e^2 = 0$ . (C3)

We note that the remaining  $\phi$  integral now contains two terms, one involving the square root of a quadratic form in  $\cos\phi$  and one free from the square root. The term free from the square root can be integrated and expressed in terms of trigonometric functions while the one involving the square root, i.e., the second term in (C2), gives rise to the elliptical integrals after suitable transformations. We now carry out the  $\phi$  integration.

(i) For the ferromagnetic and the antiferromagnetic cases (with  $J \rightarrow |J|$ ), the quadratic form in  $\cos\phi$  inside the square root sign is

$$d^2 - e^2 = S(\cos\phi - A)(\cos\phi - B), \quad (\text{C4})$$



where

$$\begin{aligned} S &\equiv 4u^2(1-u^2)(1-z^2r^2), \\ A &\equiv (1-u)/2u(1+zr) + u(1+zr)/2(1-u), \\ B &\equiv (1+u)/2u(1-zr) + u(1-zr)/2(1+u), \end{aligned} \quad (C5)$$

with

$$\begin{aligned} u &\equiv zy^2, & r &\equiv 2-y^2, \\ s &\equiv 1-y^2, & t &\equiv 1-2y^2. \end{aligned} \quad (C6)$$

It is possible to satisfy (C3) only for  $A=1$ , which leads to the critical condition (17).

The transformation into the variable

$$\omega = (\cos\phi - x)/(1 - x \cos\phi) \quad (C7)$$

with

$$\begin{aligned} x &\equiv 2u/(1-zur), & T < T_c \\ &\equiv (1-zur)/2u, & T > T_c \end{aligned}$$

then leads to the following:

$$\begin{aligned} \int_0^{2\pi} d\phi (d^2 - e^2)^{-1/2} &= \frac{k}{zu} K(k), & T < T_c \\ &= \frac{1}{zu} K(k^{-1}), & T > T_c; \\ \int_0^{2\pi} d\phi \cos\phi (d^2 - e^2)^{-1/2} &= \frac{k}{xzu} K(k) - \frac{k(1-x)}{xzu} \Pi(-x^2, k), & T < T_c \\ &= \frac{1}{xzu} K(k^{-1}) - \frac{(1-x^2)}{xzu} \Pi(-x^2, k^{-1}), & T > T_c; \\ \int_0^{2\pi} d\phi (1+v \cos\phi)^{-1} (d^2 - e^2)^{-1/2} &= \frac{kx}{(v+x)zu} K(k) + \frac{vk(1-x^2)}{zu(1+vx)^2 m} \Pi(-m^2, k), & T < T_c \\ &= \frac{x}{(v+x)zu} K(k^{-1}) + \frac{v(1-x^2)}{zu(1+vx)^2 m} \Pi(-m^2, k^{-1}), & T > T_c; \end{aligned}$$

where

$$\begin{aligned} k &\equiv 4zu[(1+zur)^2 - 4zu]^{-1}, \\ v &\equiv 2(z-u)(1-zur)^{-1}, \\ m &\equiv (v+x)(1+vx)^{-1}, \end{aligned}$$

and  $K, \Pi$  are, respectively, the complete elliptical integrals of the first and third kinds defined by:

$$K(k) = \int_0^{\pi/2} (1 - k^2 \sin^2\theta)^{-1/2} d\theta, \quad \Pi(n, k) = \int_0^{\pi/2} (1 + n \sin^2\theta)^{-1} (1 - k^2 \sin^2\theta)^{-1/2} d\theta.$$

With these formulas, we find

$$\begin{aligned} E_{T < T_c} &= -2|J| + 2J' \left( \frac{t}{s} - 2 \right) + \frac{v}{8zs(1-v^2)^{1/2}} \left[ 4|J|(1+zru) + 8J'(2zu - 1 - u^2r)/s \right] \\ &+ \left[ 4|J| \left( 2zur^2 + 2y^2 - \frac{3ut}{v} + \frac{1}{zv} - \frac{4}{ks} \right) + 8J' \left( zur^2 - u^2r + y^2 - \frac{u}{v} + \frac{3us}{v} + 2zv - \frac{2t}{ks^2} \right) \right] kK(k) \\ &+ \left[ 4|J|(1-zyr) + 8J' \left( 2ur - \frac{1}{z} - uy^2 + \frac{2t}{v} \right) \right] \left[ kK(k) - k \frac{1-x^2}{x} \Pi(-x^2, k) \right], \\ &+ \left[ \frac{16|J|}{k(1-zur)} + 16J' \left( \frac{u^2(1+3s)+1}{ks(1-zur)} + \frac{2t}{ks^2} \right) \right] \left[ \frac{kx}{v+x} K(k) + \frac{kv(1-x^2)}{(1+vx)^2 m} \Pi(-m^2, k) \right], \end{aligned} \quad (C8)$$

$$E_{T > T_c} = E_{T < T_c} \text{ with } kK(k) \rightarrow K(k^{-1}) \text{ and } k\Pi(-m^2, k) \rightarrow \Pi(-m^2, k^{-1}).$$

(ii) For the superantiferromagnetic case, it is convenient to introduce

$$u \equiv zy^{-2}, \quad r \equiv 2 - y^{-2}, \quad s \equiv 1 - y^{-2}, \quad t \equiv 1 - 2y^{-2}.$$

Again we find

$$d^2 - e^2 = S(\cos\phi - A)(\cos\phi - B)$$

but with

$$\begin{aligned} S &\equiv 4z^{-4}u^2(1-u^2)(1-z^2r^2), \\ A &\equiv z^2(1-u)/2u(1+zr) + u(1+zr)/2(1-u)z^2, \\ B &\equiv z^2(1+u)/2u(1-zr) + u(1-zr)/2(1+u)z^2. \end{aligned}$$

The phase transition occurs at  $A = 1$ , which is identical with the condition (19). The transformation (C7) is used again but with a different definition for  $x$

$$\begin{aligned} x &\equiv \frac{2(u + 2u^2 - u^2y^{-2})}{z^2 + y^{-4} - z^2u^2 - 4u^2 - u^4 + 4zu^3}, \quad T < T_c \\ &\equiv \frac{z^2 + y^{-4} - z^2u^2 - 4u^2 - u^4 + 4zu^3}{2(u + 2u^2 - u^2y^{-2})}, \quad T > T_c. \end{aligned}$$

The following formulas are used:

$$\begin{aligned} \int_0^{2\pi} d\phi (d^2 - e^2)^{-1/2} &= ky^2K(k), \quad T < T_c \\ &= y^2K(k^{-1}), \quad T > T_c; \\ \int_0^{2\pi} d\phi \cos\phi (d^2 - e^2)^{-1/2} &= \frac{ky^2}{x}K(k) - \frac{ky^2(1-x^2)}{x}\Pi(-x^2, k), \quad T < T_c \\ &= \frac{y^2}{x}K(k^{-1}) - \frac{y^2(1-x^2)}{x}\Pi(-x^2, k^{-1}), \quad T > T_c; \\ \int_0^{2\pi} d\phi (1+v\cos\phi)^{-1}(d^2 - e^2)^{-1/2} &= \frac{ky^2x}{(v+x)}K(k) + \frac{kv(1-x^2)}{(1+vx)^2m}\Pi(-m^2, k), \quad T < T_c \\ &= \frac{y^2x}{(v+x)}K(k^{-1}) + \frac{v(1-x^2)}{(1+vx)^2m}\Pi(-m^2, k^{-1}), \quad T > T_c; \end{aligned}$$

where

$$\begin{aligned} k &\equiv 4zu(z^2 + 4z^2y^{-4} + z^2y^{-8} - 4z^2y^{-6} - z^4y^{-4} - y^{-4})^{-1}, \\ v &\equiv 2zs(z^2 - y^{-2}r)^{-1}. \end{aligned}$$

The expression for the energy is then

$$\begin{aligned} E_{T < T_c} &= 2J' + \frac{4J'zt}{v(y^{-2}r - z^2)} + \frac{-|J|(z^2 + yr)v + 2J'(vz^2 - t - vy^{-2} - 3svy^{-2})}{(y^{-2}r - z^2)(1-v^2)^{1/2}} + \left\{ 4|J| \left[ y^{-2}(1+z^4) - \frac{(y^{-2}+z^2)(z^2y^{-2}r-1)}{2sz^2} \right] \right. \\ &\quad \left. - 8J' \left[ y^{-2}(1+z^4) + 2y^{-2}sr + \frac{2t}{ks^2} + \frac{(y^{-2}+3sy^{-2}-z^2)(zur-1)}{2sz^2} \right] \right\} \frac{kK(k)}{z^2} \\ &\quad + \left\{ 4|J|(zur+1) - 8J' \left[ zu(1+3s) - 1 + \frac{t(1-zur)}{s} \right] \right\} \left[ \frac{kK(k)}{xz} - \frac{(1-x^2)k}{xz}\Pi(-x^2, k) \right] \\ &\quad + \left\{ 4|J| \left( \frac{2(y^{-2}r+z^2)}{ks(z^2-y^{-2}r)} \right) - 8J' \left[ \frac{2(z^2-y^{-2}-3sy^2)}{ks(y^{-2}r-z^2)} + \frac{2t}{s^2} \right] \right\} \left[ \frac{kxK(k)}{(v+x)} + \frac{vk(1-x^2)}{(1+vx)^2m}\Pi(-m^2, k) \right], \quad (C9) \end{aligned}$$

$E_{T > T_c} = E_{T < T_c}$  with  $kK(k) \rightarrow K(k^{-1})$  and  $k\Pi(-m^2, k) \rightarrow \Pi(-m^2, k^{-1})$ .

From (C8) and (C9) we find that the coefficients of the elliptical integrals all vanish at  $T_c$  which renders continuity in the internal energy at the critical point. To investigate the nature of the singularity of the specific heat, we note that the asymptotic expression for the energy as  $T \rightarrow T_c^\pm$  is

$$E \rightarrow M(y,z)K(k),$$

where  $M(y,z)$  is regular in  $T$  and vanishes identically at  $T_c$ . The specific heat then takes the following asymptotic expression:

$$C \rightarrow \frac{dM}{dT}K(k) + M \frac{d}{dT}K(k).$$

The second term on the right-hand side is finite at  $T_c$ . Therefore, the singular behavior of  $C$  is due entirely to the first term. It can be shown that  $dM/dT$  is regular

at  $T_c$ . It follows that the singularity of the specific heat arises from that of the elliptical integral  $K$  and is logarithmic, as is understood for the usual Ising model.

*Note added in manuscript.* (1). Professor C. Domb has kindly called our attention to an earlier paper [C. Domb and R. B. Potts, Proc. Roy. Soc. **A210**, 125 (1951)], in which some of the results of Sec. II have been discussed from the point of view of the method of transfer matrix. Their approximation for the equivalent neighbor model yields  $e^{-2K} = \frac{1}{3}(\sqrt{10}-1) = 0.72076$  for the transition temperature as compared to the value 0.68946 of the present paper and the presumably exact Padé value 0.6837.

(2). We also received a preprint by N. W. Dalton and D. W. Wood in which the Padé analysis of Ising model with higher neighbor interactions of Ref. 8 is extended to include the low-temperature expansions as well as models with nonequivalent higher neighbors.

## Exact Solution for a Linear Chain of Isotropically Interacting Classical Spins of Arbitrary Dimensionality\*

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The isotropic Hamiltonian  $\mathcal{H}^{(\nu)} = -J \sum_{j=1}^{N-1} \mathbf{S}_j \cdot \mathbf{S}_{j+1}$  is considered for an open linear chain of  $N$   $\nu$ -dimensional vector spins  $\mathbf{S}_j$ ;  $\mathcal{H}^{(\nu)}$  reduces to the  $S = \frac{1}{2}$  Ising, planar, and Heisenberg models for  $\nu = 1, 2$ , and 3. The thermodynamic properties (including the susceptibility) of  $\mathcal{H}^{(\nu)}$  are found for ferromagnetic ( $J > 0$ ) and antiferromagnetic ( $J < 0$ ) exchange interactions for all temperatures  $T$  and all spin dimensionalities  $\nu$ . The manner in which the various properties depend upon  $T$  and  $\nu$  is studied; in particular we find (a) that although the chain of spins does not display long-range order except at  $T = 0$  for any value of  $\nu$ , most of the properties vary monotonically with  $\nu$  (in such a way that, e.g., the degree of "short-range order" decreases with increasing  $\nu$ ); and (b) that as the spin dimensionality increases without limit, all of the calculated properties approach precisely those predicted by the Berlin-Kac spherical model.

### I. INTRODUCTION

THERE exist comparatively few nontrivial statistical mechanical models which have been solved exactly in more than one dimension.<sup>1</sup> One motivation

for considering exactly soluble one-dimensional models is that their solutions may possibly aid in judging the validity of approximation techniques which are used in three dimensions.<sup>2</sup> A second motivation is that results discovered for one-dimensional models are sometimes generalizable to higher dimensionalities. Finally, a one-dimensional model may serve as a reasonable approximation to some special physical system. For example, there exist materials in which the magnetic ions may be considered to form "linear chains" so that interactions between spins within the chains are ap-

\* A different derivation of the partition function is presented in H. E. Stanley, Proceedings of the 1968 IUPAP Conference on Statistical Mechanics, Kyoto, J. Phys. Soc. Japan (to be published).

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<sup>1</sup> Two notable examples are the two-dimensional Ising model in zero field [L. Onsager, Phys. Rev. **65**, 117 (1944)] and, more recently, the various two-dimensional "ferroelectric" models [see, e.g., E. H. Lieb, 1968 Boulder Lectures in Theoretical Physics (to be published)]. For a comprehensive introduction to exactly soluble models of interacting particles in one-dimension, see E. H. Lieb and D. C. Mattis, *Mathematical Physics in One Dimension* (Academic Press Inc., New York, 1966).

<sup>2</sup> For example, many approximation schemes (such as extrapolation from high-temperature expansions) have been tested on the Ising model for one-dimensional and two-dimensional lattices.