

## Numerical evaluations of the critical properties of the two-dimensional Ising model\*

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Scaling transformations are used in numerical calculations of the properties of the two-dimensional Ising model near its critical point. When compared with the exact Onsager solution, the best approximation is seen to lead to 1 part in  $10^4$  accuracy for the two largest scaling indices. This rather accurate calculation is obtained by utilizing a scaling transformation which depends upon a parameter. The parameter is set by demanding that two different evaluations of the magnetic eigenvalue agree with one another. One evaluation is found via the standard eigenvalue method; the other comes from a consistency condition for the spin-spin correlation function. This condition may also be used to distinguish scaling eigenvalues from other eigenvalues.

### I. CONCEPTUAL BASIS OF THE CALCULATION

#### A. Setting up the problem

Recently, several different groups<sup>1-4</sup> have performed numerical calculations of the critical properties of spins on lattices by the direct calculation of approximate scaling transformations. In this application of the renormalization-group method,<sup>5-7</sup> one starts from a functional of all the spins in the system  $Z\{\sigma\}$ . One defines a transformation of this partition functional to a new set of spin variables  $\mu_{\vec{r}}$  on a lattice with a lattice constant larger by a factor of  $l$ . This transformation is of the form

$$Z'\{\mu\} = \sum_{\{\sigma\}} T\{\mu, \sigma\} Z\{\sigma\}. \quad (1.1)$$

Here the transformation matrix  $T$  is limited by the condition that the partition function be invariant under the scaling transform, i. e., that

$$Z = \sum_{\{\sigma\}} Z\{\sigma\} = \sum_{\{\mu\}} Z'\{\mu\}. \quad (1.2)$$

Condition (1.2) will be satisfied automatically if  $T$  obeys

$$\sum_{\{\mu\}} T\{\mu, \sigma\} = 1. \quad (1.3)$$

This condition, in turn, will be satisfied if  $T$  is a product over all sites of the  $\mu$  lattice of the form<sup>8</sup>

$$T\{\mu, \sigma\} = \prod_{\vec{r}'} \frac{1}{2} (1 + \mu_{\vec{r}'} t_{\vec{r}'}\{\sigma\}). \quad (1.4)$$

In using the transformation method, one parametrizes  $Z\{\sigma\}$  by writing it as a function of a group of coupling constants  $K_i$ . These coupling constants include a magnetic field term, nearest-neighbor interactions, next-neighbor, four-spin terms, etc. They appear in  $Z\{\sigma\}$  in the form

$$Z\{\sigma\} = \exp \sum_i K_i S_i\{\sigma\}. \quad (1.5)$$

Here the  $S_i$  are extensive functions of the  $\sigma$ 's. In general they may be represented as a sum over lattice sites of the form

$$S_i = \sum_{\vec{r}} s_i(\vec{r}). \quad (1.6)$$

For example,  $s_1$  might be  $\sigma_r$  or  $s_2$  might be a product of neighboring spins, etc.

In these terms, the transformation (1.1) can be considered to be a transformation upon the  $K_i$ 's of the form

$$K_i' = R_i(\vec{K}) \quad (1.7)$$

The fixed point is identified as a special set of  $K$ 's called  $\vec{K}^*$ , for which the transformation leaves  $K_i$  invariant,

$$K_i^* = R_i(\vec{K}^*). \quad (1.8)$$

This fixed point is identified with the critical point.

In numerical applications, an approximate form of  $R_i(\vec{K})$  is found, and the fixed point located. Then the properties of small deviations from the fixed point

$$K_i = K_i^* + h_i, \quad h_i \ll 1, \quad (1.9)$$

are investigated by evaluating the matrix  $b_{ij}$  defined by

$$h_i' = K_i' - K_i^* = \sum_j b_{ij} h_j. \quad (1.10)$$

The eigenvalues and eigenstates of  $b_{ij}$  are found. We indicate these by the notation

$$\begin{aligned} \sum_j b_{ij} u_j^\alpha &= u_i^\alpha b^\alpha, \\ \sum_i v_i^\alpha b_{ij} &= v_i^\alpha b^\alpha. \end{aligned} \quad (1.11)$$

#### B. Interpretation of eigenstates and eigenvalues

The eigenstates and eigenvalues defined by Eqs. (1.11) have a very direct physical interpretation. The eigenvalues, when written in the form

$$b^\alpha = l^{\nu\alpha}, \tag{1.12}$$

give the scaling indices directly. For example, the largest relevant odd- and even-spin eigenvalues can be directly interpreted in terms of the standard critical indices as

$$\begin{aligned} y_\alpha &= 1/\nu \quad (\text{even-spin}), \\ y_\alpha &= d - \beta/\nu \quad (\text{odd-spin}), \end{aligned} \tag{1.13}$$

with  $d$  being the dimensionality. Notice that the results (1.13) are supposed to be independent of the choice of scaling transformation.

Furthermore, the eigenstates can also be given a direct interpretation. From the right eigenstate, we can form the eigenoperator

$$s_\alpha(\vec{r}) = \sum_i u_i^\alpha s_i(\vec{r}). \tag{1.14}$$

The correlation function for these eigenoperators then has the simple scaling properties

$$\langle s_\alpha(\vec{r}) s_\beta(0) \rangle_{\vec{K}=\vec{K}^*} = A_{\alpha\beta}(\vec{r}/r) / r^{2d-y_\alpha-y_\beta}$$

for large  $r$ . The concept of conformal invariance indicates that  $A_{\alpha\beta}$  should be diagonal. Thus, this equation simplifies to the form

$$\langle s_\alpha(\vec{r}) s_\beta(0) \rangle_{\vec{K}=\vec{K}^*} = A_\alpha \delta_{\alpha\beta} / r^{2(d-y_\alpha)}. \tag{1.15}$$

In general  $A_\alpha$  will be nonvanishing for the relevant operators of the theory, but will vanish for the so-called "scaling" operators.<sup>9</sup>

Equations (1.14) and (1.15) enable us to write an asymptotic form for the correlation function  $\langle s_i(\vec{r}) s_j(0) \rangle$ . Equation (1.14) may be inverted to give

$$s_i(\vec{r}) = \sum_\alpha v_i^\alpha s_\alpha(\vec{r}), \tag{1.16}$$

so that

$$\langle s_i(\vec{r}) s_j(0) \rangle_{K^*} = \sum_{(\text{relevant})} (v_i^\alpha)^2 \frac{A_\alpha}{r^{2(d-y_\alpha)}} \tag{1.17}$$

for  $r \rightarrow \infty$ .

C. Examples of scaling transformations

In this paper, we shall discuss three specific examples of scaling transformations:

(i) Decimation. The new lattice  $r'$  is chosen to include half the sites on the old lattice, as indicated in Fig. 1. Then  $l = \sqrt{2}$ . On the new lattice, the new spins  $\mu_{r'}$  are chosen to be exactly equal to  $\sigma_{r'}$ . The remaining  $\sigma$ 's are summed over. Thus

$$t_{r'}\{\sigma\} = \sigma_{r'}. \tag{1.18}$$

(ii) Block transformation. As shown in Fig. 2, each  $\mu_{r'}$  appears in the midst of a block of four spins. Once again the increase in lattice constant  $l$  is  $\sqrt{2}$ . We choose

$$t_{r'} = \tanh \bar{K}(\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4), \tag{1.19}$$

where the four  $\sigma$ 's are those immediately surrounding the block.<sup>8</sup>

(iii) Second block transformation. The  $\mu$ 's are further spaced out, as shown in Fig. 3. Now  $l$  equals 2. We choose  $t_{r'}$  once again to have the form (1.19). This transformation can be considered to be simply the composition of the previous two.

D. Dependence upon  $\bar{K}$

According to the theory,  $y_\alpha$  should not depend on  $\bar{K}$ . Let us jump ahead and look at the results of our approximate recursion calculation to see whether this independence is indeed realized. Figure 4 plots the values of  $1/\nu$  and  $\beta$  determined from Eq. (1.13) and our most successful transformation, the second block transformation. The details of the approximation method will be developed in Secs. II and III. For now, the important point is to note that the calculated eigenvalues do appear to be roughly constant over a whole range of  $\bar{K}$ , but that some  $\bar{K}$  dependence is indeed present. It would be helpful to be able to choose some particular value of  $\bar{K}$  as "better" than the others. In some sense, this could be the value of  $\bar{K}$  for which the approximations for  $R_i(\bar{K})$  were more accurate than for other values.

For this reason, we seek another equation to determine  $\beta/\nu$ . If we can obtain an independent evaluation of this quantity, we can then compare this result with the eigenvalue. Presumably the "best" value of  $\bar{K}$  would be the one for which these quantities were most nearly equal.

E. Correlation-function determination of  $y_\alpha$

To develop this second equation for  $y_\alpha$ , we calculate the  $\mu$ - $\mu$  correlation function as

$$\langle \mu_{r'} \mu_0 \rangle_{K'} = \sum_{\{\mu\}} \mu_{r'} \mu_0 Z'\{\mu\} / \sum_{\{\mu'\}} Z'\{\mu'\}.$$

From the definitions (1.1)-(1.4) of the transformation, it immediately follows that this correlation function can also be expressed as

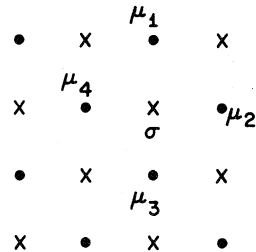


FIG. 1. Decimation transformation.  $l = \sqrt{2}$ ;  $\times = \sigma_{r'}$ ,  $\bullet = \mu_{r'}$ , and  $\sigma_{r''}$ .

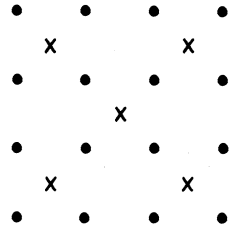


FIG. 2. Block transformation.  $l=\sqrt{2}$ ;  $\times = \mu_r$ ;  $\bullet = \sigma_r$ .

$$\langle \mu_r, \mu_0 \rangle_{K'} = \langle t_r, \{\sigma\} t_0 \{\sigma\} \rangle_K; \tag{1.20}$$

now,  $t_r$  and  $\mu_r$  can be written in terms of the basic objects  $s_i(r)$ . Let us define  $s_1(r)$  to be just the spin variable

$$\mu_r = s_1(\vec{r}'). \tag{1.21}$$

Then for decimation transformation

$$t_r \{\sigma\} = \sigma_r = s_1(\vec{r}'), \tag{1.22}$$

while for the block transformations

$$\begin{aligned} t_r \{\sigma\} &= \tanh \bar{K} (\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4) \\ &= \frac{1}{4} w_+ (\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4) \\ &\quad + \frac{1}{4} w_- (\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4) \sigma_1 \sigma_2 \sigma_3 \sigma_4, \end{aligned}$$

with

$$w_{\pm} = \frac{1}{2} (\tanh 4\bar{K} \pm 2 \tanh 2\bar{K}). \tag{1.23a}$$

The  $\sigma$ 's lie at the points immediately surrounding the  $\mu$ . If we define  $s_2(\vec{r})$  to be a product of three neighboring  $\sigma$ 's, e.g.,  $\sigma_1 \sigma_2 \sigma_3$ , we can write the result for the block transformation

$$t_r \{\sigma\} = w_+ s_1(\vec{r}') + w_- s_2(\vec{r}'). \tag{1.24}$$

Then, both transforms may be represented by (1.24) if we define

$$w_+ = 1, \quad w_- = 0 \tag{1.23b}$$

for decimation.

Now apply Eq. (1.20) at the fixed point. From (1.20) and (1.24) it follows that

$$\langle s_1(\vec{r}') s_1(0) \rangle_{K^*}$$

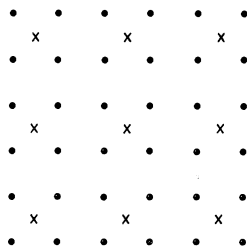


FIG. 3. Second block transformation.  $l=2$ ;  $\times = \mu_r$ ,  $\bullet = \sigma_r$ .

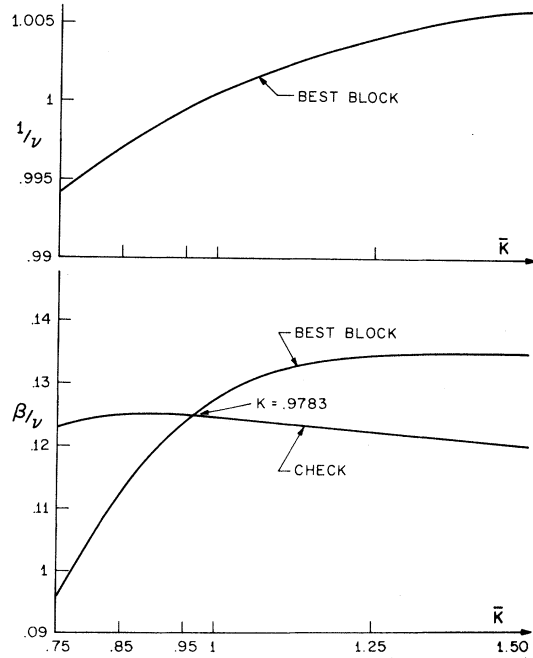


FIG. 4. Even-spin eigenvalue  $1/\nu$  and odd-spin eigenvalue  $\beta/\nu$  as obtained from the second block transformation, plotted as a function of the parameter  $\bar{K}$ . The curve labeled "check" gives the value of  $\beta/\nu$  obtained from Eq. (1.26); the curves intersect at a value of  $\bar{K} = 0.9783$ , at which point  $\beta/\nu = 0.12447$ .

$$= \langle [w_+ s_1(l\vec{r}') + w_- s_2(l\vec{r}')] [w_+ s_1(0) + w_- s_2(0)] \rangle_{K^*}. \tag{1.25}$$

Next, go to the limit of large  $r$  and apply Eq.

(1.17). Equation (1.25) becomes

$$\sum_{\alpha} \frac{A_{\alpha}}{(r/l)^{2(d-\gamma_{\alpha})}} (v_1^{\alpha})^2 = \sum_{\alpha} \frac{A_{\alpha} (v_1^{\alpha} y + v_2^{\alpha} y_-)^2}{r^{2(d-\gamma_{\alpha})}}, \tag{1.26}$$

with  $r = r'l$ . For all relevant eigenvalues,  $A_{\alpha} \neq 0$ . If there is no degeneracy,  $\gamma_{\alpha} \neq \gamma_{\beta}$ , then we can consider (1.26) to be true term by term in  $\alpha$ . This can be true if and only if

$$l^{d-\gamma_{\alpha}} = w_+ + (v_2^{\alpha}/v_1^{\alpha}) w_-. \tag{1.27}$$

Equation (1.27) is our second equation for the eigenvalue  $\gamma_{\alpha}$ . It holds for all relevant eigenvalues, but not for the scaling eigenvalues.

F. Results for eigenvalues

Let us look at the results of our calculations once more. Equation (1.27) may be used to obtain an additional determination of the odd-spin eigenvalue. Our pair of determinations was plotted in Fig. 4 and the difference curve is given in Fig. 5. The eigenvalues are identical at  $\bar{K} = 0.9783$  and have the value

$$\beta/\nu = 0.12447 \tag{1.28a}$$

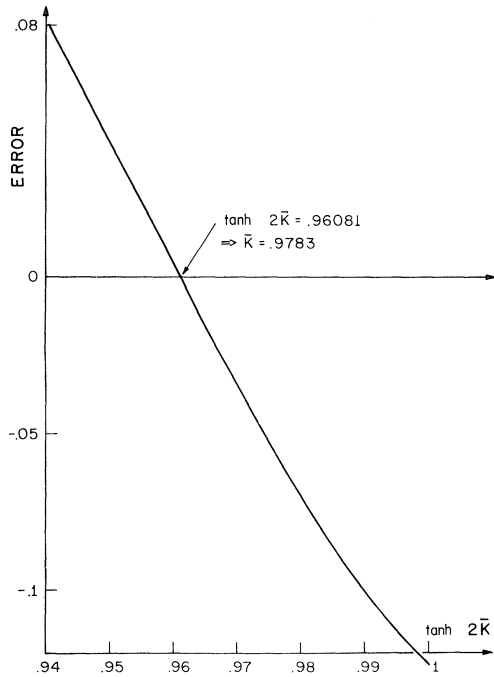


FIG. 5. Difference curve,  $(\beta/\nu)_{\text{check}} - (\beta/\nu)/(\beta/\nu)_{\text{check}}$  plotted as a function of  $\tanh 2\bar{K}$ . The two determinations of  $\beta/\nu$  are identical at  $\bar{K} = 0.9783$ .

at this point. Here  $1/\nu$  from Fig. 4 has the value

$$1/\nu = 0.999964 . \tag{1.28b}$$

These should be compared with the exact (Onsager-solution) values 0.125 and 1.0. The comparison is obviously more than satisfactory.

We conclude that the trick of adjusting  $\bar{K}$  improves immensely the accuracy of our calculational method.

All results so far have been taken from the second block transformation, which is essentially the composition of the first block transformation and a decimation.

Notice that Eq. (1.27) gives nonsense for the decimation transformation. Since  $w_+$  and  $w_-$  are, respectively, 1 and 0 for this case, we find

$$l^{d-\nu} \alpha = 1,$$

or perhaps

$$\nu_1^\alpha = 0 .$$

In either case, we cannot make much sense of our procedure. We therefore drop the pure decimation transformation as having at best a complex relationship with the physics of the two-dimensional Ising model.

On the other hand, the first block transformation does make sense. The results of this transformation are plotted in Fig. 6. Clearly this is a worse

approximation than the second block transformation. The indices are more dependent upon  $\bar{K}$ , i.e., the approximation method, and the two evaluations of  $\beta/\nu$  never intersect. However, we can choose the best value of  $\bar{K}$  as the one which minimizes the difference between these evaluations. At this value we get

$$\begin{aligned} 1/\nu &= 1.03 , \\ \beta/\nu &= 0.10 \text{ from eigenvalues ,} \\ &= 0.15 \text{ from correlation function .} \end{aligned} \tag{1.29}$$

As we expected from the figure, these values are far less accurate than values obtained from the other approximation. It would appear that our approximation method simply converges better in the case of the second block transformation.

### G. Remainder of this paper

Sections II and III have the nature of technical appendices. They detail the approximations used for constructing the recursion relation. Since the decimation transformation is simplest, we describe it in Sec. II. However, it is not used alone, only in conjunction with the block transformation to form the second block approach. The block transformation is described in Sec. III.

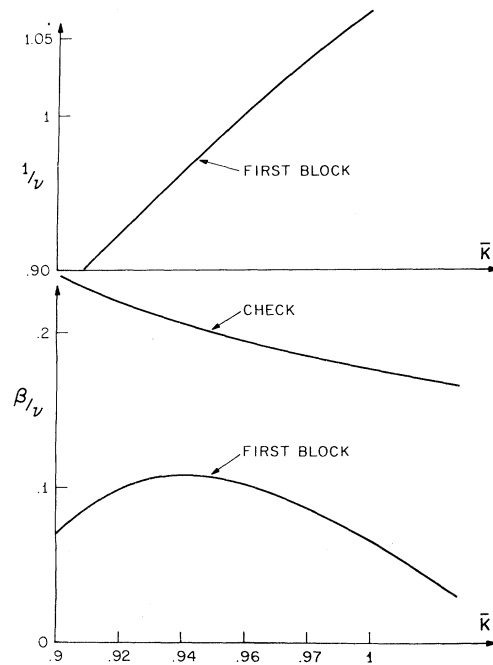


FIG. 6.  $1/\nu$  and  $\beta/\nu$  as obtained from the first block transformation. In this case the two indices are quite dependent on  $\bar{K}$  and the two evaluations of  $\beta/\nu$  never intersect.

II. DECIMATION TRANSFORMATION

A. Setting up the calculation

To begin, write the partition functionals in terms of coupling constants in the form

$$\ln Z\{\sigma\} = \sum_i K_i S_i = \mathcal{F}\{\sigma\}.$$

Then, the recursion relation becomes

$$\mathcal{F}'\{\mu\} = \ln \left( \sum_{\{\sigma_r\}} e^{\mathcal{F}\{\sigma\}} \right)_{\sigma_r = \mu_r}. \quad (2.1)$$

The actual coupling terms which we use in our calculation are shown in Figs. 7 and 8. We use for  $K_i$  the notation  $K_{n,i}$ , where  $n$  is the number of spins contained in the corresponding  $s_i$ .

The calculation of the sum in Eq. (2.1) is considerably facilitated by the fact that we can perform the sum exactly when there are only nearest-neighbor couplings present. Our basic procedure then is to perform the sum for the nearest-neighbor case and then handle all other terms in perturbation theory.

When there are only nearest-neighbor and constant terms in  $\mathcal{F}$ , the sum in (2.1) takes the form of a product of terms like

$$z = \sum_{\sigma} \exp[2K_{0,1} + \sigma K_{2,1}(\mu_1 + \mu_2 + \mu_3 + \mu_4)] = 2 \cosh K_{2,1}(\mu_1 + \mu_2 + \mu_3 + \mu_4) \exp 2K_{0,1}. \quad (2.2)$$

Here the  $\mu$ 's are the new spin variables immediately surrounding the spin  $\sigma$ . (See Fig. 1.) In performing the perturbation calculation it is also important to know the average of  $\sigma$  derived from the partial partition function (2.2). This average is

NUMBER OF SPINS $n$	COUPLING CONSTANT	DIAGRAM	NUMBER OF DIAGRAMS OVER NUMBER OF SITES = $U$
1	$K_{1,1}$	$\bullet$	1
3	$K_{3,1}$		4
	$K_{3,2}$		2
	$K_{3,3}$		4
	$K_{3,4}$		8
5	$K_{5,1}$		1

FIG. 8. Odd-spin diagrams.

$$\langle \sigma_r \rangle_{\mu} = \tanh K_{2,1}(\mu_1 + \mu_2 + \mu_3 + \mu_4). \quad (2.3)$$

With these results in hand, one can rewrite Eq. (2.1) in the form

$$\mathcal{F}'\{\mu\} = \mathcal{F}'_0\{\mu\} + \mathcal{F}'_1\{\mu\}, \quad (2.4)$$

$$\mathcal{F}'_0\{\mu\} = \sum_{\text{summation sites}} \ln z, \quad (2.5)$$

$$\mathcal{F}'_1\{\mu\} = \ln \langle e^{\mathcal{F}_{\text{rem}}\{\sigma\}} \rangle_{\mu}. \quad (2.6)$$

In Eq. (2.6)  $\mathcal{F}_{\text{rem}}$  means  $\mathcal{F}\{\sigma\}$  less the constant and nearest-neighbor terms. The average is defined by Eq. (2.3), so that the average of each summation variable depends upon the four  $\mu$ 's immediately surrounding it.

$\mathcal{F}'_0\{\mu\}$  may be evaluated exactly. It contains the coupling constants

$$(K'_{0,1})_0 = 2K_{0,1} + U_0, \quad (K'_{2,1})_0 = 2U_2, \\ (K'_{2,2})_0 = U_2, \quad (K'_{4,1})_0 = U_4, \quad (2.7)$$

with

$$U_0 = \ln 2 + \frac{1}{8} \ln \cosh 4K_{2,1} + \frac{1}{2} \ln \cosh 2K_{2,1}, \\ U_2 = \frac{1}{8} \ln \cosh 4K_{2,1}, \\ U_4 = \frac{1}{8} \ln \cosh 4K_{2,1} - \frac{1}{2} \ln \cosh 2K_{2,1}. \quad (2.8)$$

The remainder of the problem lies in the evaluation of the average (2.6). Some terms in  $\mathcal{F}_{\text{rem}}$  are trivial—those which do not involve summation variables. The first five terms in the left-hand column of Fig. 9 are the trivial ones; the remaining terms in the figure are the nontrivial terms included in our analyses. The trivial terms simply give rise to a contribution to  $\mathcal{F}'_1\{\mu\}$  of the form

$$(K'_i)_{\text{triv}} = \sum_j R_{i,j} K_j. \quad (2.9)$$

Here the following components of  $R_{ij}$  are equal to unity:

$$R_{21;22}, \quad R_{22;23}, \quad R_{41;43}, \quad R_{11;11}, \quad R_{31;33}. \quad (2.10)$$

NUMBER OF SPINS = $n$	COUPLING CONSTANT	DIAGRAM	NUMBER OF DIAGRAMS DIVIDED BY NUMBER OF LATTICE SITES = $U$
0	$K_{0,1}$		1
2	$K_{2,1}$		2
	$K_{2,2}$		2
	$K_{2,3}$		2
	$K_{2,4}$		4
4	$K_{4,1}$		1
	$K_{4,2}$		4
	$K_{4,3}$		1
	$K_{4,4}$		8
	$K_{4,5}$		4
	$K_{4,6}$		8

FIG. 7. Even-spin diagrams.

COUPLING CONSTANT	SIMPLER DIAGRAM	MORE COMPLEX DIAGRAM
$K_{2,2}$		
$K_{2,3}$		
$K_{4,3}$		
$K_{1,1}$		
$K_{3,3}$		
$K_{2,4}$		
$K_{4,1}$		
$K_{3,1}$		
$K_{3,2}$		
$K_{3,4}$		
$K_{5,1}$		

FIG. 9. Terms actually included in the analysis of the decimation recursion relation. The trivial terms are the first five in the left-hand column. In all cases, save for  $K_{2,2}$ , the terms in the right-hand column are not included in the analysis. Instead, we approximate them by doubling the size of the terms in the left-hand column. The diagrams  $K_{4,2}$  are not included in this figure because our approximation for the block transformation does not generate  $K_{4,2}$ .

All the remaining contributions from the diagrams under consideration vanish.

To complete the calculation, we need the contribution of the nontrivial couplings indicated in Fig. 9. Each term represented here may be written as a term in the sum

$$\mathcal{F}_{\text{rem}} = \sum_t K_t s_t$$

or as a product

$$e^{\mathcal{F}_{\text{rem}}} = \prod_t \cosh K_t (1 + \tanh K_t s_t) \quad (2.11)$$

since each  $s_t$  has values  $\pm 1$ . Therefore the entire set of remaining terms in the analysis can be expressed as

$$\mathcal{F}'_2\{\mu\} = \ln \left\langle \prod_t \cosh K_t (1 + s_t \tanh K_t) \right\rangle_\mu \quad (2.12)$$

In a cumulant expansion of the average Eq. (2.12) reduces to

$$\begin{aligned} \mathcal{F}'_2\{\mu\} = & \sum_t \ln \cosh K_t + \langle s_t \rangle_\mu \tanh K_t \\ & + \frac{1}{2} \sum_{tt'} \tanh K_t \tanh K_{t'} \end{aligned}$$

$$\times (\langle s_t s_{t'} \rangle_\mu - \langle s_t \rangle_\mu \langle s_{t'} \rangle_\mu) + \dots \quad (2.13)$$

Thus the remaining contributions to  $K'_i$  may be expanded in a power series in  $\tanh K_t$  of the form

$$\begin{aligned} U_i(K'_i)_2 = & \sum_j C_{ij} (\tanh K_j) U_j \\ & + \sum_{jh} D_{ijh} (\tanh K_j) (\tanh K_h) U_j U_h \end{aligned} \quad (2.14)$$

Here  $U_i$  is the number of diagrams of a given type as defined in Fig. 7. In conclusion,  $K'$  is the sum of  $K'_0$  [Eq. (2.7)],  $K'_{\text{triv}}$  [Eq. (2.9)] and  $(K')_2$ .

### B. Evaluation of nontrivial diagrams

Each nontrivial diagram involves  $\langle \sigma \rangle_\mu$ . From Eq. (2.3), this may be written

$$\langle \sigma \rangle_\mu = \frac{1}{4} S_1 (x_+ + x_- S_4) \quad (2.15)$$

with

$$\begin{aligned} S_1 = & \mu_1 + \mu_2 + \mu_3 + \mu_4, \\ S_4 = & \mu_1 \mu_2 \mu_3 \mu_4, \\ x_\pm = & \frac{1}{2} \tanh 4K_{2,1} \pm \tanh 2K_{2,1} \end{aligned} \quad (2.16)$$

A typical lowest-order contribution to (2.13) is produced by the fourth-neighbor interaction shown in the sixth line of Fig. 9.

For this case, the resulting expectation value is

$$s_t = \frac{1}{4} \mu_0 (\mu_1 + \mu_2 + \mu_3 + \mu_4) (x_+ + x_- S_4)$$

A count of terms shows that the contributions to the  $C_{ij}$  are

$$\begin{aligned} C_{24;24} = C_{21;24} = C_{22;24} = C_{23;24} = & \frac{1}{2} x_+, \\ C_{45;24} = C_{42;24} = & \frac{1}{2} x_-, \\ C_{44;24} = C_{46;24} = & \frac{1}{4} x_- \end{aligned} \quad (2.17)$$

The terms  $C_{\dots;22}$ ,  $D_{\dots;22;22}$ , and  $C_{\dots;41}$ , which are only slightly more complex, are treated in an exactly analogous fashion. Even one type of contribution  $C_{\dots;42}$  (the term shown in the right-hand column of Fig. 9) can also be handled in this way. However, there are other terms, one involves 512 terms when written out as a product that are too complicated to handle directly.

### C. Simplification from symmetry

But, why should the left- and right-hand columns of Fig. 9 give different contributions? They are physically identical terms in the original  $\sigma$  lattice. They only become distinguishable because of the symmetry breaking produced by the summation technique.

In lowest order, the difference between these diagrams should not contribute to any physical eigenvalue or eigenstate—only to redefinitions of irrelevant eigenvalues and eigenstates. Hence for all linear analyses we can replace the right-hand-

TABLE I. Odd-spin portion of the recursion relation,  $K'_i = 2 \sum_j M_{ij} K_j$ . The values of  $M_{ij}$  are listed in the table with the notation  $x = x_+ + x_-$ . The blanks represent zeroes.

$K$ value	$K_{11}$	$K_{31}$	$K_{32}$	$K_{33}$	$K_{34}$	$K_{51}$
$K'_{1,1}$	1	$\frac{1}{2}x$	$\frac{1}{2}x$		$\frac{1}{4}x_+$	$x_-$
$K'_{3,1}$		$\frac{1}{2}x$	$\frac{1}{2}x$	1	$\frac{1}{4}x_+$	$x_+$
$K'_{3,2}$					$\frac{1}{4}x_+$	
$K'_{3,3}$						
$K'_{3,4}$					$\frac{1}{4}x_+$	
$K'_{5,1}$						$x_-$

column diagrams by the simpler diagrams in the left-hand column. We make this replacement in all cases save that of  $K_{2,2}$ , which we take to second order. In this way, we are left with seven non-trivial diagrams to evaluate. Once again we replace contributions to coupling constants which are not on our list by lumping them into the highest-order coupling constant  $K'_{n,i}$  with the same  $n$  value. In this way we obtain our approximation for the decimation recursion relation. The odd-spin portion of this approximation is summarized in Table I.

### III. THE BLOCK TRANSFORMATION

#### A. Setting up the calculation

In calculating the results of the decimation transformation, we extracted the exact effects of the lowest-order interaction and took all the higher-order interactions into account as perturbations. We can apply a rather similar method for the block transformation. We start by calculating the properties of the basic block shown in Fig. 10(a). Then, we move on to calculate the interaction between two

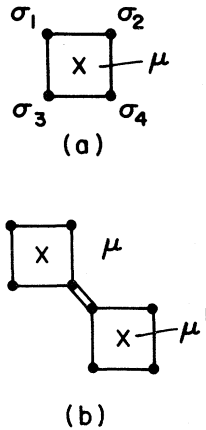


FIG. 10. (a) Basic block. (b) Two blocks together.

TABLE II. Configurations of four spins and associated values of functions of these spins.  $W_T$  represents the number of similar configurations.

Variable	Configuration					
	+++-	+-	++	+-	--	--
$W_T$	1	4	4	2	4	1
$S_1 = \sigma_1 + \sigma_2 + \sigma_3 + \sigma_4$	4	2	0	0	-2	-4
$S_{nn} = \sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_4 + \sigma_4\sigma_1$	4	0	0	-4	0	4
$S_{nnn} = \sigma_1\sigma_3 + \sigma_2\sigma_4$	2	0	-2	2	0	2
$S_3 = S_1 S_4$	4	-2	0	0	2	-4
$S_4 = \sigma_1\sigma_2\sigma_3\sigma_4$	1	-1	1	1	-1	1

blocks as shown in Fig. 10(b). When these two terms are calculated, we use the results as a starting point for a perturbation theory in which we expand in (a) the correlations among more than two blocks and (b) the interaction terms which cannot be included in the blocks.

The basic block is organized so that it contains the couplings produced by  $\bar{K}$  as well as the interaction terms listed in the first four rows of Fig. 9. Then, the zeroth-order result for the transformed free-energy function is obtained by calculating the partition function for the basic block. This is simply a sum over the  $\sigma$  variables of

$$e^{f_0} = \frac{1}{2} (1 + \tanh \bar{K} \mu S_1) \times \exp(K_{0,1} + K_{2,1} S_{nn} + K_{2,2} S_{nnn} + K_{4,1} S_4), \quad (3.1)$$

where  $S_1, S_{nn}, \dots$  are defined by Fig. 10(a) and Table II. The partition function for the basic block is then given by

$$z = \sum_{\alpha} e^{f_0(\alpha)} W_T(\alpha) \quad (3.2)$$

where the  $\alpha$  are the configurations listed in Table II.

In summing over all the basic blocks, we essentially sum over all  $\sigma$  variables twice, since each one falls into two blocks. To represent this fact, we introduce two variables  $\tau_{r'}$  for each  $\sigma_r$ . These  $\tau_{r'}$  variables are taken to be at sites halfway between the  $\sigma_r$  sites and the  $\mu'_{r'}$  sites—as indicated in Fig. 11.

Each pair of  $\tau_{r'}$  variables surround a  $\sigma_r$  variable. We define these new variables by the statement that they are equal to the  $\sigma_r$  variable and to each other, i. e.,

$$\sigma_r = \frac{1}{2}(\tau + \tau'), \quad \tau = \tau' = \sigma_r. \quad (3.3)$$

To represent this equality, a factor  $\frac{1}{2}(1 + \tau\tau')$  is introduced into the sum defining  $\mathcal{F}'$  at each  $\sigma_r$  posi-

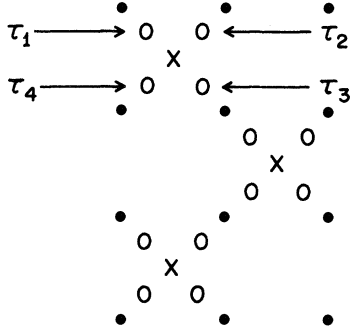


FIG. 11. Distribution of the auxiliary sites relative to the basic  $\sigma$  and  $\mu$  sites.  $\times = \mu$ ,  $\bullet = \sigma$ ;  $\circ = \tau$ .

tion. Then, the basic equation for  $\mathcal{F}'$  can be written

$$\mathcal{F}'\{\mu\} = \ln \sum_{\tau} \left[ \prod_{r''} e^{f_0(\tau_1, \tau_2, \tau_3, \tau_4; \mu_{r''})} \right] \times \left( \prod_r V_r \right) e^{\mathcal{F}_{\text{rem}}\{\sigma_r\}}. \quad (3.4)$$

Here,  $V_r$  is defined by

$$V_r = \frac{1}{2}(1 + \tau\tau') e^{K_{1,1}\tau}, \quad (3.5)$$

where  $\tau$  and  $\tau'$  are the two new summation variables surrounding the point  $r$ . The  $K_{1,1}$  term takes into account the one-spin term in  $\mathcal{F}$ . The remaining interactions in  $\mathcal{F}$  are included in  $\mathcal{F}_{\text{rem}}\{\sigma\}$ , with each of the  $\sigma$ 's replaced by a pair of  $\tau$ 's in accordance with Eq. (3.3).

Equation (3.4) permits a very convenient rewriting of  $\mathcal{F}'$ . Define  $\langle \rangle_{\mu}^0$  to mean an average of some function of the  $\tau$ 's with a weight factor

$$\prod_{r''} e^{f_0(\dots; \mu_{r''})}.$$

With this weight factor,  $\tau$ 's which fall into different blocks are uncorrelated, while  $\tau$ 's in the same block have only a weak correlation. In fact,  $\bar{K}$  is chosen to make the intrablock correlations as weak as possible. In any case, with this definition of  $\langle \rangle_{\mu}^0$ , Eq. (3.4) can be written

$$\mathcal{F}'\{\mu\} = \mathcal{F}'_0\{\mu\} + \mathcal{F}'_1\{\mu\}, \quad (3.6)$$

$$\mathcal{F}'_0\{\mu\} = \sum_{r''} \ln z + \sum_r \ln \langle V_r \rangle_{\mu}^0, \quad (3.7)$$

$$\mathcal{F}'_1\{\mu\} = \ln \left\langle \left( \prod_r \frac{V_r}{\langle V_r \rangle_{\mu}^0} \right) e^{\mathcal{F}_{\text{rem}}(\sigma)} \right\rangle_{\mu}^0. \quad (3.8)$$

Equation (3.6) represents our starting point for the calculation of  $\mathcal{F}'$ .

#### B. Lowest-order calculation

The zeroth-order partition function  $z$  is easily calculated from Eq. (3.1). This equation also permits the direct calculation of averages of the  $\tau$ 's

which lie on a single block. We define these averages as

$$\begin{aligned} \langle \tau_1 \rangle_{\mu}^0 &= L_1 \mu, & \langle \tau_1 \tau_2 \rangle_{\mu}^0 &= L_{\text{nn}}, & \langle \tau_1 \tau_3 \rangle_{\mu}^0 &= L_{\text{nnn}}, \\ \langle \tau_1 \tau_2 \tau_3 \rangle_{\mu}^0 &= L_3 \mu, & \langle \tau_1 \tau_2 \tau_3 \tau_4 \rangle_{\mu}^0 &= L_4, \end{aligned} \quad (3.9)$$

where nn and nnn stand for nearest- and next-nearest-neighbor terms.

One can also directly calculate  $\langle V_r \rangle_{\mu}^0$  as

$$\begin{aligned} \langle V_r \rangle_{\mu}^0 &= \frac{1}{2} \cosh K_{1,1} (1 + L_1^2 \mu \mu') \\ &\times [1 + \lambda \tanh K_{1,1} \frac{1}{2}(\mu + \mu')], \end{aligned} \quad (3.10)$$

with

$$\lambda = 2L_1 / (1 + L_1^2), \quad (3.11)$$

where  $\mu$  and  $\mu'$  are the (nearest-neighbor) new spin variables immediately adjacent to  $r$ . For our later work, we shall also need to know the quantity

$$\begin{aligned} \langle \sigma_r \rangle_{\mu}^1 &= \frac{\langle V_r \sigma_r \rangle_{\mu}^0}{\langle V_r \rangle_{\mu}^0} \\ &= \frac{\lambda(\mu + \mu'/2) + \tanh K_{1,1}}{1 + \lambda(\mu + \mu'/2) \tanh K_{1,1}}. \end{aligned} \quad (3.12)$$

Equation (3.8) defines the lowest-order approximation for  $\mathcal{F}'$ , i.e.,  $\mathcal{F}'$  contains constant, nearest-neighbor, and one-spin terms. In the case of small  $K_{1,1}$  these have coupling constants

$$\begin{aligned} (K'_{0,1})_0 &= \ln z + \frac{1}{4} \ln(1 - L_1^4), \\ (K'_{1,1})_0 &= 2\lambda K_{1,1}, \\ (K'_{2,1})_0 &= \frac{1}{2} \ln[(1 + L_1^2)/(1 - L_1^2)]. \end{aligned} \quad (3.13)$$

The remainder of the calculation is the estimation of  $\mathcal{F}'_1$  as defined by Eq. (3.9).

#### C. Corrections from $\mathcal{F}_{\text{rem}}$

The general structure of the terms lumped into  $\mathcal{F}_{\text{rem}}$  is a product of terms of the form  $\exp K_i \sigma_{r_1} \sigma_{r_2} \dots \sigma_{r_n}$ , where each  $\sigma$  is represented by a  $\frac{1}{2}(\tau + \tau')$ . In a first-order expansion such a term produces a contribution to  $\mathcal{F}'$  of the form

$$\delta \mathcal{F}'_1\{\mu\} = K_t \left\langle \left( \prod_{i=1}^n \frac{V_{r_i} \sigma_{r_i}}{\langle V_{r_i} \rangle_{\mu}^0} \right) \prod \frac{V_r}{\langle V_r \rangle_{\mu}^0} \right\rangle_{\mu}^0, \quad (3.14)$$

where the second product is over all  $r$ 's not in the diagram. In lowest order, we approximate such a contribution by neglecting the correlations among different  $V_r$ 's.

Then we find

$$\delta \mathcal{F}'_1\{\mu\} = K_t \prod_{i=1}^n \langle \sigma_{r_i} \rangle_{\mu}^1, \quad (3.15)$$

where  $\langle \rangle_{\mu}^1$  is defined by Eq. (3.12).

For example, a  $K_{2,4}$  term like that defined in Fig. 9 will produce a contribution to the right-hand side of (3.15) which looks like



$$\delta\mathcal{F}'_1\{\mu\} = K_{2,4} \frac{\lambda(\mu_1 + \mu_2/2) + \tanh K_{1,1}}{1 + \lambda(\mu_1 + \mu_2/2)\tanh K_{1,1}} \times \frac{\lambda(\mu_3 + \mu_4/2) + \tanh K_{1,1}}{1 + \lambda(\mu_3 + \mu_4/2)\tanh K_{1,1}}. \quad (3.16)$$

The next step is to convert (3.16) into a statement about coupling constants. Start with  $K_{1,1} = 0$ . Then the right-hand side of (3.16) takes the form  $\frac{1}{4}K_{2,4}\lambda^2(\mu_2\mu_3 + \mu_2\mu_4 + \mu_1\mu_3 + \mu_1\mu_4)$ , for odd  $n$  and even  $m$ , which includes, respectively, a nearest-neighbor term, a next-nearest-neighbor term, and a  $K'_{2,3}$  and a  $K'_{2,4}$  term. The new lattice contains, respectively,  $U_i N'$  of these terms, i. e.,  $2N'$ ,  $2N'$ ,  $2N'$ , and  $4N'$ , where  $N'$  is the number of  $\mu_r$  sites. On the other hand, there are  $4N$  or  $8N'$  terms like (3.16). Hence a direct count gives a contribution to  $K'_{2,1}K'_{2,2} \dots$ ,

$$\delta K'_{2,1} = \delta K'_{2,2} = \delta K'_{2,3} = \delta K'_{2,4} = \frac{1}{4}K_{2,4}\lambda^2 8N'/2N'. \quad (3.17)$$

In a similar way, we can assess the effects of all terms in  $\mathcal{F}_{\text{rem}}\{\sigma\}$ . The general structure we see is that the terms independent of  $K_{1,1}$  are

$$\delta K'_{j,n} = \frac{2}{U_{j,m}} \sum_{\alpha} \sum_i \sum_{m=0}^{\infty} C_{j,n;i,n+2m,\alpha} \times \left(\frac{\lambda}{2}\right)^{n+2m} K_{i,n+2m} V_{i,n+2m,\alpha}. \quad (3.18)$$

The values of the matrix  $C$  are set forth in Table III. In Eq. (3.13), the index  $\alpha$  distinguishes between different types of diagrams which may have the same coupling constant.  $V_{i,m,\alpha}$  is just the number of such diagrams divided by the number of lattice sites.

The first-order term in  $K_{1,1}$  produces effects a little more complex than those listed in Eq. (3.13). As can be seen by taking the first-order correction in  $K_{1,1}$  to Eq. (3.16), which is

TABLE III. Values of  $C_{ni:mj\alpha}$  for even  $n$ .

Row index $n$		Column $m$		2		3		4		4		4	
		index $j$	$\alpha$	2	3	4	1	2	3	1	2	3	1
0	1								2			1	1
2	1			2	1	1			8			5	4
	2			2	2	1			4			3	
	3					1						1	2
	4					1	1					1	
4	1								1			1	2
	2											1	
	3												
	4											1	4
	5											1	2
	6											1	
Other												1	

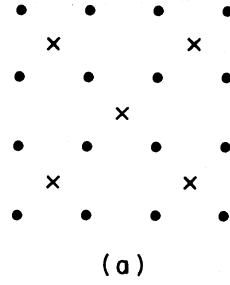
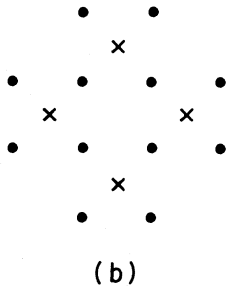


FIG. 12. Correlation corrections.



$$K_{2,4}K_{1,1} \left[ \frac{1}{2}\lambda(\mu_1 + \mu_2 + \mu_3 + \mu_4) - \frac{1}{4}\lambda^3(1 + \mu_1\mu_2)(\mu_3 + \mu_4) - \frac{1}{4}\lambda^3(1 + \mu_3\mu_4)(\mu_1 + \mu_2) \right],$$

these terms have the structure

$$\delta K'_{j,n} = \frac{2}{U_{j,n}} \sum_{i\alpha m} K_{1,1} K_{i,m,\alpha} V_{i,m,\alpha} \left(\frac{\lambda}{2}\right)^{m-1} \times \left[ M_{jn;im\alpha}^1 \left(1 - \frac{\lambda^2}{2}\right) - \frac{\lambda^2}{2} M_{jn;im\alpha}^2 \right]. \quad (3.19)$$

Values of the matrices  $M^1$  and  $M^2$  are easily determined by a direct count.

D. Correlation corrections

Figure 12(a) shows four vertex functions arrayed about a single block. This arrangement leads to an important correction to  $\mathcal{F}'_1$ , namely, a term of the form

$$\delta\mathcal{F}_1 = \ln \left\langle \frac{V_1 V_2 V_3 V_4}{\langle V_1 \rangle_{\mu}^0 \langle V_2 \rangle_{\mu}^0 \langle V_3 \rangle_{\mu}^0 \langle V_4 \rangle_{\mu}^0} \times \exp[K_{3,1}\sigma_1\sigma_2\sigma_3\sigma_4(\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4)] \right\rangle_{\mu}^0. \quad (3.20)$$

Note that we have included a  $K_{3,1}$  term (type  $\alpha = 1$ ) in  $\delta\mathcal{F}_1$ . The evaluation of (3.20) is not materially impeded by this inclusion, and the inclusion of  $K_{3,1}$  here gives a more accurate evaluation of its effect than the calculation outlined in Sec. III C. Consequently, we handle the  $K_{3,1}^{(\alpha=1)}$  terms in Eq. (3.20)

and do not include them in the sums in Eqs. (3.13) and (3.14). The major interblock correlation effects upon the response to  $K_{3,1}$  are thus taken into account.

Because of the highly symmetrical structure of Fig. 12(a), the average in (3.20) is easily computed and its effects upon  $K'$  assessed. An evaluation of the averages gives

$$\begin{aligned} \delta\mathcal{F}'_1 = & \ln(L'_0 + \mu S_1 L'_1 + S_{nn} L'_{nn} + S_{mn} L'_{mn} + S_3 L'_3 \mu + S_4 L'_4) \\ & - 4 \ln \cosh K_{1,1} - (2 + \frac{1}{2} \mu S_1) \ln(1 + L_1^2) \\ & \times (1 + \mu \lambda \tanh K_{1,1}) - (2 - \frac{1}{2} \mu S_1) \ln(1 - L_1^2). \end{aligned} \quad (3.21)$$

Here  $S_1$  and  $S_{nn}$  are the variables defined in Table II, except that they are functions of  $\mu_1, \mu_2, \mu_3$ , and  $\mu_4$  instead of  $\sigma$ 's. The functions  $L'_0, L'_1, \dots$  are defined as averages on the basic block, with

$$\begin{aligned} L'_0 &= \langle e^{K_{11} S_1 + K_{31} S_3} \rangle_\mu^0, \\ \mu L'_1 &= \langle e^{K_{11} S_1 + K_{31} S_3} \frac{1}{4} S_1 \rangle_\mu^0, \\ L'_{nn} &= \langle e^{K_{11} S_1 + K_{31} S_3} \frac{1}{4} S_{nn} \rangle_\mu^0. \end{aligned} \quad (3.22)$$

In Eq. (3.22) the  $S$ 's are once again of the form defined by Table II, but now they are functions of the four  $\tau$ 's which appear in the basic block.

The contributions to the coupling constants may now be evaluated by a process of projection applied

to Eq. (3.21). For example

$$\delta K'_{4,2} = \frac{1}{128} \sum_\alpha \sum_{\mu=\pm 1} W_T(\alpha) S_3(\alpha) \delta\mathcal{F}'_1(\alpha, \mu) \mu,$$

where the sum over  $\alpha$  is a sum over the configurations of the four variables  $\mu_1, \mu_2, \mu_3$ , and  $\mu_4$ .

Another set of blocks whose correlations can be evaluated is shown in Fig. 12(b). However, all three-block correlation effects are already included in expression (3.15). Thus, the correlations in Fig. 12(b) have, in the main, already been taken into account. We use this diagram to get a more accurate assessment of the  $\alpha=2$  effects of  $K_{2,2}, K_{4,1}$ , and  $K_{3,1}$  by calculating these effects from

$$\delta\mathcal{F}'_1 = \langle V_a V_b V_c V_a X X \rangle_\mu^0 / \langle V_a V_b V_c V_a \rangle_\mu^0, \quad (3.23)$$

with

$$\begin{aligned} X &= K_{2,2}(\sigma_a \sigma_c + \sigma_b \sigma_d) + \sigma_a \sigma_b \sigma_c \sigma_d \\ &\times [K_{4,1} + K_{3,1}(\sigma_a + \sigma_b + \sigma_c + \sigma_d)]. \end{aligned} \quad (3.24)$$

Once again the numerical calculation of the sum is relatively easy. Using (3.23), we can completely drop  $K_{3,1}, K_{4,1}$ , and  $K_{2,2}$  from the perturbation theoretic calculations of the previous section—and instead have a more accurate result in which a variety of correlation effects upon the results of these terms are included.

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