Series Expansions from Corner Transfer Matrices: The Square Lattice Ising Model

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Received February 6, 1979

The corner transfer matrix formalism is used to obtain low-temperature series expansions for the square lattice Ising model in a field. This algebraic technique appears to be far more efficient than conventional methods based on combinatorial enumeration.

KEY WORDS: Lattice models; series expansions; corner transfer matrices.

1. INTRODUCTION

Exact series expansions have been of considerable importance in the investigation of the critical behavior of lattice models in statistical mechanics. In spite of the large number of techniques which have been devised, the derivation of significant numbers of series coefficients is a formidable problem. Most techniques are based on combinatorial enumeration ("graph-counting") and the number of series terms which can be obtained is limited mainly by the rate at which graph embeddings can be counted using digital computers. The present paper describes an algebraic technique for obtaining series expansions for various Ising models on the square lattice using an algebraic method based on the work of Baxter⁽¹⁾ (hereafter referred to as I). Wortis⁽²⁾ has commented that the most efficient techniques for obtaining series expansions tend to replace combinatorial complexity by algebraic complexity.

Baxter^(1,3) has described a hierarchy of variational approximations for the partition functions of lattice models. The approximations involve matrix expressions for the eigenvectors of the transfer matrix. The lowest order approximation (using 1×1 matrices) is that described by Kramers and Wannier,⁽⁴⁾ who showed that the approximation gives the first few series

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coefficients correctly. As $n \to \infty$ the formalism becomes exact and the equations [(1a)-(1c)] are the variational expressions for the corner transfer matrices described by Baxter.^(5,6)

Throughout this paper we work with the exact equations, which involve infinite matrices. Fortunately, for the purposes of obtaining a finite number of coefficients in the series expansion of the reduced partition function κ , only a small number of rows and columns of the matrices need be considered explicitly. This reduction does depend on choosing an appropriate basis for the matrices.

The following sections outline the procedures for obtaining series expansions for κ from the corner transfer matrix equations. The low-temperature expansion for the square lattice Ising model in a magnetic field is considered as a test case.

Section 2 describes the variational expressions for the (infinite) corner transfer matrices (as given in I) and shows how the matrix equations can be transformed into a more unified form. In obtaining solutions of the equations we are at liberty to change the basis, specify various normalization conditions, and introduce various scale factors. We make use of all these "degrees of freedom" to simplify the calculations. Section 3 carries out the iterative solution of the equations for the nearest-neighbor Ising model, using the procedure described in I, but expressing the results as a power series. This example exhibits an important general property, namely that the equations are dominated by certain leading order terms and so it is possible to obtain the leading power of the eigenvalues of the corner transfer matrices explicitly as described in Section 4. This result forms the basis for a considerable simplification of the iterative procedure. This is described in Section 5, which gives a complete specification of which matrix equations can be used to solve for any required matrix element. Once this is known it is possible to work through the equations iteratively, obtaining solutions for the leading powers of the matrix elements. Once the leading powers are known, the equations can be examined to determine the order to which a matrix element must be obtained if some other matrix element is to be given to a specified order. These procedures are outlined in Section 6. They form the basis for the sequence of computations described in Sections 8 and 9. (Section 7 describes, for completeness, the precise way in which we have transformed the equations to simplify the calculations. These transformations are purely for computational convenience and do not affect the structure described in Sections 5 and 6.)

The results tabulated in the appendix show that the algebraic technique is particularly efficient. We have been able to expand the reduced partition function κ to order 23 in the low-temperature variable *u*. The longest series previously obtained extended only to u^{11} (Sykes *et al.*⁽⁷⁾). Similar series

expansion techniques should be possible for other square lattice models. These are currently under investigation.

2. THE MATRIX EQUATIONS

The variational equations for the corner and half-row transfer matrices are given in Eq. (30) of I. For an isotropic system they are

$$\sum_{b} F(a, b)A^{2}(b)F(b, a) = \xi A^{2}(a)$$
(1a)
$$\sum_{b,b'} w(a, b, a', b')F(a, b)A(b)F(b, b')A(b')F(b', a')$$
$$= \eta A(a)F(a, a')A(a')$$
(1b)

$$A^{T}(a) = A(a), \qquad F^{T}(a, b) = F(b, a)$$
 (1c)

Here a, b, a', and b' have values +1 and -1; each of F(+, +), F(+, -), F(-, +), F(-, -), A(+), A(-) is a matrix; ξ and η are positive real numbers; and w(a, b, a', b') is the Boltzmann weight of a face of the square lattice with spins a, b, a', and b' at the bottom left, bottom right, top left, and top right corners, respectively. Thus the partition function Z is

$$Z = \sum_{\sigma} \prod w(\sigma_i, \sigma_j, \sigma_k, \sigma_l)$$
(2)

where the product is over all faces (i, j, k, l) of the lattice and the sum is over the value +1 or -1 of every spin.

If there are N spins, then in I it is shown that

$$\kappa = Z^{1/N} = \eta/\xi \tag{3}$$

where η and ξ are given by the appropriate solution of the matrix equations (1).

In general this solution will be one in which the matrices are infinitedimensional. However, quite good approximations to κ can be obtained by truncating these matrices and keeping only a few rows and columns. Such approximations correctly give the first few terms in a low- (or high-) temperature expansion. The more rows and columns are kept, the more terms are given correctly. This is the essential idea of this paper.

Here we consider the usual nearest-neighbor Ising model in a magnetic field, with

$$w(a, b, a', b') = \exp\{\frac{1}{2}K(ab + bb' + b'a' + a'a - 4) + \frac{1}{4}L(a + b + b' + a' - 4)\}$$
(4)

where K and L are positive, being given by

$$K = J/kT, \qquad L = H/kT \tag{5}$$

Here the ground-state energy has been subtracted from the Hamiltonian to ensure that

$$w(+, +, +, +) = 1 \tag{6}$$

This is convenient for our purposes, since we shall be obtaining lowtemperature expansions, which is equivalent to perturbing about the state in which all spins are positive.

Substituting the expression (4) for w into (1), the resulting equations can be somewhat simplified by defining

$$\overline{F}(a, b) = e^{K(ab-1)/2 + L(a+b-2)/8} A^{1/2}(a) F(a, b) A^{1/2}(b)$$

$$\overline{A}(a) = e^{(K+L/4)(1-a)} A(a)$$
(7)

and

$$\bar{\tau}(+, +) = \bar{\tau}(+, -) = \bar{\tau}(-, +) = 1, \quad \bar{\tau}(-, -) = u$$

$$\bar{\rho}(+) = 1, \qquad \qquad \bar{\rho}(-) = \mu u^2$$
(8)

where

$$u = e^{-4K}, \quad \mu = e^{-2L}$$
 (9)

(12)

The equations then become

$$\sum_{b} \bar{\tau}(a, b) \bar{F}(a, b) \bar{A}(b) \bar{F}(b, a) = \xi \bar{\rho}(a) \{ \bar{A}(a) \}^{3}$$

$$\sum_{b,b'} \bar{F}(a, b) \bar{F}(b, b') \bar{F}(b', a') = \eta \bar{\tau}(a, a') \bar{A}(a) \bar{F}(a, a') \bar{A}(a')$$
(10)

for a, a' = +1 or -1.

It is convenient to introduce the enlarged matrices

$$C = \begin{pmatrix} \overline{A}(+) & 0\\ 0 & \overline{A}(-) \end{pmatrix}, \quad H = \begin{pmatrix} \overline{F}(+, +) & \overline{F}(+, -)\\ \overline{F}(-, +) & \overline{F}(-, -) \end{pmatrix}, \quad S = \begin{pmatrix} I & 0\\ 0 & -I \end{pmatrix}$$
(11)

where I is the identity matrix. Let the elements i, j of C, H, and S be c_{ij} , h_{ij} , and $s_{ij} = s_i \delta_{ij}$, respectively. Then s_i has value +1 or -1 depending on the block in which the row and column *i* lie. Define

 $\tau_{ij} = 1 \quad \text{if} \quad s_i \quad \text{or} \quad s_j = +1$ $= u \quad \text{if} \quad s_i = s_j = -1$

and

$$\rho_i = 1 \qquad \text{if} \quad s_i = +1 \\ = \mu u^2 \qquad \text{if} \quad s_i = -1$$

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Then Eqs. (10) can be written

$$\sum_{k} \tau_{ik} (HC)_{ik} h_{kj} = \xi \rho_i (C^3)_{ij} \quad \text{if} \quad s_i = s_j$$

$$(H^3)_{ij} = \eta \tau_{ij} (CHC)_{ij}, \quad \text{all } i \text{ and } j$$
(13)

From (1c), both C and H are symmetric matrices.

In I it was shown that a basis can normally be chosen in which A(+) and A(-) are diagonal matrices. In most of this paper we shall use this representation, so C is also diagonal, with elements $c_{ij} = c_i \delta_{ij}$. Introducing the matrix $V = H^2$, we can write Eqs. (13) explicitly as

$$\sum_{k} \tau_{ik} h_{ik} c_k h_{kj} = \xi \rho_i c_i^{3} \delta_{ij} \quad \text{if} \quad s_i = s_j \tag{14a}$$

$$\sum_{k} v_{ik} h_{kj} = \eta \tau_{ij} c_i h_{ij} c_j \tag{14b}$$

$$\sum_{k} h_{ik} h_{kj} = v_{ij} \tag{14c}$$

If the matrices C, H, and V are n by n, then i and j take the values 1,..., n, and the k-summations are from k = 1 to k = n.

The normalization of C and H is still undetermined. A convenient way to fix it is to require that

$$c_1 = h_{11} = 1 \tag{15}$$

3. ITERATIVE DIAGONALIZATION PROCEDURE

In I an iterative method for solving the equations was proposed. In terms of our present notation it can be expressed as follows.

Define R, U^+ , and U^- to be the matrices with elements

$$r_{ij} = (\tau_{ij}c_i/\xi\rho_j c_j^{3})^{1/2}h_{ij}$$
(16a)

$$u_{ij}^+ = v_{ij} / (c_i c_j)^{1/2} \tag{16b}$$

$$u_{ij} = v_{ij} / [v_i v_j (c_i c_j)^{1/2}],$$
(16c)

where

$$\nu_i = 1 ext{if } s_i = +1 \\
= u^{1/2} ext{if } s_i = -1 ext{(17)}$$

Then Eqs. (14a) and (14b) can be written (using the symmetry of H)

$$\sum_{k} r_{ki} r_{kj} = \delta_{ij} \quad \text{if} \quad s_i = s_j \tag{18a}$$

$$\sum_{k} u_{ik}^{+} r_{kj} = r_{ij}(\eta c_j) \quad \text{if} \quad s_j = +1$$

$$\sum_{k} u_{ik}^{-} r_{kj} = r_{ij}(\eta c_j) \quad \text{if} \quad s_j = -1$$
(18b)

From (18b) it is apparent that each ηc_j is an eigenvalue of U^+ (if $s_j = +1$) or of U^- (if $s_j = -1$). The column vector j of the matrix R is the

corresponding eigenvector. Equation (18a) merely states that eigenvectors of the same matrix should be chosen to be orthonormal.

Given an initial guess at ξ , η , C, H, and V, the iteration procedure is as follows:

(i) Calculate U^+ and U^- from (16b).

(ii) Diagonalize U^+ and U^- to obtain the r_{ij} and ηc_j in (18). Use (15) to obtain η , and hence c_2, c_3, \dots

(iii) Calculate $\xi^{-1/2}h_{ij}$ from (16a). Use (15) to obtain ξ , and hence the h_{ij} . If h_{ii} is "more accurate" than h_{ii} , then set $h_{ii} = h_{ii}$.

(iv) Calculate v_{ii} from (14c). Then repeat.

Note that if C, H, and V are initially n by n, then so are both U^+ and U^{-} , so (18) gives 2n eigenvalues c_i , and 2n column vectors for R. To obtain the correct infinite-dimensional solution, all of these should in principle be kept, so the new C and R are 2n by 2n matrices. The rows of R corresponding to the *n* new eigenvalues should at this stage be set to zero.

Thus the matrices should double in size at each iteration. However, in practice it is useful to repeat each iteration once before expanding the matrices, so as to obtain the correct leading order behavior of the lower elements of R, and the lower-right elements of H, V, U^+ , and U^- .

To see how this works, suppose that u is small, as it is for low temperatures.

If u is in fact zero, then all spins must be up, and from Section 5 of I it is obvious that only F(+, +) and A(+) are nonzero, and that they are one by one matrices, acting only on the state with all spins up. Thus C, H, and Vare one by one, with $s_1 = +1$, and (14) has the trivial solution

$$\xi = \eta = c_1 = h_{11} = v_{11} = 1 \tag{19}$$

Now use this as input to the above iteration procedure, with u small but nonzero. Keeping only the leading small-u behavior of each matrix element, and setting

$$t = \mu^{1/2}$$
 (20)

we obtain

 c^{γ}

(i)
$$U^+ = U^- = (1)$$

(ii) $C = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad R = \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}$

(iii)
$$H = \begin{pmatrix} 1 & tu \\ tu & 0 \end{pmatrix}$$

(iv)
$$V = \begin{pmatrix} 1 & tu \\ tu & t^2u^2 \end{pmatrix}$$

The next steps would be to calculate the four by four matrices V, U^+ , and U^- , then the eight by eight matrices C, R, and so on. Note that doubling the size of the matrices does not affect the leading terms of the elements already obtained: for instance, the two by two matrix H given above is the top-left block of the four by four matrix H.

One very useful fact emerges from this procedure: the rows and columns can always be ordered so that

$$s_i = (-1)^{i-1} \tag{22}$$

and, to leading order in u,

the dots denoting elements that vanish when u = 0. These two requirements actually fix the ordering of the rows and columns. We shall call this the "natural" ordering.

For a given integer i, let i' be defined by

$$i' = \operatorname{Int}[\frac{1}{2}(i+1)]$$
 (24)

Then, from (23),

$$r_{i',i} = 1 + \mathcal{O}(u)$$

$$r_{ji} = o(u) \quad \text{if} \quad j \neq i'$$
(25)

4. LEADING ORDER EQUATIONS FOR THE c_i

From (25), for j = i the summation in (18a), and therefore also in (14a), is dominated for small u by the term k = i'. Using the symmetry of H, and the fact that $\xi = 1 + \mathcal{O}(u)$, to leading order (14a) therefore gives

$$\tau_{ii'} c_{i'} h_{ii'}^2 = \rho_i c_i^{\ 3} \tag{26a}$$

Further, if j = i in (14b), or if j = i' in (14b) or (14c), the summation on the rhs is again dominated by the term k = i'. Since $\eta = 1 + O(u)$, it follows that to leading order

$$v_{ii'}h_{ii'} = \tau_{ii}c_ih_{ii}c_i$$

$$v_{ii'}h_{i'i'} = \tau_{ii'}c_ih_{ii'}c_{i'}$$

$$h_{ii'}h_{i'i'} = v_{ii'}$$
(26b)

These equations can be solved sequentially, giving the leading order behavior of $c_1, c_2, c_3,...$ The natural way to write the result is to go back to the original matrices A(+) and A(-), whose diagonal elements are $\rho_i^{1/4}c_i$, and to use a binary, or spin, representation of the indices, setting

$$i = \{\sigma_1, \sigma_2, \sigma_3, ...\}$$

= 1 + $\frac{1}{2}[(1 - \sigma_1) + 2(1 - \sigma_2) + 4(1 - \sigma_3) + 8(1 - \sigma_4) + \cdots]$ (27)

where $\sigma_1, \sigma_2, \sigma_3,...$ take the values +1 or -1. Thus the value 1 of the index *i* corresponds to $\sigma_1 = \sigma_2 = \sigma_3 = \cdots = +1$, i.e., all spins up. The value 2 corresponds to σ_1 being down, the rest up; and so on.

From (24) it follows that if i is given by (27), then

$$i' = \{\sigma_2, \sigma_3, \sigma_4, ...\}$$
(28)

and the solution of (26) is found to be

$$\rho_{i}^{1/4}c_{i} = \exp\left\{\frac{1}{4}L(\sigma_{1}-1) + \sum_{r=1}^{\infty} \left[(2r-1)K(\sigma_{r}\sigma_{r+1}-1) + 2rL(\sigma_{r+1}-1)\right]\right\}$$
(29)

Note that when L = 0 (no magnetic field) this expression can be written as a direct product in terms of the spins $\mu_r = \sigma_r \sigma_{r+1}$, giving

$$\mathscr{A} = \rho^{1/4}C = \begin{pmatrix} 1 & 0 \\ 0 & u^{1/2} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & u^{1\frac{1}{2}} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & u^{2\frac{1}{2}} \end{pmatrix} \otimes \cdots$$
(30)

It has been shown⁽⁶⁾ that this result is exact for all temperatures T less than T_c , provided u is replaced by the nome of the elliptic functions that occur in the exact solution of the zero-field Ising model.⁽⁹⁾

5. SIMPLIFIED ITERATIVE PROCEDURE

The iterative method of solution given in Section 3 is quite general, but rather cumbersome. Fortunately we found that for the nearest-neighbor Ising model it can be enormously simplified. First write Eq. (14a), with j = i, as

$$\tau_{ii'}c_{i'}h_{ii'}^2 = \xi \rho_i c_i^3 - \sum_{k \neq i'} \tau_{ik} h_{ik} c_k h_{ki}$$
(31a)

and write (14b) and (14c) as

$$v_{ij}h_{jj} - \eta \tau_{ij}c_ih_{ij}c_j = -\sum_{k \neq j} v_{ik}h_{kj}$$

$$v_{ij} - h_{ij}h_{jj} = \sum_{k \neq j} h_{ik}h_{kj}$$
 (31b)

First calculate the c_i , $h_{ii'}$ (up to some maximum value of *i*) from (15) and the leading order equations (26). Set $h_{i'i} = h_{ii'}$ and set all other matrix elements to zero. Now proceed as follows:

- (i) Calculate v_{11} from (14c).
- (ii) Calculate η from (14b), with i = j = 1.
- (iii) Calculate ξ from (14a), with i = j = 1.
- (iv) Calculate $\kappa = \eta/\xi$.

Set i = 2.

- (v) Calculate $v_{ii'}$ from (14c). Set $v_{i'i} = v_{ii'}$.
- (vi) Calculate c_i from (14b), with i = i'.
- (vii) Calculate $h_{ii'}$ from (31a). Set $h_{i'i} = h_{ii'}$.

(viii) Regard (31b) as two linear equations for the v_{ij} and h_{ij} explicitly occurring on the lhs, with "known" coefficients involving c_i , c_j , and h_{jj} . For j = 1, ..., i, but not equal to i', solve these equations for v_{ij} and h_{ij} . Set $v_{ji} = v_{ij}$ and $h_{ji} = h_{ij}$.

Now increase i by one, and repeat steps (v)-(viii) up to the desired maximum value of i. Then go back to (i) and repeat the whole procedure.

Basically, this is the procedure we have used to obtain the perturbation expansion solution of the equations in powers of u, except that we did not necessarily use precisely the sequence indicated.

6. EXPANSION IN POWERS OF u

As is well known,⁽¹⁰⁾ κ can be expanded in a power series in u:

$$\kappa = 1 + \mu u^{2} + 2\mu^{2}u^{3} + (\mu^{4} + 6\mu^{3} - 2\mu^{2})u^{4} + \cdots$$
$$= \sum_{r=0}^{\infty} a_{r}u^{r}$$
(32)

where each coefficient a_r is a polynomial in μ with integer coefficients. The other variables ξ , η , h_{11} , h_{12} ,..., v_{11} , v_{12} ,... in our equations can similarly be expanded; for instance, any element h_{ij} of H can be expanded in the form

$$h_{ij} = u^{l_{ij}} \{ h_{ij0} + h_{ij1}u + h_{ij2}u^2 + \cdots \}$$
(33)

where l_{ij} is a nonnegative integer and the coefficients h_{ijr} are functions only of μ . The procedure of Section 5 can be used to systematically obtain all such coefficients, in particular the coefficients a_r in (32).

The usefulness of the present approach lies in the fact that to obtain the first *m* coefficients in (32) it is only necessary to expand a finite number of elements of *H* and *V* (all the rest can be taken to be zero), and no more than *m* coefficients are needed in any element. To see this, consider, for example, Eq. (14a) with i = j = 1. This equation can be regarded as defining ξ . Using (15), we can write it as

$$\xi = 1 + c_2 h_{21}^2 + c_3 h_{31}^2 + c_4 h_{41}^2 + \cdots$$
(34)

Using the small-u behavior given in Section 3, we obtain the orders of magnitude of the various terms in (34) as

$$\xi = 1 + \mathcal{O}(u^2) + \mathcal{O}(u^{10}) + \mathcal{O}(u^7) + \cdots$$
(35)

Variable	Maximum number of terms needed	Variable	Maximum number of terms needed	Variable	Maximum number of terms needed
 v ₁₁	8	<i>c</i> ₂	6	h ₁₄	2
η	8	h_{22}	5	c_{14}	2
ξ	8	v_{22}	4	h_{44}	1
v_{12}	6	v_{24}	2	v_{14}	1
h_{12}	6	h_{24}	2		

Table 1.	Variables	Needed	in Calo	culating	ж to	Order	7 ^a	and	the	Maximum
	Number of	Terms N	eeded	in the E	Expans	sion of	Ea	ch V	arial	ble

^a I.e., the first eight terms. Recall that c_1 and h_{11} are fixed to be one.

The general trend is for the powers of u to increase: the largest term omitted in (35) is actually of order u^{12} . Thus, if we wish to obtain ξ to order u^7 (say) from this equation, we shall need

 c_2 and h_{21} to relative order u^5 (first six coefficients)

 c_4 and h_{41} to leading order only (first coefficient)

All other matrix elements occurring in this equation (including c_3 and h_{31}) are negligible to this order.

Of course, to obtain κ to order u^{γ} , we need both ξ and η to this order, so it is also necessary to look at the equation used to calculate η , and then at the equations used to determine all the variables that are needed in calculating ξ and η , and so on. Even so, we find that only 14 variables are needed, and for many of these only the first one or two terms in their expansions are needed, as is shown in Table I.

Note in particular that only elements occurring in rows and columns one, two, and four are needed. All other elements can be taken to be zero. Thus, in using the iterative procedure of Section 5 we could stop at i = 4, and ignore i (or j) = 3, provided we need κ only to order u^7 .

If we want κ to a higher order, then we of course need more rows and columns of the matrices. For instance, to order u^{11} we need elements in rows and columns one, two, three, four, and eight. Any element c_i , h_{ij} , v_{ij} with either *i* or *j* not equal to one of these values can be ignored.

More generally, we found empirically the following simple rule: to calculate κ to order u^{2m+1} we need only those rows and columns *i* for which $\rho_i^{1/2}c_i^2 \ge u^m$. From (29), this implies that the $\sigma_1, \sigma_2, \dots$ in (27) must satisfy

$$\alpha_i \equiv \sum_{r=1}^{\infty} (2r-1)(1-\sigma_r \sigma_{r+1}) \ge 2m \tag{36}$$

i	α_i	i	α_i	i	α _i	i	αί
1	0	7	12	32	18	9	24
2	2	16	14	13	20	29	24
4	6	5	16	31	20	63	24
3	8	15	16	14	22	10	26
8	10	6	18	64	22		

Table 2. The First 19 Values of α_i in Nondecreasing Order^a

^a This α_i is the leading power of *u* in the expansion of $\rho_i c_i^4$.

This rule makes good sense. The variational expression (31a) for κ in I contains a factor

$$r_1 = \sum_a \operatorname{Tr} A^4(a) \tag{37}$$

which in our present notation becomes

$$r_1 = \sum_i \rho_i c_i^4 \tag{38}$$

Thus the rule (36) is equivalent to stating that if the contribution of c_i to r_1 is negligible (to the required order u^{2m+1}), then row *i* and column *i* may be deleted from the matrices.

In Table II the first 19 values of α_i , arranged in nondecreasing order, are given. It can be seen that to obtain κ to order u^{23} we needed 15 rows and columns of the matrices. To obtain κ to order u^{25} we would need 18 rows and columns.

7. TECHNICAL MODIFICATIONS

The coefficients in the expansion of κ are themselves polynomials in μ , with integer coefficients. It would obviously be a considerable computational simplification if this were true of all coefficients of powers of u that occur, for instance, the h_{iir} in (33).

We ensured this by overcoming two obstacles. The first is that step (vii) of Section 5 involves taking a square root, which can produce half-integer leading powers of u and μ (as is evident in Section 3), and noninteger coefficients. To avoid this we replaced H and V in (14) by $P^{1/2}HP^{1/2}$ and $P^{1/2}VP^{1/2}$, where P is a diagonal matrix. The elements $h_{ii'}$ can then be chosen arbitrarily, and (31a) regarded instead as a linear equation for p_i .

The other difficulty is in step (viii), which involves dividing by the determinant of the coefficients of v_{ij} and h_{ij} in (31b), namely

$$\Delta_{ij} = \eta \tau_{ij} c_i c_j - h_{jj}^2 \tag{39}$$

Let k = 2j if i is even, 2j + 1 if i is odd. Then j = k', and from (26b) it follows that to leading order

$$\Delta_{ij} = \tau_{ij}c_ic_j - \tau_{kj}c_kc_j = \tau_{ij}c_j(c_i - c_k) \tag{40}$$

since $s_i = s_k$.

Provided that c_i is not of the same order as c_k , Δ_{ij} is to leading order of the form $\pm \mu^{2p} u^n$, and there is no problem in dividing by it.

Since $s_i = s_k$, it is also true that $\rho_i = \rho_k$. Thus c_i is of the same order as c_k iff $\alpha_i = \alpha_k$, where α_i is given by (36). Since j = i' is excluded in step (viii), *i* and *k* are distinct.

From Table II it is apparent that the lowest seven α_i are unequal. To order 15 in κ , only the rows and columns corresponding to these α_i are needed in the calculation, so c_i and c_k in (40) are always of different orders, and all is well. In fact, (31b) becomes effectively two independent equations: one for h_{ij} , the other for v_{ij} .

However, when calculating κ to higher order, values of *i* and *k* for which $\alpha_i = \alpha_k \ (i \neq k)$ are needed; the first are 5 and 15. In these cases we allowed the off-diagonal element $c_{ik} \ (=c_{ki})$ of *C* to be nonzero, and set h_{ij} (for i < k) to zero. For i < k, step (viii) was then replaced by a calculation of v_{ij} and c_{ik} . For i > k, h_{ij} was calculated from (14a), v_{ij} from (14c).

Since C is no longer diagonal, the equations were of course appropriately modified, starting from the basis-independent equations (13). Fortunately it remained true that C was "near-diagonal," in the sense that to leading order in u its diagonal elements were its eigenvalues. Thus the discussion of Section 4, for instance, remains true, provided c_i is understood to be the diagonal element c_{ii} of C.

8. COMPUTATIONAL PROCEDURE

The procedure for obtaining series coefficients breaks up into seven main stages

(i) Determine the "structure" of the equations and the leading powers of the c_i , as described in Section 4.

(ii) Obtain a specification for which equations determined which matrix elements. This is given in Section 5. For each new matrix element introduced in Section 7, one of the original matrix elements is fixed and this is done in such a way as to preserve the essential structure of the iterative procedure described in Section 5.

These first two stages were carried out by hand.

(iii) Work through the equations as in Section 5 to determine the leading powers of u in the expansion of each matrix element.

(iv) Determine the relative order needed in each matrix element to obtain κ to the desired order m.

(v) Determine the sequence in which the individual steps (one for each variable) in Section 5 should be performed. This sequence was required to produce one new term in one matrix element at each step.

These three stages were carried out using a DEC-10 computer. The calculations required only short runs of comparatively small Fortran programs. Steps (iii) and (iv) were carried out using up to 50 rows and columns of the matrices so as to be reasonably sure that no significant elements had been ignored.

(vi) Calculate successive coefficients of the matrix elements in the order obtained from (v).

(vii) As a check, substitute the solutions obtained into every matrix equation [including those which were not needed in steps (iii)–(vi)] to check that each equation is satisfied to the appropriate order in u.

By dividing the calculations into stages in this way we ensured that only the short calculations of stages (iii)–(v) involved iterative procedures. In the longer calculations of stage (vi) each coefficient in each matrix element was calculated directly rather than being obtained as the limit of a sequence of improvements.

9. COMPUTATIONAL DETAILS

The most critical part of any computer calculation involving algebraic manipulation is normally the design of the data structures. Dividing the problem into stages as described in Section 8 enabled us to achieve some considerable simplifications.

For stages (iii)–(v) only a limited amount of information was needed for each matrix element (leading power, required order, known order) and so the various properties could be conveniently stored using Fortran arrays. Each of the stages (iii)–(v) involved iterative procedures. Each equation from Section 5 was examined in turn and, if possible, used to refine the current quantity being calculated. This whole process was repeated until no further refinements occurred.

Stage (iii) calculated leading powers [e.g., l_{ij} in (33)]. The starting point for the iteration was to assume that the leading powers were arbitrarily large in all variables except the "fixed" variables and the c_i .

Stage (iv) calculated the required orders. The initial stage was a specified required order for κ . Other variables were initially specified as being not required at all.

Stage (v) operated by assuming that all earlier calculations had been

performed to specified orders. The program then searched cyclically through the equations, applying the following procedure:

(a) Is the variable needed to one more order? If not, go on to the next equation.

(b) Can the variable be calculated to one more order at this stage? (I.e., are all the other variables in the equation known to sufficiently higher order?) If so, record this as the next step in the sequence of calculations and regard the variable as having been calculated.

Since the procedure of Section 5 is purely empirical, it could have happened at some stage that there were variables to update but no single equation which determined any one of them (i.e., we would have had to solve simultaneous equations in order to proceed). Fortunately this did not occur.

The knowledge of this iteration sequence for obtaining coefficients was exploited in the design of stage (vi).

The calculation of κ to order 23 involved about 270 matrix elements (and the variables κ , ξ , and η). Each of these quantities was a power series in u with from one to 24 terms. The coefficients were expressions of the form $\mu^a \sum_{m=0}^n c_m \mu^m$ with *n* ranging from zero to over 100 (the leading power *a* was allowed to be negative). The number of c_m in all the terms of all the matrix elements grew roughly exponentially with the order to which κ was calculated. 70,000 numbers being required at order 23. Because of the sequential nature of the calculation it was possible to store these numbers in a linear array so that $\mu^a \sum_{m=0}^n c_m \mu^m$ was represented by the sequence $(n, a, c_0, ..., c^n)$ and this sequence was stored immediately after the previous such sequence. Since each such polynomial was calculated correctly without any subsequent revisions and required for all subsequent orders, there was no need of any complicated memory management to allow for reuse of space formerly occupied by temporary intermediate quantities. The polynomials for various powers of *u* were located by an array of pointers associated with each matrix element.

Like the memory requirements, the execution time and the maximum integers occurring grew exponentially with the order of the calculation. It took about 16 sec of CPU time to reproduce the results of Sykes *et al.*⁽⁷⁾ and slightly more than an hour to obtain κ to order 23. At order 18 certain coefficients exceed $2^{35} - 1$, the maximum integer allowed by our Fortran system. The calculations were therefore performed using modular arithmetic. The whole program was run twice, once with calculations being performed modulo 2^{35} and once with calculations being performed modulo 3937, so that the results in the appendix are correct modulo $2^{35} \times 3937$. If the observed exponential growth in the size of the maximum coefficient is preserved through to order 23, then the values tabulated will be correct without any additional

multiples of $2^{35} \times 3937$. An additional reason for believing that such multiples are absent is that for $\mu = \pm 1$, both κ and $\partial \kappa / \partial \mu$ agree with the known exact solutions.^(9,11,12)

10. VARIATIONAL APPROXIMATIONS

We emphasize again that we have used the exact infinite-dimensional matrix equations (1), calculating all matrix element coefficients necessary to obtain κ to order u^{23} .

At the same time, it is interesting to use our methods to test the variational approximations proposed in I. These are obtained by restricting the matrices in (1) to be of finite size. The natural sequence of such approximations is to take the matrices to be 1 by 1, 2 by 2, 4 by 4, 8 by 8, etc.; and to be given at low temperatures as in Section 3. Tsang⁽⁸⁾ has investigated these approximations numerically for the zero-field Ising model, and has found that they converge rapidly (extremely rapidly away from the critical point) to the known exact values.

We can now answer the question: how many terms in the expansion of κ does a given approximation correctly reproduce?

It was easy to modify our program so as to keep only elements occurring in a given approximation, and to then compare the resulting series for κ with the exact one.

The 1 by 1 approximation is that of Kramers and Wannier.⁽⁴⁾ This correctly gives κ to order u^5 , and gives the coefficient of u^6 correctly except that it omits the term $\mu^9 u^6$. Thus

$$\kappa_{\text{exact}} - \kappa_{1 \times 1} = \mu^9 u^6 + \mathcal{O}(u^7) \tag{41a}$$

Similarly, we have found that

$$\kappa_{\text{exact}} - \kappa_{\times 22} = \mu^{25} u^{10} + \mathcal{O}(u^{11})$$

$$\kappa_{\text{exact}} - \kappa_{4 \times 4} = \mu^{49} u^{14} + \mathcal{O}(u^{15})$$

$$\kappa_{\text{exact}} - \kappa_{8 \times 8} = \mu^{81} u^{18} + \mathcal{O}(u^{19})$$
(41b)

From these results it is apparent that the leading error in the 2^{n-1} by 2^{n-1} approximation is $\mu^{(2n+1)^2} u^{4n+2}$. Graphically, this is the contribution to κ of a 2n + 1 by 2n + 1 square, consisting entirely of reversed spins.

APPENDIX

The series expansion for κ is of the form

$$\kappa = 1 + \sum_{n=2}^{\infty} \sum_{m} C(n, m) u^{n} \mu^{m}$$

The nonzero C(n, m) have

$$j \le m \le j^2, \qquad n = 2j$$

$$j \le m \le j(j-1), \qquad n = 2j - 1$$

At $\mu = 1$ (H = 0) both κ and the magnetization $M [= 1 + (\partial/\partial H)(kT \ln \kappa)]$ are known exactly. The zero-field susceptibility is

$$\begin{split} \chi &= (\partial^2 / \partial H^2) (kT \ln \kappa) |_{H=0} \\ &= 4(kT)^{-1} (u^2 + 8u^3 + 60u^4 + 416u^5 + 2791u^6 + 18296u^7 \\ &+ 118016u^8 + 752008u^9 + 4746341u^{10} + 29727472u^{11} \\ &+ 185016612u^{12} + 1145415208u^{13} + 7059265827u^{14} \\ &+ 43338407712u^{15} + 265168691392u^{16} + 1617656173824u^{17} \\ &+ 9842665771649u^{18} + 59748291677832u^{19} \\ &+ 361933688520940u^{20} + 2188328005246304u^{21} \\ &+ 13208464812265546u^{22} + 79600379336505342u^{23} \\ &+ \cdots) \end{split}$$

	1	C	2(2,1)				
	2	C	2(3,2)				
	-2 C	(4,2) TO 6	C(4,4)	1			
	-14	(5,3) то 18	C(5,6)	8	2		
8	C -77	(6,3) то 44	C(6,9) 40	22	6	1	
98 2	-370	(7,4) то 40	C(7,12) 138	134	72	30	8
-40 151	C 799 68	(8,4) то -1556 22	C(8,16) -424 6	221 1	546	462	310
-706 1342	C 5304 864	(9,5) TO -5470 456	C(9,20) -3708 218	-1222 88	1230 30	1896 8	1902 2
225 7557 187	-7672 7444 68	C(10,5) 30348 6426 22	TO C(10,2 -13598 4572 6	5) -18964 2979 1	-14444 1728	-2696 914	3699 426

5204 -65 13272 25 4472 2 2	C(11,6) TO 104 151574 458 31394 408 1208	C(11,30) -694 -65862 28974 24000 560 238	-87948 -4978 17746 1217 88 3	86 ~17472 26 7574 10 8
-1362 70 -242384 -83 75882 55 1054	C(12,6) TO 850 -467359 6 084 12470 076 37234 470 187	C(12,36) 49535 262160 88700 119884 23814 14364 68 22	-87840 -37839 128778 11776 8238 441 6	93 -337810 66 99290 00 2244 1
~39030 7: -1545118 -16: 522638 5: 133968 5: 2816 2816 2	C(13,7) TO 32764 -2932576 25216 -1051706 49068 504642 88290 55970 1332 584	C(13,42) 2228858 2029 -589506 -100 435766 350 33738 19 238	9462 874668 0010 213582 0336 267222 5574 10784 88 30	-1014862 429998 193180 5664 8
8670 9549646 -3337080 2382596 768638 58838 1106 1	C(14,7) TO -639433 66 762288 -42 -1518502 2255598 22 546306 3 33768 470	C(14,49) 311938 -162447 249586 -76955 97156 11642 306540 16822 375856 2491 18664 98 187	768 4560830 965 -6881592 996 1945588 952 1352688 954 159636 966 5014 68 22	10051601 ~5583312 2281417 1037676 98522 2408 6
296652 59058342 -27241336 8391488 6980988 1227956 75440 1360 2	C(15,8) TO -7804442 47: 31112876 49 -19920878 -111 9972394 10 5647102 49 828890 9 42520 584	C(15,56) 256224 -787788 952616 -237434 449760 -47912 580136 102799 426656 33565 544458 3469 23178 12 238	300 -10768506 438 -31567608 266 1316882 976 9481042 992 2473336 994 215208 160 6136 88 30	32372408 -33797354 5415648 8287220 1766316 129258 2960 8
-57253 -186465885 -597278 -108483798 22564319 45256582 20273390 4529332 578554 38620 1106 6	C(16,8) TO 5685542 12493642 -86868766 -78593018 35587123 41190974 15829110 3182598 355542 , 20524 470 1	C(16,64) -78352726 261194858 -148295915 -44988760 43185150 36188632 12041549 2154074 212810 10558 187	313892342 238197716 -153278297 -18303116 47169002 30705631 8948590 1423134 124132 5202 68	-322579472 159972553 -140530480 5156834 47364155 25323304 6487288 918726 70233 2468 22
-2278538 -1251265124 635252528 -681225430 -90986820 208594416 165178696 61956052 13746848 1877982 151632 6300 888	C(17,9) TO 80310676 -764445582 127063826 -601802848 8428644 217550716 142441448 47670848 9600928 1186826 85244 2992 30	C(17,72) -679161356 724510014 -379872674 -462203986 84160308 215438532 119644950 35977028 6574570 734714 46600 1360 8	$1863094888\\1183548008\\-616220230\\-333441648\\144560572\\203846368\\98244398\\26611628\\4418162\\444422\\24738\\584\\2824738\\584\\2824738\\584\\2828\\2838\\2838\\2838\\2838\\2838\\2838\\28$	-993191542 1274083894 -729611390 -202229512 183938370 186544548 78820104 19314722 2909010 262906 12696 238

	C(18.9) TO C(18.)	81)	
388802	-50032548	916955220	-5217511816
9834974207	-1089145506	-5657415098	-7098109106
-487090066	3635914388	6838712692	5540059481
3680485502	831342834	-1147699828	-2666288478
-3197910140	-3404412644	-3082431138	-2656113322
-2087698748	-1546743800	-993051812	-521524459
-87170874	259626592	547690090	756159946
902055898	981708972	1011770298	995157736
946239371	871933652	783431182	686674998
589385362	2 495302608	408530636	330685268
263068892	2 205658638	158148838	119586158
89003823	65162530	46959374	33290564
2322970	1 15940820	10762790	7143314
4660592	2 2986678	1879750	1160328
702578	3 416448	241610	136848
75685	5 40712	21304	10770
5270	2468	1106	470
187	7 68	22	6
1	t		

C (19,10) TO C(19,9	0)	
17649910	-797698944	9016362186	-36018566176
45188788806	13621335208	-14707405668	-42179699380
-22532767840	-1569288086	25232887974	30719299520
29745477974	18615039164	7925920732	-3076407410
-9591429048	-14406378468	-15739114470	-15741068066
-14212502540	-12318554234	-9873794544	-7587998260
-5225244528	-3152960096	-1216458316	414413968
1814578926	2900487922	3739479444	4297607820
4629244778	4741404944	4686737324	4486638124
4188731988	3817870916	3409991942	2986345974
2569772506	2173560256	1809591182	1482920164
1197509370	952833304	747583408	578263006
441254780	332060818	246552076	180569152
130470700	92978850	65362432	45302620
30963148	20855388	13843842	9049282
5824898	3688490	2297646	1405942
845040	498056	287682	162568
89800	48344	25338	12880
6336	2992	1360	584
238	88	30	8
2			

C	C(20.10) TO C(2	0,100)	
-2699202	436976042	-10273440219	78353373965
-224603332620	170177308196	137645380565	30290040193
-181767876286	-176499399732	-118585422851	33966625668
113112711312	162942828110	144892167071	109025803836
52019575364	7935035690	-33346637431	-57056817287
-72044727940	-75529606284	-74313139558	-67156106274
-58949700218	-48584738492	-38697422840	-28508502848
-19224958776	-10399824286	-2738436906	4111367087
9755582174	14392370794	17858017887	20343275756
21812028152	22462088640	22349550232	21655588075
20482940924	18984024358	17260822518	15431749461
13571789098	11760048162	10042540600	8460370720
7032090196	5771299776	4676825349	3744177562
2961346430	2314740106	1788009488	1365272026
1030329734	768675138	566798557	413139584
297596928	211864634	149017209	103558802
71074110	48172590	32228382	21278938
13857418	8899228	5631354	3510146
2153196	1299326	770133	448272
255710	142900	78009	41580
21540	10846	5270	2468
1106	470	187	68
22	6	1	

	С(21,11) ТО С	(21,110)	
-137674532	7785746552	-112888535288	612376056680
-1261409345442	423106621732	801825413332	704180055914
-472416181748	-889395776028	-1021024867678	-395226054492
115128451484	611780411810	769125941340	778247147438
581264541660	378018576704	130274078330	-56645505196
-210575498342	-298783105656	-354043993498	-363169036964
~355447107466	-324809631118	-289243215724	-245498356166
-202439064366	-157512872880	-115950878666	-75563836072
-39213719214	-5815541354	22949974670	47885535776
67989446690	83954158250	95419796290	103015575062
106861414854	107591334036	105552425648	101387623842
95499032950	88445155468	80608543682	72415666818
64153016790	56108367452	48459035782	41360450420
34893724540	29112899304	24024038986	19615962248
15848336942	12673741034	10031524258	7860845428
6098011504	4683766622	3561595390	2681586246
1998818468	1475082080	1077583166	779248172
557695446	395006668	276808518	19190-360
131574666	89207692	59782024	39593052
25900410	16731882	10666906	6709210
4159626	2541224	1528112	903944
525376	299750	167600	91728
49008	25542	12920	6336
2992	1360	584	238
88	30	8	2

(C(22,11) TO C	(22,121)	
19076006	-3794770713	111304562027	-1092704834228
4346652233232	-6291768217070	-376126004360	3129928307620
5592658217298	679016122604	-2724759534469	-5789007505314
-4382809075566	-2307752907687	794745448158	2699292204678
3954323197056	3850259185456	3375918830835	2306290801088
1282990166282	242272413516	-526697708097	-1153904785370
-1502912104262	-1721524481865	-1758761536061	-1722633811538
-1597795341798	-1447506956370	-1259323433439	~1072381885192
-874903651924	-686995664340	-501395669362	-330299440430
-168407379252	-23992189363	106238437455	217467942226
311633846638	386664886313	444402432861	484449002118
509133385060	519203696700	517094841000	504300209966
483195403146	455421545217	423067326875	387633978474
350726691968	313517449971	277107077201	242244854088
209576736204	179469511693	152190239266	127815919430
106347020794	87667941990	71620746856	57986981032
46537111248	37020720378	29195990553	22825821468
17692629696	13595524004	10357675690	7822695960
5857133378	4347091080	3198142752	2331913666
1685113960	1206603136	856029487	601590324
418753076	288625076	196956187	133019854
88896396	58762848	38411074	24816062
15841458	9985054	6212410	3811952
2305732	1373310	805061	463756
262362	145456	78965	41840
21624	10846	5270	2468
1106	470	187	68
22	6	1	

C	C(23,12) TO C	(23,132)	
1080178538	-74731542218	1351003453762	-9503167548524
28127939528142	-26891781363918	~13207067538620	4522686599434
31141664581778	18139538680866	1880468249182	-22904276527452
-27190235998138	-24436947953846	-10650936005412	1549143457220
13254410978582	18180037905140	20432280600446	18055038292228
14386260860398	9206832077992	4572222975832	30735576280
-3250077587556	-5895167942722	-7413342739388	-8349691212982
-8563692206672	-8453916232204	-7947721447958	-7322910909586
-6528694002232	-5714827391066	-4841269003308	-3997099216886
-3145744362890	-2344094195940	-1568811393958	-854735681794
-191459054670	399873582720	925320442076	1371356526908
1744588408594	2038992013684	2261547377836	2412463077942
2500308625556	2529044171728	2507995388538	2443452302656
2344334766176	2217554998498	2071056094176	1910986572650
1743783003478	1574261974430	1407015953008	1245329036872
1092038934718	948961018146	817468033792	698172964190
591348668150	496769408092	413983573728	342261568638
280767712426	228541284508	184612447588	147993501574
117745607452	92974018006	72865154256	56676557478
43754944118	33524837122	25493281372	19238482582
14407761188	10706769444	7894797574	5775520084
4191594878	3017463414	2154461718	1525425028
1070902030	745270346	514072144	351367848
237929952	159565440	105960218	69643618
45293968	29134370	18528374	11642842
7226144	4426312	2674384	1592464
933808	538576	305258	169712
92456	49232	25586	12920
6336	2992	1360	584
238	88	30	8
2			

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