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Hard-Square Lattice Gas

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We have studied the hard-square lattice gas, using corner transfer matrices. In particular, we have obtained the first 24 terms of the high-density series for the order parameter $\rho_2 - \rho_1$. From these we estimate the critical activity to be 3.7962 ± 0.0001. This is in excellent agreement with the earlier work of Gaunt and Fisher. It conflicts with the value 4.0 given by Müller-Hartmann and Zittartz's formula for the critical point of the antiferromagnetic Ising model in a field, so we conclude that this formula, while a good approximation, is not exact.

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

1. INTRODUCTION

It has been known for some years that good numerical estimates of the thermodynamic properties of simple two-dimensional lattice models can be obtained using the "corner transfer matrix" (CTM) formalism.[1-4] Very recently it has also been shown that this method can be used to obtain series expansions[5] longer than those previously obtained by graphical methods.

Until now, the CTM method has been applied only to "ferromagnetic" systems in which the thermodynamic states are translation invariant. Here we consider an "antiferromagnetic" system: the hard-square lattice gas. In this model the translation invariance symmetry is broken at sufficiently high densities, one or the other of the two sublattices being preferentially occupied.

The hard-square lattice gas is an interesting model in its own right and was studied by series expansions by Gaunt and Fisher[6] in 1965 and numerically by Runnels and Combs[7] in 1966. From our point of view it has the advantage that there is only one parameter (usually the activity z), so we only

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have to handle single (rather than multiple) series on the computer. This has meant that our computer time was measured in minutes, rather than hours.

Added interest has also been given to the problem by Müller-Hartmann and Zittartz.[8] They considered the antiferromagnetic square-lattice Ising model with spins $\sigma_i = \pm 1$ at sites i, and Hamiltonian

$$\mathscr{H} = J \sum_{\langle ij \rangle} \sigma_i \sigma_j - H \sum_i \sigma_i, \qquad J > 0 \tag{1.1}$$

the first summation being over all nearest neighbor pairs $\langle ij \rangle$ of sites. By considering the interfacial tension, they obtained the formula

$$\cosh(H/kT) = \sinh^2(2J/kT) \tag{1.2}$$

for the position of the critical point (for the antiferromagnetic model there is a critical point even for nonzero H).

Although their derivation of the interfacial tension was approximate, the formula (1.2) is exact[9] for $H = 0$. It has been conjectured[10] that it may be exact for all H, and Lin and Wu[11] have extended the conjecture to the triangular-lattice Ising model.

If one lets J/kT and H/kT both tend to infinity, keeping

$$z = \exp[(8J - 2H)/kT] \tag{1.3}$$

fixed, then the antiferromagnetic Ising model becomes the hard-square lattice gas with activity z. The formula (1.2) then gives the critical activity z_c of z to be

$$z_c = 4 \tag{1.4}$$

This is fairly close to the numerical estimate 3.80 ± 0.02 of Gaunt and Fisher. Indeed, it was tempting to speculate that Gaunt and Fisher may have been overoptimistic in their error bounds, and that (1.4) is correct.

For this reason we have been particularly interested in locating z_c. Our best estimate was obtained from the large-z (high-density) expansion of the order parameter $\rho_2 - \rho_1$. Gaunt and Fisher had obtained the first 10 terms in this series: we have extended the number of known terms to 24. Our conclusion is that Gaunt and Fisher were remarkably accurate in their best estimate, and properly conservative in their error bounds: in their equation (5.31) they quote a value 0.7915 ± 0.0010 of $z_c/(1 + z_c)$, giving $z_c = 3.7962 \pm 0.0230$. We find that

$$z_c = 3.7962 \pm 0.0001 \tag{1.5}$$

It therefore appears that (1.2) is not an exact result. Even so, it is a remarkably simple and reasonably accurate approximation.

2. THE CTM EQUATIONS

To each site λ of a square lattice of N sites assign a "spin," or "occupation number" a_λ. If each spin interacts only with spins on a common face, then the partition function is

$$Z = \sum_{\{a\}} \prod_{(\lambda,\mu,\nu,\tau)} w(a_\lambda, a_\mu, a_\nu, a_\tau) \tag{2.1}$$

where the product is over all faces $(\lambda, \mu, \nu, \tau)$ of the lattice (such as that shown in Fig. 1), the sum is over all allowed values of $a_1,\ldots,a_N$, and $w(a_\lambda, a_\mu, a_\nu, a_\tau)$ is the Boltzmann weight of a face.

In particular, for the hard-square lattice gas, we can take

$$\begin{aligned} a_\lambda &= 0 \quad \text{if site } \lambda \text{ is empty} \\ &= 1 \quad \text{if site } \lambda \text{ is occupied} \end{aligned} \tag{2.2}$$

We require that no two adjacent sites be occupied, and assign an activity z to each occupied site. Sharing out these activities among the four surrounding squares, it follows that

$$w(a, b, c, d) = z^{(a+b+c+d)/4} g_{ab} g_{bd} g_{dc} g_{ca} \tag{2.3}$$

where

$$g_{00} = g_{01} = g_{10} = 1, \qquad g_{11} = 0 \tag{2.4}$$

We want to calculate the thermodynamic properties, in particular the partition function per site:

$$\kappa = \lim_{N\to\infty} Z^{1/N} \tag{2.5}$$

and the mean density at site λ

$$\rho_\lambda = \langle a_\lambda \rangle \tag{2.6}$$

For a translation-invariant system the corner transfer matrix equations are given in Eqs. (30) and (47) of Ref. 3. However, translation-invariance symmetry is spontaneously broken in the hard-squares model: one or the other of the two sublattices is preferentially occupied.

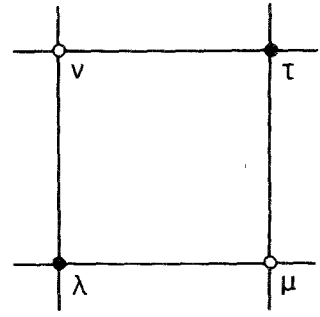


Fig. 1. A typical face of the square lattice, with corner sites λ, μ, ν, τ.

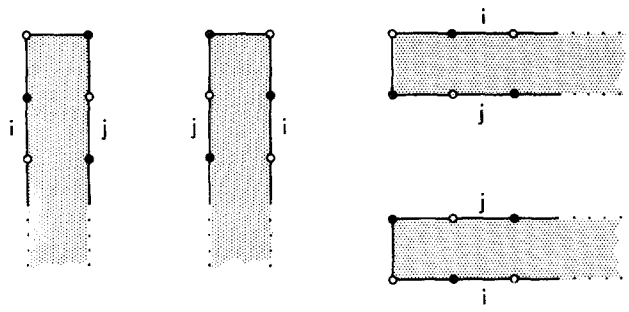


Fig. 2. Typical half-column and half-row segments of the infinite square lattice. Their weights are the elements F_{ij} of the matrix F.

To obtain sensible high-density approximations we must allow for this lack of symmetry. Divide the lattice into two sublattices 1 and 2 (open circles and filled circles) such that sites 1 are adjacent only to sites of type 2, and vice versa.

The easiest way to derive the CTM equations is to generalize the graphical interpretation given in Figs. 2–4 of Ref. 3. First consider all the possible half-row and half-column segments that can be formed in the infinite lattice. Four such are shown in Fig. 2. To each a label i is associated with the long edge ending in an open circle, and a label j to the one ending in a filled circle. This $i(j)$ denotes all the occupation numbers of the sites on its edge [it replaces the pair (a, λ) of Ref. 3].

Even allowing for a distinction between the sublattices, it is evident that all the four segments shown in Fig. 2 are equivalent, in that we expect the probability distribution $P(i, j)$ to be the same for each. Four other equivalent segments can be obtained by rotating the figure through 180°. With each such segment we therefore associate a weight F_{ij}.

Similarly, we consider the eight possible quadrants that can be formed in the infinite lattice. Three such are shown in Fig. 3. Labels i or i' are associated

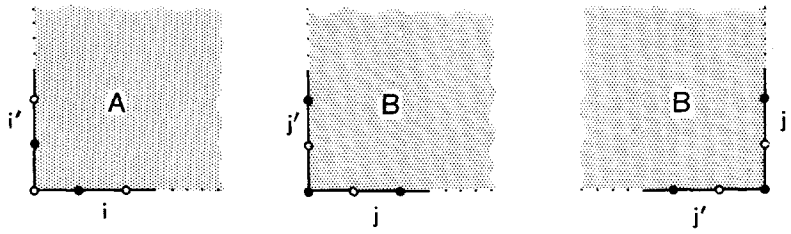


Fig. 3. Typical quadrants, or "corners," of the infinite square lattice, with weights $A_{ii'}$ and $B_{jj'}$; A and B are the "corner transfer matrices."

with edges ending in an open circle; j or j' with ones ending in a filled circle. It is evident that there are only two distinct quadrants: ones with an open circle at the corner, and ones with a filled circle. With the first we associate a weight $A_{ii'}$, with the second a weight $B_{jj'}$. Plainly they satisfy the symmetry conditions

$$A_{ii'} = A_{i'i}, \qquad B_{jj'} = B_{j'j} \tag{2.7}$$

The indices i and i' denote all the occupation numbers on the corresponding two edges in Fig. 3. Since the corner site is common to both edges, they are not quite independent. For an edge of type i, ending in an open circle, let s_i be the occupation number (0 or 1) of the end site. Similarly, for an edge of type j, let t_j be the occupation number of the end site. Then $A_{ii'}$ ($B_{jj'}$) is defined only if $s_i \times s_{i'}$ ($t_j = t_{j'}$).

It is convenient to extend the definition and to set

$$\begin{aligned} A_{ii'} &= 0 \qquad \text{if } s_i \neq s_{i'} \\ B_{jj'} &= 0 \qquad \text{if } t_j \neq t_{j'} \end{aligned} \tag{2.8}$$

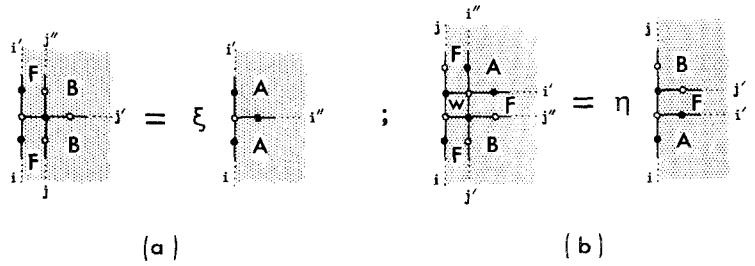
Now consider the analog of Fig. 4 of Ref. 3. In our case we obtain the two diagrams in our Fig. 4, plus two others obtained by interchanging filled and open circles.

First consider Fig. 4a, which contains two graphs, one on either side of the equals sign. The occupation numbers i, i' on the left-hand vertical edges are to be regarded as given; all others are to be summed over. For each graph this gives the unnormalized probability distribution $P(i, i')$ of spins on the left of a semi-infinite lattice. Since this is independent of the manner in which the lattice is built up, both sides must be the same, to within a normalization factor ξ. Thus

$$\sum_{j,j',j''} F_{ij} B_{jj'} B_{j'j''} F_{i'j''} = \xi \sum_{i''} A_{ii''} A_{i''i'} \tag{2.9a}$$

Since the edges i and i' end in the same site, this equation is valid for all i, i' such that

$$s_i = s_{i'} \tag{2.9b}$$



(a) (b)

Fig. 4. Diagrammatic representation of Eqs. (2.9) and (2.11).

A similar equation can be obtained by interchanging filled and open circles in Fig. 4a. From Figs. 2 and 3, the effect of this is to interchange the indices of F, and to interchange A with B. Also interchanging i with j, we obtain

$$\sum_{ii'i''} F_{ij}A_{ii'}A_{i'i''}F_{i''j'} = \xi' \sum_{j''} B_{jj''}B_{j''j'} \tag{2.10a}$$

for all j, j' such that

$$t_j = t_{j'} \tag{2.10b}$$

In the same way, Fig. 4b leads to the equation

$$\sum_{j'j''i'i''} w(s_i, t_{j'}, t_j, s_{i'})F_{ij'}B_{j'j''}F_{i'j''}A_{i'i''}F_{i''j} = \eta \sum_{i'j'} A_{ii'}F_{i'j'}B_{j'j} \tag{2.11}$$

for all i and j. Interchanging filled and open circles in Fig. 4b merely leads again to (2.11) with the products in reverse order, so (2.9)–(2.11) are the complete generalization of Eqs. (30) and (47) of Ref. 3.

It is obvious from (2.9) and (2.10) that it is useful to regard $A_{ii'}$, $B_{jj'}$, and F_{ij} as elements of infinite-dimensional matrices A, B, F (the corner and half-column transfer matrices). Further, by inserting the diagonals in the quadrants of Fig. 3, one can define matrices X, Y such that

$$A = X^T X, \qquad B = Y^T Y \tag{2.12}$$

where $X(Y)$ has the same block-diagonal property as $A(B)$, i.e.,

$$\begin{aligned} X_{ii'} &= 0 \qquad \text{if } s_i \neq s_{i'} \\ Y_{jj'} &= 0 \qquad \text{if } t_j \neq t_{j'} \end{aligned} \tag{2.13}$$

If $s_i = t_j = 1$, then F_{ij} is the weight of a half-column with the two end sites both occupied. Since this is not allowed, F_{ij} must be zero for all such i and j. From (2.4) it follows that

$$g(s_i, t_j)F_{ij} = F_{ij} \tag{2.14}$$

Equations (2.9)–(2.11) can now be simplified a little by defining

$$H_{ij} = z^{(s_i+t_j)/8}(XFY^T)_{ij}, \qquad C_{ii'} = z^{-s_i/4}(XX^T)_{ii'}, \qquad D_{jj'} = z^{-t_j/4}(YY^T)_{jj'} \tag{2.15}$$

They then become

$$\begin{aligned} (HDH^T)_{ii'} &= \xi z^{s_i}(C^3)_{ii'} \qquad \text{if } s_{i'} = s_i \\ (H^T CH)_{jj'} &= \xi' z^{t_j}(D^3)_{jj'} \qquad \text{if } t_{j'} = t_j \\ g(s_i, t_j)(HH^T H)_{ij} &= \eta(CHD)_{ij}, \qquad \text{all } i, j \end{aligned} \tag{2.16}$$

If we also define W, $\overline{W}$ by

$$W_{ii'} = z^{s_i}\delta_{ii'}, \qquad \overline{W}_{jj'} = z^{t_j}\delta_{jj'} \tag{2.17}$$

then the CTM equations (2.16) can be written in the simple form

$$HDH^T = \xi WC^3, \quad [C] \tag{2.18a}$$

$$H^TCH = \xi'\overline{W}D^3, \quad [D] \tag{2.18b}$$

$$HH^TH = \eta CHD, \quad [H] \tag{2.18c}$$

$$C^T = C, \qquad D^T = D \tag{2.18d}$$

where $[U]$ after a matrix equation (any U) means that if an element of U is defined to be zero by (2.13)–(2.15), then the corresponding element of the equation is to be ignored.

3. THE FREE ENERGY AND SUBLATTICE DENSITIES

Define

$$r_1 = \operatorname{Tr} WC^4, \qquad \bar{r}_1 = \operatorname{Tr} \overline{W}D^4, \qquad r_2 = \operatorname{Tr} CHDH^T, \qquad r_3 = \operatorname{Tr} HH^THH^T \tag{3.1}$$

Then it is evident from (2.18) that

$$\xi = r_2/r_1, \qquad \xi' = r_2/\bar{r}_1, \qquad \eta = r_3/r_2 \tag{3.2}$$

Further, if we define κ_2 by

$$\kappa_2 = \eta^2/\xi\xi' = r_1\bar{r}_1 r_3^2/r_2^4, \tag{3.3}$$

then κ_2 is stationary with respect to variations in the matrices C, D, and H, provided that (2.18) is satisfied.

By considering large, but finite, lattice segments, as in Eq. (65) of Ref. 3, one can establish that κ_2 is related to the partition function per site κ (which is the exponential of the negative free energy) by

$$\kappa = \kappa_2^{1/2} \tag{3.4}$$

A partial verification of this result can be obtained by differentiating (3.3) with respect to z. Since κ_2 is stationary with respect to C, D, and H, we can ignore the increments induced in these, leaving

$$z\frac{\partial}{\partial z}\ln\kappa_2 = \frac{\operatorname{Tr}' WC^4}{\operatorname{Tr} WC^4} + \frac{\operatorname{Tr}' \overline{W}D^4}{\operatorname{Tr} \overline{W}D^4} \tag{3.5}$$

the primes indicating that the traces are only over diagonal elements (i, i) or (j, j) for which $s_i = 1$ or $t_j = 1$.

From (2.17), (2.15), and (2.12),

$$\frac{\operatorname{Tr}' WC^4}{\operatorname{Tr} WC^4} = \frac{\operatorname{Tr}' A^4}{\operatorname{Tr} A^4} \tag{3.6}$$

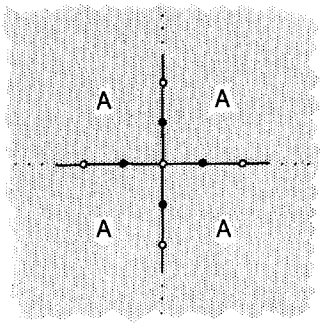


Fig. 5. Diagrammatic representation of Tr A^4.

As is evident from Fig. 5, Tr A^4 is the unnormalized partition function of an infinite lattice centered on an open circle site. Further, Tr′ A^4 is the same sum-over-states, but restricted to states where the central site is occupied. Their ratio is simply the mean density on a site on sublattice 1, as defined by (2.6). Thus

$$\rho_1 = \text{Tr}'\ WC^4/\text{Tr}\ WC^4 \tag{3.7a}$$

and similarly

$$\rho_2 = \text{Tr}'\ \overline{W}D^4/\text{Tr}\ \overline{W}D^4 \tag{3.7b}$$

Thus (3.4) and (3.5) give

$$z(\partial/\partial z)\ln\kappa = \tfrac{1}{2}(\rho_1 + \rho_2) \tag{3.8}$$

and this is indeed the correct thermodynamic formula.

A stronger test is also available. Since we have consistently distinguished between the two sublattices, we could assign different activities z_1 and z_2 to the sublattices 1 and 2, respectively. The only change in (2.17)–(3.4) is that the first z in (2.17) becomes z_1, the second z_2. Differentiating (3.3) then gives the correct result

$$z_i(\partial/\partial z_i)\ln\kappa = \tfrac{1}{2}\rho_i, \qquad i = 1, 2 \tag{3.9}$$

From now on we return to the case $z_1 = z_2 = z$.

4. SOLVING THE EQUATIONS

Equations (2.18) define C, D, H to within normalization factors and to within the orthogonal transformations

$$C \to P^T C P, \qquad D \to Q^T D Q, \qquad H \to P^T H Q \tag{4.1}$$

where P, Q are orthogonal matrices satisfying

$$\begin{aligned} P_{ti'} &= 0 \quad \text{if } s_t \neq s_{t'} \\ Q_{jj'} &= 0 \quad \text{if } t_j \neq t_{j'} \end{aligned} \tag{4.2}$$

Thus P and Q, like C and D, are block-diagonal. It follows that they can be chosen to ensure that C and D are strictly diagonal. With some slight modifications, this is the representation we use.

The equations are exact, but the matrices are infinite dimensional. The essence of the CTM method is that very good approximations can be obtained by truncating the matrices to finite size. The equations can then either be solved numerically for given values of z, or they can be used to obtain series expansions for the elements of the matrices, and hence for κ, ρ_1, and ρ_2.

The larger the matrices, the more accurate are the numerical results,[4] and the larger the number of correct terms in the series expansions.[5]

Given a reasonable initial guess for small or large z, the equations can be solved numerically by the Newton–Raphson method. The results can then be extrapolated to less extreme values of z and the procedure repeated. Alternatively, if the leading powers of all the matrix elements are known, then series expansions can be obtained by successively solving the equations to leading order, next leading order, etc.

To obtain such initial guesses, or leading powers, we adapted the method given in Section 3 of Ref. 3. Define U by

$$H^T H = U \tag{4.3a}$$

Then (2.18c) becomes

$$HU = \eta CHD \tag{4.3b}$$

Suppose η, C, and the first H on the LHS of (4.3) are known. If D is diagonal, then any column j of (4.3) is a coupled pair of eigenvalue equations with eigenvalue D_{jj}, columns j of H and U being the corresponding eigenvectors. The normalization of these vectors is given by the (j, j) element of (2.18b).

Similar equations for C_{ii} and rows i of H can be obtained by transposing (2.18c), defining $HH^T = V$, and using (2.18a) as the normalization condition.

Solving these eigenvalue equations, with the solution of a given truncation, one obtains not only the original diagonal elements of C and D, but also some new ones. The largest (or group of largest) of these should be kept and the matrices appropriately expanded. In this way one can build up larger and larger truncations: a similar procedure is exhibited in Section 3 of Ref. 5.

5. ACCURACY OF A GIVEN TRUNCATION

It is obviously important to know how accurate a particular truncation is. This is particularly true of series expansions, where one needs to know how many of the coefficients are correct.

In the absence of a rigorous treatment of the infinite-dimensional

matrices, we are forced to look for simple patterns in the sequence of approximations obtained by successively larger truncations. This can be done in two ways: either by merely comparing successive truncations and observing which coefficients change; or by considering a subtruncation of a larger one and seeing at what order the "outer" terms enter the "inner" equations.

Fortunately some very simple patterns emerge. To discuss them it is useful to define

$$\Gamma_i = (WC^4)_{ii}/(WC^4)_{11}, \qquad \Delta_j = (\overline{W}D^4)_{jj}/(\overline{W}D^4)_{11} \tag{5.1}$$

and to tighten the expansion rule at the end of Section 4 to become: Locate the largest new Γ_i or Δ_j. Keep this and all Γ_i or Δ_j of the same order, as well as all the original Γ_i, Δ_j.

We then find empirically that:

(i) All new Γ_i, Δ_j encountered in enlarging a truncation are at least one order higher than all the old ones. The old ones are unchanged to leading order (so in general are all the old matrix elements). Thus the sequence of truncations groups the collated set (Γ_i, Δ_j) in strictly increasing order.

(ii) If the largest Γ_i or Δ_j not included in a given truncation is of order n, then κ is accurate to relative order $n - 1$.

As was emphasized in Refs. 4 and 5, rule (ii) makes good sense. From (3.1), neglecting a Γ_i or Δ_j of order n introduces a relative error into r_1 or $\bar{r}_1$, and hence into κ, of order n. Of course this is a naive simplification, since truncating the matrices alters all elements at some order. Even so, it appears to have some validity: so far we have not found an exception to it in any of the models we have considered.

6. HIGH-DENSITY LEADING-ORDER SOLUTION

As $z \to \infty$, all sites of one sublattice (say 2) become occupied, all sites of the other (1) empty. There is then only one allowed state of the occupation numbers on a segment edge. Taking this to be state "one," it follows that $s_1 = 0$ and $t_1 = 1$, so

$$W = (1), \qquad \overline{W} = (z) \tag{6.1}$$

The matrices C, D, H are one-by-one. Their normalization is arbitrary, so we can choose

$$C = (1), \qquad D = (1), \qquad H = (1) \tag{6.2}$$

Then (2.18) gives

$$\xi = 1, \qquad \xi' = z^{-1}, \qquad \eta = 1 \tag{6.3}$$

and (3.3), (3.4), and (3.7) give the expected close-packed results

$$\kappa = z^{1/2}, \qquad \rho_1 = 0, \qquad \rho_2 = 1 \tag{6.4}$$

We build up from this one-by-one solution in the manner given in Sections 4 and 5. Taking (6.2) to be the first, the eleventh truncation gives C, D, H to be 7 by 7, 6 by 6, and 7 by 6 matrices. Set

$$x = z^{-1} \tag{6.5}$$

$$S = (s_1, s_2, s_3, \ldots), \qquad T = (t_1, t_2, t_3, \ldots) \tag{6.6}$$

and

$$H = L^{1/2} G M^{1/2} \tag{6.7}$$

where L and M are diagonal matrices that are at our disposal. Writing the diagonal matrices C, D, L, and M in row-vector form, we find that, to leading order,

$$\begin{aligned}
S &= (0 \quad 1 \quad 1 \quad 0 \quad 1 \quad 0 \quad 1) \\
C &= (1 \quad x \quad x^2 \quad 2x^2 \quad x^3 \quad 1\tfrac{1}{2}x^3 \quad x^4) \\
L &= (1 \quad x \quad x^2 \quad 4x^5 \quad x^3 \quad \tfrac{9}{16}x^6 \quad x^4) \\
T &= (1 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0) \\
D &= (1 \quad 1 \quad x \quad x^2 \quad 2x^3 \quad x^3) \\
M &= (1 \quad x \quad x^2 \quad x^3 \quad x^2 \quad x^4)
\end{aligned} \tag{6.8}$$

$$G = \begin{bmatrix}
1 & 1 & -x^2 & x^4 & 0.x^6 & -2x^6 \\
0 & 1 & 1 & -x^2 & 0 & 2x^4 \\
0 & -x^2 & 1 & 1 & 0 & 0.x^2 \\
-x & 1 & x^{-1} & \frac{1}{2}x^{-1} & 1 & -\frac{1}{4} \\
0 & x^4 & -x^2 & 1 & 0 & 1 \\
x^2 & -x & 1 & 2x^{-1} & \frac{8}{3} & \frac{4}{3}x^{-1} \\
0 & -x^6 & x^4 & -x^2 & 0 & 1
\end{bmatrix}$$

Elements of G denoted simply by 0 are exactly zero. Elements such as $0.x^6$ are only zero to the order given.

The largest Γ_i or Λ_j omitted in this truncation are Γ_8, Γ_9, and Δ_7, which are all of order x^{16}. Thus we expect this truncation to give κ correctly to order 15. This was borne out by our subsequent calculations of larger truncations. Also, to go to order 16 we must include Γ_8, Γ_9, and Δ_7, i.e., go to a 9 by 7 truncation of H.

A complication arises in this next step: C_{88} and C_{99} are eigenvalues of the same matrix equation, and are of the same order. This means that, to leading

order, one has a genuine two-by-two matrix to diagonalize, thereby introducing nonrational numbers. To avoid this we modify the requirement that C be strictly diagonal, and allow C_{89} ($=C_{98}$) to be nonzero.

The corresponding H-eigenvectors have dominant elements in positions 4 and 6, respectively, and these in turn correspond to H_{84} and H_{96}. Since from (4.1) we are free to premultiply H by a two-by-two orthogonal matrix P mixing rows 8 and 9, we can and do choose H_{86} to be zero. This fixes the representation.

Continuing to the 17th truncation, similar complications arise with rows 11 and 12, columns 9 and 10, and columns 11 and 12. The matrix H is then 13 by 12. The values of S and T, and the leading powers of the nonzero elements of C, D, L, M, G, are given in Appendix A.

The next largest Γ_i, Δ_j are Γ_{14}, Γ_{15}, Γ_{16}, Δ_{13}, and Δ_{14}, which are all of order x^{24}. We therefore expect the 13 by 12 truncation to give κ correctly to order 23. To obtain the next order we would have had to go to a 16 by 14 truncation, so it was convenient to stop at order 23.

7. LOW-DENSITY LEADING-ORDER SOLUTION

At low densities ($z < z_c$), the sublattice symmetry is not broken, so from Figs. 2 and 3 it is apparent that $F^T = F$ and $B = A$. It follows from (2.12)–(2.15) and (3.7) that

$$H^T = H, \qquad D = C, \qquad t_i = s_i, \qquad \rho_1 = \rho_2 \tag{7.1}$$

Equations (2.18) are then a special case of Eqs. (13) of Ref. 5.

When $z = 0$, all sites are empty, so there is only one allowed state i of the occupation numbers on a segment edge. Taking this to be state "one," it follows that $s_1 = t_1 = 0$, and

$$W = \overline{W} = (1) \tag{7.2}$$

The matrices C, D, H are one-by-one, so again we can choose them to be

$$C = D = (1), \qquad H = (1) \tag{7.3}$$

Then (2.18), (3.3), (3.4), and (3.7) give

$$\xi = \xi' = \eta = \kappa = 1, \qquad \rho_1 = \rho_2 = 0 \tag{7.4}$$

and these are indeed the zero-density values of κ, ρ_1, ρ_2.

We build up from this one-by-one truncation as in Sections 4 and 5. At the seventh truncation all matrices are 7 by 7. Again it is convenient to write H in the form (6.7), only now we naturally choose

$$M = L \tag{7.5}$$

To leading order we obtain

$$
\begin{aligned}
S &= (0 \quad 1 \quad 0 \quad 0 \quad 1 \quad 0 \quad 1) \\
C &= (1 \quad 1 \quad z^2 \quad z^4 \quad 2z^4 \quad z^6 \quad 1\tfrac{1}{2}z^6) \\
L &= (1 \quad z \quad z^5 \quad z^5 \quad 8z^6 \quad z^9 \quad 3\tfrac{3}{8}z^{10})
\end{aligned}
\tag{7.6}
$$

$$
G = \begin{bmatrix}
1 & 1 & -z & -z^5 & -z^7 & -z^7 & -\tfrac{1}{2}z^9 \\
1 & 0 & 1 & z^4 & 0 & z^6 & 0 \\
-z & 1 & z^{-2} & 1 & 1 & z^2 & \tfrac{1}{2}z^2 \\
-z^5 & z^4 & 1 & -1 & -\tfrac{1}{2} & 1 & 1 \\
-z^7 & 0 & 1 & -\tfrac{1}{2} & 0 & \tfrac{1}{4} & 0 \\
-z^7 & z^6 & z^2 & 1 & \tfrac{1}{4} & -z^{-2} & -\tfrac{2}{3}z^{-2} \\
-\tfrac{1}{2}z^9 & 0 & \tfrac{1}{2}z^2 & 1 & 0 & -\tfrac{2}{3}z^{-2} & 0
\end{bmatrix}
$$

The largest Γ_i, Δ_j omitted in this truncation are $\Gamma_8 = \Delta_8$ and $\Gamma_9 = \Delta_9$, which are of order z^{32}. Thus this truncation should give κ correctly to order 31.

We continued to the 11th truncation, when the matrices are 13 by 13. The largest Γ_i or Δ_j then omitted are of order z^{48}, so we expect this truncation to be accurate to order 47 in κ. In fact we have only calculated κ to order 42.

Since C_{88} and C_{99} have the same order, and $s_8 = s_9$, we allowed C_{89} to be nonzero and set H_{86} to zero. Similarly $C_{11,11}$ and $C_{12,12}$ have the same order and s value: we let $C_{11,12}$ be nonzero and set $H_{11,9}$ to zero. The values of S, and the leading powers of the nonzero elements of C, L, G, are given in Appendix A.

8. DERIVATION OF SERIES EXPANSIONS

We used (2.18) to expand ξ, ξ', η, and the matrix elements in increasing powers of x (for high densities) or z (for low densities).

The diagonal elements of (2.18a) and (2.18b) act as quadratic normalization conditions on the rows and columns of H. To solve them as written would involve taking square roots. We avoided this by substituting the form (6.7) of H into (2.18) and using the resulting extra freedom to fix certain "dominant" elements of G (those denoted by an asterisk in Appendix A) to be unity. Then (2.18a) and (2.18b) became linear equations for the corresponding elements of L and M.

We also fixed C_{11}, D_{11}, L_{11}, M_{11} all to be unity. Then the (1, 1) elements of (2.18) serve to define ξ, ξ', η.

We then found that Eqs. (2.18) could be solved sequentially for all the variables. Each step consisted only in solving one or two linear equations for one or two variables, and gave one more correct term in the expansion of this (these) variable(s).

The procedure was similar to that of Ref. 5, the main difference being that we used an appropriate diagonalization procedure to compute the leading powers from (4.3), and then let the computer decide which equation(s) to solve for which variable(s). Given the leading powers, the procedure was as follows:

(*i*) *Basic sequence.* Initially regard the leading coefficients of all variables (except those fixed to be unity) as unknown.

Examine each matrix element equation at leading order. Does it contain only one variable whose leading coefficient is unknown? Is the factor multiplying this variable nonzero at leading order? If both answers are yes, then solve for the leading coefficient of this variable, and record that this variable is determined by this equation.

It is sometimes necessary to generalize this procedure and to look at selected pairs of equations, seeing if a pair can be solved linearly for two variables at once.

Keep iterating through the equations until all leading coefficients are known (some may be zero). This gives a basic sequence for solving the equations.

(*ii*) *Required orders.* To calculate κ to a given order n, it is only necessary to calculate any variable to some relative order $n - r$, where r is nonnegative and independent of n. This r we call the "required order" of the variable. The program calculates these iteratively as follows.

First set the required orders of κ, ξ, ξ', η to zero, the rest to infinity. Now go through the basic sequence of equations and variables. At each step the variable v to be evaluated has a current value of r. Examine every other variable in the equation and determine to what required order it is needed for v to be calculated with required order r. If necessary, modify the required order of this other variable accordingly.

Repeat this procedure until a complete cycle through the basic sequence produces no modifications.

The purpose of calculating the required orders is to ensure that each variable is finally calculated only to the minimum order necessary: if a variable has $r = 17$ and we want κ to order 21, then the variable only has to be calculated to relative order 4.

The required orders can also be used to determine the accuracy of a subtruncation of a larger truncation, and hence to estimate the accuracy of successive truncations. We found they were sometimes overconservative,

presumably because we were not using the optimal route for solving the equations.

(*iii*) *Ordered search procedure.* The next phase of the program is similar to (i), except that first it finds a subsequence of the basic sequence to calculate all variables with $r = 0$, then all those with $r = 1$, and so on.

(*iv*) *Execution.* Following (iii), the actual calculation of coefficients begins. All variables with $r = 0$ are calculated to leading order. Then those with $r = 1$ are calculated to leading order, those with $r = 0$ to next-plus-leading. Then those with $r = 2, 1, 0$ are calculated to leading, next-plus-leading, and second relative order, respectively; and so on. This stops when κ is calculated to the order desired. At each step it is verified that the other variables in the equation are in fact known to the orders needed to determine the variable being evaluated.

(*v*) *Check.* Finally, since there are more equations than unknowns, it is checked that each is satisfied to the order available.

9. SERIES ANALYSIS

Our series calculations have been restricted to the case of a uniform activity ($z_1 = z_2 = z$). This means that all the calculations involve series in only one variable rather than the two-variable series involved in our earlier work,[5] so that we avoid many of the technical problems which we described in connection with memory management. Restricting our calculations to $z_1 = z_2$ prevents us from calculating the staggered susceptibility χ^+, but does not prevent us from calculating the staggered density $R = \rho_2 - \rho_1$ since Eq. (3.7) enables us to obtain ρ_2 and ρ_1 individually.

The coefficients occurring in some of the matrix elements involve rational fractions. These were handled by mapping the fractions onto the field of integers modulo p_i for various primes p_i. This procedure has been described by Borosh and Fraenkel[13] and we have used it in obtaining high-field Ising model series.[14]

The first 43 series terms in $\kappa(z)$ and $\kappa(\rho)$, and the first 24 terms of $\kappa(x)$ and $R(x)$, are tabulated in Appendix B. In view of the conjecture (1.2), we have concentrated on using these series to estimate z_c.

In the absence of series for χ^+ we have been unable to extract any useful estimates for z_c from the low-density series. When attempting to fit Padé approximants to series for $\kappa(z)$ and $\rho(z)$ we find that the higher order approximants cannot be determined uniquely with available machine accuracy. In other words, the 43 available coefficients can be represented to the available machine accuracy by using low-order approximants, and these approximants

give no indication of any physical singularity. Gaunt and Guttmann[15] have pointed out that the method of N-point fits is less prone to such numerical instabilities than is the construction of Padé approximants. We found the improvement insufficient to enable us to ever construct a fit based on all of the 43 coefficients. The results that we obtained represented the series in terms of a large number of poles on the negative z axis. Gaunt and Fisher[6] noted this type of behavior and remarked that it suggested a branch cut on part of the negative z axis.

We also tried transforming the variable and examining the series for $\kappa(u)$ and $\kappa(\rho)$, where $u = z/(1 + z)$ is a variable used by Gaunt and Fisher[6] and ρ is the density. The former seemed to be no improvement on the z series; the latter has some advantages (the coefficients are smaller), but we are unable to add significantly to previous comments [paragraph containing Eq. (5.4) of Ref. 6]. Our estimates of z_c come from the high-density series for the order parameter $R = \rho_2 - \rho_1$. We constructed Padé approximants for $(d/dx) \ln R(x)$ and $R(x)^{-8}$. We also analyzed the series for $R(x)^{-8}$, using the ratio method.

The series for $(d/d\rho') \ln R(\rho')$ were analyzed by Padé approximants to give estimates of ρ_c and the exponent ratio $\beta/(1 - \alpha)$. We also attempted to analyze the series given by Gaunt and Fisher for $\chi^+(\rho)$ using our improved estimate of ρ_c, but this was inconclusive.

The results of the Padé approximant analysis are given in Table 1, which gives the (physical) poles and residues for approximants to the three functions:

(i) $(d/dx) \ln R(x)$. These approximants give particularly consistent estimates for $\chi_c \approx 0.26341$ and $\beta \approx \frac{1}{8}$. Even the fact that some of the approximants are not uniquely defined is an indication of the consistency of the approximants, since it indicates that the series can be fitted to machine accuracy by using lower order approximants. We then used Padé approximants to look for the singularities of $R(x)^{-8}$ and $R(x)^8$. The former has the expected singularity at x_c, but the latter shows no sign of any singularity in this vicinity. For these reasons we follow Gaunt and Fisher and hereafter assume $\beta = \frac{1}{8}$ exactly.

(ii) $R(x)^{-8}$. If $\beta = \frac{1}{8}$, this function should have a simple pole (assuming that the physical singularity has no logarithmic corrections). The residues are tabulated as an indication of how consistently the approximants are representing the behavior near x_c. Although the variation in the estimates of x_c is small, there does appear to be a slight trend toward smaller values of x_c. From these figures we estimate $x_c = 0.263415 \pm 0.000015$ or $z = 3.7963 \pm 0.0002$.

(iii) $(d/d\rho') \ln R(\rho')$, where $\rho' = 1 - 2\rho$. Both the estimates of the poles and the residues show quite a strong trend toward smaller values as the order of the approximant is increased. If we assume $(\rho_c' - \rho') \sim (x_c - x)^{1-\alpha'}$, then we expect $R(\rho') \sim (\rho_c' - \rho')^{\beta/(1-\alpha')}$, so that the residues will be estimates of

Table I. Padé Approximants

	$(d/dx)\ln R(x)$		$R(x)^8$		$(d/d\rho')\ln R(\rho')$	
$[D, N]$	Pole	Residue	Pole	Residue	Pole	Residue
[6, 7]	0.26334	−0.12430	—	—	0.26586	−0.1562
[7, 6]	0.26334	−0.12431	—	—	0.26585	−0.1562
[7, 7]	0.263344	−0.12434	0.263458	0.46490	0.26564	−0.1552
[7, 8]	[a]	—	0.263434	0.46434	0.26508	−0.1512
[8, 7]	0.263399	−0.12473	0.263433	0.46430	0.26498	−0.1504
[8, 8]	[a]	—	0.263431	0.46425	0.26483	−0.1488
[8, 9]	[a]	—	0.263438	0.46444	0.26489	−0.1495
[9, 8]	0.263390	−0.12466	0.263433	0.46432	0.26488	−0.1498
[9, 9]	0.263410	−0.12486	0.263411	0.46333	0.26488	−0.1493
[9, 10]	0.263406	−0.12481	0.263424	0.46400	0.26490	−0.1495
[10, 9]	0.263406	−0.12481	0.263423	0.46394	0.26488	−0.1494
[10, 10]	0.263408	−0.12483	0.263421	0.46385	0.26481	−0.1486
[10, 11]	0.263410	−0.12487	0.263421	0.46384	0.26476	−0.1483
[11, 10]	0.263411	−0.12487	0.263421	0.46384	0.26475	−0.1477
[11, 11]	0.263415	−0.12494	0.263421	0.46386	0.26466	−0.1463
[11, 12]	—	—	0.263418	0.46372	—	—
[12, 11]	—	—	0.263418	0.46367	—	—

[a] These approximants are not uniquely defined, i.e., to machine accuracy the truncated series can be fitted by lower order approximants.

$-\beta/(1-\alpha')$. We have attempted to extrapolate the trends by plotting the estimates from the $[D, N]$ approximants against $y = 1/(D+N)$, $N = D$, $N = D \pm 1$, and extrapolating to $y = 0$. The resulting graphs are not particularly regular and so we have not reproduced them. We estimate $\rho_c' = 0.264 \pm 0.002$ or $\rho_c = (0.736 \pm 0.002)\rho_{\max}$. This is a slight improvement on the estimates that Gaunt and Fisher obtained from the series for $\chi^+(\rho')$. The exponent estimates extrapolate to give $\beta/(1-\alpha') = 0.138 \pm 0.008$ or $\alpha' = 0.09 \pm 0.05$, assuming $\beta = \frac{1}{8}$.

These exponent estimates are particularly interesting if three-exponent scaling is assumed. The estimates of $\beta/(1-\alpha')$ would seem to preclude the possibility that $\alpha' = 0$ as in the Ising model and so scaling precludes the Ising model result of $\delta = 15$. The α' estimate above gives $13.88 < \delta < 14.68$. If δ were an integer, then scaling would give $\alpha = \alpha' = \frac{1}{8}, \beta = \frac{1}{8}, \gamma' = \gamma = 1\frac{5}{8}$, $\delta = 14$, $\beta/(1-\alpha') = \frac{1}{7}$, and $\gamma/(1-\alpha) = 1\frac{6}{7}$. Unfortunately, when we analyze $\chi^+(\rho)$ by the ratio method to obtain estimates for the exponent $\gamma/(1-\alpha)$ we find that the exponent estimate is of the order of 2.3, which is much greater than the scaling prediction. Assuming that scaling is not violated,

Table II. Ratio Method Analysis for $[R(x)]^{-8} = \sum_{n=0}^{\infty} R_n x^n$

n	R_n	$r_n = R_n/R_{n-1}$	$t_n = (R_n/R_{n-2})^{1/2}$
0	1		
1	8	8	
2	28	3.5	5.29150
3	96	3.4286	3.46410
4	366	3.8125	3.61544
5	1,392	3.8033	3.80789
6	5,312	3,8161	3.80968
7	19,976	3.7605	3.78822
8	76,285	3.8188	3.78958
9	288,096	3.7766	3.79764
10	1,097,428	3.8092	3.79287
11	4,152,976	3.7843	3.79674
12	15,799,082	3.8043	3.79427
13	59,862,320	3.7890	3.79662
14	227,546,756	3.8011	3.79507
15	862,775,120	3.7916	3.79640
16	3,278,079,614	3.7995	3.79555
17	12,434,266,488	3.7932	3.79631
18	47,230,647,652	3.7984	3.79578
19	179,198,915,584	3.7941	3.79627
20	680,552,451,060	3.7977	3.79593
21	2,582,531,487,080	3.7948	3.79625
22	9,806,668,461,772	3.7973	3.79603
23	37,218,005,665,832	3.7952	3.79624

we can only conclude that, because the singularity in ρ is rather weak, the series in ρ are not long enough to give reliable estimates of exponents.

Returning to our primary concern of estimating z_c, we have analyzed the series for $R(x)^{-8}$ using the ratio method. Table II gives the coefficients R_n, the ratios $r_n = R_n/R_{n-1}$, and also $t_n = (R_n/R_{n-2})^{1/2}$. The ratios r_n show a regular oscillation, with the even ratios converging to z_c from above and the odd-numbered ratios converging to z_c from below. This odd–even oscillation is somewhat reduced if one looks at t_n, the geometric mean of r_n and r_{n-1}. Taking into account the fact that the odd t_n values are varying more slowly than the even t_n, we obtain our best estimate (1.5) of z_c.

10. NUMERICAL SOLUTION OF THE EQUATIONS

We also solved three truncations of Eqs. (2.18) numerically, using appropriate subtruncations of (6.8) as initial guesses for high values of z, and of (7.6) for low values. Initial guesses for intermediate values were obtained by extrapolation.

In the low-density regime we used the two-by-two, three-by-three, and five-by-five top-left truncations of (7.6), since the corresponding series expansions are accurate to orders 7, 15, and 23 respectively. These truncations are also "natural" in that the first is the Kramers–Wannier approximation[12] and to leading order the second (third) is obtained from the first (second) by keeping *all* eigenvalues in the buildup procedure of Section 4.

Presumably the exact infinite-dimensional solution is asymmetric ($D \neq C$, $H^T \neq H$) for $z > z_c$, but becomes symmetric at $z = z_c$ (this ensures that the transition is continuous). To observe this effect for the truncated matrices, one must make a truncation that permits it to occur. The values of s_i and t_j should therefore be the same, at least to within permutations of the s_i (or t_j), i.e., reordering rows and columns.

At high densities we therefore truncated the matrices by selecting the following rows and columns of H and G and the corresponding diagonal entries of C, L, D, M (a) two-by-two: rows 1, 2; columns 2, 1; (b) three-by-three: rows 1, 2, 4; columns 2, 1, 3; (c) five-by-five: rows 1, 2, 4, 6, 3; columns 2, 1, 3, 4, 5.

These truncations have the same s_i, t_j values as the corresponding low-density ones. We found that they did indeed become symmetric at a value z_t of z, and that they were then the same as their low-density counterparts. The values of z_t for the three truncations are

$$2.8729, \quad 3.4575, \quad 3.7066 \tag{10.1}$$

For such small truncations, these results are really quite good: presumably the sequence is converging to the value 3.796 of z_c predicted in Section 9.

The asymmetric (high-density) solution exists only for $z \geqslant z_t$. The symmetric (low-density) one exists for $z \leqslant z_t$, and also a little way into the interval $z > z_t$. Presumably this penetration is an effect of the finite truncation and will disappear as the truncations increase in size. In any event, κ is maximized by using the asymmetric solution for $z > z_t$ and the symmetric one for $z \leqslant z_t$, and this is what we have done.

Away from z_c, the truncations appear to be converging rapidly, as has been observed for the CTMs of other models.[1,3,4] For instance, for $z = 2.8$ they give $\kappa = 1.9838, 1.9884, 1.9886$ and $\rho = 0.3146, 0.3216, 0.3222$, respectively.

In Fig. 6 the order parameter $R = \rho_2 - \rho_1$ is plotted against z^{-1} for the three approximations, indicating how the asymmetric ($R \neq 0$) solutions become symmetric ($R = 0$) as z is decreased to z_t. Also plotted is $\ln \kappa$: to this scale the three approximations for it are almost indistinguishable!

We have also plotted $\ln \kappa$ (referred to as Γ in Ref. 6) against ρ. The resulting graphs are not reproduced here, since the 2 by 2 and 3 by 3 results

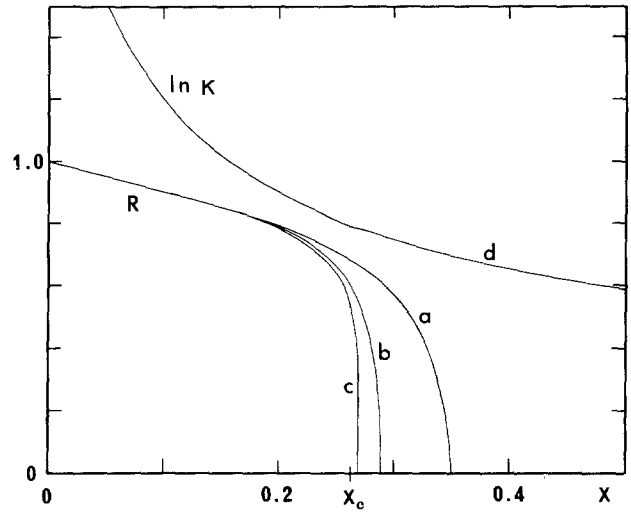


Fig. 6. Plots of $R(x)$ for (a) the 2 by 2 truncation, (b) the 3 by 3, (c) the 5 by 5. Also shown is the "exact" critical point x_c and the graph (d) of ln κ.

can barely be distinguished from the exact curve of Fig. 14 of Ref. 6, and the 5 by 5 cannot be distinguished.

11. SUMMARY

We have used the truncated corner transfer matrix equations (2.18) to obtain the low-density series expansion of $\kappa(z)$ to order 42, and the high-density expansions of $\kappa(z^{-1})$ and $R(z^{-1})$ to order 23. We have also solved some smaller truncations numerically.

From the series for $R(z^{-1})$ we have confirmed Gaunt and Fisher's[6] result $\beta = \frac{1}{8}$, and considerably reduced the error bounds on their estimate of z_c. The central estimate is unchanged.

These results are clearly in conflict with the conjecture (1.2) of Müller-Hartmann and Zittartz,[8] which gives $x_c = 0.25$, $z_c = 4.0$. It would take an extraordinary systematic bias to reconcile the sequences of Tables I and II with these values.

We have also obtained from $R(\rho')$ the moderately improved estimate $\rho_c = (0.736 \pm 0.002)\rho_{\max}$.

Our attempts to determine other critical exponents produce results which seem to be distinct from the Ising model values, but we have been unable to obtain a consistent set of exponents α, β, and γ which satisfy scaling.

The numerical results are interesting in that they indicate how the solution of (2.18) behaves, but the series expansions provide more accurate estimates of z_c and the critical properties.

APPENDIX A. LEADING POWERS

The vectors S and T and the leading powers of the elements of C, L, D, M, and G are given here. Asterisks denote elements that may be chosen to be unity; elements indicated by a dot are zero. The powers of the diagonal elements of C, D, L, and M are given in row vector form. Those of nonzero off-diagonal elements of C and D are listed individually after G.

High density (powers of $x = z^{-1}$)

$S = (0 \quad 1 \quad 1 \quad 0 \quad 1 \quad 0 \quad 1 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 1)$

C: $(0^* \quad 1 \quad 2 \quad 2 \quad 3 \quad 3 \quad 4 \quad 4 \quad 4 \quad 5 \quad 5 \quad 5 \quad 6)$

L: $(0^* \quad 1 \quad 2 \quad 5 \quad 3 \quad 6 \quad 4 \quad 7 \quad 5 \quad 5 \quad 10 \quad 6 \quad 6)$

$T = (1 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 1 \quad 0 \quad 1 \quad 1 \quad 0 \quad 0)$

D: $(0^* \quad 0 \quad 1 \quad 2 \quad 3 \quad 3 \quad 4 \quad 4 \quad 5 \quad 5 \quad 5 \quad 5)$

M: $(0^* \quad 1 \quad 2 \quad 3 \quad 2 \quad 4 \quad 3 \quad 5 \quad 4 \quad 6 \quad 9 \quad 6)$

$$G: \begin{bmatrix} 0^* & 0^* & 2 & 4 & 6 & 6 & 8 & 7 & 10 & 9 & 6 & 8 \\ . & 0^* & 0^* & 2 & . & 4 & . & 5 & . & . & 4 & 6 \\ . & 2 & 0^* & 0^* & . & 2 & . & 3 & . & . & 2 & 4 \\ 2 & 0^* & -1 & -1 & 0^* & 0 & 2 & 1 & 4 & 3 & 0^* & 2 \\ . & 4 & 2 & 0^* & . & 0^* & . & 2 & . & . & 1 & 3 \\ 2 & 1 & 0^* & -1 & 0 & -1 & 0^* & 0 & 2 & 1 & -1 & 1 \\ . & 6 & 4 & 2 & . & 0^* & . & 0^* & . & . & 0 & 2 \\ 3 & 2 & 1 & 0^* & 0 & . & 0 & -1 & 0^* & -1 & -2 & 0 \\ 4 & 3 & 2 & 1 & 1 & 0^* & 1 & 0 & . & 0^* & -1 & 1 \\ . & 8 & 7 & 4 & . & 2 & . & 0^* & . & . & . & 0^* \\ 3 & 2 & 1 & 0 & 0^* & -1 & -1 & . & -1 & -2 & -3 & -2 \\ 5 & 4 & 3 & 2 & 2 & 1 & 1 & 0^* & 1 & 0 & -1 & 0 \\ . & 10 & 8 & 6 & . & 4 & . & 2 & . & . & -1 & 0^* \end{bmatrix}$$

C_{89}, C_{98}: 4

$C_{11,12}$, $C_{12,11}$, $D_{9,10}$, $D_{10,9}$, $D_{11,12}$, $D_{12,11}$: 5

Low density (powers of z)

$T = S, \quad D = C, \quad M = L, \quad G^T = G$

$S = (0 \quad 1 \quad 0 \quad 0 \quad 1 \quad 0 \quad 1 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 1)$

C: (0* 0 2 4 4 6 6 8 8 8 10 10 10)

L: (0* 1 5 5 6 9 10 14 9 10 14 13 14)

G:

$$\begin{bmatrix}
0^* & & & & & & & & & & & \\
0^* & . & & & & & & & & & & \\
1 & 0^* & -2 & & & & & & & & & \\
5 & 4 & 0^* & 0 & & & & & & & & \\
7 & . & 0^* & 0 & . & & & & & & & \\
7 & 6 & 2 & 0^* & 0 & -2 & & & & & & \\
9 & . & 2 & 0^* & . & -2 & . & & & & & \\
8 & 7 & 3 & 1 & 0^* & . & -2 & -4 & & & & \\
11 & 10 & 6 & 4 & 3 & 0^* & 0 & -2 & 0 & & & \\
13 & . & 6 & 4 & . & 0^* & . & -2 & 0 & . & & \\
12 & 11 & 7 & 5 & 4 & 1 & 0^* & -2 & . & 0 & -2 & \\
13 & 12 & 8 & 6 & 5 & 2 & 1 & -2 & 0^* & 0 & -2 & -2 \\
15 & . & 8 & 6 & . & 2 & . & -2 & 0^* & . & -2 & -2 \quad .
\end{bmatrix}$$

(only the powers of the lower-left elements of G are shown)

C_{89}, C_{98}: $8\frac{1}{2}$

$C_{11,12}, C_{12,11}$: $10\frac{1}{2}$

[In solving (2.18) we actually worked with $L^{1/2}CL^{-1/2}$ rather than C. All powers are then integers.]

APPENDIX B. SERIES COEFFICIENTS

High-Density: Coefficients of x^n in the Expansion of $x[\kappa(x)]^2$ and $R(x)$

n	$x[\kappa(x)]^2$	$R(x)$
0	1	1
1	1	−1
2	0	1
3	1	−6
4	−1	9
5	5	−60
6	−10	116
7	39	−685
8	−95	1,465
9	353	−8,197
10	−960	18,770
11	3,532	−101,730
12	−10,284	244,592
13	37,725	−1,294,636
14	−114,966	3,229,643
15	421,569	−16,775,859
16	−1,327,087	43,075,617
17	4,868,771	−220,289,362
18	−15,701,346	578,991,935
19	57,660,914	−2,922,618,856
20	−189,473,994	7,832,501,622
21	696,676,438	−39,099,055,551
22	−2,323,894,060	106,531,725,770
23	8,555,724,782	−526,655,410,908

Low-Density: Coefficients of z^n and ρ^n in the Expansions of $\kappa(z)$ and $\kappa(\rho)$

n	$\kappa(z)$	$\kappa(\rho)$
0	1	1
1	1	1
2	−2	3
3	8	7
4	−40	13
5	225	17
6	−1,362	5
7	8,670	−51
8	−57,253	−180
9	388,802	−376
10	−2,699,202	−650
11	19,076,006	−1,634
12	−136,815,282	−6,536
13	993,465,248	−23,576
14	−7,290,310,954	−59,032
15	53,986,385,102	−70,664
16	−402,957,351,939	154,964
17	3,028,690,564,108	1,115,828
18	−22,904,845,414,630	3,187,198
19	174,175,863,324,830	4,791,554
20	−1,331,044,586,131,594	453,494
21	10,217,222,223,168,657	−9,631,530
22	−78,746,146,809,812,974	26,321,436
23	609,153,211,886,323,748	260,559,872
24	−4,728,123,941,310,119,629	599,839,326
25	36,812,657,530,897,835,053	−1,287,997,722
26	−287,439,461,791,025,474,818	−14,636,454,872
27	2,250,314,840,062,625,743,472	−54,542,259,400
28	−17,660,572,072,127,314,002,800	−91,252,751,468
29	138,917,347,311,377,551,474,338	147,076,485,384
30	−1,095,044,102,004,611,782,219,794	1,487,978,128,638
31	8,649,079,543,673,381,406,386,578	4,704,052,980,990
32	−68,441,069,128,808,194,161,922,385	5,079,849,028,514
33	542,528,768,962,390,004,584,576,547	−23,738,147,507,286
34	−4,307,673,277,782,673,209,498,570,830	−143,783,668,419,110
35	34,255,913,017,196,256,622,645,849,406	−357,511,314,224,066
36	−272,811,973,711,116,137,449,858,922,289	−86,517,671,744,353
37	2,175,663,718,003,877,171,512,666,515,965	3,077,284,192,138,255
38	−17,373,555,504,340,949,646,557,187,291,612	13,682,193,414,479,531
39	138,907,228,460,715,779,361,866,368,091,340	28,258,373,296,286,175
40	−1,111,918,671,840,441,187,102,586,337,375,728	−9,315,888,451,955,854
41	8,910,623,138,600,432,871,714,003,453,719,826	−300,653,929,789,475,442
42	−71,483,639,721,296,620,300,995,136,065,253,668	−1,180,466,383,460,671,734

NOTE ADDED IN PROOF

We cannot exclude the possibility that α, ν, δ have their Ising values 0,1,15. This has recently and convincingly been argued.[16,17]

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REFERENCES

1. R. J. Baxter, *J. Math. Phys.* **9**:650 (1968).
2. S. B. Kelland, *Can. J. Phys.* **54**:1621 (1976).
3. R. J. Baxter, *J. Stat. Phys.* **19**:461 (1978).
4. R. J. Baxter and S. K. Tsang, Entropy of hard hexagons, to be published in *J. Phys. A: Math. Gen.*
5. R. J. Baxter and I. G. Enting, *J. Stat. Phys.* **21**:103 (1979).
6. D. S. Gaunt and M. E. Fisher, *J. Chem. Phys.* **43**:2840 (1965).
7. L. K. Runnels and L. L. Combs, *J. Chem. Phys.* **45**:2482 (1966).
8. E. Müller-Hartmann and J. Zittartz, *Z. Phys. B* **27**:261 (1977).
9. L. Onsager, *Phys. Rev.* **65**:117 (1944).
10. T. W. Burkhardt, *Z. Phys. B* **29**:129 (1978).
11. K. Y. Lin and F. Y. Wu, *Z. Phys. B* **33**:181 (1979).
12. H. A. Kramers and G. H. Wannier, *Phys. Rev.* **60**:263 (1941).
13. I. Borosh and A. S. Fraenkel, *Math. Comp.* **20**:107 (1966).
14. I. G. Enting and R. J. Baxter, An investigation of the high-field series expansions for the squares lattice Ising model, submitted to *J. Phys. A: Math. Gen.*
15. D. S. Gaunt and A. J. Guttmann, in *Phase Transitions and Critical Phenomena, Vol. 3*, C. Domb and M. S. Green, eds. (Academic, New York, 1974).
16. Z. Racz, preprint, Phase boundary of Ising antiferromagnets. . .
17. D. W. Wood and M. Goldfinch, Vertex models for the hard square and hard hexagon gases, . . ., to be published in *J. Phys. A. Math. Gen.*