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Inclusion-exclusion relations on the triangular lattice

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Received 17 March 1986

Abstract. The combinatorial factors required for performing finite lattice series expansions on the triangular lattice are discussed. Series expansions can be obtained from a linear combination of free energies for finite convex hexagonal regions. An algorithm for calculating the combinatorial weights is given. A number of results are presented, showing that many cancellations occur and that not all convex hexagons of less than a given size are required. For a given degree of computational complexity (as given by the size of the largest transfer matrix) the expansion using hexagons of less than a certain perimeter and exploiting the full triangular symmetry gives 50% more series terms than the earlier approach which adds second-neighbour bonds to the square lattice and only exploits square lattice symmetries.

1. Introduction

The finite lattice method of series expansion has recently proved to be a very powerful technique for deriving series expansions for lattice statistics problems on the square lattice. The basic principle is that F_N/N , the free energy per site in the limit $N \rightarrow \infty$, can be expressed as a linear combination of f_{mn} , free energies for $m \times n$ rectangles:

$$F_N / N = \sum_{mn} a(m, n) f_{mn}(x) + O(x^{c(m+n)})$$
(1.1)

where x is some appropriate expansion variable. The principle has long been known by many workers in the field of series expansions but it was apparently de Neef (1975) who first exploited the great efficiency of the technique which comes from the fact that the f_{mn} can be easily evaluated using transfer matrix techniques. The combinatorial basis for (1.1) was described by Hijmans and de Boer (1955) in the context of closed form approximations. If a finite maximal connected graph α_0 is taken then the set of graphs required to give optimal corrections for finite-size effects will be A = $\{\alpha_i : i = 0 \dots m\}$ where the set A contains α_0 and all connected graphs that are intersections of other pairs α_i , α_j with all possible relative displacements of the graphs. The set of all rectangles less than a certain size forms a set A with such a closure property under intersections.

The weights assigned to the graphs α_i are obtained by inverting the matrix of incidence counts as described in § 3 and as pointed out by de Neef and Enting (1977). The overall approach of the finite lattice method is, as described by Wortis (1974) in the context of renormalised expansions, to substitute algebraic complexity for combinatorial complexity.

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Since Hijmans and de Boer (1955) only considered low-order examples they failed to note that many cancellations occur in that many of the graphs α_i in set A have zero weights and so need not be evaluated.

The earliest square lattice calculations were for the three-site Potts model (de Neef and Enting 1977) and the limit of chromatic polynomials (Kim and Enting 1979). These cases replaced α_0 by a maximal set of graphs: those rectangles with perimeter k. The other graphs in set A were smaller rectangles since the intersection of two rectangles always gives a rectangle. Subsequently Enting (1978a) was able to produce an explicit expression for the a(m, n):

$$a(m, k-m) = 1$$
 $m = 1$ to $k-1$ (1.2a)

$$a(m, k-m-1) = -3$$
 $m = 1$ to $k-2$ (1.2b)
 $a(m, k-m-2) = 2$ $m = 1$ to $k-2$ (1.2c)

$$a(m, k-m-2) = 3$$
 $m = 1 \text{ to } k-3$ (1.2c)
 $a(m, k-m-3) = -1$ $m = 1 \text{ to } k-4$ (1.2d)

$$(m, \kappa - m - 3) = -1$$
 $m = 1 \text{ to } \kappa - 4$ (1.2*a*)

$$a(m, n) = 0$$
 otherwise. (1.2e)

If *m* and *n* are taken as giving the dimensions of the rectangles in numbers of bonds then the high-temperature expansions of the Ising and Potts model zero-field free energies will be correct to order 2k and 2k+1, respectively. Equations (1.2a)-(1.2d)show that only the four largest sizes of rectangles are needed.

An even more extreme example of such cancellations was the case considered by Enting and Baxter (1977) which was suggested by analogy with the variational method of Baxter (1968, 1978). It has

$$a(m, m) = 1$$
 m fixed (1.3a)

$$a(m-1, m) = a(m, m-1) = -1$$
 m fixed (1.3b)

$$a(m-1, m-1) = 1$$
 m fixed (1.3c)

$$a(j,k) = 0$$
 otherwise. (1.3*d*)

This will give the Ising and Potts high-temperature zero-field free energies correct to order 2m+2 and 2m+3, respectively.

For the triangular lattice, the variational method suggests an expansion based on six hexagons (or three distinct hexagons in the case of full triangular symmetry). The proof of the combinatorial expression (equation (4.1) below) is given by Enting (1980a). However, actual calculations on the triangular lattice have usually been carried out by representing the lattice as a square lattice with half the second-neighbour bonds present and using the combinatorial weights (1.2a)-(1.2e) (Enting 1980b, Enting and Wu 1982).

The present paper concerns generalising the approach of de Neef and Enting (1977) to take full advantage of the symmetry of the triangular lattice. Although it has not been possible to obtain a general explicit formula for the weights corresponding to equations (1.2n)-(1.2e) an algorithm for calculating the weights is presented. In addition the results are presented for two particular cases and for other cases the numbers of graphs required is tabulated. These results show that there are also considerable cancellations in this triangular case and so the calculations should prove manageable. The layout of the remainder of the paper is as follows. Section 2 discusses various lattice statistics problems on the triangular lattice, determines the number of series terms that can be obtained from various orders of finite hexagon expansions

and defines the notation used to represent the various finite hexagons. Section 3 defines the incidence relations and the way in which the solution gives the combinatorial weights required for the finite lattice expansion. It also gives the overall algorithm for calculating these weights. Section 4 presents the results for the numbers of hexagons required and the actual combinatorial weights for two particular cases. The possible applications are summarised in § 5.

2. Series groupings

The set of finite lattices to be considered in this paper are convex hexagons on the triangular lattice. These will be described by a set of numbers $[n_1, n_2, \ldots, n_6]$ that give the lengths of the sides in various directions as shown in figure 1(a) which corresponds to [2, 2, 2, 3, 1, 3]. The other examples show how various degenerate cases have sides of length zero. Such cases must be included as they can be generated by the intersection of pairs of hexagons or other graphs derived from intersecting hexagons. Throughout this paper the term 'hexagons' will be taken to include such degenerate cases. The graphs that are considered are classified by their perimeters and only convex graphs are required. The following properties are important:



Figure 1. Examples of convex hexagonal graphs showing notation and including degenerate cases. (a) General notation, (b)-(e) various degenerate cases.

(i) any convex graph α which is a subgraph of another convex graph β will have its perimeter $p_{\alpha} \leq p_{\beta}$, and the equality only holds if $\alpha = \beta$;

(ii) the intersection of two convex graphs with an arbitrary relative displacement is a convex graph (or the empty set); therefore

(iii) the set of graphs of perimeter p can be used as a maximal set: all graphs derived from this set will have perimeters less than p;

(iv) any non-convex graph α of perimeter p_{α} is a subgraph of a convex graph β of perimeter $p_{\beta} \leq p_{\alpha}$.

The expansions that we consider here are the low-temperature and high-temperature expansions of the q-state Potts model with the Ising model as a special case. The low-temperature graphs are sets of perturbed sites. In terms of the variable $u = \exp(\Delta J/kT)$, a connected set of perturbed sites α gives a contribution of order u^n where

$$n = 6 + 2p_{\alpha} + d_{\alpha}. \tag{2.1}$$

The term d_{α} is the length of the internal boundaries between sites perturbed into different states. For the q = 2 case (i.e. the Ising model) d_{α} vanishes, *n* is always even

and so the low-temperature series can be expressed in powers of u^2 . Enting (1978b) has described the linked-cluster expansion for low-temperature series, has shown that the leading powers are the same as for conventional expansions and that, as described by de Neef and Enting (1977), the linked cluster expansion can be resummed into a finite lattice form. It follows that the first power given incorrectly by a finite lattice expansion is the lowest power associated with any of the connected graphs that do not fit into any of the maximal set used in the finite lattice expansions. For the Potts model the lowest powers are associated with Ising-like graphs, i.e. $d_{\alpha} = 0$, and so if the maximal set is the graphs with perimeter p then the first incorrect power is 2p+8. Thus Potts model series are correct to order u^{2p+7} and Ising series correct to $(u^2)^{p+3}$.

Similarly, for high-temperature expansions, the lowest graphs in the expansion of the free-energy are Ising-like with a loop of length p giving a power w^p with

$$w = (1 - u)/(1 + (q - 1)u)$$
(2.2a)

or

$$w = \tanh(\frac{1}{2}\Delta J/kT)$$
 for $q = 2$. (2.2b)

Thus a finite lattice expansion with maximal perimeter p will, by virtue of property (iv) above, be correct to order w^{p} . (For expansions in powers of w, degenerate 'straight-line' graphs such as in figure 1(c) make no contribution.)

A useful property to describe the various hexagons is the breadth perpendicular to each of the three bond directions. Thus we define

$$b_1 = n_1 + n_2 = n_4 + n_5 \tag{2.3a}$$

$$b_2 = n_2 + n_3 = n_5 + n_6 \tag{2.3b}$$

$$b_3 = n_3 + n_4 = n_6 + n_1. \tag{2.3c}$$

As well as defining the b_i , equations (2.4a)-(2.4c) represent constraints on the set of n_i . However only two of the constraints are independent. The importance of the b_i is that the partition function for a q-state model on a graph of breadth b can be generated by a transfer matrix of size q^{b+1} for the low-temperature representation and size q^b for the high-temperature form. (Each of these factors can be reduced by utilising any equivalences between states as in the standard Potts model for example.) From (2.1a)-(2.1c) it follows that

$$p = \sum_{i=1}^{6} n_i = \sum_{j=1}^{3} b_j.$$
(2.4)

Thus a transfer matrix calculation for graphs of maximum width b can calculate the partition functions for all graphs of $p \le 3b+2$. The general hexagonal graph has 11 other equivalent graphs that can be derived from it by combinations of rotations and reflection. In order to make maximum use of the symmetry it is desirable to pick a canonical representative from each equivalence class and calculate its partition function. We do this by defining an index $\langle b_1, n_2, n_5, n_6 \rangle$ and selecting the smallest values of b_1 , and in cases of equality the smallest n_2 and so on. The reasons for this choice are

(i) smallest breadth so as to give the most efficient transfer matrix;

(ii) smallest n_2 , n_5 so that, as shown in figure 2(a), the graph is as near as possible to rectangular, thus reducing the number of 'corner-truncation' modifications to the transfer matrix formalism;



Figure 2. (a) Square lattice orientation and definition of breadths b_i . (b) Incidence relations between graphs n and m. The incidence number W(m, n) is the number of integer x, y displacements for which m lies within n.

(iii) n_6 is chosen because it is independent of b_1 , n_2 and n_5 (as is n_3) while $n_4 = b_1 - n_5$.

The numbers b_1 , n_2 , n_5 and n_6 uniquely characterise a hexagon since the other n_i can be derived from equations (2.3a)-(2.3c).

3. Incidence relations and computational techniques

In this section the various hexagons are denoted by vectors n, m, etc, representing $[n_1, n_2, \ldots, n_6]$. The finite lattice expansions have an irreducible contribution to g(n) for each finite lattice n. These g(n) are summations of conventional connected graph expansions using graphs α with irreducible weights $c(\alpha)$

$$g(n) = \sum_{\alpha: h(\alpha) = n} c(\alpha)$$
(3.1)

where $h(\alpha)$ is the convex hull of graph α , i.e. the smallest hexagon that can bound graph α . Formally the free energy per site is

$$F/N = \sum_{\alpha} c(\alpha) \tag{3.2a}$$

$$=\sum_{n}g(n) \tag{3.2b}$$

since each α contributes to one and only one g(n). When deriving series expansions the summations are truncated; the effect of this truncation is described in the previous section. The finite lattice method calculates the free energies f(n) where

$$f(\mathbf{n}) = \sum_{\mathbf{m}} g(\mathbf{m}) W(\mathbf{m}, \mathbf{n})$$
(3.3)

where W(m, n) is the number of ways *m* occurs as a subgraph of *n*. The g(m) are not required explicitly. What is required is a set of weighting factors a(n) such that

$$\sum_{n \le n_{\max}} a(n) f(n) = \sum_{n,m \le n_{\max}} g(m) W(m,n) a(n)$$
(3.4*a*)

$$=\sum_{m\leq n_{\max}}g(m) \tag{3.4b}$$

$$\approx F/N. \tag{3.4c}$$

Thus it is necessary to solve

$$\sum_{n \le n_{\max}} W(m, n) a(n) = 1 \qquad \forall m \le n_{\max}$$
(3.5)

where \leq refers to an ordering of the graphs in which each graph succeeds all its subgraphs. With such an ordering W(m, n) is an upper triangular matrix with 1 on each diagonal element and so equations (3.5) can be solved by direct elimination and all the a(n) will be integers. Furthermore, the elimination can be performed one column at a time and so it is not necessary to have the whole matrix W accessible at any one time. The equations can be solved by generating each column and completing the reductions before generating the next column.

The procedure for generating the weights a(n) is thus

(i) generate a list of all possible *n* ordered by perimeter up to some maximum p_{max} ;

(ii) set up a vector e(m) = 1 for all *m* corresponding to the right-hand side of equation;

(iii) for each column *n*, generate W(m, n) and then perform the eliminations

$$e(m) \leftarrow e(m) - e(n) W(m, n) \quad \forall m < n$$

(when complete e(m) will have been set to a(m));

(iv) for symmetric cases, combine the a(n) for the graphs in each equivalence class, associating the sum with the canonical representative defined in the previous section.

The list of vectors described in (i) above can be generated by letting p run over the ranges

$$0 \le p \le p_{\max} \tag{3.6a}$$

$$0 \le n_1 \le \frac{1}{2}p \tag{3.6b}$$

$$0 \le n_2 \le \frac{1}{2}p - n_1 \tag{3.6c}$$

$$0 \le n_3 \le \frac{1}{2}p - n_2 \tag{3.6d}$$

subject to the constraints

$$n_4 = p - n_1 - 2(n_2 + n_3) \ge 0 \tag{3.7a}$$

$$n_5 = n_1 + n_2 - n_4 \ge 0 \tag{3.7b}$$

$$n_6 = n_3 + n_4 - n_1 \ge 0. \tag{3.7c}$$

The evaluation of W(m, n) is illustrated in figure 2(b). Each possible incidence corresponds to a displacement (x, y) of the origin such that each boundary of m lies on the 'inside' of the corresponding boundary of n.

These conditions are

$y \ge 0$	boundary 1	(3.8a)
$m_1 + x - y \le n_1$	boundary 2	(3.8 <i>b</i>)
$x+m_1+m_2 \le n_1+n_2$	boundary 3	(3.8c)
$y+m_5+m_6 \le n_5+n_6$	boundary 4	(3.8d)
$y+m_6-x \le n_6$	boundary 5	(3.8e)
$x \ge 0$	boundary 6.	(3.8f)

W(m, n) is given by the number of integer (x, y) pairs satisfying these conditions and can be evaluated by using (3.8a), (3.8d) and (3.8f), (3.8c) to define a pair of nested loops to run through x, y pairs checking constraints (3.8b), (3.8e).

4. Results

The main results are presented in table 1. The column under 'all hexagons' gives the number of hexagons of each perimeter. The cumulation of these values in the following column gives the size of the matrix W required at each order and the growth in these numbers emphasises the importance of being able to reduce each row in isolation without having to store the whole matrix. The column 'No' under 'distinct hexagons' gives the number of distinct hexagons at each order for systems with full triangular symmetry. The cumulation of these numbers in the following column is the number of finite lattices that would need to be evaluated if all possible hexagons contributed. The final column gives the number of hexagons that are actually required, i.e. the number of non-zero a(n) at each order p.

The a(n) are given for the cases p = 14 and p = 17 in tables 2(a) and 2(b), respectively. These cases are of the form p = 3b+2 where b is the maximum width required and the two cases represent the highest order that can be calculated using strips up to four bonds and five bonds wide, respectively.

These results should be contrasted to the expression given by Enting (1980a) which, for the reduced form of the fully symmetric case, is

$$a([k, k-1, k, k-1, k, k-1]) = 2$$
 for one particular k (4.1a)

$$a([k-1, k-1, k, k-1, k-1, k]) = -3$$
(4.1b)

$$a([k-1, k-1, k-1, k-1, k-1]) = 1$$
(4.1c)

$$a(n) = 0$$
 for all other *n*. (4.1*d*)

Table 1. Hexagon counts for various perimeters. No denotes number with perimeter p. Cum is the cumulative total of the preceding column. 'Distinct' treats hexagons related by symmetry operations as equivalent.

	A	ll hexagons	Dis	tinct hexagons			
р	No	Cum	No	Cum	- Non-zero a(n)		
0	1	1	1	1	1		
1	0	1	0	1	1		
2	3	4	1	2	2		
3	2	6	1	3	3		
4	6	12	2	5	5		
5	6	18	1	6	6		
6	12	30	4	10	8		
7	12	42	2	12	10		
8	21	63	5	17	13		
9	22	85	4	21	15		
10	33	118	7	28	20		
11	36	154	5	33	24		
12	50	204	11	44	28		
13	54	258	7	51	34		
14	72	330	13	64	41		
15	78	408	11	75	47		
16	99	507	17	92	55		
17	108	615	13	105	64		

(a) (b)										 (b) cc	nti	nue	d						
2	1	2	1	2	1	-2	0	0	6	0	0	6	-3	3	0	5	3	0	5	-18
0	0	5	0	0	5	3	1	1	4	1	1	4	-3	3	0	6	1	2	4	-48
1	1	3	1	1	3	15	2	1	3	2	1	3	-6	3	1	4	3	1	4	-30
2	1	2	2	1	2	15	2	2	2	2	2	2	-1	3	1	5	1	3	3	-30
3	0	3	1	2	1	6	3	1	3	1	3	1	-2	3	2	3	3	2	3	-15
1	0	5	0	1	4	-6	2	0	5	1	1	4	12	4	0	4	4	0	4	-9
2	0	4	1	1	3	-48	2	1	4	1	2	3	30	4	0	5	2	2	3	-48
2	1	3	1	2	2	-60	3	0	4	2	1	3	12	4	0	6	0	4	2	-18
3	0	3	2	1	2	-24	3	1	3	2	2	2	30	4	1	4	2	3	2	-30
3	0	4	0	3	1	-6	4	0	4	1	3	1	6	5	0	5	1	4	1	-24
0	0	6	0	0	6	-6	0	0	7	0	0	7	6	1	0	8	0	1	7	6
1	0	5	1	0	5	18	1	0	6	1	0	6	-6	2	0	7	1	1	6	12
1	1	4	1	1	4	30	1	1	5	1	1	5	-30	2	1	6	1	2	5	6
2	0	4	2	0	4	18	2	0	5	2	0	5	-6	3	0	6	2	1	5	12
2	0	5	0	2	3	18	2	0	6	0	2	4	-6	3	0	7	0	3	4	6
2	1	3	2	1	3	60	2	1	4	2	1	4	-60	3	1	5	2	2	4	12
2	2	2	2	2	2	10	2	2	3	2	2	3	-30	3	2	4	2	3	3	6
3	0	3	3	0	3	9	3	0	4	3	0	4	-6	4	0	5	3	1	4	12
3	0	4	1	2	2	72	3	0	5	1	2	3	-48	4	0	6	1	3	3	12
3	1	3	1	3	1	20	3	1	3	3	1	3	-30	4	1	4	3	2	3	6
4	0	4	0	4	0	2	3	1	4	1	3	2	-60	4	1	5	1	4	2	6
1	0	6	0	1	5	-18	4	0	4	2	2	2	-24	5	0	5	2	3	2	6
2	0	5	1	1	4	-48	4	0	5	0	4	1	-6	5	0	6	0	5	1	6
2	1	4	1	2	3	-30	1	0	7	0	1	6	18							
3	0	4	2	1	3	-48	2	0	6	1	1	5	72							
3	0	5	0	3	2	-18	2	1	5	1	2	4	60							
3	1	3	2	2	2	-30	3	0	5	2	1	4	72							
4	0	4	1	3	1	-24	3	0	6	0	3	3	18							
0	0	7	0	0	7	3	3	1	4	2	2	3	120							
1	0	6	1	0	6	6	3	2	3	2	3	2	20							
1	1	5	1	1	5	3	4	0	4	3	1	3	36							
2	0	5	2	0	5	6	4	0	5	1	3	2	72							
2	0	6	0	2	4	6	4	1	4	1	4	1	20							
2	1	4	2	1	4	6	5	0	5	0	5	0	2							
2	2	3	2	2	3	3	0	0	8	0	0	8	3							
3	0	4	3	0	4	6	1	0	7	1	0	7	-18							
3	0	5	1	2	3	12	1	1	6	1	1	6	-15							
3	1	3	3	1	3	3	2	0	6	2	0	6	-18							
3	1	4	1	3	2	6	2	0	7	0	2	5	-18							
4	0	4	2	2	2	6	2	1	5	2	1	5	-30							
4	0	5	0	4	1	6	2	2	4	2	2	4	-15							

Table 2. Weighting factors for hexagons of perimeters $p \le 14$ (a) and $p \le 17$ (b) expressed as n_1 , n_2 , n_3 , n_4 , n_5 , n_6 in canonical order, followed by w_i .

This choice involves graphs of breadth $\leq b = 2k - 1$ and will give low-temperature Potts model series correct to $u^{8k+5} = u^{4b+9}$. The use of rectangular lattice graphs with weights given by (1.2a)-(1.2e) and breadth $\leq b$ will give low-temperature Potts model series correct to u^{4b+7} . The more general form discussed in this paper, allowing the use of graphs of breadth $\leq b$ and perimeters $\leq p = 3b+2$, gives Potts model series correct to $u^{2p+7} = u^{6b+11}$. However, the apparent advantage of the general triangular formalism over the simpler form is reduced and possibly negated by the fact that the partition functions for the highly regular hexagons involved in (4.1a)-(4.1c) can be calculated by taking traces of corner-transfer matrix expressions (see Baxter 1978). This reduces (by a power of $\frac{1}{2}$) the size of the vectors that need to be stored at any one time (R J Baxter personal communication) although the overall complexity of the calculation appears to be comparable to that of conventional transfer matrix techniques. If this is so then the corner-transfer matrix approach is most suitable for problems where the computational effort is dominated by storage access times.

5. Summary and applications

The main results of this paper are the algorithm for calculating the weights a(n) and the table of numbers of non-zero elements, indicating that the reductions due to combinatorial cancellations and the application of symmetry have reduced the calculations required by more than 30%.

The lack of an explicit expression for the a(n) does not provide a limitation on the possible calculations for regular systems since, for example, the work of de Neef and Enting (1977) and Kim and Enting (1979) preceded the derivation of equations (1.2a)-(1.2e).

However the simple explicit expressions (1.2a)-(1.2e) were of considerable utility in generalising the finite lattice formalism to calculate surface susceptibilities (Enting and Guttmann 1980) and to count polygons on the square lattice (Enting 1980c) and on directed lattices (Enting and Guttmann 1985). All of these problems will be harder to formulate on triangular lattices and the most practical approach may be to use the appropriate generalisations of equations (4.1a)-(4.1d).

As a point of computational detail, equations (1.1) or (3.4) are usually replaced by their exponentials, thus expressing $Z^{1/N}$, the partition function per site, as a product of powers of finite lattice partition functions. This usually leads to expressions involving only integer coefficients.

The discussion of the number of terms that can be derived has concentrated on the Potts/Ising models but is of greater generality because many models have their lowest order contributions from any given graph equivalent to an Ising model term. The enumeration of polygons presents a number of problems, the most serious arising from the requirement of connectedness. Enting (1980c) introduced an asymmetry by forcing the loops to span the lengths of the rectangles, thereby changing the combinatorial factors. For the triangular lattice a more appropriate technique might be to follow the formulation of Nienhuis (1982, 1984) and label each loop with one of qstates and take the $q \rightarrow 0$ limit to select single loops.

The calculations of combinatorial factors apply directly to the triangular lattice but the same factors can also be applied to the honeycomb lattice, i.e. the dual of the triangular lattice. Figure 3 shows the correspondence between the triangular lattice graphs and the honeycomb lattice graphs. An expansion on the honeycomb lattice can also be related to the triangular lattice by the star-triangle relation but except for



Figure 3. Duality relations—the honeycomb lattice graphs corresponding to various convex hexagons on the triangular lattice.

the zero-field Ising model or the Potts model at criticality, the star-triangle transformation breaks the triangular symmetry and so the combinatorial factors will be more complicated than those presented here.

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