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Generating functions for connected embeddings in a lattice: II. Weak embeddings

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Abstract. The method of partial generating functions is developed to enumerate connected weak embeddings in a lattice. For the body-centred cubic lattice the number of connected weak embeddings of clusters with up to 14 bonds is derived.

1. Introduction

In a previous paper (Sykes 1986), hereafter referred to as I, we have described a method of generating the number of connected *strong* embeddings in a lattice; in this paper we describe the necessary modifications to generate the number of connected *weak* embeddings. (For precise definitions of these graph theoretical terms see Essam and Fisher (1970).) Direct computer enumeration of the number of connected strong embeddings of n sites in a lattice for ascending n is very time consuming; the direct enumeration of connected weak embeddings of n bonds is even more so. For example, for the body-centred cubic lattice we quote the following sequence for the numbers of weak embeddings of connected clusters of n bonds, B_n, grouped by bonds†.

Bonds n	Number of clusters B_n
0	1
1	4
2	28
3	252
4	2582
5	28 648
6	335 272
7	4077 228
8	51 033 970
9	653 295 948
10	8514 628 368
11	112 616 865 088
12	1507 834 338 200
13	20 398 243 646 604
14	278 402 821 091 304

(1.1)

† It is, of course, possible to consider also the number of *strong* embeddings grouped by bonds; these are trivially obtained by regrouping the polynomials $A_n(b)$ of I, appendix 1.

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In I we have taken the counting rate of 200 clusters every millisecond, achieved by Redelmeier (1981), as a measure of the likely efficiency of direct machine cluster enumeration; at this rate the direct counting of B_{14} would require about 400 000 hours, or some 46 years of CPU time. Using the method we describe below the results (1.1), together with information on the number of sites in the clusters, required about 20 min of Cray time to perform some algebra. We comment more fully on the validity of this comparison in our concluding section.

The bare numbers of (1.1) are usefully supplemented by more detailed properties. We denote by B_n the number of connected weak embeddings, or subgraphs, of n bonds. Following the same pattern as I we now define a generating function

$$F(b) = B_0 + B_1 b + B_2 b^2 + \dots \tag{1.2}$$

and more generally

$$F(b, x) = \sum_r B_r(x) b^r \tag{1.3}$$

where in (1.3) each polynomial $B_r(x)$ records the site content of the clusters of r bonds. For the body-centred cubic lattice the expansion starts

$$F(b, x) = x + 4x^2 b + 28x^3 b^2 + 252x^4 b^3 + (2570x^5 + 12x^4) b^4 + \dots \tag{1.4}$$

and the coefficient of b^4 records the fact that out of 2582 connected clusters of four bonds, 2570 have five sites and therefore cyclomatic index 0, and 12 have four sites and therefore cyclomatic index 1. We give the values of the B_r through B_{14} in appendix 1.

2. Method of partial generating functions

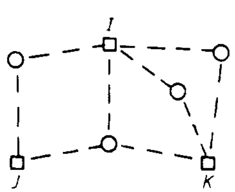
The method described in I and by Sykes *et al* (1965, 1973) for exploiting the equivalence of the two sublattices of an infinite loose-packed lattice is immediately applicable to weak embeddings. It is only necessary to characterise the bond embeddings by the sublattice distribution of their *sites*. Thus equation (1.5) of I has an analogue:

$$2F(x, y) = B_{1,0}x + B_{0,1}y + B_{1,1}xy + B_{2,1}x^2 y + \dots \tag{2.1}$$

The subscripts in (2.1) now refer to the *sites* and each $B_{r,s}$ is a polynomial in b; the whole of the formation of § 2 of I can then be applied, *mutatis mutandis*. A knowledge of the first n partial generating functions enables the number of weak embeddings with $(2n+1)$ *sites* to be deduced.

3. Restricted and unrestricted generating functions

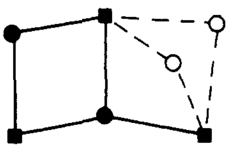
We begin this section by taking as example the finite graph G used before in I to illustrate restricted and unrestricted generating functions for strong embeddings:

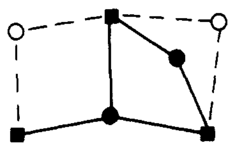


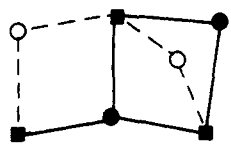
For this graph we can immediately derive an *unrestricted subgraph enumerator* which we write

$$
\begin{aligned}
G(IJK) &= (1+2by+b^2y)^3(1+3by+3b^2y+b^3y)\\
&= 1+(9b+6b^2+b^3)y+(30b^2+39b^3+18b^4+3b^5)y^2\\
&\quad +(44b^3+84b^4+63b^5+22b^6+3b^7)y^3\\
&\quad +(24b^4+60b^5+62b^6+33b^7+9b^8+b^9)y^4.
\end{aligned} \tag{3.1}
$$

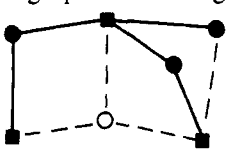
It summarises the site and bond content of all the 512 subgraphs obtained by selecting any number of B sites and any (non-zero) number of bonds from each chosen site. Again we assume the A sites are *always* occupied. In using round brackets on the left-hand side (3.1) we follow the fairly widespread convention of representing weak embeddings by round brackets and strong embeddings by square brackets. As an example the term $3b^5y^2$ now corresponds to the subgraphs (a), (b) and (c) illustrated below.


(a)


(b)


(c)

All of these are as it happens also section graphs; an example of an embedding which is not a section graph is the subgraph:


(d)

and this will contribute to the coefficient of b^5y^3. The derivation of (3.1) only differs from that of the corresponding strong embedding in the replacement of each *strong auxiliary polynomial* $(1+b^ry)$ for any r-vertex star by a *weak auxiliary polynomial* $(1+\{(1+b)^r-1\}y)$.

The *restricted (connected) subgraph enumerator* for G can also be written down by inspection (although the work is now quite detailed):

$$
\begin{aligned}
G^*(IJK) &= b^3y+(14b^4+3b^5)y^2+(46b^5+21b^6+3b^7)y^3\\
&\quad +(44b^6+31b^7+9b^8+b^9)y^4.
\end{aligned} \tag{3.2}
$$

Again we now define *partitioned* subgraph enumerators exactly analogous to the partitioned section graph enumerators of I; for our example these can be written down by inspection as†

$$
\left.
\begin{aligned}
G(I,JK) &= (1+2by)^3(1+3by+b^2y)\\
G(J,IK) &= (1+2by)(1+2by+b^2y)^2(1+3by+b^2y)\\
G(K,IJ) &= (1+2by)^2(1+2by+b^2y)(1+3by+b^2y)\\
G(I,J,K) &= (1+2by)^3(1+3by).
\end{aligned}
\right\} \tag{3.3}
$$

† Exercises of this kind can be performed with facility by anyone with a practical familiarity with generating functions; for further guidance see the article by Fisher (1962).

Now the whole of the formal argument of I can be repeated simply by *replacing square brackets by round brackets throughout*; we thus have immediately from (3.8) of I:

$$G^*(IJK) = G(IJK) - G(I, JK) - G(J, IK) - G(K, IJ) + 2G(I, J, K) \tag{3.4}$$

and it can be verified by substitution of (3.3) in (3.4) that (3.2) is correct.

The results (3.3) illustrate an important difference between the partitioned section graph and the partitioned subgraph enumerators. While the former can be written as products of the simple auxiliary polynomials that occur in the unpartitioned enumerator, the latter require the introduction of extra auxiliary polynomials. These polynomials are of quite simple structure and we give a full prescription in the next section.

4. Prescription for auxiliary unrestricted subgraph enumerators

We begin by writing down the auxiliary polynomials that correspond to the first four vertex stars.

First-order vertex star; one A site I:

$$\psi_1 = (1 + by) \qquad \text{always.}$$

Second-order vertex star; two A sites I, J

$\psi_{2,1} = (1 + 2by + b^2y)$ if I, J in same subset of partitioned set

$\psi_{2,2} = (1 + 2by)$ if I, J in different subsets of partitioned set.

Third-order vertex star; three A sites I, J, K:

$\psi_{3,1} = (1 + 3by + 3b^2y + b^3y)$ if I, J, K in same subset

$\psi_{3,2} = (1 + 3by + b^2y)$ if I, J, K intersect two subsets

$\psi_{3,3} = (1 + 3by)$ if I, J, K intersect three subsets.

Fourth-order vertex star; for A sites I, J, K, L:

$\psi_{4,1} = (1 + 4by + 6b^2y + 4b^3y + b^4y)$ if I, J, K, L in same set

$\psi_{4,2} = (1 + 4by + 3b^2y + b^3y)$ if I, J, K, L intersect two subsets with division 1-3

$\psi_{4,3} = (1 + 4by + 2b^2y)$ division 2-2

$\psi_{4,4} = (1 + 4by + b^2y)$ three subsets

$\psi_{4,5} = (1 + 4by)$ four subsets.

The form of the general prescription should now be clear. For each partition of the $I, J, K \ldots$ into connectively disjoint subsets, say

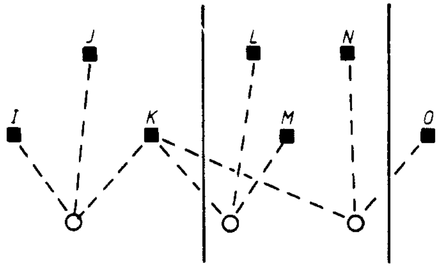
$$IJK, MN, PQ \ldots, \ldots = S_1, S_2, S_3, \ldots, S_i, \ldots$$

and a vertex star spanning some set V of $I, J, K, \ldots$ denote the cardinality of $S_i \cap V$ by C_i. Then the corresponding auxiliary polynomial is just

$$\psi = 1 + \sum_{\text{All } i} [(1 + by)^{C_i} - 1]y \tag{4.1}$$

and the corresponding enumerator for the partition is the continued product of all such ψ over all the vertex stars.

For example consider the specific partition illustrated below of seven A sites and three B sites, each latter forming a vertex star of order 3 spanning the A sites as drawn:



Applying the above prescription

$$G(IJK, LMN, O) = (1+3by+3b^2y+b^3y)(1+3by+b^2y)(1+3by).$$

5. Application to the body-centred cubic lattice

We have applied the technique of the preceding sections to the body-centred cubic lattice. The procedure is a straightforward generalisation of that described in § 5 of I for the enumeration of strong embeddings. The same basic configurational data are required: the specification of all the arrangements of up to six cubes determines the first six partial generating functions and these, following § 2 of I and of the present paper, determine all the embeddings with up to 13 *sites.* The actual determination of all the products appropriate to each arrangement of cubes is rather more intricate and is conveniently done by computer. The partial generating functions for strong embeddings were expressed in I as sets of weighted codes $\{\alpha, \beta, \gamma \ldots\}$ wherein by convention the successive parameters denoted the exponents of the simple auxiliary polynomials of § 3 of I. For weak embeddings the prescription of § 4 results in a weighted set of codes of the more general form:

$$(\alpha, \beta, \beta', \gamma, \gamma', \gamma'', \delta \ldots) = (\psi_1)^\alpha (\psi_{2,1})^\beta (\psi_{2,2})^{\beta'} (\psi_{3,1})^\gamma (\psi_{3,2})^{\gamma'} \ldots \tag{5.1}$$

each code corresponding to some product of auxiliary polynomials of type (4.1).

The number of these *weak* codes (5.1) at each stage increases more rapidly than the corresponding number of strong codes (5.7) of I; for the body-centred cubic the first six partial generating functions contain 1, 6, 33, 206, 1497, 12 205 codes respectively. The derivation of these codes requires very little extra computing time; however the substitution (4.1) and the subsequent expansion of the products of the auxiliary polynomials takes longer. The 12 205 sixth-order codes took 20 min to expand using the University of London Cray. By exploiting the sublattice symmetry the number of weak embeddings with up to 13 sites then follows. The only embeddings of up to 14 bonds with more than 13 sites correspond to graphs with cyclomatic index 0 or 1; it is possible to obtain the number of these by techniques based on the theory of bond percolation which we describe in subsequent papers. For completeness we quote the full values of B_n through $n = 14$ in the appendix.

6. Conclusions

The work described in this paper continues the feasibility study begun in I. By using the method of partial generating functions we have been able to produce a table of connected weak embeddings for the body-centred cubic lattice through B_{14}. As we have noted in our introduction a direct enumeration by computer would require some 46 *years* of CPU time; recently it has proved possible to rederive all the relevant details of the arrangements of six cubes used in this paper on the London University Cray in 45 *minutes* CPU time (J L Martin and M K Wilkinson, private communication); the effective counting rate achieved is thus some 500 000 times faster. Our general conclusion reaffirms that of I: If a large amount of machine time is available it would be more efficient to use it to derive partial generating functions than to count clusters directly.

Appendix. Weak embeddings of clusters in the body-centred cubic lattice grouped by bond and site content

$B_0 = x$

$B_1 = 4x^2$

$B_2 = 28x^3$

$B_3 = 252x^4$

$B_4 = 2570x^5 + 12x^4$

$B_5 = 28\,360x^6 + 288x^5$

$B_6 = 329\,892x^7 + 5368x^6 + 12x^5$

$B_7 = 3986\,292x^8 + 90\,408x^7 + 528x^6$

$B_8 = 49\,568\,107x^9 + 1451\,694x^8 + 14\,142x^7 + 27x^6$

$B_9 = 630\,277\,520x^{10} + 22\,704\,304x^9 + 312\,700x^8 + 1424x^7$

$B_{10} = 8158\,745\,828x^{11} + 349\,603\,020x^{10} + 6232\,256x^9 + 47\,192x^8 + 72x^7$

$$B_{11} = 107\,168\,136\,392x^{12} + 5330\,879\,928x^{11} + 116\,596\,608x^{10} + 1247\,456x^9 + 4704x^8$$

$$B_{12} = 1424\,941\,392\,516x^{13} + 80\,772\,408\,610x^{12} + 2091\,391\,256x^{11} + 28\,963\,354x^{10} + 1822\,214x^9 + 250x^8$$

$$B_{13} = 19\,142\,538\,495\,540x^{14} + 1218\,664\,333\,920x^{13} + 36\,417\,087\,944x^{12} + 618\,185\,200x^{11} + 5525\,940x^{10} + 18\,056x^9 + 4x^8$$

$$B_{14} = 259\,435\,941\,941\,340x^{15} + 18\,333\,838\,574\,748x^{14} + 620\,449\,516\,128x^{13} + 12\,445\,699\,084x^{12} + 144\,569\,688x^{11} + 789\,264x^{10} + 1052x^9$$

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