Generating functions for connected embeddings in a lattice: V. application to the simple cubic and body-centred cubic lattices

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Generating functions for connected embeddings in a lattice: V. Application to the simple cubic and body-centred cubic lattices

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Abstract. The method of partial generating functions is used to derive, for the simple cubic lattice, the number of connected strong embeddings through 13 sites, the number of connected weak embeddings through 14 bonds and three new bond perimeter polynomials D_{10}, D_{11}, D_{12} for the bond percolation problem. For the body-centred cubic and simple cubic lattices an expression is derived for the mean number of clusters for the site percolation problem in powers of the probabilities of occupation of A and B sites.

1. Introduction

In this paper we report some applications of the techniques developed in previous papers (Sykes 1986a, b, c, d, hereafter referred to as I–IV respectively) to the simple cubic and body-centred cubic lattices. In I–III the method of partial generating functions was developed using the body-centred cubic lattice as an example; by repeating the calculations for the simple cubic lattice we have obtained the number of connected strong embeddings with details of their bond content through 13 sites, the number of connected weak embeddings with details of their site content through 14 bonds and the bond perimeter polynomials through D_{12}. We give these results, in the notation of I and II, in appendices 1, 2 and 3, respectively. The expansion of the generating function for the simple cubic lattice for the most complicated case, the bond perimeter substitution using the auxiliary polynomials (2.3) of III, took only 8 min of CPU time on the Cray.

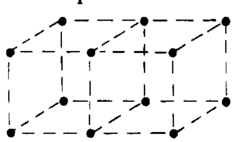
The pilot study of I and II was based on a classification of all the arrangements of up to six cubes; the classification was achieved manually by exhaustive enumeration of all the possibilities using the shadow lattice techniques developed originally for a study of the Ising model (Sykes *et al* 1965, 1973a, b, Sykes 1979). The classification of arrangements of cubes is visually simple; the analogous classification of arrangements of octahedra required to duplicate the calculations of I–III for the simple cubic lattice is rather less so, although the total number of configurations is smaller. We have made an exhaustive manual enumeration of all the arrangements of up to six octahedra; the corresponding shadow lattice is the face-centred cubic lattice with second neighbours (Sykes *et al* 1973a). We have been able to check both the above enumerations by computer, using a program developed by J L Martin (private communication); this required 250 min for the body-centred cubic problem and 75 min for the simple cubic problem on the Cray. We shall not give any details of these calculations since they are likely to be superseded by improved routines currently being developed.

Our chief objective is to apply the alternative procedure developed in IV to the derivation of series expansions for the site percolation problem. Since site perimeter polynomials are available for the simple cubic lattice up to eleven sites and for the body-centred cubic up to ten sites (Sykes *et al* 1976) it suffices to derive expansions for the mean number of clusters only; expansions for other quantities of interest can then be deduced indirectly (Sykes and Wilkinson 1986). In § 2 we investigate how to develop the mean number expansion when there are two species of site. In § 3 we apply similar ideas to the mean number of clusters for the bond percolation problem and obtain a partial verification of the expansions given in III (equations (4.1) and (4.2)). Finally, although we have not had to use the techniques explicitly, for the reason stated above, we give in § 4 some indication of how the exploitation of sublattice symmetry can be applied to the expansion of the mean size of finite clusters.

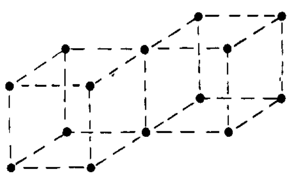
This paper reports new data; most of the theoretical background is covered by the references cited.

2. Bipartite percolation: expansion for the mean number of clusters

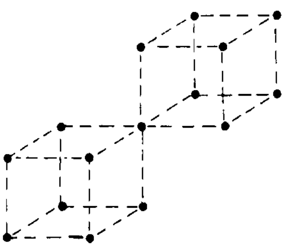
The generalisation of the site problem on a bipartite graph, by the introduction of separate probabilities α, β for the presence of A and B sites respectively, has already been made in IV. A general prescription for obtaining the mean number of clusters by the use of unrestricted generating functions is given there. To illustrate how these ideas can be used to exploit the sublattice symmetry of the simple cubic and body-centred cubic lattices we quote below the results of applying the techniques of IV, § 3, to the finite graphs G_1, G_2, G_3 which correspond in each case to a connected configuration of two cubic shadows on the body-centred cubic system when all the A and B sites are present:

G_1  $(3N)$

$$K_1 = 2\alpha + 12\beta - 16\alpha\beta + 6\alpha^2\beta^2 - 4\alpha^2\beta^3 + \alpha^2\beta^4 \tag{2.1}$$

G_2  $(6N)$

$$K_2 = 2\alpha + 14\beta - 16\alpha\beta + \alpha^2\beta^2 \tag{2.2}$$

G_3  $(4N)$

$$K_3 = 2\alpha + 15\beta - 16\alpha\beta. \tag{2.3}$$

If we weight the functions K_1, K_2, K_3 by the number of occurrences of each shadow pattern we obtain a total contribution (per lattice site) of

$$26\alpha+180\beta-208\alpha\beta+24\alpha^2\beta^2-12\alpha^2\beta^3+3\alpha^2\beta^4. \tag{2.4}$$

In (2.4) the last three terms, which make up the coefficient of α^2, are identical (apart from a factor of 2 due to our working per sublattice site) with the terms in α^2 for the expansion for the infinite lattice (equation (1.4) of IV). It is easy to see why this has to be the case: the mean number function has a connected graph expansion (Essam and Sykes 1966); any embedding with a non-zero weight that contributes to the coefficient of α^2 must have two A sites and these can be taken as defining some embedding of the shadows illustrated above. But all the connected graphs which are associated with the same embedding must contribute also to the coefficient of α^2 for the finite graph and conversely. For the same reason we need not consider any arrangement of shadows that is disconnected.

We can therefore exploit the symmetry of the two sublattices in the usual way to deduce the coefficient of any term $\alpha^x\beta^y$ with $x>y$ from that of $\alpha^y\beta^x$. Using the configurational data for all the possible contacts of up to six octahedral shadows for the simple cubic lattice and for up to six cubic shadows for the body-centred cubic lattice, we have derived all the terms in the mean number expansions for these two lattices through p^{13} in general form (the calculation was performed on the University of London Cray computer in under 2 min CPU time):

simple cubic lattice:

$$\begin{aligned}K=&\tfrac{1}{2}(\alpha+\beta)-3\alpha\beta+3\alpha^2\beta^2+4\alpha^3\beta^3-4\alpha^3\beta^3(\alpha+\beta)+30\alpha^4\beta^4-37\tfrac{1}{2}\alpha^4\beta^4(\alpha+\beta)\\&+294\alpha^5\beta^5+15\alpha^4\beta^4(\alpha^2+\beta^2)-522\alpha^5\beta^5(\alpha+\beta)+3193\alpha^6\beta^6\\&+378\alpha^5\beta^5(\alpha^2+\beta^2)-6777\alpha^6\beta^6(\alpha+\beta)-117\alpha^5\beta^5(\alpha^3+\beta^3)+\ldots\end{aligned} \tag{2.5}$$

body-centred cubic lattice:

$$\begin{aligned}K=&\tfrac{1}{2}(\alpha+\beta)-4\alpha\beta+12\alpha^2\beta^2-6\alpha^2\beta^2(\alpha+\beta)+4\alpha^3\beta^3+\tfrac{3}{2}\alpha^2\beta^2(\alpha^2+\beta^2)-4\alpha^3\beta^3(\alpha+\beta)\\&+220\alpha^4\beta^4-474\alpha^4\beta^4(\alpha+\beta)+3108\alpha^5\beta^5+485\alpha^4\beta^4(\alpha^2+\beta^2)\\&-8212\alpha^5\beta^5(\alpha+\beta)-281\alpha^4\beta^4(\alpha^3+\beta^3)+65\,304\alpha^6\beta^6\\&+10\,468\alpha^5\beta^5(\alpha^2+\beta^2)+96\alpha^4\beta^4(\alpha^4+\beta^4)-209\,372\alpha^6\beta^6(\alpha+\beta)\\&-7411\tfrac{1}{2}\alpha^5\beta^5(\alpha^3+\beta^3)-18\alpha^4\beta^4(\alpha^5+\beta^5)+\ldots.\end{aligned} \tag{2.6}$$

Setting $\alpha=\beta=p$ we obtain the corresponding expansions for the one-variable problem:

$$\begin{aligned}K_{\mathrm{SC}}=&p-3p^2+3p^4+4p^6-8p^7+30p^8-75p^9+324p^{10}\\&-1044p^{11}+3949^{12}-13\,788p^{13}+\ldots\end{aligned} \tag{2.7}$$

$$\begin{aligned}K_{\mathrm{BCC}}=&p-4p^2+12p^4-12p^5+7p^6-8p^7+220p^8-948p^9+4078p^{10}\\&-16\,986p^{11}+86\,432p^{12}-433\,603p^{13}+\ldots.\end{aligned} \tag{2.8}$$

We make a detailed application of these two expansions in a companion paper (Sykes and Wilkinson 1986). By using the generating functions of IV we have been able to avoid having to list all the strong embeddings through 13 sites on these two lattices.

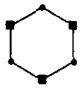
3. Bond percolation: expansion for the mean number of clusters

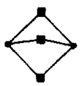
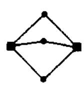
The correctness of the data derived for weak embeddings is dependent upon that of the expansion of the mean number of bond clusters used in their derivation. We now show how to apply the theory developed in IV, § 4, to check the series given in III, § 4, which were used in II to complete the data for the body-centred cubic lattice (in the appendix) and in the present paper to complete the corresponding data for the simple cubic lattice (appendix 2).

Direct expansion of the mean number of clusters in a bond mixture calls for a *bond*-grouped list of *weak* star embeddings (see Essam and Sykes (1966) for a detailed treatment); for the body cubic lattice the expansion begins

$$K(p)=1-4p+12p^4+136p^6-192p^7+2307p^8+\dots \qquad (3.1)$$

In (3.1) we have adopted the null-cluster convention, which allows isolated sites; the expected number of clusters per site then approaches unity as p approaches zero. The coefficient of p^6, for example, corresponds to weak embeddings of two star graphs:

the hexagon  (148 embeddings per site) $k-wt$: +1

and the theta graph  or  (6 embeddings each per site) $k-wt$: −1.

For a bipartite lattice the distribution of the vertices of these weak embeddings on the two sublattices plays no significant role in the theory of the star expansion, but we can include information on this distribution in a purely formal way by introducing variables, a and b, and writing the coefficient of p^6 illustrated above:

$$148a^3b^3-6a^3b^2-6a^2b^3. \qquad (3.2)$$

By inspection of the star data used in the original derivation of (3.1) to p^{14} given in II, § 4, equation (4.2) we have re-derived the expansion in this detailed form as

$$\begin{aligned}K(p)={}&\tfrac{1}{2}(a+b)-4abp+12a^2b^2p^4+[148a^3b^3-6(a^3b^2+a^2b^3)]p^6-192a^3b^3p^7\\
&+[2736a^4b^4-240(a^4b^3+a^3b^4)+48a^3b^3+\tfrac{3}{2}(a^4b^2+a^2b^4)]p^8\\
&+[-7012a^4b^4+332(a^4b^3+a^3b^4)]p^9+[61\,896a^5b^5-9342(a^5b^4+a^4b^5)\\
&+7636a^4b^4+144(a^5b^3+a^3b^5)-96(a^4b^3+a^3b^4)]p^{10}\\
&+[-237\,468a^5b^5+24\,756(a^5b^4+a^4b^5)-4092a^4b^4\\
&-216(a^5b^3+a^3b^5)]p^{11}+[1579\,324a^6b^6-352\,578(a^6b^5+a^5b^6)\\
&+468\,096a^5b^5+12\,127(a^6b^4+a^4b^6)-26\,292(a^5b^4+a^4b^5)\\
&-30(a^6b^3+a^3b^6)+1016a^4b^4+72(a^5b^3+a^3b^5)]p^{12}\\
&+[-8124\,192a^6b^6+1395\,996(a^6b^5+a^5b^6)-559\,128a^5b^5\\
&-32\,880(a^6b^4+a^4b^6)+13\,332(a^5b^4+a^4b^5)\\
&+48(a^6b^3+a^3b^6)-64a^4b^4]p^{13}\\
&+[43\,702\,920a^7b^7-13\,119\,462(a^7b^6+a^6b^7)+23\,424\,960a^6b^6\\
&+777\,060(a^7b^5+a^5b^7)-2611\,548(a^6b^5+a^5b^6)-7548(a^7b^4+a^4b^7)\\
&+411\,804a^5b^5+35\,346(a^6b^4+a^4b^6)\\
&-3156(a^5b^4-a^4b^5)-18(a^6b^3+a^3b^6)]p^{14}\\
&+\dots\end{aligned} \qquad (3.3)$$

Some 340 star graphs contribute to the final coefficient in (3.3); the introduction of the variables a and b enables us to provide some check on the accuracy of the derivation. In IV, § 4, a prescription is given for the derivation of the mean number function $K(p)$ for a bipartite graph; there it is shown how to extract that part of $K(p)$ that corresponds to the contribution of stars with a full complement of A sites. By applying this prescription successively to all the arrangements of 1-6 cubes we have been able to obtain expansions that are consistent with (3.3). Thus for example the coefficient of p^{14} with a full complement of A sites derived from six cubes is found to be 7729 278 and this is in agreement with the contribution indicated by (3.3) which is just the sum of the coefficients of $a^6b^3p^{14}$, $a^6b^4p^{14}$, $a^6b^5p^{14}, \ldots$ to exhaustion. Effectively we obtain a consistency check on all the coefficients a^rb^s for which either $r \leq 6$ or $s \leq 6$; the only term not checked is therefore that in a^7b^7 which must have cyclomatic index unity and corresponds simply to the fourteen-sided polygon.

4. Bipartite percolation: expansion for the mean size of clusters

The methods of § 2 can also be used to derive an expansion for the mean size, $S(p)$, of clusters; we define this latter concept precisely in a companion paper (Sykes and Wilkinson 1986); for our present objective it suffices to notice that interest centres on the expansion of the unnormalised second moment, $pS(p)$, which we denote by $S^*(p)$. For the body-centred cubic lattice the expansion begins (Sykes *et al* 1976):

$$S^*(p) = p + 8p^2 + 56p^3 + 248p^4 + 1232p^5 + \ldots . \tag{4.1}$$

The corresponding expansion for the bipartite lattice mixture is

$$S^*(\alpha, \beta) = \tfrac{1}{2}(\alpha + \beta) + 8\alpha\beta + 28\alpha\beta(\alpha + \beta) + 248\alpha^2\beta^2 + 616\alpha^2\beta^2(\alpha + \beta) + \ldots . \tag{4.2}$$

Using elementary methods the corresponding moments for the three shadow graphs of § 2 are readily found to be

$$S_1^* = 2\alpha + 12\beta + 32\alpha\beta + 8\alpha^2\beta + 112\alpha\beta^2 + 40\alpha^2\beta^2 + 40\alpha^2\beta^3 - 130\alpha^2\beta^4 + 112\alpha^2\beta^5 - 32\alpha^2\beta^6 \tag{4.3}$$

$$S_2^* = 2\alpha + 14\beta + 32\alpha\beta + 4\alpha^2\beta + 112\alpha\beta^2 + 44\alpha^2\beta^2 + 120\alpha^3\beta^3 - 72\alpha^2\beta^4 \tag{4.4}$$

$$S_3^* = 2\alpha + 15\beta + 32\alpha\beta + 2\alpha^2\beta + 112\alpha\beta^2 + 28\alpha^2\beta^2 + 98\alpha^2\beta^3. \tag{4.5}$$

The weighted total

$$3S_1^* + 6S_2^* + 4S_3^* = \ldots + 496\alpha^2\beta^2 + 1232\alpha^2\beta^3 - 822\alpha^2\beta^4 + 336\alpha^2\beta^5 + \ldots \tag{4.6}$$

corresponds in an analogous manner to the coefficients of the infinite lattice (apart from a factor of 2) for all the terms of the form $\alpha^2\beta^r$, $r \geq 2$.

For the simple cubic lattice and body-centred cubic lattice it is not necessary to apply the methods of the present section to the derivation of the second moment since, as we show in Sykes and Wilkinson (1986), there are enough perimeter polynomials available for this to be obtained indirectly using (4.1) or (4.2). The whole process of obtaining second moments by the use of generating functions follows the general pattern used for the mean number function but is of necessity more complicated in its detailed application. We hope to develop it further subsequently.

Acknowledgments

We thank Dr J L Martin for his constructive advice and criticism throughout this series of papers.

Appendix 1. Strong embeddings of clusters in the simple cubic lattice grouped by site and bond content

$A_1 = 1$

$A_2 = 3b$

$A_3 = 15b^2$

$A_4 = 83b^3 + 3b^4$

$A_5 = 486b^4 + 48b^5$

$A_6 = 2967b^5 + 496b^6 + 18b^7$

$A_7 = 18\,748b^6 + 4368b^7 + 378b^8 + 8b^9$

$A_8 = 121\,725b^7 + 36\,027b^8 + 4854b^9 + 306b^{10} + b^{12}$

$A_9 = 807\,381b^8 + 288\,732b^9 + 51\,030b^{10} + 5544b^{11} + 159b^{12} + 24b^{13}$

$A_{10} = 5447\,203b^9 + 2280\,792b^{10} + 488\,976b^{11} + 72\,244b^{12} + 5103b^{13} + 396b^{14} + 24b^{15}$

$$A_{11} = 37\,264\,974b^{10} + 17\,866\,896b^{11} + 4463\,316b^{12} + 801\,396b^{13} + 89\,715b^{14} + 7568b^{15} + 660b^{16} + 24b^{17}$$

$$A_{12} = 257\,896\,500b^{11} + 139\,239\,286b^{12} + 39\,546\,852b^{13} + 8179\,476b^{14} + 1197\,481b^{15} + 132\,681b^{16} + 12\,546b^{17} + 1080b^{18} + 3b^{20}$$

$$A_{13} = 1802\,312\,605b^{12} + 1081\,555\,008b^{13} + 343\,288\,410b^{14} + 79\,574\,192b^{15} + 13\,869\,918b^{16} + 1929\,048b^{17} + 215\,204b^{18} + 23\,976b^{19} + 864b^{20} + 96b^{21}.$$

Appendix 2. Weak embeddings of clusters in the simple cubic lattice grouped by bond and site content

$B_0 = x$

$B_1 = 3x^2$

$B_2 = 15x^3$

$B_3 = 95x^4$

$B_4 = 678x^5 + 3x^4$

$B_5 = 5229x^6 + 48x^5$

$B_6 = 42\,464x^7 + 622x^6$

$B_7 = 357\,987x^8 + 7308x^7 + 18x^6$

$B_8 = 3104\,013x^9 + 81\,981x^8 + 450x^7$

$B_9 = 27\,511\,300x^{10} + 895\,536x^9 + 7958x^8 + 8x^7$

$$B_{10}=248\,160\,162x^{11}+9627\,966x^{10}+119\,520x^{9}+372x^{8}$$

$$B_{11}=2270\,927\,307x^{12}+102\,460\,488x^{11}+1640\,634x^{10}+9036x^{9}+12x^{8}$$

$$B_{12}=21\,032\,126\,627x^{13}+1083\,057\,959x^{12}+21\,266\,068x^{11}+172\,345x^{10}+447x^{9}+x^{8}$$

$$\begin{aligned}B_{13}=&\,196\,774\,731\,204x^{14}+11\,396\,143\,092x^{13}+265\,101\,684x^{12}\\&+2857\,182x^{11}+12\,447x^{10}+24x^{9}\end{aligned}$$

$$\begin{aligned}B_{14}=&\,1857\,077\,730\,393x^{15}+119\,533\,011\,852x^{14}\\&+3213\,321\,288x^{13}+43\,317\,237x^{12}+274\,419x^{11}+756x^{10}.\end{aligned}$$

Appendix 3. Bond perimeter polynomials for the simple cubic lattice (for earlier terms see Sykes *et al* (1981))

$$\begin{aligned}D_{10}=&\,37\,264\,974q^{46}+73\,034\,952q^{45}+70\,171\,248q^{44}\\&+45\,126\,408q^{43}+17\,533\,428q^{42}+4004\,592q^{41}\\&+3200\,472q^{40}+3690\,624q^{39}+2699\,952q^{38}+843\,138q^{37}\\&+177\,060q^{36}+41\,280q^{35}+51\,030q^{34}+53\,736q^{33}\\&+9666q^{32}+5088q^{31}+306q^{28}+66q^{26}\end{aligned}$$

$$\begin{aligned}D_{11}=&\,257\,896\,500q^{50}+570\,616\,752q^{49}+627\,603\,288q^{48}\\&+469\,676\,808q^{47}+240\,021\,897q^{46}+80\,393\,760q^{45}\\&+37\,531\,818q^{44}+38\,028\,048q^{43}+30\,675\,228q^{42}\\&+15\,418\,152q^{41}+4226\,472q^{40}+1151\,064q^{39}+636\,984q^{38}\\&+713\,568q^{37}+321\,738q^{36}+90\,744q^{35}+25\,608q^{34}\\&+5544q^{32}+1908q^{31}+1584q^{30}+12q^{25}\end{aligned}$$

$$\begin{aligned}D_{12}=&\,1802\,312\,605q^{54}+4442\,485\,104q^{53}\\&+5494\,079\,484q^{52}+4654\,566\,416q^{51}+2850\,265\,746q^{50}\\&+1261\,429\,248q^{49}+532\,476\,318q^{48}+412\,747\,008q^{47}\\&+333\,878\,916q^{46}+213\,839\,986q^{45}+85\,344\,114q^{44}\\&+24\,531\,618q^{43}+11\,524\,284q^{42}+8047\,308q^{41}\\&+5990\,499q^{40}+2112\,640q^{39}+713\,256q^{38}\\&+106\,104q^{37}+72\,244q^{36}+62\,553q^{35}+27\,660q^{34}\\&+9888q^{33}+159q^{30}+288q^{29}+q^{24}.\end{aligned}$$

References

Essam J W and Sykes M F 1966 *J. Math. Phys.* **7** 1573-81
Sykes M F 1979 *J. Phys. A: Math. Gen.* **12** 879-92
—— 1986a *J. Phys. A: Math. Gen.* **19** 1007-25
—— 1986b *J. Phys. A: Math. Gen.* **19** 1027-32
—— 1986c *J. Phys. A: Math. Gen.* **19** 2425-9
—— 1986d *J. Phys. A: Math. Gen.* **19** 2431-8
Sykes M F, Essam J W and Gaunt D S 1965 *J. Math. Phys.* **6** 293-8
Sykes M F, Gaunt D S, Essam J W, Heap B R, Elliott C J and Mattingly S R 1973a *J. Phys. A: Math., Nucl. Gen.* **6** 1498-506
Sykes M F, Gaunt D S, Essam J W and Hunter D L 1973b *J. Math. Phys.* **14** 1060-5
Sykes M F, Gaunt D S and Glen M 1976 *J. Phys. A: Math. Gen.* **9** 1075-12
—— 1981 *J. Phys. A: Math. Gen.* **14** 287-93
Sykes M F and Wilkinson M K 1986 *J. Phys. A: Math. Gen.* **19** 3415-24

Erratum

In paper IV of this series, an error appeared at the printing stage. The three lines after equation (3.5) should be replaced by the following:

'This is a strikingly simple result; for connected clusters each unrestricted generating function appears with weight $(-1)^{m+1}(m-1)!$ and for the mean number this is replaced by $(-1)^m(m-2)!$.'