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Generating functions for connected embeddings in a lattice: IV. Site percolation

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Abstract. The method of partial generating functions is applied to the problem of site percolation. It is concluded that the direct generation of site perimeter polynomials, although feasible, is likely to be less efficient than the corresponding generation of bond perimeter polynomials. The theory of percolation on a bipartite graph is developed and an alternative method of expanding the mean number of clusters for both site and bond mixtures without recourse to perimeter polynomials is described; a general prescription for the required generating functions is given.

1. Introduction

In this paper we examine the application of the techniques described in three previous papers (Sykes 1986a, b, c, hereafter referred to as I, II and III respectively), to the site percolation problem. In III we used the method of partial generating functions to derive perimeter polynomials for bond mixtures. For site mixtures perimeter polynomials for the more usual crystal lattices are given by Sykes and Glen (1976) and Sykes *et al* (1976); these data were obtained by machine enumeration and as we have stressed previously such enumerations are very demanding of computer time. A detailed introduction to the site problem is given in the papers cited.

In III, § 2 we gave an expression for the bond perimeter of a weak embedding; the simple form of this expression enabled the required perimeter polynomials to be generated by the introduction of a single auxiliary variable. This auxiliary variable recorded the number of *deficit* bonds; the usefulness of the concept rested on the fact that in every case the deficit bonds for a weak embedding all lay in the corresponding associated section graph.

Suppose a strong embedding in a lattice of coordination number Z has S sites and B bonds; then from each site there radiate Z lattice bonds each of which leads to a perimeter site unless the lattice bond contributes to B. If no perimeter site were adjacent to more than one cluster site the required site perimeter would be $SZ-2B$. Extending the ideas of III we can define a *deficit site* of degree ν to be a site adjacent to $(\nu+1)$ sites of the cluster; if λ_ν denotes the number of these, the analogue of (2.2) of III is an expression for the site perimeter in the form

$$SZ-2B-\sum_{\nu=1}^{Z-1}\nu\lambda_\nu. \tag{1.1}$$

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Unlike deficit bonds, which lie inside the associated section graph, deficit sites lie *outside* the associated section graph (the latter now identified with the strong embedding itself). It is still possible to write down unrestricted generating functions for all the clusters and their site perimeters but such functions have to carry much more detail and call for the use of labelled ancillary variables; the algebraic computing problem is much more intricate and correspondingly slower. The fundamental inversion of I is, however, still applicable and the derivation of perimeter polynomials with its aid would probably prove more efficient than direct enumeration if the initial investment in programming were thought worthwhile. However, for the type of applications we have in mind (the development of series expansions for the mean number and size of clusters, for example) recourse to perimeter polynomials can be avoided and we shall instead develop alternative procedures.

Since the method of partial generating functions exploits the sublattice symmetry of bipartite lattices it is convenient to generalise the site percolation problem and consider bipartite percolation; that is, to allow the two sublattices of A and B sites to be occupied with probability α and β respectively, the case $\alpha = \beta = p$ corresponding to the simple site problem for which every site is occupied with probability p. To illustrate one general method of deriving series expansions without recourse to perimeter polynomials we shall study as a detailed example the expansion for the mean number of clusters; the coefficients in this case have a well known graphical interpretation (a star expansion, treated in detail by Essam and Sykes (1966)). For example, on the body-centred cubic the initial terms of the expansion of the mean number of clusters, $K(p)$, at low densities, for the symmetric case $\alpha = \beta$ are

$$K = p - 4p^2 + 12p^4 - 12p^5 + 7p^6 + \ldots \tag{1.2}$$

and we illustrate the graphical interpretation of these coefficients below.

Graph	Number of strong embeddings (per site)	Strong $K-wt$
•	1	1
——	4	−1
	12	+1
	12	−1
	4	+1
	3	+1.

(1.3)

Since the two sets of A and B sites are symmetric, the detailed analysis above enables the corresponding expansion for the bipartite problem to be written down by inspection

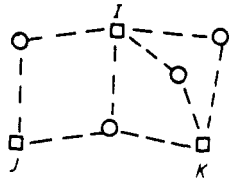
as

$$K = \tfrac{1}{2}(\alpha+\beta) - 4\alpha\beta + 12\alpha^2\beta^2 - 6\alpha^2\beta^2(\alpha+\beta) + 4\alpha^3\beta^3 + \tfrac{3}{2}\alpha^2\beta^2(\alpha^2+\beta^2) + \ldots . \qquad (1.4)$$

The direct application of the star expansion method to the series (1.2) calls for a vertex grouped list of strong embeddings of stars in the lattice; such a list is quite difficult to prepare. We have therefore sought to extend the general theory of sublattice symmetry developed in I-III to the derivation of the mean number expansion in its bipartite form (1.4) by providing appropriate partial generating functions. We show in § 2 how expansions for the mean number of clusters on a bipartite graph can be obtained by the use of generating functions.

2. The mean number of site clusters on a bipartite graph

We take as a specific example the bipartite graph of the figure which we have already used in I-III.



We first consider the situation when all three A sites, I, J, K are *occupied.* The results of § 3 of I enable a complete description of all the possible embeddings that could arise to be generated by use of the restricted *section graph* enumerators; for our present purpose each embedding is to be weighted by the number of its connected components. The variable b may be omitted from the generating function and the work can be set out as follows:

$$\begin{aligned}
&G^*[IJK] = \{y + 5y^2 + 4y^3 + y^4\} && \text{weight 1} \\
&G^*[I, JK] = \{\quad\quad\} \\
&G^*[J, IK] = \{2y + y^2\} && \text{weight 2} \qquad (2.1) \\
&G^*[K, IJ] = \{y\quad\quad\} \\
&G^*[I, J, K] = \{1\} && \text{weight 3}
\end{aligned}$$

and we obtain as the weighted total

$$3 + 7y + 7y^2 + 4y^3 + y^4. \qquad (2.2)$$

Alternatively the calculation may be performed using unrestricted enumerators. In this case the weights can be derived by applying the fundamental inversion of I and we find for our example

$$\begin{aligned}
&G[IJK] = \{1 + 4y + 6y^2 + 4y^3 + y^4\} && \text{weight 1} \\
&G[I, JK] = \{1\quad\quad\} \\
&G[J, IK] = \{1 + 2y + y^2\} && \text{weight 1} \qquad (2.3) \\
&G[K, IJ] = \{1 + y\quad\quad\} \\
&G[I, J, K] = \{1\} && \text{weight } -1
\end{aligned}$$

and these yield the same weighted total (2.1). The probability that I, J and K are all occupied is α^3; the probability that every B site that occurs in the above enumeration is occupied, while the remainder are unoccupied, is obtained by replacing y^n everywhere by $\beta^n(1-\beta)^{4-n}$ since there are four B sites. We thus obtain for the mean number of clusters when I, J and K are occupied:

$$K_{IJK} = \alpha^3\{3-5\beta+4\beta^2-\beta^3\}. \tag{2.4}$$

By repeating the logic for all three cases when only *two* of the A sites are occupied we readily obtain corresponding polynomials:

$$\begin{aligned} K_{IJ} &= \alpha^2(1-\alpha)\{2-2\beta+\beta^2\} \\ K_{JK} &= \alpha^2(1-\alpha)\{2-3\beta+3\beta^2-\beta^3\} \\ K_{JK} &= \alpha^2(1-\alpha)\{2-\beta\}. \end{aligned} \tag{2.5}$$

To obtain (2.5) we have only to use enumerators, restricted or unrestricted with appropriate weights, applied in turn to the graph obtained by deleting from G the unoccupied A site and any incident edges, and then make the appropriate probability substitutions. Likewise we can obtain expressions for the cases when only one A site is occupied:

$$\begin{aligned} K_I &= \alpha(1-\alpha)^2\{1\} \\ K_J &= \alpha(1-\alpha)^2\{1+2\beta\} \\ K_K &= \alpha(1-\alpha)^2\{1+\beta\} \end{aligned} \tag{2.6}$$

and finally if no A site is occupied

$$K_0 = (1-\alpha)^3\{4\beta\}. \tag{2.7}$$

By collecting together all these contributions we thus obtain finally

$$K = 3\alpha+4\beta-9\alpha\beta+4\alpha^2\beta^2-\alpha^2\beta^3. \tag{2.8}$$

This result is readily verified to be in agreement with the graphical interpretation we have quoted earlier; the term $4\alpha^2\beta^2$, for example, corresponding to the four four-sided polygons that can be embedded in G. In subsequent applications, when we exploit the sublattice symmetry of crystal lattices, only the coefficient of α^3 will be found to make a significant contribution for a graph with three A sites; in our particular example this turns out to be zero. Notice however that this latter result cannot be deduced from (2.4) alone; it is necessary to consider the contribution from cases where fewer than three A sites are occupied; this is only to be expected since A sites that are not occupied can occur as perimeter sites of some embeddings.

3. General prescription for the mean number of clusters in terms of unrestricted enumerators

To apply the method of the previous section to other examples we require a general prescription for the weights (2.3) which enable the calculation to be performed in terms of *unrestricted* enumerators; as we have shown in earlier applications made in I, II and III it is these latter enumerators that are most easily obtained in practice.

Consider first the general case of four occupied A sites set out in the form (2.1) and using the notation of I, § 3, (3.13):

$$\begin{aligned}
f_4^* &= f_4 - f_{1,3} - f_{2,2} + 2f_{2,1,1} - 6f_{1,1,1,1} && \text{weight 1}\\
f_{1,3}^* &= \quad f_{1,3} \quad - 2f_{2,1,1} + 8f_{1,1,1,1} && \text{weight 2}\\
f_{2,2}^* &= \qquad f_{2,2} - \ f_{2,1,1} + 3f_{1,1,1,1} && \text{weight 2}\\
f_{2,1,1}^* &= \qquad\quad f_{2,1,1} - 6f_{1,1,1,1} && \text{weight 3}\\
f_{1,1,1,1}^* &= \qquad\qquad f_{1,1,1,1} && \text{weight 4.}
\end{aligned} \tag{3.1}$$

From the treatment of I, § 4, the sum of all the coefficients of the elements in the above array that correspond to *restricted* partitioned enumerators of m parts and any one *unrestricted* partitioned enumerator of n parts is just $S^*(n, m)$, the Stirling number of the first kind. For example if we take $m = 2$ the coefficients in (3.1) above that correspond to $f_{1,3}^*$, $f_{2,2}^*$ and $f_{2,1,1}$ sum to -3 or $S^*(3, 2)$; likewise those that correspond to $f_{1,3}^*$, $f_{2,2}^*$ and $f_{1,1,1,1}$ sum to 11 or $S^*(4, 2)$.

By taking the unweighted sum of the equations (3.1)

$$f_4^* + f_{1,3}^* + f_{2,2}^* + f_{2,1,1}^* + f_{1,1,1,1}^* = f_4 \tag{3.2}$$

and we recover the starting point of the logical procedures of I, § 3, where the relation (3.2) is taken as evident. The cancellation of all the coefficients except that of f_4 on the right-hand side of (3.2) is ensured by the elementary identity

$$\sum_{m=1}^{m} S^*(n, m) = 0 \qquad m > 1. \tag{3.3}$$

For the mean number each entry on the left-hand side of (3.1) has to be weighted by the number of components; on the right-hand side each coefficient in the total will now be

$$\sum_{m=1}^{m} mS^*(n, m) = (-1)^m (m-2)! \qquad \text{for } m > 1 \tag{3.4}$$

and we obtain at order 4

$$f_4 + f_{3,1} + f_{2,2} - f_{2,1,1} + 2f_{1,1,1,1}. \tag{3.5}$$

The procedure of the last two sections can be modified to derive the mean number of bond clusters. For the graph of our example the possible embeddings are now summarised by the restricted *subgraph enumerators*:

4. The mean number of bond clusters on a bipartite graph

The procedure of the last two sections can be modified to derive the mean number of bond clusters. For the graph of our example the possible embeddings are now summarised by the restricted *subgraph enumerators*:

$$\begin{aligned}
G^*(IJK) &= b^3 + 14b^4 + 49b^5 + 65b^6 + 34b^7 + 9b^8 + b^9\\
G^*(I, JK) &= b^2 + 6b^3 + 12b^4 + 8b^5\\
G^*(J, IK) &= 3b^2 + 20b^3 + 47b^4 + 45b^5 + 15b^6 + 2b^7\\
G^*(K, IJ) &= 2b^2 + 13b^3 + 29b^4 + 24b^5 + 4b^6\\
G^*(I, J, K) &= 1 + 9b + 30b^2 + 44b^3 + 24b^4.
\end{aligned} \tag{4.1}$$

In (4.1) we have omitted the variable x, which is no longer relevant, and the unweighted total reduces to $(1+b)^9$. If we adopt the null cluster convention, under which a bond cluster is defined as a connected choice of sites (and therefore includes isolated sites), we can form as before the weighted sum of the enumerators (4.1) to obtain

$$3+27b+102b^2+211b^3+262b^4+203b^5+103b^6+38b^7+9b^8+b^9 \qquad (4.2)$$

and the only clusters excluded from the enumeration will be isolated B sites. To convert to the probabilities p, that a bond is occupied, and $q=1-p$, that a bond is unoccupied, we make the substitution $p^x q^{9-x}$ for b^x in (4.2). On adding the mean number of isolated B sites which for example is $3q^2+q^3$ we obtain finally

$$K(p)=7-9p+4p^4+p^6-2p^7+p^8+p^9. \qquad (4.3)$$

This result could equally well be obtained using the more convenient *unrestricted* generators; the appropriate weights are those already found in § 3 for the site problem. If desired, the correction for isolated B sites could be made by redefining appropriate enumerators to include them. The derivation of the mean number of bond clusters in a bond mixture that we have given above is not restricted to bipartite graphs. The whole logical procedure we have described in I-III can be appropriately recast to study the connectivity of embeddings in a general graph (for an example of this alternative formulation see Uhlenbeck and Ford (1962)). Although the two classes of A and B sites do not appear in the final result (4.3) it is possible to exploit the fact that the graph is bipartite. The coefficients in (4.3) have a well known graphical interpretation (a star expansion, treated in Essam and Sykes (1966)); the constant term is given by the number of sites; thereafter every star of n bonds contribute to p^n with a weight (the *weak* $k-wt$ of the star). In our example the coefficient of p^6 comes from two stars:

the hexagon:  (2 embeddings) $k-wt=+1$

the theta graph:  (1 embedding) $k-wt=-1$.

The first of these contains three A sites and the second only two. By applying the principle of inclusion and exclusion and evaluating the mean number function in turn for all the graphs obtained by deleting from G every choice of A sites and any incident edges we can distinguish between the two contributions above. The procedure follows the same general pattern as that of the previous section; modifying the notation so that K_{IJ} denotes the mean number for the graph with I and J *deleted* the work can be set out as follows:

$$\begin{aligned} K_{IJK} &= 7-9p+4p^4+p^6-2p^7-p^8+p^9 \quad -K_{JK}=-6+5p \\ &\quad -K_{IK}=-6+7p-3p^4+p^6 \quad -K_{JK}=-6+6p-p^4 \quad +K_I=5-4p \\ &\quad +K_J=5-2p \quad +K_K=5-3p \quad -K_0=-4 \end{aligned} \qquad (4.4)$$

and the total

$$2p^6-2p^7-p^8+p^9 \qquad (4.5)$$

corresponds to the contribution from star graphs with *three* A *sites*; the contribution of the theta graph to p^6 in our example has been deleted.

5. Summary and conclusions

We have found the direct generation of site perimeter polynomials is likely to be less efficient than the corresponding generation of bond perimeter polynomials described in III. We have developed an alternative method, without recourse to perimeter polynomials, of expanding the mean number of clusters for both site and bond mixtures. For site mixtures we have shown how to derive the function $K(\alpha, \beta)$ explicitly for a bipartite graph; in a subsequent paper this will enable us to exploit the sublattice symmetry of the body-centred cubic and simple cubic lattices and derive the function $K(p)$ without the use of a *site* grouped list of *strong* star embeddings. For bond mixtures we have shown how to derive the function $K(p)$ explicitly for a bipartite graph and also how to obtain that part of $K(p)$ that corresponds to the contribution of star embeddings with a full complement of A sites; in a subsequent paper this will enable us to check the accuracy of the bond grouped list of *weak* star embeddings used to derive the mean number expansions ((4.1) and (4.2) of III).

The methods we have used to derive expansions for the mean number function can be generalised in a straightforward way to derive expansions for other properties of interest such as the mean size of finite clusters. We have not described such generalisations because the series for the mean number combined with the data already available on perimeter polynomials has proved sufficient for the applications we have made so far.

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