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Generating functions for connected embeddings in a lattice: III. Bond percolation

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Abstract. The method of partial generating functions is developed to obtain bond perimeter polynomials for percolation processes. Four new polynomials, D_9-D_{12}, are given for the body-centred cubic lattice.

1. Introduction

In this paper we examine the application of the techniques described in two previous papers, Sykes (1986a, b, hereafter referred to as I and II respectively), to the bond percolation problem. Specifically we shall describe the necessary modifications that enable the method to be used for the derivation of *perimeter polynomials.* Data for these polynomials for the more usual crystal lattices are given by Sykes *et al* (1981); the data were obtained by machine enumeration. As we have already stressed in I and II such enumerations are very demanding of computer time.

2. The bond perimeter of a weak embedding

We first recall the essential concepts and definitions by an example: consider the free graph with four bonds, G, of figure 1(a) and a weak embedding, figure 1(b), thereof in the plane triangular lattice. (In general the lattice, L, in which G is embedded could just as well be a finite graph.) The embedding illustrated has a *bond* perimeter of 15.

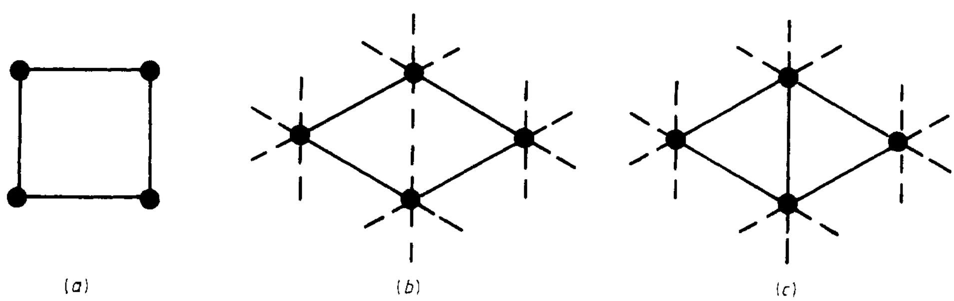

Figure 1. (a) Free graph G; (b) a weak embedding of G in a triangular lattice; (c) associated section graph.

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To obtain the fourth-order perimeter polynomial we have essentially to summarise the average environmental situation for all connected graphs with four bonds that can be embedded in the lattice (if the bond probability is p and $q=1-p$, each embedding of four bonds with a bond perimeter of σ will contribute a term p^4q^σ to $D_4(q)$); notice however that the concepts of weak embedding and bond perimeter apply equally well to graphs with more than one component. Any weak embedding of G in a lattice (or finite graph) L defines another graph: the associated section graph of the embedding. (In our example the associated section graph is the graph (c) of figure 1. For definitions of this and other theoretical terms see Essam and Fisher (1970).)

In II the method of partial generating functions was developed to provide the number of connected weak embeddings (or subgraphs) of b bonds together with information on their site content. Now the site content is a property of the free graph while the bond perimeter is a property of the embedding. However, provided the total valency of every site of L is known (which is a trivial requirement for an infinite crystal lattice), the bond perimeter of any embedding will be determined if we also know the number of bonds in the associated section graph.

Suppose the free graph has S sites and b bonds; suppose the associated section graph of some embedding has B bonds and further that the lattice has coordination number Z. Then from each site of the associated *section* graph of the embedding there radiate Z lattice bonds and these will all be perimeter bonds of the section graph unless a pair of sites are neighbours; the number of perimeter bonds of the section graph is thus just $(SZ-2B)$. The weak embeddings will have an augmented perimeter of $(SZ-2B)+B-b$. We define the quantity

$$\Lambda = B - b \qquad (2.1)$$

as the *bond deficit* of the embedding. The bond perimeter can now be written

$$SZ - 2b - \Lambda. \qquad (2.2)$$

Expression (2.2) relates the perimeter of each embedding of a free graph to the number of sites and bonds in the free graph and the bond deficit; furthermore, the *deficit bonds*, $B-b$ in number, all lie in the associated section graph. As we show in § 3, the above considerations make it possible to modify the method of partial generating functions to provide the necessary extra information. The essential point is that all the above results hold even if G is *not* connected.

3. Subgraph enumerators with explicit bond deficit parameter

In II, § 3 we have described how an unrestricted subgraph enumerator can be written down as a continued product of certain auxiliary generating polynomials; the product is taken over all the vertex stars that correspond to B sites having at least one A site as neighbour. Each vertex star can be considered in isolation. To take a specific example, three A sites and a B site contribute a factor

$$(1+3by+3b^2y+b^3y) \qquad (3.1)$$

which is no more than the general polynomial given in II evaluated for a 3-vertex star. Since the enumerator is *unrestricted* the embeddings generated are not necessarily connected; in fact the term $3by$ above corresponds simply to the three ways of embedding a bond in the vertex star.

Now in writing down (3.1) we have simply recorded the number of bonds for each embedding chosen; but we notice that all the other bonds in the vertex star must necessarily be *deficit bonds*. It therefore suffices to write in place of (3.1)

$$(1+3b\lambda^2y+3b^2\lambda y+b^3y) \tag{3.2}$$

and the number of deficit bonds generated (i.e. the contribution to Λ) will be recorded by the power of λ. The appropriate auxiliary polynomial for an r-vertex star is thus seen to be

$$\{1+[(\lambda+b)^r-\lambda^r]y\}. \tag{3.3}$$

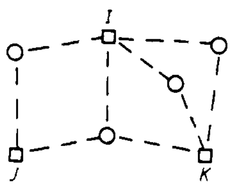
The substitution required for the auxiliary polynomials that arise in *partitioned* enumerations is now simply obtained by replacing the expression

$$[(1+by)^{C_i}-1] \tag{3.4}$$

of (4.1) of II by

$$[(\lambda+by)^{C_i}-\lambda^{C_i}]. \tag{3.5}$$

Thus taking as example the graph



which we have used in I and II we can immediately write down the complete set of unrestricted subgraph enumerators:

$$\begin{aligned}
G(IJK) &= (1+2\lambda by+b^2y)^3(1+3\lambda^2by+3\lambda b^2y+b^3y)\\
G(I,JK) &= (1+2\lambda by)^3(1+3\lambda^2by+\lambda b^2y)\\
G(J,IK) &= (1+2\lambda by)(1+2\lambda by+b^2y)^2(1+3\lambda^2by+\lambda b^2y)\\
G(K,IJ) &= (1+2\lambda by)^2(1+2\lambda by+b^2y)(1+3\lambda^2by+\lambda b^2y)\\
G(I,J,K) &= (1+2\lambda by)^3(1+3\lambda^2by)
\end{aligned} \tag{3.6}$$

from which we deduce

$$\begin{aligned}
G^*(IJK) = {} & b^3y+[(2+12\lambda)b^4+3b^5]y^2+[(4\lambda+42\lambda^2)b^5+(1+20\lambda)b^6+3b^7]y^3\\
& +(44\lambda^3b^6+31\lambda^2b^7+9\lambda b^8+b^9)y^4
\end{aligned} \tag{3.7}$$

which can be verified by inspection (although the task is now of some complexity).

The result (3.7) summarises all the connected subgraphs of G with information on their site content, bond content and bond deficit; the primary sites are assumed to be always occupied.

4. Applications

The results of the previous section can be applied to the body-centred cubic lattice by simply repeating the formal processes of II and using the *same basic configurational data*; it is only necessary to retain the extra parameter, λ, throughout the calculation. In this way we obtain four new perimeter polynomials $D_9(q)$-$D_{12}(q)$ which we give in the appendix. The detailed information provided by the partial generating functions enables us to obtain also a more general perimeter polynomial $D_{s,b}(q)$ which summarises the average environmental situation of all subgraphs with s sites and b bonds. These perimeter polynomials, which are too extensive to be quoted here, have two important applications. First, by developing the general theory of balance tables (which we shall describe subsequently (Sykes and Wilkinson 1986a)) it is possible to complete the polynomials $B_{13}(x)$ and $B_{14}(x)$ quoted in II; second, they greatly facilitate the derivation of series expansions for the mean size of bond clusters when measured by site content. We shall report this second application for the simple cubic and body-centred cubic lattices subsequently (Sykes and Wilkinson 1986b); there it will be shown that the data for perimeter polynomials are usefully supplemented by a knowledge of the expansion of the mean number, $K(p)$, of clusters at low densities. We have therefore derived these expansions using the cluster method of Essam and Sykes (1966) and find

$$K_{sc} = 1-3p+3p^4+22p^6-18p^7+183p^8-328p^9+2034p^{10}-5142p^{11} +26\,539p^{12}-81\,183p^{13}+381\,222p^{14}\ldots \quad (4.1)$$

$$K_{bcc} = 1-4p+12p^4+136p^6-192p^7+2307p^8-6348p^9+50\,944p^{10}-192\,480p^{11} +1315\,034p^{12}-5930\,392p^{13}+37\,681\,032p^{14}\ldots \quad (4.2)$$

The number of star graphs that contribute to the final coefficient in (4.2) is 340 of which 147 have cyclomatic index 5 or more. The listing of these star graphs and the determination of the number of their weak embeddings is a task of some complexity; it is therefore desirable to find some independent means of checking the derivation; we shall go some way to providing this in the next paper.

5. Conclusions

We have shown that the derivation of perimeter polynomials can be made to depend on the determination, for each embedding, of one parameter: the bond deficit. Because this dependency applies both to connected and disconnected graphs the whole of the formal procedure described in I and II can be used to generate perimeter polynomials of connected graphs only. As a byproduct we have obtained at the same time information on the site content of all the subgraphs.

Appendix. Bond perimeter polynomials for the body-centred cubic lattice (for earlier terms see Sykes *et al* (1981))

$$D_9 = 70\,545\,284q^{62}+139\,356\,264q^{61}+154\,046\,760q^{60}+121\,832\,944q^{59} +78\,940\,680q^{58}+41\,397\,648q^{57}+18\,049\,700q^{56}+5309\,952q^{55} +4131\,640q^{54}+6144\,216q^{53}+6011\,064q^{52}+4253\,616q^{51} +2145\,912q^{50}+747\,768q^{49}+68\,376q^{48}+72\,096q^{46} +110\,360q^{45}+90\,144q^{44}+37\,512q^{43}+2588q^{42}+704q^{38}+720q^{37}$$

$$D_{10}=638\,589\,820q^{68}+1438\,759\,872q^{67}+1810\,272\,744q^{66}+1637\,483\,904q^{65}$$
$$+1220\,529\,240q^{64}+758\,618\,640q^{63}+407\,983\,040q^{62}+176\,859\,312q^{61}$$
$$+92\,582\,784q^{60}+85\,552\,664q^{59}+86\,639\,664q^{58}+73\,216\,992q^{57}$$
$$+47\,253\,480q^{56}+24\,364\,644q^{55}+8251\,344q^{54}+1390\,704q^{53}$$
$$+898\,692q^{52}+1734\,808q^{51}+1821\,672q^{50}+1206\,288q^{49}+515\,284q^{48}$$
$$+55\,512q^{47}+12\,844q^{44}+20\,664q^{43}+12\,564q^{42}+1120q^{41}+72q^{36}$$
$$D_{11}=5847\,741\,388q^{74}+14\,797\,602\,912q^{73}+20\,839\,131\,300q^{72}+21\,115\,886\,128q^{71}$$
$$+17\,597\,289\,060q^{70}+12\,444\,614\,544q^{69}+7723\,757\,976q^{68}$$
$$+4128\,654\,192q^{67}+2209\,169\,832q^{66}+1528\,628\,832q^{65}+1309\,205\,652q^{64}$$
$$+1145\,162\,592q^{63}+864\,426\,480q^{62}+549\,560\,904q^{61}+274\,192\,416q^{60}$$
$$+101\,453\,280q^{59}+32\,437\,224q^{58}+25\,257\,960q^{57}+30\,788\,352q^{56}$$
$$+26\,139\,360q^{55}+16\,597\,248q^{54}+6634\,608q^{53}+1280\,688q^{52}$$
$$+195\,120q^{50}+406\,056q^{49}+396\,168q^{48}+220\,832q^{47}+29\,280q^{46}$$
$$+2016q^{42}+2376q^{41}+312q^{40}$$
$$D_{12}=54\,073\,952\,472q^{80}+151\,836\,363\,792q^{79}+236\,264\,310\,264q^{78}$$
$$+264\,433\,527\,616q^{77}+242\,265\,305\,232q^{76}+189\,919\,078\,224q^{75}$$
$$+131\,635\,620\,752q^{74}+80\,760\,938\,880q^{73}+47\,285\,290\,554q^{72}$$
$$+30\,227\,447\,316q^{71}+22\,541\,800\,296q^{70}+18\,328\,034\,200q^{69}$$
$$+14\,480\,868\,684q^{68}+10\,407\,987\,408q^{67}+6392\,920\,728q^{66}$$
$$+3236\,660\,160q^{65}+1395\,723\,836q^{64}+642\,799\,844q^{63}$$
$$+501\,455\,592q^{62}+471\,239\,104q^{61}+369\,622\,912q^{60}$$
$$+218\,193\,936q^{59}+92\,778\,288q^{58}+22\,361\,744q^{57}+3586\,806q^{56}$$
$$+6681\,144q^{55}+8392\,632q^{54}+6997\,780q^{53}+3433\,236q^{52}+782\,304q^{51}$$
$$+38\,370q^{48}+73\,344q^{47}+60\,012q^{46}+10\,488q^{45}+198q^{40}+52q^{39}.$$

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