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Percolation processes in two dimensions III. High density series expansions

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Abstract. The derivation of high density series expansions for the percolation probability and mean cluster size in random site and bond mixtures on a two-dimensional lattice is described. New data are given for the triangular, simple quadratic and honeycomb lattices.

1. Introduction

In this paper we describe the derivation of series expansions required for a study of random mixtures of sites (or bonds)† in the high density region on a two-dimensional lattice. We have given a general introduction in a previous paper (Sykes and Glen 1976, to be referred to as I) which described the elementary practical theory of the derivation of series expansions valid in the low density region $p < p_c$. The mean number of clusters K was there expanded in the form:

$$K(p, q) = \sum_s \langle n_s \rangle = \sum_s D_s(q) p^s. \quad (1.1)$$

We use $K(p, q)$ to denote the formal expansion in p and q that results from application of the perimeter method. (Since p and q are *dependent* variables, other expansions can be obtained with p and q as arguments; we follow Sykes and Essam (1964) in adopting the above convention.) In the low density region all the clusters are *finite*; the formal relation

$$p = \sum_s s \langle n_s \rangle \quad p < p_c \quad (1.2)$$

expresses the probability that a site will be black as a sum over the expectations that it will belong to a black cluster of a particular size. If the restriction $p < p_c$ is relaxed, the sum (1.2) becomes the expectation that a site will belong to a *finite* cluster of black sites. As p approaches unity almost all the black sites will belong to one cluster: *the infinite cluster*. We denote the density of black sites that belong to an infinite cluster by p_∞ , and to a finite cluster by p_f . Then

$$p = p_f + p_\infty \quad p > p_c \quad (1.3)$$

$$p = p_f \quad p < p_c. \quad (1.4)$$

† In general, the observations of this section apply, *mutatis mutandis*, to bond mixtures; we shall not restate every result for bond mixtures.

The *percolation probability* is defined as the probability that a black site belongs to the infinite cluster:

$$P(p) = p_\infty/p = 1 - p_t/p. \tag{1.5}$$

The method proposed by Domb (1959) for the study of the high density region rests on the observation that the relation (1.2) can be made universally valid by simply writing:

$$p_t = \sum_s \langle n_s \rangle \quad 0 \leq p \leq 1. \tag{1.6}$$

Since each $\langle n_s \rangle$ is positive and $p_t < 1$, the infinite summation on the right-hand side is convergent.

In the low density region, the natural arrangement of the environmental data is the site grouping or p grouping (1.1). In the high density region the natural arrangement is a (site) perimeter grouping or q grouping:

$$K(p, q) = \sum_s \xi_s(p) q^s. \tag{1.7}$$

We notice a formal analogy between these two data groupings and the two data groupings that arise in the Ising model of a ferromagnet (Sykes *et al* 1965, 1973 a,b,c,d,e, 1975 a,b,c, to be referred to as I* to IX*): the p grouping polynomials correspond to the μ grouping or ordering of the data by the number of *overturned spins* regarded as *black sites* (and denoted by $L(z)$ in II*); the q grouping polynomials correspond to the z grouping or ordering of the data by the number of energy linkages between overturned spins and ordered spins (and denoted by $\psi(\mu)$ in II*). The second analogy is not exact because the Ising perimeter (the power of z) and the site perimeter (the power of q) are not identical, but we have found the analogy a useful one and made it the basis of our treatment.

The specification of clusters contributing to successive p grouped polynomials (1.1) is a practically convenient one: the number of sites; the specification of clusters contributing to successive q grouped polynomials (1.7) is much less convenient: the site perimeter.

To derive q grouped polynomials we have modified many of the graph theoretic methods developed earlier for the Ising problem and described in I*-IX* (especially IV* and VIII*). The optimum method in each case is dictated by the structure of the lattice studied. In §§ 2 and 3 we describe the methods we have used for the site and bond problem on the triangular lattice as these examples illustrate the general nature of the problems encountered. To obtain a useful amount of data for any lattice it is usually necessary to make a detailed configurational study; for this purpose we have drawn extensively on data collected for earlier studies of the Ising model.

The q grouped polynomials (1.7) are the source of high density expansions in powers of q which are obtained by making the substitution $p = 1 - q$. For example, on the triangular lattice:

$$K(p, q) = pq^6 + 3p^2q^8 + 2p^3q^9 + \dots \tag{1.8}$$

and using (1.6) and substituting after the formal differentiation:

$$p_t = p \partial K / \partial p = q^6 - q^7 + 6q^8 - 6q^9 + \dots \tag{1.9}$$

and on substitution in (1.5) the percolation probability is

$$P(p) = 1 - q^6 - 6q^8 + O(q^{10}) \dots \tag{1.10}$$

At high densities, the mean size of *finite* clusters, defined as the mean number of black sites connected to any black site that is not in the infinite cluster, is given by a generalization of (2.10) of I to be

$$S(p) = \frac{1}{p_t} \sum_s s^2 \langle n_s \rangle. \quad (1.11)$$

We give the expansions for $P(p)$ and $S(p)$ we have derived for the more usual two-dimensional lattices in the appendix. The analysis of these data is given in a companion paper (Sykes *et al* 1976).

2. Site problem for the triangular lattice

By regrouping the perimeter polynomials D_s through D_{14} (given in the appendix of I) we obtain the expansion of the key distribution function $K(p, q)$ as a q grouping through ξ_{16} :

$$\begin{aligned} K(p, q) &= \sum_s \xi_s(p) q^s \\ &= (p)q^6 + (3p^2)q^8 + (2p^3)q^9 + (9p^3 + 3p^4)q^{10} + (12p^4 + 6p^5)q^{11} \\ &\quad + (29p^4 + 21p^5 + 14p^6 + p^7)q^{12} + (66p^5 + 43p^6 + 30p^7 + 6p^8)q^{13} \\ &\quad + (93p^5 + 153p^6 + 111p^7 + 69p^8 + 27p^9 + 3p^{10})q^{14} \\ &\quad + (298p^6 + 366p^7 + 291p^8 + 166p^9 + 86p^{10} + 24p^{11} + 2p^{12})q^{15} \\ &\quad + (306p^6 + 840p^7 + 957p^8 + 803p^9 + 492p^{10} + 255p^{11} + 117p^{12} + 27p^{13} \\ &\quad + 3p^{14})q^{16} + \dots \end{aligned} \quad (2.1)$$

It is to be noticed that the only contributions the polynomials D_{12}, D_{13}, D_{14} make to the last coefficient ξ_{16} in (2.1) correspond to a very few clusters of 12, 13 and 14 sites with site perimeter as low as 16; thus only a very small fraction of the summary of the environmental situation provided by the D_s is made use of at first in the regrouping. This inefficient use of p grouped polynomials in the derivation of q grouped polynomials is closely analogous to that which occurs in forming the z grouped Ising polynomials from the corresponding μ grouped polynomials. For the Ising model, the μ grouping is essentially an area grouping, the area being measured by the number of overturned spins (the power of μ) and the energy of a cluster of n overturned spins cannot exceed $3n$; the length of the μ grouped polynomials therefore increases at most linearly with n . In contrast the z grouping is an energy grouping and the area of a configuration with m energy linkages (the power of z) increases as m^2 ; the length of the z grouped polynomials increases quadratically. Likewise in the present context, the site perimeter of a cluster of n sites cannot exceed $2n + 4$ and the growth of the p grouped polynomials is therefore at most linear with n . In contrast the site area of a cluster of fixed site perimeter m increases as m^2 ; the length of the q grouped polynomials increases quadratically.

To make the analogy more specific, we contrast the two polynomials

$$\xi_{12} = 29p^4 + 21p^5 + 14p^6 + p^7 \quad (2.2)$$

$$\psi_9 = 19\frac{1}{3}\mu^3 + 5\mu^4 + 21\mu^5 + 14\mu^6 + \mu^7. \quad (2.3)$$

In (2.3) ψ_9 is the corresponding z grouped polynomial for the triangular lattice taken from IV*. The coefficients of the higher powers of p and μ are seen to be identical; if we delete from ψ_9 contributions from clusters with more than one component and substitute for (2.3) the *connected* z grouping

$$\psi_9^c = 29\mu^4 + 21\mu^5 + 14\mu^6 + \mu^7 \quad (2.4)$$

the identity is complete. However the next polynomial

$$\psi_{10}^c = 66\mu^5 + 42\mu^6 + 30\mu^7 + 6\mu^8 \quad (2.5)$$

is not identical with

$$\xi_{13} = 66p^5 + 43p^6 + 30p^7 + 6p^8 \quad (2.6)$$

but differs only in the coefficient of p^6 . The source of small discrepancies can be explained on the basis of the graph theoretic description we have given of the ψ polynomials in VIII*. The higher powers of μ are there shown to correspond to connected and essentially convex clusters. The highest power of μ always corresponds to an absolutely convex cluster. For this convex region (characterized by near maximum powers of μ and defined more precisely in VIII*) there exists a simple relation between the site perimeter (σ) and the Ising perimeter ($\omega = \text{power of } z^2$). From theorem (3.3) of VIII*:

$$\sigma = \omega + 3 \quad (2.7)$$

and this relation can be used to transform the result (2.5) of VIII* for the general pattern of the convex end of the ψ polynomials into the general pattern for the convex end of ξ polynomials:

$$\begin{aligned} \xi_{6m} &= p^{3m^2-3m+1}(1+14p^{-1}+87p^{-2}+\dots) \\ \xi_{6m+1} &= p^{3m^2-2m}(6+42p^{-1}+216p^{-2}+\dots) \\ \xi_{6m+2} &= p^{3m^2-m}(3+27p^{-1}+147p^{-2}+\dots) \\ \xi_{6m+3} &= p^{3m^2}(2+24p^{-1}+128p^{-2}+\dots) \\ \xi_{6m+4} &= p^{3m^2+m}(3+27p^{-1}+147p^{-2}+\dots) \\ \xi_{6m+5} &= p^{3m^2+2m}(6+42p^{-1}+216p^{-2}+\dots). \end{aligned} \quad (2.8)$$

Following closely the ideas of VIII*, we define an (essentially) convex cluster as one for which (2.7) holds. The more general result

$$\sigma \leq \omega + 3 \quad (2.9)$$

enables the *concavity* of a cluster to be characterized by writing

$$\sigma = \omega + 3 - \delta. \quad (2.10)$$

We adopt the value of δ as a measure of the concavity and describe a cluster as δ -concave. With this convention, clusters that contribute to ξ_σ divide into two classes:

- (a) convex clusters in the Ising polynomial $\psi_{\sigma-3}^c$;
- (b) δ concave clusters in the Ising polynomials $\psi_{\sigma-3+\delta}^c$ for all $\delta > 0$.

The enumeration of these two classes corresponds to two operations: for (a) the deletion of concave terms from $\psi_{\sigma-3}^c$; for (b) the selection of all the required concave terms in all $\psi_{\sigma-3+\delta}^c$. The second task involves an inspection of the ψ^c in ascending order

and this is inconvenient as the amount of configurational information increases rapidly with each new ψ^c while the amount of significant information in the present context becomes very small. We therefore recast the problem in such a way that the required information can be found from an inspection of all ψ_s^c with $s \leq \sigma - 3$. The method is based on a classification of the concavities that occur first in practice.

As the power of p (or μ) declines from the absolutely convex end we can define a *first zone of mild concavity* where departures from concavity correspond to single holes and faults of the type illustrated in figure 1. If the objective is ξ_σ , clusters with a concavity of

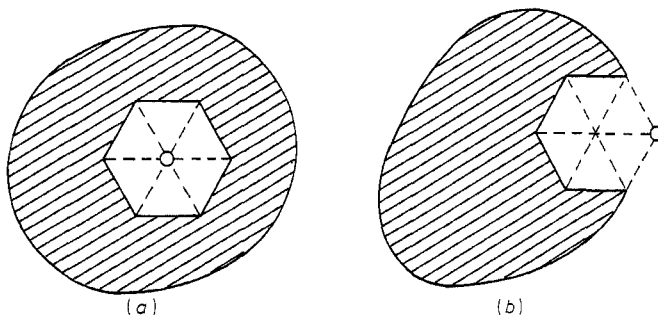


Figure 1. Concavities that characterize the first zone of (mild) concavity in ψ_ω^c . (a) Simple hole of unit area (2-concave). (b) An f fault (1-concave). \circ , Rogue site or spin.

either type must be deleted from $\psi_{\sigma-3}^c$ and clusters with a concavity of type (a) selected from $\psi_{\sigma-1}^c$, those with a concavity of type (b) from $\psi_{\sigma-2}^c$. The failure of the equality in (2.7) is due to the presence of a perimeter site (or spin) marked in the figure with an open circle and which we call a *rogue site*. If, for any cluster with a concavity of type (a), the rogue site is removed by adding an extra site to the cluster in its place, the new cluster so formed must lie in $\psi_{\omega-3}^c$ (or $\psi_{\sigma-4}^c$): that is one *below* rather than two *above* originally. In other words the holes that occur in $\psi_{\sigma-1}^c$ can be regarded as lying in $\psi_{\sigma-4}^c$ and found by an examination of this. The task is further simplified by the fact that the presence of the hole (a) implies that the new in-filled cluster is all the more likely to be convex; the number of possible holes that lie in $\psi_{\sigma-4}^c$ can then be determined by using the formula for the number of internal points given in VIII* (equation (2.4)).

If an f fault (b) occurs in ψ_ω^c , then, on adding an extra site to the cluster to suppress the rogue site, a hole of type (a) will result (in $\psi_{\omega+1}^c$) and a new rogue site will be created; on in-filling again we obtain a cluster in $\psi_{\omega-2}^c$. Since for ξ_σ we require f faults in $\psi_{\sigma-2}^c$ we can instead examine $\psi_{\sigma-4}^c$ for external obtuse angles in the contour.

In summary, the convex terms required for ξ_σ lie in $\psi_{\sigma-3}^c$; the details of clusters that constitute the first zone of mild concavity and contribute to ξ_σ can be obtained by an analysis of $\psi_{\sigma-4}^c$.

A second zone of somewhat more severe concavity we define by the presence of the concavities illustrated in figure 2. (This schematic classification describes the faults that occur in the order they first appear as we move down ψ_ω^c ; the resultant hierarchy of faults does not correspond to an ordering by the parameter δ .) By an extension of the arguments already used for the first zone and by adding sites to the cluster to suppress the rogue sites and any rogue sites thereby created, it can be shown that clusters with any of the three types of concavity (c), (d) and (e) required to complete ξ_σ can all be found by an examination of $\psi_{\sigma-5}^c$.

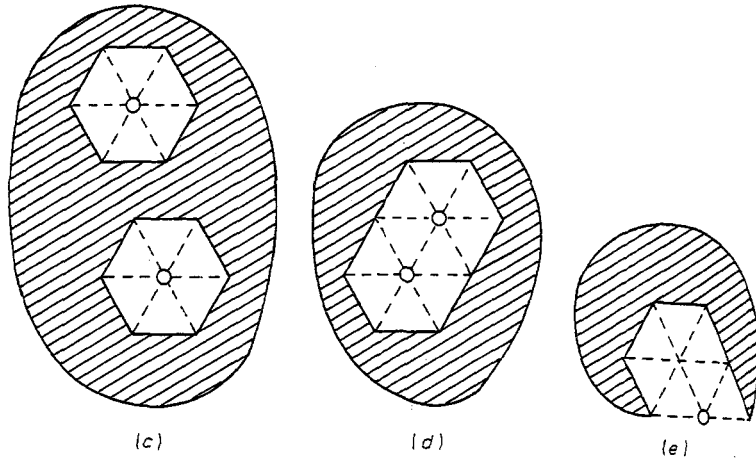


Figure 2. Concavities that characterize the second zone of (stronger) concavity in ψ_{σ}^c . (c) Two holes of unit area (4-concave). (d) Hole of area 2 (3-concave). (e) f^* fault (1-concave). \circ , Rogue site or spin.

Concavities that characterize successively higher zones may be reduced along similar lines; the work becomes more intricate but involves no new difficulty in principle. Using these techniques, we have obtained the polynomials

$$\begin{aligned}
 \xi_{17} &= 1290p^7 + 2349p^8 + 2592p^9 + 2157p^{10} + 1542p^{11} + 801p^{12} + 426p^{13} + 168p^{14} \\
 &\quad + 42p^{15} + 6p^{16} \\
 \xi_{18} &= 1014p^7 + 4299p^8 + 6734p^9 + 7484p^{10} + 6111p^{11} + 4771p^{12} + 2858p^{13} + 1524p^{14} \\
 &\quad + 759p^{15} + 290p^{16} + 87p^{17} + 14p^{18} + p^{19} \\
 \xi_{19} &= 5310p^8 + 13\,634p^9 + 19\,416p^{10} + 21\,810p^{11} + 18\,608p^{12} + 14\,442p^{13} + 10\,029p^{14} \\
 &\quad + 5774p^{15} + 3147p^{16} + 1458p^{17} + 613p^{18} + 198p^{19} + 42p^{20} + 6p^{21} \\
 \xi_{20} &= 3408p^8 + 20\,469p^9 + 42\,963p^{10} + 58\,164p^{11} + 63\,804p^{12} + 58\,902p^{13} + 46\,119p^{14} \\
 &\quad + 34\,164p^{15} + 21\,924p^{16} + 13\,074p^{17} + 6864p^{18} + 3273p^{19} + 1449p^{20} \\
 &\quad + 507p^{21} + 147p^{22} + 27p^{23} + 3p^{24}. \tag{2.11}
 \end{aligned}$$

To extend the data we have modified the computer generation of perimeter polynomials used in I to obtain the polynomials that correspond to clusters of a given perimeter. It is straightforward to arrange for an enumeration to reject clusters whose site perimeter exceeds some number σ and to continue with an increasing number of sites to exhaustion; unfortunately this procedure does not generate all the clusters in the q grouping (ξ_{σ}) since the addition of a site to a cluster may in certain circumstances reduce the perimeter.

To complete ξ_{σ} by successive addition of sites it is therefore necessary to generate clusters with perimeters in excess of σ and this results in an appreciable loss of efficiency. The theory and classification of the situations illustrated in figure 3 is closely linked with the theory of concavities we have already described. By making a specialized study, we have combined the two techniques and added two further

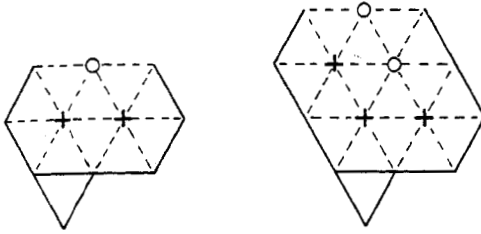


Figure 3. Examples of clusters for which the addition of extra sites (O) reduces the site perimeter when using the computer cluster generation technique of Martin (1974). (The addition of sites marked (+) produces clusters generated in a different sequence under the algorithm on which the technique is based.)

polynomials:

$$\begin{aligned} \xi_{21} = & 21\,372p^9 + 72\,256p^{10} + 133\,380p^{11} + 179\,186p^{12} + 192\,626p^{13} + 185\,220p^{14} \\ & + 153\,406p^{15} + 117\,632p^{16} + 81\,606p^{17} + 52\,419p^{18} + 31\,288p^{19} \\ & + 16\,461p^{20} + 8292p^{21} + 3685p^{22} + 1488p^{23} + 496p^{24} + 128p^{25} \\ & + 24p^{26} + 2p^{27} \end{aligned} \quad (2.12)$$

$$\begin{aligned} \xi_{22} = & 11\,562p^9 + 93\,747p^{10} + 247\,974p^{11} + 417\,270p^{12} + 554\,523p^{13} + 605\,766p^{14} \\ & + 589\,094p^{15} + 514\,503p^{16} + 411\,546p^{17} + 305\,656p^{18} + 206\,904p^{19} \\ & + 134\,598p^{20} + 79\,309p^{21} + 44\,010p^{22} + 22\,419p^{23} + 10\,574p^{24} \\ & + 4614p^{25} + 1743p^{26} + 579p^{27} + 147p^{28} + 27p^{29} + 3p^{30}. \end{aligned}$$

From the polynomials through ξ_{22} summarized in (2.1), (2.11) and (2.12) the expansions of $P(p)$ and $S(p)$ in powers of q given in the appendix follow by the substitutions described in § 1.

To obtain corresponding expansions for the simple quadratic and honeycomb lattices we have made detailed configurational studies along essentially similar lines.

3. Bond problem for the triangular lattice

For the bond problem on the triangular lattice, we are again confronted with the situation that the p grouped polynomials require supplementation if a useful number of q grouped polynomials are to be derived. However for the bond problem the characterization of the clusters required can be made much more systematic and the relationship with the Ising z grouping is capable of explicit statement.

We first observe that bond clusters may be divided into two mutually disjoint classes (illustrated in figure 4). (1) Weak embeddings which are also strong embeddings (conveniently called saturated clusters). (2) Weak embeddings which are not strong embeddings (conveniently called unsaturated clusters).

We already have a complete listing of the saturated clusters in the connected z grouping since the power of z is identical with the *bond* perimeter; further any unsaturated cluster can be formed by deletion of bonds from some saturated cluster

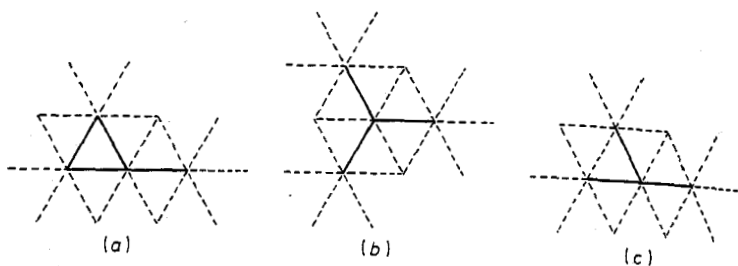


Figure 4. Examples of bond clusters on the triangular lattice. (a), (b) saturated clusters, (c) unsaturated cluster.

with a lower power of z . This is readily seen by taking as example the terms in ψ_8^c of which there are only two, illustrated in figure 5. Each corresponds to a saturated cluster of bond perimeter 16: the first with bond area 7, the second with bond area 4. (The bond areas (r) are related to the spin areas (s) by the linkage rule: $\omega = 3s - r$). By removing bonds in every way that leaves the sites at least simply connected, we can enumerate all the unsaturated clusters associated with the site embeddings defined by the vertices of (1) and (2). Each bond removed decreases the bond area by unity and increases the bond perimeter by unity. By inspection the results for the example are readily found to be:

$$(1) \quad 6(p^7 q^{16})[1 + 7(q/p) + 19(q/p)^2 + 21(q/p)^3]. \quad (3.1)$$

$$(2) \quad 12(p^4 q^{16})[1 + 3(q/p)]. \quad (3.2)$$

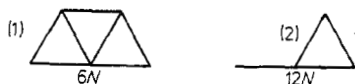


Figure 5. The connected terms in $\psi_8^c(\mu)$ for the triangular lattice.

The technique is perfectly general. Thus if G is any graph of s spins strongly embedded in a lattice L of any dimension with corresponding lattice constant $[G; L]$ and lying in ψ_ω^c we will obtain a contribution of the form

$$[G; L] p^{3s-\omega} q^{2\omega} [1 + Y_1(q/p) + Y_2(q/p)^2 + \dots] \quad (3.3)$$

where the Y are combinatorial factors (conveniently called *yield factors*). A variety of methods can be developed for calculating yield factors and by an analysis of the strong embeddings on the triangular lattice that contribute to the ψ^c through ψ_{15}^c we have obtained the ξ through ξ_{30} .

The yield factors are independent of the lattice and the present method can be used without modification for any lattice (including three-dimensional lattices) for which the connected z grouping is known in detail. We have used it to derive the expansions for the simple quadratic and honeycomb bond mixtures given in the appendix.

Direct enumeration of the ξ can be achieved along the same general lines described for the site problem; however the efficiency is much reduced because examples of bond

perimeters falling on addition of an extra bond are more numerous. We have however been able to use the method as a check on the polynomials obtained by the yield factor method.

Acknowledgment

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Appendix

Coefficients for expansion of $P(p) = 1 + q^{\theta} \sum a_r q^{r-1}$

	Triangular site problem	Square site problem	Honeycomb site problem	Triangular bond problem	Square bond problem	Honeycomb bond problem
θ	6	4	3	10	6	4
a_1	-1	-1	-1	-1	-1	-1
a_2	0	0	-3	0	0	-4
a_3	-6	-4	-6	-2	-8	-12
a_4	0	-8	-28	0	+6	-34
a_5	-27	-23	-36	-9	-48	-76
a_6	+6	-28	-360	+6	+66	-212
a_7	-111	-186	-203	-24	-279	-538
a_8	+72	+48	-4362	+20	+508	-1192
a_9	-534	-1301	+4626	-82	-1695	-3961
a_{10}	+638	+1412	-54 347	+100	+3788	-7824
a_{11}	-2868	-12 292	+105 309	-243	-11 495	-24 919
a_{12}	+5004	+30 384		+326	+28 396	-67 230
a_{13}	-17 408	-142 441		-781	-79 820	-138 908
a_{14}	+36 162			+1182	+200 686	
a_{15}	-106 035			-2559		
a_{16}	+233 190			+4496		
a_{17}	-626 439			-9231		
a_{18}				+14 946		
a_{19}				-27 324		
a_{20}				+48 360		
a_{21}				-97 099		

Coefficients for expansion of $S(p) = 1 + \sum b_r q^r$

	Triangular site problem	Square site problem	Honeycomb site problem	Triangular bond problem	Square bond problem	Honeycomb bond problem
b_1	0	0	0	0	0	+4
b_2	+6	+4	+3	+4	+12	+18
b_3	+6	+20	+6	-4	-12	+42
b_4	+30	+76	+87	+18	+74	+106
b_5	+24	+100	-54	-18	-104	+614
b_6	+138	+764	+2484	+48	+480	+1038
b_7	-24	-196	-3996	-56	-802	+4102
b_8	+1050	+6480	+58 818	+198	+3060	+17 790

Coefficients for expansion of $S(p) = 1 + \sum b_i q^i$ —continued.

	Triangular site problem	Square site problem	Honeycomb site problem	Triangular bond problem	Square bond problem	Honeycomb bond problem
b_9	-918	-9316	-186 783	-260	-6964	+20 852
b_{10}	+7128	+91 524	+1 277 136	+522	+25 278	+183 606
b_{11}	-12 366	-240 248	-5 173 485	-888	-62 968	+285 510
b_{12}	+53 418	+1 259 944		+2386	+184 996	+1 138 548
b_{13}	-104 004			-3124	-432 864	
b_{14}	+339 750			+5446		
b_{15}	-692 016			-11 292		
b_{16}	+2 090 490			+29 068		
b_{17}				-46 924		
b_{18}				+78 896		
b_{19}				-137 014		
b_{20}				+297 280		

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