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Derivation of series expansions for a study of percolation processes

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Abstract. The derivation of series expansions for a study of percolation processes for both site and bond mixtures is reviewed. For the bond problem, low density expansions for the mean size of clusters on the simple cubic and body-centred cubic lattices are given through p^{14} . High density expansions for the mean number and size of finite clusters and the percolation probability are given for the simple cubic through q^{41} and for the body-centred cubic through q^{61} .

1. Introduction

In this paper we review the derivation of series expansions that are used to study percolation processes in site and bond mixtures. We assume a general familiarity with the problem; there are reviews by Shante and Kirkpatrick (1971), Essam (1971, 1972, 1980), Kirkpatrick (1973), de Gennes (1976), Welsh (1977), Wu (1978), Stauffer (1979) and Domb (1983). Sykes and Glen (1976) and Sykes *et al* (1976a, b, c) (hereafter referred to as I*-IV* respectively) derived series expansions for the more usual crystal lattices. They used the technique of perimeter polynomials introduced by Domb (1959); for an elementary introduction reference should be made to I*, § 2. Recently, Sykes (1986a, b, c, d) and Sykes and Wilkinson (1986) (hereafter referred to as I**-V** respectively) have used partial generating functions and exploited sublattice symmetry to provide new data for bond perimeter polynomials and the expansion of the mean number of clusters in site mixtures for the simple cubic and body-centred cubic lattices. We use these new data to derive extended series expansions for the mean size of finite clusters at high and low densities and also for the percolation probability. We begin by treating both site and bond mixtures together. The starting point of Domb's treatment is to consider the expectation of clusters of a certain size. For the site problem a natural measure of the size of a cluster is the number of its sites; in early work on the bond problem the measure was usually taken to be the number of its bonds. Essam and Sykes (1966) noticed that a simplification often resulted if, for bond mixtures, the bonds were primarily considered as connections between sites. They introduced the *null-cluster convention* under which an isolated site (that is, one with no incident bonds) is also treated as a cluster. Later, Essam (1971) in his studies of the pair connectedness developed this approach further and measured the size of a bond cluster by the number of its sites.

We allow for both these conventions by generalising the method used in I*-IV* and denoting the expectation (or mean number) per lattice site of clusters with s sites and b bonds by $\langle n_{s,b} \rangle$. At low density the principal moments of interest are

$$\begin{aligned} m_0 &= \sum \langle n_{s,b} \rangle & m_{ss} &= \sum s^2 \langle n_{s,b} \rangle \\ m_s &= \sum s \langle n_{s,b} \rangle & m_{sb} &= \sum sb \langle n_{s,b} \rangle \\ m_b &= \sum b \langle n_{s,b} \rangle & m_{bb} &= \sum b^2 \langle n_{s,b} \rangle \end{aligned} \quad (1.1)$$

where the summations are taken over all s and b . At low densities all the above moments can be expanded in powers of p . For site problems p denotes the probability that a site is occupied; for bond problems p denotes the probability that a bond is occupied.

For the zeroth moment we shall write

$$m_0 = K(p) = \sum_{r=0}^{\infty} k_r p^r. \quad (1.2)$$

The coefficients in this expansion have been studied in detail by Essam and Sykes (1966) for both site and bond mixtures. Notice that (1.2) determines two different functions and two distinct sets of coefficients; one for site mixtures, the other for bond mixtures. No confusion should arise since we shall treat the two problems separately later.

At low densities the first-order moments all reduce to finite polynomials in p :

$$m_s = \begin{cases} p & \text{(site problem)} \\ 1 & \text{(bond problem)} \end{cases} \quad (1.3)$$

$$m_b = \begin{cases} \frac{1}{2} z p^2 & \text{(site problem)} \\ \frac{1}{2} z p & \text{(bond problem)} \end{cases} \quad (1.4)$$

where in (1.4) z denotes the coordination number of the lattice. (We follow the usual convention of working per lattice site for both site and *bond* mixtures.)

The *mean size* of clusters at low densities can be defined in various ways and is usually related to the expansion of one of the three moments:

$$m_{ss} = \sum a_r^{ss} p^r \quad (1.5)$$

$$m_{sb} = \sum a_r^{sb} p^r \quad (1.6)$$

$$m_{bb} = \sum a_r^{bb} p^r. \quad (1.7)$$

The first moment (1.5) is the one usually studied for site mixtures; for these the mean size is defined to be the expected number of sites connected to an occupied site:

$$S_{ss}(p) = m_{ss}/p. \quad (1.8)$$

For bond mixtures the mean size studied in I*-IV* is defined as the expected number of bonds connected to an occupied bond:

$$S_{bb}(p) = m_{bb}/\frac{1}{2}zp. \quad (1.9)$$

We shall derive expansions for the mean size by sites; for bond problems this function is identical with m_{ss} of (1.5), since now all the sites are treated as occupied and $m_s = 1$.

The cross-moment (1.6) can be used to expand the expected number of bonds connected to an occupied site or, alternatively, the expected number of sites connected to an occupied bond. The former is the simpler concept and for bond mixtures the corresponding mean size is identical with m_{sb} .

To derive expansions for the moments (1.1) we follow III** and generalise the concept of perimeter polynomials of I*-IV* by writing

$$\langle n_{s,b} \rangle = D_{s,b}(q)p^s \quad (\text{site problem}) \quad (1.10)$$

$$= D_{s,b}(q)p^b \quad (\text{bond problem}) \quad (1.11)$$

where $q = 1 - p$ and the polynomial on the right-hand side summarises the average environmental situation for all clusters with s sites and b bonds. Notice that (1.10) and (1.11) define different functions; the clusters summarised in (1.10) are strong embeddings, those in (1.11) are weak embeddings.

We shall not develop the general theory of the polynomials $D_{s,b}$ for the site problem since we have made no application of it. Although bond problems can be treated as site problems on a suitably defined covering lattice, there exists no simple equivalence between sites and bonds; if a cluster has s sites it must have $(s - 1)$ or *more* bonds; if a cluster has b bonds it must have $(b + 1)$ or *fewer* sites. As we show below, when we introduce the concept of a balance table, this last condition can be usefully exploited for bond problems.

2. Site problem: perimeter polynomials and balance tables

In this section we consider the site problem separately. Series expansions for the mean size of clusters, defined by (1.8), are given in I*-IV*; perimeter polynomials D_s (see below) are first obtained for all clusters through some number, N , of sites; direct expansion then yields the expansion of m_{ss} through p^N . Further coefficients can then be added by the procedures we now describe; for an elementary introduction reference should be made to I*.

For the purpose of this section we particularise to the *site* problem and denote the expectation of a cluster of size s (by sites) by $\langle n_s \rangle$; we follow I* and write

$$\langle n_s \rangle = D_s(q)p^s \quad (2.1)$$

where D_s is now the simple site perimeter polynomial which corresponds to the contraction of the more general $D_{s,b}$ defined by (1.10):

$$D_s(q) = \sum_b D_{s,b}(q). \quad (2.2)$$

From these the mean number of clusters can be expanded in an ascending array:

$$\begin{aligned} \langle n_1 \rangle &= \sum_n \alpha_{1,n} p^n \\ \langle n_2 \rangle &= \sum_n \alpha_{2,n} p^n \\ &\dots \quad \dots \end{aligned} \quad (2.3)$$

At low densities we have the formal relation of (1.3) from which it follows that

$$\sum_{i=1}^N i \alpha_{i,N} = 0 \quad \text{if } N > 1. \quad (2.4)$$

Because of this condition the set of contributions $\alpha_{1,N}, \alpha_{2,N}, \dots, \alpha_{N,N}$ is conveniently called the *Nth balance table*. We denote the total number of connected clusters of n sites by A_n and note the trivial relation:

$$A_N = \alpha_{N,N}. \quad (2.5)$$

If the perimeter polynomials are known through D_N , then, by application of (2.4) to the $(N + 1)$ th balance table, $\alpha_{N+1,N+1}$ and therefore A_{N+1} , k_{N+1} and a_{N+1}^{ss} are determined.

In many cases the low density expansion for the mean number, (1.2), can be derived independently by special methods (Essam and Sykes 1966, III*). Then, still assuming that N perimeter polynomials are available, we can first evaluate the quantities

$$\sum_{i=1}^N \alpha_{i,N+2} = \eta_0 \quad \sum_{i=1}^N i\alpha_{i,N+2} = \eta_1 \quad \sum_{i=1}^N i^2\alpha_{i,N+2} = \eta_2 \quad (2.6)$$

and then by application of (2.4) to the $(N + 2)$ th balance table, together with the relation

$$\sum_{i=1}^{N+2} \alpha_{i,N+2} = k_{N+2} \quad (2.7)$$

we can determine the last two elements of the balance table and the next mean size coefficient. Explicitly:

$$\begin{aligned} \alpha_{N+1,N+2} &= \eta_1 + (N + 2)(k_{N+2} - \eta_0) \\ \alpha_{N+2,N+2} &= -\eta_1 - (N + 1)(k_{N+2} - \eta_0) \\ a_{N+2}^{ss} &= \eta_2 - (2N + 3)\eta_1 - (N + 1)(N + 2)(k_{N+2} - \eta_0). \end{aligned} \quad (2.8)$$

In summary: a knowledge of N perimeter polynomials, together with k_{N+2} , determines A_{N+2} and a_{N+2}^{ss} . If A_{N+2} is independently known, it serves as a check on the data; alternatively if A_{N+2} is known and k_{N+2} is not known we may use the relations

$$\begin{aligned} a_{N+2}^{ss} &= \eta_2 - (N + 1)\eta_1 + (N + 2)A_{N+2} \\ k_{N+2} &= \eta_0 - (\eta_1 + A_{N+2}) / (N + 1). \end{aligned} \quad (2.9)$$

If we further suppose that the mean number expansion is available through k_{N+3} and also that the total number of clusters A_{N+3} is known, then, by first evaluating

$$\sum_{i=1}^N \alpha_{i,N+3} = \zeta_0 \quad \sum_{i=1}^N i\alpha_{i,N+3} = \zeta_1 \quad \sum_{i=1}^N i^2\alpha_{i,N+3} = \zeta_2 \quad (2.10)$$

we can exploit the relations

$$\begin{aligned} \alpha_{N+1,N+3} &= \zeta_1 - (N + 2)(\zeta_0 - k_{N+3}) + A_{N+3} \\ \alpha_{N+2,N+3} &= -\zeta_1 + (N + 1)(\zeta_0 - k_{N+3}) - 2A_{N+3} \\ \alpha_{N+3,N+3} &= A_{N+3} \end{aligned} \quad (2.11)$$

to add a further coefficient to the second moment. Explicitly:

$$a_{N+3}^{ss} = \zeta_2 - (2N + 3)\zeta_1 + (N + 1)(N + 2)(\zeta_0 - k_{N+3}) + 2A_{N+3}. \quad (2.12)$$

3. Site problem: specific applications

The extent to which the results of the previous section can be usefully applied varies from lattice to lattice. In two dimensions, because of the special methods (Essam and Sykes 1966) that can be used to derive the mean number expansion (1.2), series of sufficient length are usually available to enable the results (2.9) to be exploited. The expansions given by Sykes and Glen (I*) for the triangular, simple quadratic and

honeycomb lattices were all extended in this way. More recently Margolina *et al* (1983) have obtained a further perimeter polynomial (D_{15}) for the triangular lattice; using the value $k_{17} = -1194$ extracted from the data of Sykes *et al* (III*), they obtained the value $A_{17} = 12\,866\,153\,748$. Using their data and (2.9) gives an extra coefficient for the mean size defined by (1.5) and (1.8):

$$a_{17}^{ss} = 2383\,596 \quad (\text{triangular lattice}). \quad (3.1)$$

To exploit (2.12) when N perimeter polynomials are available requires the number of connected clusters with $(N+2)$ sites; Sykes and Glen (I*) concluded that direct enumeration of the total number of clusters, although faster than the direct enumeration of perimeter polynomials, was not fast enough to make this procedure worthwhile; it would in general be more efficient to derive the next perimeter polynomial instead. Their conclusion still holds but, in one instance, because of the very large amount of computer time used by Redelmeier (1981) the extra total is already available; using his $A_{20} = 22\,964\,779\,660$ for the simple quadratic lattice and the value $k_{20} = 9894$, obtained by the methods of Essam and Sykes (1966) and III*, equation (2.12) yields the extra coefficient:

$$a_{20}^{ss} = -702\,592 \quad (\text{simple quadratic lattice}). \quad (3.2)$$

That this coefficient would be *negative* was predicted by Sykes *et al* (1973).

In three dimensions the methods available for the independent derivation of the mean number expansion are more restricted. The theory of strong K weights (Essam and Sykes 1966) requires an exhaustive listing of strong embeddings of star graphs which is quite difficult to provide.

For the simple cubic lattice we have used the mutually consistent results $k_{13} = -13\,788$ and $A_{13} = 3322\,769\,321$ of V** to derive

$$a_{13}^{ss} = 10\,375\,770 \quad (\text{simple cubic lattice}). \quad (3.3)$$

This result corrects a small error in the value given by Gaunt *et al* (1976).

Direct expansion of $K(p)$ for the body-centred cubic lattice is more difficult. Sykes *et al* (IV*) give the perimeter polynomials through D_{10} ; using the data of IV* and (2.12) we obtain the new results

$$\begin{aligned} k_{12} &= 86\,432 & k_{13} &= -433\,603 \\ a_{12}^{ss} &= 40\,355\,260 & a_{13}^{ss} &= 203\,033\,932 \end{aligned} \quad (\text{body-centred cubic lattice}). \quad (3.4)$$

The derivation of high density expansions for site problems is not advanced by the above observations; all the available expansions are summarised by Gaunt and Sykes (1983).

4. Bond problem: perimeter polynomials and balance tables

In this section we treat the bond problem separately. It is possible to treat the bond problem as a site problem on the covering lattice; simple bond perimeter polynomials can be defined and extra coefficients then added by the methods of § 2; however, extra information can be obtained by a direct study of the more general perimeter polynomials (1.11).

Suppose the perimeter polynomials $D_{s,b}$ of (1.11) are known for all $s \leq N$; then there can be no clusters with fewer than N bonds whose perimeter is not known. Consequently the $(N - 1)$ th balance table, which we now take to be all the contributions to the coefficient of p^{N-1} from all the $\langle n_{s,b} \rangle$ when the right-hand side of (1.11) is expanded for each, is complete. Writing as a generalisation of (2.3)

$$\langle n_{s,b} \rangle = \sum_n \Delta_{s,b,n} p^n \tag{4.1}$$

the partial contribution to the moments from the incomplete N th balance table can be obtained as

$$\begin{aligned} \sum \Delta_{s,b,N} &= \eta_0 & \sum s \Delta_{s,b,N} &= \eta_s & \sum b \Delta_{s,b,N} &= \eta_b \\ \sum s^2 \Delta_{s,b,N} &= \eta_{ss} & \sum sb \Delta_{s,b,N} &= \eta_{sb} & \sum b^2 \Delta_{s,b,N} &= \eta_{bb} \end{aligned} \tag{4.2}$$

where the summations are taken over all s and b with $s \leq N$. We denote the number of connected clusters of s sites and b bonds by $B_{s,b}$ and note the trivial relation

$$B_{N,N-1} = \Delta_{N,N-1,N-1} \tag{4.3}$$

Now using (4.2) with either (1.3) or (1.4) we obtain $B_{N+1,N}$ and also

$$\begin{aligned} k_N &= \eta_0 + B_{N+1,N} \\ a_N^{ss} &= \eta_{ss} - (N + 1)\eta_s \\ a_N^{sb} &= \eta_{sb} - N\eta_s = \eta_{sb} - (N + 1)\eta_b \\ a_N^{bb} &= \eta_{bb} - N\eta_b. \end{aligned} \tag{4.4}$$

In most cases the mean number expansion (1.2) can be derived by independent methods (Essam and Sykes 1966). Then, still assuming that all the perimeter polynomials are known through $s \leq N$, the partial contributions to the $(N + 1)$ th balance table that corresponds to replacing N by $N + 1$ on every left-hand side of (4.2) *without* increasing the range of summation, and which we denote by $\zeta_0, \zeta_s, \zeta_b, \zeta_{ss}, \zeta_{sb}, \zeta_{bb}$ respectively, together with the value of k_{N+1} , determine

$$\begin{aligned} B_{N+2,N+1} &= (N + 1)\zeta_0 - \zeta_s - (N + 1)k_{N+1} \\ B_{N+1,N+1} &= -\zeta_0 + \zeta_s - \zeta_b + k_{N+1} \\ a_{N+1}^{ss} &= \zeta_{ss} + (N + 1)(N + 2)(\zeta_0 - k_{N+1}) - (2N + 3)\zeta_s \\ a_{N+1}^{sb} &= \zeta_{sb} + (N + 1)^2(\zeta_0 - k_{N+1}) - (N + 1)(\zeta_s + \zeta_b) \\ a_{N+1}^{bb} &= \zeta_{bb} + N(N + 1)(\zeta_0 - k_{N+1}) - (2N + 1)\zeta_b. \end{aligned} \tag{4.5}$$

In summary: a knowledge of the perimeter polynomials through $s \leq N$, together with k_{N+1} , determines the $(N + 1)$ th coefficient for all three moments and also the total numbers of clusters with $(N + 1)$ bonds of cyclomatic number 0 and 1 respectively. This last result is an especially useful one: the methods described in III** for the derivation of perimeter polynomials provide the general perimeter polynomials quite naturally as a site grouping; by using the above relations the total number of bond clusters through $(N + 1)$ can be obtained with details of their site content. This technique was used in II** to complete the values of $B_{13}(x)$ and $B_{14}(x)$ for the

body-centred cubic and again in V^{**} to complete the values of $B_{13}(x)$ and $B_{14}(x)$ for the simple cubic.

5. Bond problem: specific applications

The results (4.5) of the previous section, combined with the general perimeter polynomials $D_{s,b}$ grouped by sites obtained by the methods described in III^{**} for the body-centred cubic lattice and in V^{**} for the simple cubic lattice, enable the low density expansion for the three moments (1.5)-(1.7) to be obtained through the coefficient of p^{14} . We give these coefficients in table 1.

The general perimeter polynomials also enable a significant number of terms to be added to high density expansions. The expansion for the mean number of clusters, K_{BCC} , on the body-centred cubic lattice is given by Gaunt and Sykes (1983), appendix 1, through q^{47} . (If the null-cluster convention is adopted the term q^8 should be prefixed to their expansion.) By expanding the $D_1^*-D_{13}^*$ obtained in III^{**} and including some contributions from clusters with more than 13 sites we have added 14 further coefficients:

$$\begin{aligned}
 K_{BCC} = & q^8 + 4q^{14} - 4q^{15} + \dots + 1388\ 810q^{48} - 1301\ 132q^{49} \\
 & + 2048\ 224q^{50} - 3898\ 076q^{51} + 7880\ 628q^{52} \\
 & - 15\ 330\ 876q^{53} + 21\ 794\ 812q^{54} - 23\ 218\ 900q^{55} \\
 & + 29\ 208\ 826q^{56} - 51\ 146\ 912q^{57} + 95\ 338\ 772q^{58} \\
 & - 181\ 108\ 576q^{59} + 299\ 949\ 212q^{60} - 385\ 858\ 764q^{61} \\
 & + \dots
 \end{aligned}
 \tag{5.1}$$

Gaunt and Sykes (1983) also give the expansion for the bond percolation probability P_{BCC}^b , defined as the probability that a given occupied bond lies in the infinite cluster,

Table 1. Coefficients for second moment expansions at low densities (bond problem).

r	Body-centred cubic†			Simple cubic		
	a_r^{ss}	a_r^{sb}	a_r^{bb}	a_r^{ss}	a_r^{sb}	a_r^{bb}
1	8	8	4	6	6	3
2	56	56	56	30	30	30
3	392	392	392	150	150	150
4	2 504	2 552	2 600	690	702	714
5	16 232	16 520	16 808	3 246	3 294	3 342
6	99 152	101 888	104 648	14 250	14 622	14 994
7	621 608	636 920	652 616	64 770	66 210	67 686
8	3 698 942	3 816 656	3 936 416	277 734	286 074	294 522
9	22 752 088	23 396 648	24 062 048	1 239 322	1 271 490	1 304 682
10	132 890 344	137 475 328	142 163 312	5 222 538	5 392 710	5 566 038
11	808 503 496	833 161 984	858 717 856	23 053 710	23 703 378	24 376 170
12	4 652 182 268	4 821 607 024	4 995 332 464	95 780 740	99 078 330	102 447 990
13	28 147 030 544	29 042 197 232	29 972 440 432	420 269 004	432 707 748	445 619 106
14	159 780 956 360	165 846 265 328	172 075 348 544	1724 854 200	1786 662 060	1849 957 488

† The entry for a_{10}^{bb} corrects a small error in Gaunt *et al* (1976).

and to this we have likewise added a further 14 coefficients:

$$\begin{aligned}
 P_{\text{BCC}}^b = 1 - 2M_b/ zp = & 1 - q^{14} - 14q^{20} + \dots - 1253\ 651q^{48} \\
 & + 1633\ 854q^{49} - 3338\ 428q^{50} + 6150\ 082q^{51} \\
 & - 12\ 002\ 184q^{52} + 21\ 001\ 056q^{53} - 26\ 102\ 578q^{54} \\
 & + 29\ 661\ 750q^{55} - 49\ 806\ 320q^{56} + 93\ 109\ 946q^{57} \\
 & - 167\ 927\ 241q^{58} + 301\ 733\ 826q^{59} - 454\ 706\ 045q^{60} \\
 & + 565\ 744\ 398q^{61} + \dots
 \end{aligned} \tag{5.2}$$

In (5.2) M_b denotes the appropriate high density analogue of m_b for finite clusters. If the site-weighting convention is adopted it is more natural to study the corresponding site percolation probability P_{BCC}^s defined as the probability that a given site lies in the infinite cluster:

$$P_{\text{BCC}}^s = 1 - M_s \tag{5.3}$$

and we give this expression through q^{61} in appendix 1. We have also extended the expansion of the second moment by bonds given by Gaunt and Sykes (1983) which for consistency we denote by χ^{bb} and obtain:

$$\begin{aligned}
 \chi_{\text{BCC}}^{bb} = & 4q^{14} - 4q^{15} + \dots + 85\ 761\ 588q^{48} - 113\ 562\ 380q^{49} \\
 & + 204\ 796\ 872q^{50} - 385\ 245\ 024q^{51} + 703\ 838\ 400q^{52} \\
 & - 1219\ 752\ 264q^{53} + 1788\ 156\ 568q^{54} \\
 & - 2382\ 368\ 704q^{55} + 3727\ 278\ 288q^{56} - 6727\ 066\ 224q^{57} \\
 & + 12\ 017\ 966\ 196q^{58} - 20\ 817\ 051\ 084q^{59} + 33\ 231\ 499\ 436q^{60} \\
 & - 47\ 679\ 991\ 988q^{61} + \dots
 \end{aligned} \tag{5.4}$$

We give the expansion for the second moment by sites, χ_{BCC}^{ss} , through q^{61} in appendix 2.

For the simple cubic lattice we have added a further five coefficients to the expansions given by Gaunt and Sykes (1983):

$$\begin{aligned}
 K_{\text{SC}} = & q^6 + 3q^{10} - 3q^{11} + \dots - 2465\ 541q^{37} + 4197\ 528q^{38} - 6603\ 214q^{39} \\
 & + 12\ 030\ 048q^{40} - 23\ 763\ 903q^{41} \\
 & + \dots
 \end{aligned} \tag{5.5}$$

$$\begin{aligned}
 P_{\text{SC}}^b = & 1 - q^{10} - 10q^{14} + \dots + 5225\ 024q^{37} - 8633\ 109q^{38} \\
 & + 14\ 942\ 110q^{39} - 30\ 199\ 449q^{40} + 59\ 412\ 948q^{41} \\
 & + \dots
 \end{aligned} \tag{5.6}$$

$$\begin{aligned}
 \chi_{\text{SC}}^{bb} = & 3q^{10} - 3q^{11} + \dots - 242\ 839\ 461q^{37} + 441\ 301\ 659q^{38} \\
 & - 802\ 060\ 923q^{39} + 1583\ 927\ 781q^{40} - 3173\ 009\ 517q^{41} \\
 & + \dots
 \end{aligned} \tag{5.7}$$

We give the expressions of P_{SC}^s and χ_{SC}^{ss} through q^{41} in appendices 1 and 2 respectively.

Appendix 1. Expansions for the site percolation probability for the body-centred and simple cubic lattices

$$\begin{aligned}
 P_{\text{BCC}}^s &= 1 - q^8 - 8q^{14} + 8q^{15} - 84q^{20} + 168q^{21} - 84q^{22} - 48q^{24} \\
 &\quad - 528q^{26} + 2064q^{27} - 2364q^{28} + 816q^{29} - 900q^{30} + 1560q^{31} \\
 &\quad - 3112q^{32} + 17\,560q^{33} - 36\,912q^{34} + 30\,448q^{35} - 17\,014q^{36} \\
 &\quad + 31\,392q^{37} - 51\,328q^{38} + 150\,336q^{39} - 428\,676q^{40} + 607\,304q^{41} \\
 &\quad - 479\,768q^{42} + 548\,280q^{43} - 1055\,172q^{44} + 2064\,272q^{45} \\
 &\quad - 4923\,372q^{46} + 8968\,792q^{47} - 10\,031\,712q^{48} + 9941\,088q^{49} \\
 &\quad - 16\,429\,748q^{50} + 31\,557\,632q^{51} - 64\,006\,974q^{52} + 125\,015\,136q^{53} \\
 &\quad - 179\,526\,940q^{54} + 197\,079\,480q^{55} - 260\,507\,334q^{56} \\
 &\quad + 466\,001\,256q^{57} - 872\,212\,792q^{58} + 1663\,589\,824q^{59} \\
 &\quad - 2779\,049\,638q^{60} + 3641\,311\,608q^{61} + \dots
 \end{aligned}$$

$$\begin{aligned}
 P_{\text{SC}}^s &= 1 - q^6 - 6q^{10} + 6q^{11} - 45q^{14} + 90q^{15} - 57q^{16} \\
 &\quad - 260q^{18} + 900q^{19} - 1200q^{20} + 572q^{21} - 1098q^{22} \\
 &\quad + 6360q^{23} - 14\,332q^{24} + 15\,444q^{25} - 12\,450q^{26} \\
 &\quad + 39\,366q^{27} - 124\,284q^{28} + 218\,028q^{29} - 256\,649q^{30} \\
 &\quad + 394\,470q^{31} - 1010\,484q^{32} + 2176\,628q^{33} \\
 &\quad - 3455\,013q^{34} + 5239\,008q^{35} - 10\,100\,470q^{36} \\
 &\quad + 20\,506\,812q^{37} - 35\,739\,483q^{38} + 59\,103\,742q^{39} \\
 &\quad - 112\,279\,041q^{40} + 224\,644\,212q^{41} + \dots
 \end{aligned}$$

Appendix 2. High density expansions for the second moment by sites for the body-centred and simple cubic lattices

$$\begin{aligned}
 \chi_{\text{BCC}}^{ss} &= q^8 + 16q^{14} - 16q^{15} + 252q^{20} - 504q^{21} + 252q^{22} + 192q^{24} \\
 &\quad + 2112q^{26} - 8256q^{27} + 9516q^{28} - 3264q^{29} + 4500q^{30} \\
 &\quad - 7800q^{31} + 15\,722q^{32} - 87\,800q^{33} + 186\,072q^{34} \\
 &\quad - 154\,688q^{35} + 94\,778q^{36} - 188\,352q^{37} + 311\,784q^{38} \\
 &\quad - 908\,400q^{39} + 2595\,258q^{40} - 3711\,800q^{41} + 3043\,048q^{42} \\
 &\quad - 3782\,952q^{43} + 7452\,324q^{44} - 14\,644\,336q^{45} \\
 &\quad + 34\,901\,388q^{46} - 63\,851\,304q^{47} + 72\,754\,608q^{48} \\
 &\quad - 76\,396\,656q^{49} + 132\,075\,324q^{50} - 255\,875\,272q^{51} \\
 &\quad + 520\,884\,846q^{52} - 1021\,901\,664q^{53} + 1483\,792\,940q^{54} \\
 &\quad - 1681\,198\,800q^{55} + 2332\,150\,178q^{56} - 4254\,281\,880q^{57} \\
 &\quad + 7995\,286\,856q^{58} - 15\,317\,533\,168q^{59} + 25\,828\,803\,698q^{60} \\
 &\quad - 34\,506\,131\,544q^{61} + \dots
 \end{aligned}$$

$$\begin{aligned}
\chi_{SC}^{ss} = & q^6 + 12q^{10} - 12q^{11} + 135q^{14} - 270q^{15} + 183q^{16} + 1040q^{18} \\
& - 3600q^{19} + 5040q^{20} - 2528q^{21} + 5598q^{22} \\
& - 31\,800q^{23} + 74\,124q^{24} - 83\,664q^{25} + 74\,748q^{26} \\
& - 239\,488q^{27} + 765\,288q^{28} - 1390\,884q^{29} + 1748\,315q^{30} \\
& - 2838\,720q^{31} + 7287\,936q^{32} - 15\,958\,108q^{33} \\
& + 26\,519\,679q^{34} - 42\,634\,812q^{35} + 84\,119\,742q^{36} \\
& - 171\,513\,372q^{37} + 306\,443\,793q^{38} - 532\,935\,148q^{39} \\
& + 1053\,827\,307q^{40} - 2135\,689\,788q^{41} + \dots
\end{aligned}$$

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