Generating functions for connected embeddings in a lattice. I. Strong embeddings



1986 J. Phys. A: Math. Gen. 19 1007

(http://iopscience.iop.org/0305-4470/19/6/028)

J. Phys. A: Math. Gen. 19 (1986) 1007-1025. Printed in Great Britain

# Generating functions for connected embeddings in a lattice: I. Strong embeddings

M F Sykes

Wheatstone Physics Laboratory, King's College, University of London, Strand, London WC2R 2LS, UK

Received 15 July 1985

**Abstract.** The method of partial generating functions developed to derive high field expansions for the Ising model enumerates unrestricted strong embeddings in a lattice. The method is modified to enumerate connected embeddings only. An explicit general receipt is given for the relation between unrestricted and restricted generating functions. For the body-centred cubic lattice the number of connected strong embeddings of clusters with up to 13 sites is derived.

## 1. Introduction

In a recent paper, Redelmeier (1981) reports the enumeration of all the polyominoes containing 24 squares or less on an unbounded chessboard; the enumeration used ten months of computer time. He concludes that any technique that actually generates every polyomino is unlikely to get much further. The enumeration of square polyominoes is only one of a large number of enumeration problems that arise in the study of what may be rather loosely called lattice animals; they arise in the graph theoretic treatment of the cell growth problem (see Harary (1967) for a bibliography) and also in lattice statistics and the percolation problem (see the reviews by Shante and Kirkpatrick 1971, Essam 1971, 1972, 1980, Kirkpatrick 1973, de Gennes 1976, Welsh 1977, Wu 1978 and Stauffer 1979), and in many other physical applications. The mathematical problem presented by polyominoes in general has been considered, among others, by Klarner (1967), Lunnon (1971, 1972) and Golomb (1967).

We shall treat Redelmeier's problem as equivalent to the enumeration, for ascending $n$, of the number of connected clusters (per site) of $n$ sites on the simple quadratic (or plane square) lattice; the number of connected clusters of $n$ sites is identical to the number of connected strong embeddings (or section graphs) of $n$ sites. (For precise definitions of these graph theoretical terms see Essam and Fisher (1970)).

As a single result in computer enumeration the achievement of Redelmeier is impressive. He finds a total of 5239 988 770 268 polyominoes of size 24 and these were counted on a PDP-11/70 computer at a rate of approximately 200 every millisecond. For many applications it would seem desirable to retain more information than just the bare number of clusters; such requirements are likely to reduce the effective counting rate. Using the methods developed by Heap (1963) and Martin (1974) the number of connected clusters on the triangular lattice (hexagonal polyominoes) together with information on their site perimeter, has been obtained by Margolina *et al* (1983) using an IBM 370/168. A total of 918 837 374 clusters were enumerated in 55 hours, which corresponds to a counting rate of 5 every millisecond; this is some 40 times slower than Redelmeier's enumeration of the bare numbers for the simple quadratic. These two counting rates are not strictly comparable because of the different symmetries of the two lattices. Margolina *et al*'s counting rate could probably be increased by writing a specialised program restricted to the triangular lattice; but one conclusion can be drawn with confidence: the counting of connected clusters is a very time consuming computer task. For two-dimensional lattices extra terms can sometimes be added by using the special techniques of percolation theory described by Sykes and Glen (1976) and Sykes *et al* (1976a, b, c), hereafter referred to as I*-IV* respectively, and references cited therein.

The difficulty of enumerating connected clusters for three-dimensional lattices is increased by the inapplicability of many of the special techniques available in two dimensions and the very rapid growth rate of the totals. For example, for the body-centred cubic we quote the following sequence for the number of connected clusters grouped by sites:

| Sites $n$ | Number of clusters $A_n$ |
|---|---|
| 1 | 1 |
| 2 | 4 |
| 3 | 28 |
| 4 | 216 |
| 5 | 1 790 |
| 6 | 15 587 |
| 7 | 140 746 |
| 8 | 1305 920 |
| 9 | 12 374 069 |
| 10 | 119 223 556 |
| 11 | 1164 465 225 |
| 12 | 11 502 924 648 |
| 13 | 114 721 053 058 |

(1.1)

The values up to $n = 11$ can be obtained from the data given in IV*, based on computer enumeration of clusters with up to 10 sites; the total for 11 sites then follows by the methods described in I*-IV*. The last two terms have been added by the method described in this paper. A computer routine as fast as that of Redelmeier would require approximately 150 hours to complete $n = 13$; using the method we describe below a table of binomial coefficients and a desk calculator would suffice. To obtain the same total, together with information on the number of bonds in the clusters, required about 27 seconds of CDC 7600 time to perform some algebra.

This paper reports a feasibility study: we investigate whether the method of partial generating functions used by Sykes *et al* (1965, 1973a, b, c, d, e, 1975a, b, c) and Sykes (1979), hereafter referred to as $\mathrm{I}^+$-$\mathrm{X}^+$ respectively, can be applied to the present problem.

Before describing the theory of partial generating functions, and the necessary modifications thereto, we particularise our objectives more precisely. We denote the number of connected $n$-site clusters (per site) on an infinite lattice by $A_n$; and define a generating function

$$F(x) = A_1x + A_2x^2 + A_3x^3 + \dots \qquad (1.2)$$

As noted above these bare numbers are usefully supplemented by more detailed information. One parameter of interest is the bond content; any strong embedding of $n$ sites must be connected by at least $(n-1)$ bonds. We introduce a dummy variable, $b$, to record the bond content and write

$$F(x, b)=\sum_r A_r(b)x^r \tag{1.3}$$

where $A_r(b)$ is a polynomial in $b$ and $A_r(1)=A_r$. Since we shall only use functional expressions of this kind formally, to represent data grouped in a conventional way, we shall allow ourselves a certain licence and use the same symbol, $F$, on the left-hand side throughout; whether any particular ancillary parameter such as $b$, or any other that we later introduce, is explicitly written into the right-hand side is immaterial. Often a particular parameter which is not explicitly written in can be regarded as being carried silently; no confusion should arise: the sense should always be clear from the context.

For the body-centred cubic the expansion begins

$$F(x, b)=x+4bx^2+28b^2x^3+(204b^3+12b^4)x^4+\ldots \tag{1.4}$$

and the coefficient of $x^4$ records the fact that out of 216 connected clusters of four sites, 204 have three bonds and 12 have four. The method of partial generating functions will be developed to supplement the information in (1.1) in this way; we give the values of $A_r(b)$ through $A_{13}(b)$ in appendix 1.

The method of partial generating functions is most efficient when applied to bipartite (or loose-packed) lattices; the bipartite lattices usefully studied divide into two equivalent sublattices, A and B. We adopt the convention (of $\mathrm{I}^+$-$\mathrm{X}^+$) that each of these sublattices has $N$ sites. We can then regroup the data in a modified form, and rewrite the generating function as

$$2F(x, y)=A_{1,0}x+A_{0,1}y+A_{2,0}x^2+A_{1,1}xy+A_{0,2}y^2+\ldots. \tag{1.5}$$

In (1.5) each coefficient $A_{r,s}$ is the number of connected clusters (per sublattice site) of $r+s$ sites of which $r$ are A sites and $s$ are B sites. For the body-centred cubic the expansion begins

$$2F(x, y)=x+y+8xy+28x^2y+28xy^2+56x^3y+320x^2y^2+56xy^3+\ldots. \tag{1.6}$$

Graphical information sufficient to derive the expansion in this form up to five sites, by direct inspection of the clusters, is given by Domb (1960, appendix IV). The two extra parameters considered above can be taken together in a generating function

$$F(x, y, b)=\sum_{r,s} A_{r,s}(b)x^ry^s \tag{1.7}$$

where the coefficient of $x^ry^s$ is a finite polynomial in $b$ that records, in the conventional way, the bond content of all the connected clusters of $r$ A sites and $s$ B sites.

## 2. Method of partial generating functions

The analogue of the method described in $\mathrm{I}^+$ and $\mathrm{VI}^+$ is to provide partial generating functions $F_n$ for the polynomials $A_{r,s}$ of (1.7); each $F_n$ corresponds to the solution when the number of sites on one sublattice, which we shall take to be the A sublattice, is equal to $n$. The partial generating function $F_n$ provides the polynomials $A_{n,m}$ for fixed $n$. We shall call the A sites *primary* sites and the B sites *secondary* sites; notice that our convention is the *opposite* to that used in $I^+$-$X^+$. The contributions can be set out in an array:

$$
\begin{aligned}
F_0 &= A_{0,1} \\
F_1 &= A_{1,0} + A_{1,1} + A_{1,2} + A_{1,3} + A_{1,4} + \dots \\
F_2 &= \qquad\qquad A_{2,1} + A_{2,2} + A_{2,3} + \dots \\
F_3 &= \qquad\qquad\qquad A_{3,1} + A_{3,2} + \dots \\
F_4 &= \qquad\qquad\qquad\qquad A_{4,1} + \dots
\end{aligned}
\tag{2.1}
$$

where $A_{r,0} = 0$ if $r > 1$ and $A_{0,s} = 0$ if $s > 1$.

An important step is to exploit the symmetry condition

$$A_{r,s} = A_{s,r} \tag{2.2}$$

which holds because the two sublattices are equivalent; it follows that the first $n$ partial generating functions are sufficient to determine all $A_{r,s}$ for $r + s \leqslant 2n + 1$.

To take a specific example, the clusters with five sites can be determined from the partial generating functions through $F_2$ only. In the sequence

$$2A_5 = A_{1,4} + A_{2,3} + A_{3,2} + A_{4,1} \tag{2.3}$$

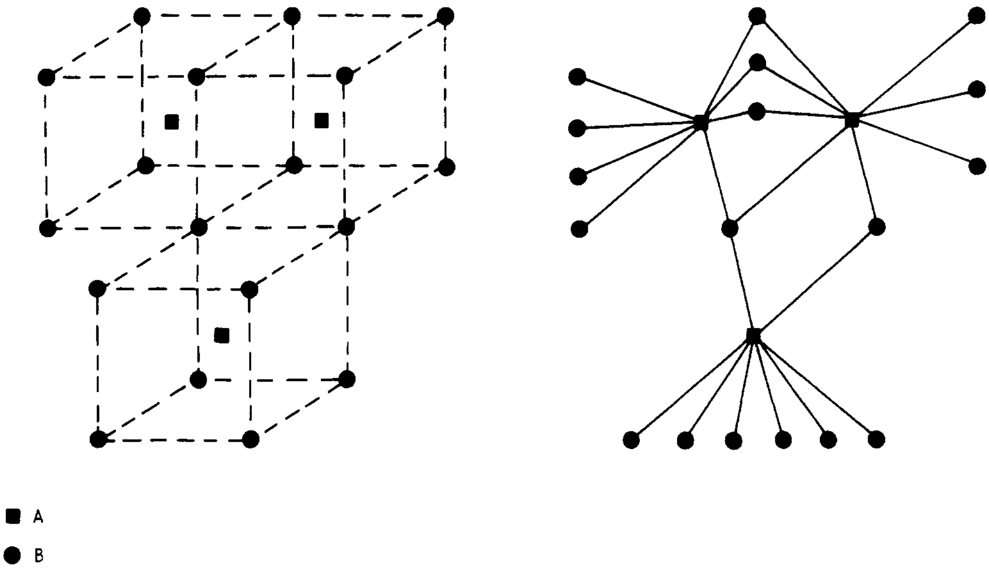
the last two contributions follow from the symmetry condition (2.2); the factor 2 on the left-hand side allows for our convention that the number of sites on each sublattice is $N$.

Partial generating functions for strong embeddings, or section graphs as we shall call them throughout our treatment, which are *unrestricted* (i.e. not necessarily connected) and their application to the Ising problem are described in detail in $I^+$-$X^+$. To illustrate that part of the theory that is relevant to our objective we take as an example the derivation of the partial generating function of third order for the body-centred cubic lattice. To obtain this, Sykes *et al* (1965, $I^+$) classified all the distinct choices of three primary or A sites on the lattice. Each chosen A site has eight nearest neighbours (on the B sublattice) which are described as its shadow; each shadow defines a cube; the interactions of the three cubes corresponding to any particular choice of A sites is significant.

We consider one possible choice illustrated below. We have to provide a generating function for all possible choices of B sites; the generating function is to provide information on the number of nearest-neighbour linkages, or bonds, for each choice.

The number of arrangements of three cubes of the above configuration on a conventional $2N$ site lattice (i.e. $N$ A sites, $N$ B sites) is $24N$. The three A sites collectively cast shadows which affect 18 distinct B sites. There will be $(N-18)$ B sites that are not neighbours of any of the chosen A sites and these will not contribute any bonds if chosen. These can all be accounted for by a factor $(1+y)^{N-18}$. There are 13 B sites which are first neighbours of only one A site; these can be accounted for by a factor $(1+by)^{13}$. There remain four B sites which are first neighbours of two A sites and one B site which is a first neighbour of three A sites; these can be accounted for by factors $(1+b^2y)^4$ and $(1+b^3y)$ respectively. All the possibilities are therefore generated by the product

$$(1+y)^{N-18}(1+by)^{13}(1+b^2y)^4(1+b^3y) \tag{2.4}$$




which we regard as a contribution to the *unrestricted* partial generating function in the special sense that the connectivity of the embeddings generated is unrestricted.

The contribution of the product (2.4) to the free energy of the Ising model is treated in detail in I⁺ and III⁺. The significant part of the product is there shown to correspond formally to the terms independent of $N$, i.e. those generated by

$$(1+by)^{13}(1+b^2y)^4(1+b^3y)/(1+y)^{18} \tag{2.5}$$

which is conveniently denoted by the code (18, 13, 4, 1). More generally, any code corresponding to any choice of any number, $r$, of cubes can be interpreted by the substitution

$$(\lambda, \alpha, \beta, \gamma, \ldots) = (1+by)^{\alpha}(1+b^2y)^{\beta}(1+b^3y)^{\gamma}\ldots/(1+y)^{\lambda} \tag{2.6}$$

where

$$\lambda = \alpha+\beta+\gamma\ldots \tag{2.7}$$

and, after expansion of the right-hand side, the coefficient of $y^s b^t$ represents the number of choices of $r$ A sites and $s$ B sites, having $t$ nearest-neighbour bonds between them, that correspond to the chosen configuration of $r$ A sites.

As a matter of convention, since we will be concerned ultimately with the enumeration of *connected* embeddings, we shall henceforth omit from any partial generating function all those terms which correspond to an isolated B site; it is evident that such terms cannot contribute to any connected component. We thus shorten the product (2.4) to

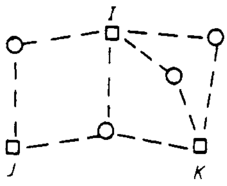
$$(1+by)^{13}(1+b^2y)^4(1+b^3y) \tag{2.8}$$

which can be regarded as a *partially* restricted generating function; no embeddings generated will contain any isolated B sites. Isolated A sites are *not* excluded.

To complete our task we have further to delete from (2.8) any embeddings that are not connected. We describe a method of achieving this in the next section.

## 3. Restricted and unrestricted generating functions

We begin this section by taking as examples the finite graph $G$ below:

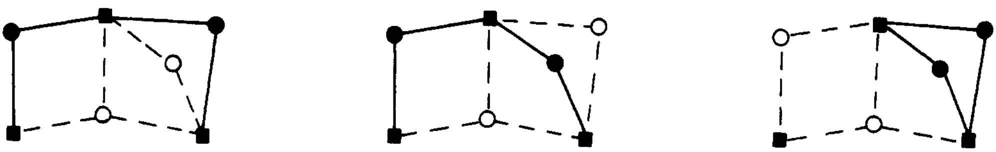



which we regard as representing a possible mapping of shadow intersections as described in the previous section. For convenience we have chosen a mapping which is neither too degenerate not too complicated; it evidently does not correspond to a realisable arrangement of cubes. We shall study the connectivity of the (primary) A sites for different choices of the (secondary) B sites. Regarded as a finite graph the sets of A and B sites of $G$ are obviously not equivalent but for our present purpose this is immaterial; we shall restore the symmetry later in applications. We regard the A sites as *always* occupied and label them $I$, $J$, $K$. By the methods of the previous section we can immediately derive an *unrestricted* section graph enumerator which we write

$$G[IJK] = (1+b^2y)^3(1+b^3y)$$
$$= 1+(3b^2+b^3)y+(3b^4+3b^5)y^2+(b^6+3b^7)y^3+b^9y^4. \quad (3.1)$$

Essentially the unrestricted enumerator is seen to be a product of simple polynomials *auxiliary generating polynomials*, each associated with an individual B site. Each auxiliary polynomial is determined only by the number, $r$ say, of neighbours of the B site and can be provided in isolation. The graphs that map the environment always have the same characteristic structure of $r$ edges radiating from a central vertex; such graphs are usually called *vertex stars* (Essam and Fisher 1970). The general rule is that an $r$-vertex star yields a factor $(1+b^ry)$. The unrestricted generating function for any bipartite graph can thus be written down by inspection, *currente calamo.*

To return to the unrestricted enumerator (3.1) we note that it summarises the site and bond content of all the 16 section graphs obtained by selecting any number of B sites while the A sites are *always* occupied. For example the term $3b^4y^2$ corresponds to the three possible section graphs with two B sites and four bonds illustrated below.



(*a*) (*b*) (*c*)

We now define a *restricted* (that is, connected) section graph enumerator in an analogous way; for our example:

$$G^*[IJK] = b^3y+(2b^4+3b^5)y^2+(b^6+3b^7)y^3+b^9y^4. \quad (3.2)$$

It summarises all the section graphs that *connect* the three A sites. The coefficient of $b^4y^2$ is now two because the section graph ($c$) does not connect the A sites. For elementary examples the restricted enumerator can be written down by inspection; we shall always denote *restricted quantities* by an *asterisk*.

We now introduce more detailed section graph enumerators (partitioned enumerators) in the following way. For any partition of the A sites into mutually disjoint subsets we define corresponding *unrestricted* enumerators that summarise all the section graphs which *do not connect* any pair of A sites in *different subsets*. In our example, excluding $IJK$, there are four possible partitions of the B sites and we find by inspection

$$\begin{aligned} G[I, JK] &= 1 \\ G[J, IK] &= (1+b^2y)^2 \\ G[K, IJ] &= (1+b^2y) \\ G[I, J, K] &= 1. \end{aligned} \tag{3.3}$$

In (3.3) the commas in the arguments of each function $G$ separate disjoint sets of A sites. Notice that in $G[J, IK]$ the essential condition is that $J$ is *not* connected to $I$ or $K$; $I$ and $K$ may or may not be connected. Unrestricted partitioned enumerators are readily written down by deleting from the full product of auxiliary polynomials any that correspond to vertex stars any pair of whose A sites lie in disjoint sets.

In an analogous way we introduce *restricted* partitioned enumerators denoted by an asterisk. Thus, while $G[J, IK]$ enumerates all section graphs subject to the restriction above, $G^*[J, IK]$ enumerates only those section graphs for which (in addition) *any* two A sites in the same set *are connected.*

We find on inspection

$$\begin{aligned} G^*[I, JK] &= 0 \\ G^*[J, IK] &= 2b^2y + b^4y^2 \\ G^*[K, IJ] &= b^2y \\ G^*[I, J, K] &= 1. \end{aligned} \tag{3.4}$$

Notice that the zero corresponds to the fact that it is not possible to connect $J$ to $K$ by a section graph that does not also connect these to $I$. Our objective is to obtain expressions for the partitioned $G^*$ in terms of the partitioned $G$; our procedure is perfectly general.

We take it as *evident* that

$$G[IJK] = G^*[IJK] + G^*[I, JK] + G^*[J, IK] + G^*[K, IJ] + G^*[I, J, K] \tag{3.5}$$

where the right-hand side is an exhaustive enumeration of all the possible partitions of the vertex set $I$, $J$, $K$ into subsets. Likewise

$$\begin{aligned} G[I, JK] &= G^*[I, JK] + G^*[I, J, K] \\ G[J, IK] &= G^*[J, IK] + G^*[I, J, K] \\ G[K, IJ] &= G^*[K, IJ] + G^*[I, J, K] \end{aligned} \tag{3.6}$$

and finally

$$G[I, J, K] = G^*[I, J, K]. \tag{3.7}$$

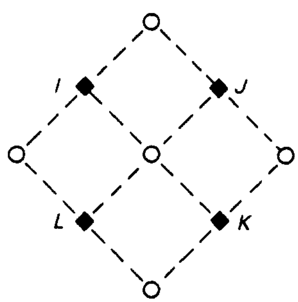
The essential point is that any section graph belongs to one, and only one, restricted partitioned enumerator.

The above equations are easily inverted to obtain corresponding expressions for the restricted enumerators in terms of the unrestricted enumerators. In particular we find for the total connected enumerator

$$G^*[IJK]=G[IJK]-G[I,JK]-G[J,IK]-G[K,IJ]+2G[I,J,K]. \qquad (3.8)$$

The importance of the above inversion lies in the fact that the unrestricted enumerators, as we have noticed above, are easily written down with the aid of the auxiliary polynomials; the value of $G^*[IJK]$ then follows from (3.8).

The above arguments are readily generalised to any number of A sites. To take a more ambitious example we consider the mapping:




with four primary sites. The unrestricted enumerators are readily seen on inspection to be

$$\begin{aligned}
&G[IJKL]=(1+b^2y)^4(1+b^4y)\\
&G[I,JKL]=G[J,IKL]=G[K,IJL]=G[L,IJK]=(1+b^2y)^2\\
&G[IJ,KL]=G[IL,JK]=(1+b^2y)^2\\
&G[IK,JL]=1\\
&G[IJ,K,L]=G[JK,I,L]=G[KL,I,J]=G[IL,J,K]=(1+b^2y)\\
&G[IK,J,L]=G[JL,I,K]=1\\
&G[I,J,K,L]=1.
\end{aligned} \qquad (3.9)$$

By extending the logical procedure used for three sites we obtain the result

$$\begin{aligned}
G^*[IJKL]=G[IJKL]&-\sum_4 G[I,JKL]-\sum_3 G[IJ,KL]\\
&+2\sum_6 G[IJ,K,L]-6G[I,J,K,L]
\end{aligned} \qquad (3.10)$$

where the subscripts denote the number of distinct terms in each summation. On substituting (3.9) in (3.10) we obtain

$$G^*[IJKL]=b^4y+4b^6y^2+(4b^6+6b^8)y^3+(b^8+4b^{10})y^4+b^{12}y^5. \qquad (3.11)$$

In this particular example, because of the symmetry of the graph chosen, it is easily verified that (3.11) describes the connected section graphs exhaustively. To simplify the general treatment we now introduce a contracted notation; we denote the summation

$$\sum_{3} G[IJ, KL] = G[IJ, KL] + G[IK, JL] + G[IL, JK] \qquad (3.12)$$

by $f_{2,2}$, the suffixes on $f$ simply recording the fact that it represents the sum of all enumerators corresponding to divisions of the A-vertex site into two sets, each of cardinality 2. In general $f_{r,s,t},\ldots$ will denote the sum of all the enumerators that correspond to distinct unordered partitions of the A-vertex set into sets of cardinality $r, s, t, \ldots$. In this notation our results so far may be summarised as follows

$$\begin{array}{llll}
1 \text{ A site} & f_1 = f_1^* & \text{and inversely} & f_1^* = f_1 \\
2 \text{ A sites} & f_2 = f_2^* + f_{1,1}^* & & f_2^* = f_2 - f_{1,1} \\
 & f_{1,1} = f_{1,1}^* & & f_{1,1}^* = f_{1,1} \\
3 \text{ A sites} & f_3 = f_3^* + f_{1,2}^* + f_{1,1,1}^* & & f_3^* = f_3 - f_{1,2} + 2f_{1,1,1} \\
 & f_{1,2} = f_{1,2}^* + 3f_{1,1,1}^* & & f_{1,2}^* = f_{1,2} - 3f_{1,1,1} \\
 & f_{1,1,1} = f_{1,1,1}^* & & f_{1,1,1}^* = f_{1,1,1}.
\end{array} \qquad (3.13)$$

In principle the problem is now completely solved. The set of equations for unrestricted enumerators can always be written down and inverted by successive substitutions. The outcome can be further contracted by recording only the coefficients in the above equations in the form of a matrix, it being understood that the rows and columns are ordered in some conventional dictionary ordering of the partitions of $n$ (such as for example, Riordan (1958) ch 6, table 1.)

We thus summarise the solution for 4 A sites by

| $M_4$ | 4 | 13 | $2^2$ | $21^2$ | $1^4$ | $M_4^*$ | 4 | 13 | $2^2$ | $21^2$ | $1^4$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 4 | 1 | 1 | 1 | 1 | 1 | 4 | 1 | −1 | −1 | 2 | −6 |
| 13 | | 1 | 0 | 2 | 4 | 13 | | 1 | 0 | −2 | 8 |
| $2^2$ | | | 1 | 1 | 3 | $2^2$ | | | 1 | −1 | 3 |
| $21^2$ | | | | 1 | 6 | $21^2$ | | | | 1 | −6 |
| $1^4$ | | | | | 1 | $1^4$ | | | | | 1. |

(3.14)

We give in appendix 2 the values of $M_5$-$M_7$ together with their respective inverses $M_5^*$-$M_7^*$. Although straightforward in principle, the direct derivation of these results is heavy; we give in the next section a general receipt for the matrix elements of $M_n$ and $M_n^*$.

## 4. General prescription for the fundamental inversion

The general expressions for the elements of the matrices $M$ and $M^*$ of the previous section are equivalent to those derived by Craig (1928) and Meeron (1957) in their studies of the relation between moments and cumulants in the statistics of independent variables introduced by Thiele (1907); that their results are immediately applicable to the present inversion and the extensions thereto we shall later make, which are more general in that they correspond also to the probabilities associated with dependent variables, is evident from the treatise of Fréchet (1940). The arguments of the previous section are a direct application of the simple principle of inclusion and exclusion in its more advanced form; the basic ideas are developed by Whitney (1932), Jordan (1933, 1934), Bonferroni (1936), Broderick (1937), Gumbel (1938), Geiringer (1938) and at length by Fréchet (1940, 1943). The inversion can be treated rigorously by the method of exponential generating functions (see, for example, Riordan (1958), ch 2) and particularly the treatise of MacMahon (1915, 1916). Essentially it rests on the advanced theory of Stirling numbers, which, like the Stirling numbers themselves, is constantly being rediscovered. An important application is to the determination of the derivatives of composite functions (Riordan 1946, Teixeira 1880). There exists an extensive literature; among modern articles that may profitably be consulted are Sherman (1964), Kubo (1962), Good (1961), Uhlenbeck and Ford (1962), Spitzer (1956) and Lukacs (1955); also relevant are the paper by Bell (1934) on exponential polynomials and those on exponential integers by Levin and Dalton (1962) (see also Becker and Riordan 1948, Broggi 1933). The theoretical background is adequately covered by the articles cited; we therefore simply give an explicit general receipt for the elements of $M$ and $M^*$.

The problem is one of distribution and occupancy. At seventh order the partitions of seven into six parts and into seven parts are assigned to the three partitions of seven into four parts in the following way

| | in $M_7$ | | in $M_7^*$ | |
|---|---|---|---|---|
| | $(21^5)$ | $(1^7)$ | $(21^5)$ | $(1^7)$ |
| $(41^3)$ | 10 | 35 | 20 | −210 |
| $(321^2)$ | 40 | 210 | 50 | −420 |
| $(2^31)$ | 15 | 105 | 15 | −105 |
| | 65 | 350 | 85 | −735 |

(4.1)

Following Riordan (1953, ch 5, § 6) the number of ways of assigning $n$ different objects into $m$ like cells, with no cells empty, is $S(n, m)$, the Stirling number of the *second* kind. The totals for the first two columns in our example correspond to the values $S(6, 4) = 65$ and $S(7, 4) = 350$ respectively. Further, following Riordan (1958, ch 2, § 7), if we denote by $S^*(n, m)$ the Stirling member of the *first* kind, the corresponding totals for the inverse matrix will be $S^*(6, 4) = 85$ and $S^*(7, 4) = -735$ respectively.

To obtain the column elements in detail we first notice that the explicit formulae of Ettinghausen (1826, see also Ginsburg 1929) for the Stirling numbers:

$$S(n, m) = \sum n!/(A_1)!(A_2!)(A_3!)\dots(1!)^{A_1}(2!)^{A_2}(3!)^{A_3}\dots \tag{4.2}$$

$$(-1)^{n-m}S^*(n, m) = \sum n!/(A_1!)(A_2!)(A_3!)\dots(1)^{A_1}(2)^{A_2}(3)^{A_3}\dots \tag{4.3}$$

for all integer solutions of

$$\begin{aligned} A_1 + A_2 + A_3 + \dots &= m \\ A_1 + 2A_2 + 3A_3 + \dots &= n \end{aligned} \tag{4.4}$$

give the required matrix elements explicitly when the objects to be assigned (all regarded as distinguishable) are of one kind (in our example all the same integer:

seven ones). Carrying out the above receipt gives the results

$$S(7,4)=35+210+105=350$$
$$S(6,4)=20+45=65.$$

The first of these gives the entries required, the correct assignment of each being indicated by the values of the solution of (4.4); the second corresponds to the entries in $M_6$ where the partition of six into six parts (all ones) is assigned to the two partitions of six into four parts. In our example the first column of entries in (4.1) corresponds to distributing six distinct objects of *two* kinds (ones and twos and in our instance five ones and one two) into four cells.

The required generalisation of the first formula of Ettinghausen is just

$$S(n_1, n_2, m)=\sum n_1!\,n_2!/A_{10}!\,A_{01}!\,A_{20}!\,A_{11}!\ldots(1!0!)^{A_{10}}\ldots \tag{4.5}$$

for all integer solutions of

$$\begin{aligned} A_{10}+A_{01}+\ A_{20}+A_{11}+\ A_{02}+\ldots &=\sum A_{rs}=m\\ A_{10}\qquad +2A_{20}+A_{11}\qquad +\ldots &=\sum rA_{rs}=n_1\\ A_{01}\qquad +A_{11}+2A_{02}+\ldots &=\sum sA_{rs}=n_2. \end{aligned} \tag{4.6}$$

For each solution the value of $A_{rs}$ will correspond to the number of cells which contain $r$ objects of the first kind and $s$ of the second. The general factors in the denominator are $(A_{rs}!)$ for the first run and $(r!s!)^{A_{rs}}$ for the second run. To obtain $S^*(n_1, n_2, m)$ it is only necessary to divide every factor inside brackets in the second run by $(r+s-1)!$ and give the final outcome the sign of $(-1)^{n_1+n_2-m}$. For the case $s=0$ every factor inside brackets in the second run will reduce to $r!/(r-1)!=r$ and the second formula of Ettinghausen is recovered identically.

In our example we find four distinct solutions

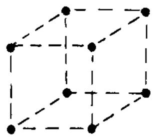
| Solution | Corresponding assignment | Corresponding partition | Contribution to $S$ | Contribution to $S^*$ | |
|---|---|---|---|---|---|
| $A_{10}=3, A_{21}=1$ | (211)(1)(1)(1) | $41^3$ | 10 | 20 | |
| $A_{10}=2, A_{20}=1, A_{11}=1$ | (21)(11)(1)(1) | $321^2$ | 30 | 30 | (4.7) |
| $A_{10}=2, A_{30}=1, A_{01}=1$ | (111)(2)(1)(1) | $321^2$ | 10 | 20 | |
| $A_{10}=1, A_{20}=2, A_{01}=1$ | (2)(11)(11)(1) | $2^31$ | 15 | 15 | |

which collectively sum to $S(6,4)$ and $S^*(6,4)$ with the required divisions.

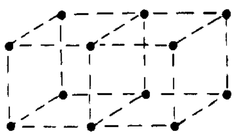
More generally, the formula for three kinds of object is the natural generalisation of that for two; for the Stirling number of the second kind the first run in the denominator consists of all the factors $A_{rst}!$ and the second of all the factors $(r!s!t!)^{A_{rst}}$. To invert the matrix every factor inside brackets in the second run must be divided by $(r+s+t+1)!$ and the whole product given the sign of $(-1)^{n_1+n_2+n_3-m}$. The generalisation to any number of objects is evident.

## 5. Application to body-centred cubic problem

We now apply the techniques described in §§ 2 and 3 to the body-centred cubic lattice. To obtain the first two partial generating functions we illustrate below all the arrangements of one and two cubes together with the full set of partitioned unrestricted enumerators for each.

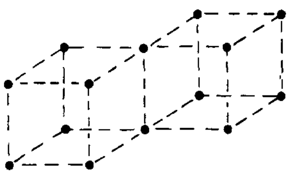


$(N)\quad f_1=(1+b_2y)^8$

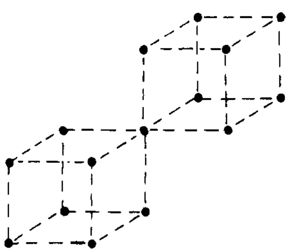


$(3N)\quad f_2=3(1+b^2y)^4(1+by)^8 \qquad f_{11}=3(1+by)^8$

(5.1)



$(6N)\quad f_2=6(1+b^2y)^2(1+by)^{12} \qquad f_{11}=6(1+by)^{12}$



$(4N)\quad f_2=4(1+b^2y)(1+by)^{14} \qquad f_{11}=4(1+by)^{14}.$

Now the partial generating function for restricted clusters can be obtained by substitution in

$$F_1=\sum f_1^*=\sum f_1$$
$$F_2=\sum f_2^*=\sum (f_2-f_{11}) \tag{5.2}$$

where the summations are taken over all distinct arrangements of one and two cubes respectively. If we adopt the convention of writing $(1+by)^\alpha(1+b^2y)^\beta\ldots$ as $\{\alpha,\beta\ldots\}$ the result may be written:

$$F_1=\{4\}$$
$$F_2=3\{8,4\}+6\{12,2\}+4\{14,1\}-3\{8\}-6\{12\}-4\{14\}. \tag{5.3}$$

In (5.3) we have suppressed the factor $N$ to obtain the partial generating functions following the conventions of § 2. These functions expand (after allowing for the primary sites represented by the variable $x$) as

$$F_1=x+8bxy+28b^2xy^2+56b^3xy^3+70b^4xy^4+\ldots \tag{5.4}$$

$$F_2=28b^2x^2y+296b^3x^2y^2+24b^4x^2y^2+1492b^4x^2y^3+216b^5x^2y^3+12b^6x^2y^3+\ldots. \tag{5.5}$$

The symmetry condition (2.2) is satisfied by the coefficients of $xy^2$ in (5.4) and $x^2y$

in (5.5); collecting the terms with appropriate weighting gives the values

$$A_1(b)=1 \qquad A_2(b)=4b \qquad A_3(b)=28b^2$$
$$A_4(b)=204b^3+12b^4 \qquad A_5(b)=1562b^4+216b^5+12b^6. \tag{5.6}$$

By inspection of all the 237$N$ possible connected arrangements of three cubes the next partial generating function is readily obtained in terms of 31 distinct codes

$$\begin{aligned}F_3=&12\{10,4,2\}+24\{13,4,1\}+8\{15,3,1\}-6\{8,4\}+3\{8,8\}-24\{10,2\}-24\{12,2\}\\&-24\{12,4\}+24\{12,6\}-24\{13,1\}-24\{13,3\}-24\{14,1\}-24\{14,4\}\\&+24\{14,5\}-24\{15,1\}-84\{16,2\}+42\{16,4\}-72\{18,1\}-72\{18,2\}\\&+72\{18,3\}-56\{20,1\}+28\{20,2\}+3\{8\}+12\{10\}+24\{12\}+24\{13\}\\&+24\{14\}+16\{15\}+42\{16\}+72\{18\}+28\{20\}.\end{aligned} \tag{5.7}$$

By listing all the 4995$N$ arrangements of four cubes, 114 219$N$ arrangements of five cubes and 2753 781$N$ arrangements of six cubes the author has obtained corresponding expressions for $F_4$, $F_5$ and $F_6$ in terms of 124, 434 and 1456 codes respectively. From these the polynomials in appendix 1 were obtained by expansion on a CDC 7600 in about 27 seconds of CPU time.

If we keep only the essential variable $y$ and set the ancilliary variable $b$ equal to unity the results (5.3) and (5.7) may be written in terms of the new variable $Y=1+y$ as

$$\begin{aligned}F_1&=Y^8\\F_2&=4Y^{15}+2Y^{14}-3Y^{12}-3Y^8\\F_3&=28Y^{22}+16Y^{21}-2Y^{20}-40Y^{19}+12Y^{18}-15Y^{16}-8Y^{15}\\&\quad-24Y^{14}+24Y^{13}-6Y^{12}+12Y^{10}+3Y^8.\end{aligned} \tag{5.8}$$

In this form $F_4$, $F_5$ and $F_6$ have only 19, 28 and 35 coefficients respectively and we quote these expressions in appendix 3.

## 6. Conclusions

The work described in this paper was undertaken as a feasibility study. By using the method of partial generating functions we have been able to produce a table of connected clusters on the body-centred cubic lattice through $A_{13}$. The expressions for $F_1$–$F_6$ of appendix 3 used to provide this could easily be expanded using a desk calculator and a table of binomial coefficients; in contrast, as noted in our introduction, direct enumeration of the bare numbers seems likely to require some 150 hours of CPU time. It is difficult to make a direct comparison since the complicated sequence of operations we have undertaken cannot be usefully measured in CPU time. However, consider the problem of obtaining the values of the next two entries in (1.1), $A_{14}$ and $A_{15}$ respectively. The direct enumeration would certainly seem to require CPU times of the order of some 600 days; preliminary trials indicate that using a computer instead to enumerate all the arrangements of seven cubes and to perform at the same time all the summations required to derive the partial generating function $F_7$ would need about 12 hours of CPU time. The present method should thus prove effectively a factor of 1000 times faster. Our general conclusion is that if a large amount of machine time is available it would be far more efficient to use it to derive partial generating functions than to count clusters directly.

## Appendix 1. Strong embeddings of clusters in the body-centred cubic lattice grouped by site and bond content

$$A_1 = 1$$

$$A_2 = 4b$$

$$A_3 = 28b^2$$

$$A_4 = 204b^3 + 12b^4$$

$$A_5 = 1562b^4 + 216b^5 + 12b^6$$

$$A_6 = 12\,544b^5 + 2704b^6 + 312b^7 + 27b^8$$

$$A_7 = 104\,756b^6 + 29\,952b^7 + 5262b^8 + 704b^9 + 72b^{10}$$

$$A_8 = 900\,168b^7 + 318\,594b^8 + 72\,096b^9 + 12\,844b^{10} + 2016b^{11} + 198b^{12} + 4b^{13}$$

$$A_9 = 7901\,843b^8 + 3333\,352b^9 + 898\,692b^{10} + 195\,120b^{11} + 38\,370b^{12} + 5976b^{13} + 692b^{14} + 24b^{15}$$

$$A_{10} = 70\,545\,284b^9 + 34\,547\,832b^{10} + 10\,698\,912b^{11} + 2\,676\,258b^{12} + 612\,060b^{13} + 120\,060b^{14} + 20\,576b^{15} + 2418b^{16} + 156b^{17}$$

$$A_{11} = 638\,589\,820b^{10} + 355\,920\,072b^{11} + 123\,953\,660b^{12} + 34\,643\,968b^{13} + 8\,846\,736b^{14} + 2009\,480b^{15} + 418\,789b^{16} + 72\,168b^{17} + 9720b^{18} + 800b^{19} + 12b^{20}$$

$$A_{12} = 5847\,741\,388b^{11} + 3653\,334\,942b^{12} + 1409\,307\,172b^{13} + 432\,705\,076b^{14} + 120\,462\,316b^{15} + 30\,389\,128b^{16} + 7161\,624b^{17} + 1503\,868b^{18} + 274\,704b^{19} + 40\,338b^{20} + 3924b^{21} + 168b^{22}$$

$$A_{13} = 54\,073\,952\,472b^{12} + 37\,417\,241\,256b^{13} + 15\,804\,769\,740b^{14} + 5270\,953\,664b^{15} + 1578\,040\,191b^{16} + 431\,637\,408b^{17} + 111\,103\,536b^{18} + 26\,355\,984b^{19} + 5715\,468b^{20} + 1090\,672b^{21} + 171\,636b^{22} + 19\,680b^{23} + 1327b^{24} + 24b^{25}.$$

## Appendix 2. Conversion matrices relating restricted and unrestricted generating functions

| $M_5$ | 5 | 41 | 32 | $31^2$ | $2^21$ | $21^3$ | $1^5$ |
|---|---|---|---|---|---|---|---|
| 5 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 41 | | 1 | 0 | 2 | 1 | 3 | 5 |
| 32 | | | 1 | 1 | 2 | 4 | 10 |
| $31^2$ | | | | 1 | 0 | 3 | 10 |
| $2^21$ | | | | | 1 | 3 | 15 |
| $21^3$ | | | | | | 1 | 10 |
| $1^5$ | | | | | | | 1 |

| $M_5^*$ | 5 | 41 | 32 | $31^2$ | $2^21$ | $21^3$ | $1^5$ |
|---|---|---|---|---|---|---|---|
| 5 | 1 | −1 | −1 | 2 | 2 | −6 | 24 |
| 41 | | 1 | 0 | −2 | −1 | 6 | −30 |
| 32 | | | 1 | −1 | −2 | 5 | −20 |
| $31^2$ | | | | 1 | 0 | −3 | 20 |
| $2^21$ | | | | | 1 | −3 | 15 |
| $21^3$ | | | | | | 1 | −10 |
| $1^5$ | | | | | | | 1 |

| $M_6$ | 6 | 51 | 42 | $3^2$ | $41^2$ | 321 | $2^3$ | $31^3$ | $2^21^2$ | $21^4$ | $1^6$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 6 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 51 | | 1 | 0 | 0 | 2 | 1 | 0 | 3 | 2 | 4 | 6 |
| 42 | | | 1 | 0 | 1 | 1 | 3 | 3 | 3 | 7 | 15 |
| $3^2$ | | | | 1 | 0 | 1 | 0 | 1 | 2 | 4 | 10 |
| $41^2$ | | | | | 1 | 0 | 0 | 3 | 1 | 6 | 15 |
| 321 | | | | | | 1 | 0 | 3 | 4 | 16 | 60 |
| $2^3$ | | | | | | | 1 | 0 | 1 | 3 | 15 |
| $31^3$ | | | | | | | | 1 | 0 | 4 | 20 |
| $2^21^2$ | | | | | | | | | 1 | 6 | 45 |
| $21^4$ | | | | | | | | | | 1 | 15 |
| $1^6$ | | | | | | | | | | | 1 |

| $M_6^*$ | 6 | 51 | 42 | $3^2$ | $41^2$ | 321 | $2^3$ | $31^3$ | $2^21^2$ | $21^4$ | $1^6$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 6 | 1 | −1 | −1 | −1 | 2 | 2 | 2 | −6 | −6 | 24 | −120 |
| 51 | | 1 | 0 | 0 | −2 | −1 | 0 | 6 | 4 | −24 | 144 |
| 42 | | | 1 | 0 | −1 | −1 | −3 | 3 | 5 | −18 | 90 |
| $3^2$ | | | | 1 | 0 | −1 | 0 | 2 | 2 | −8 | 40 |
| $41^2$ | | | | | 1 | 0 | 0 | −3 | −1 | 12 | −90 |
| 321 | | | | | | 1 | 0 | −3 | −4 | 20 | −120 |
| $2^3$ | | | | | | | 1 | 0 | −1 | 3 | −15 |
| $31^3$ | | | | | | | | 1 | 0 | −4 | 40 |
| $2^21^2$ | | | | | | | | | 1 | −6 | 45 |
| $21^4$ | | | | | | | | | | 1 | −15 |
| $1^6$ | | | | | | | | | | | 1 |

| $M_7$ | 7 | 61 | 52 | 43 | $51^2$ | 421 | $3^21$ | $32^2$ | $41^3$ | $321^2$ | $2^31$ | $31^4$ | $2^21^3$ | $21^5$ | $1^7$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 7 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 61 | | 1 | 0 | 0 | 2 | 1 | 1 | 0 | 3 | 2 | 1 | 4 | 3 | 5 | 7 |
| 52 | | | 1 | 0 | 1 | 1 | 0 | 2 | 3 | 2 | 3 | 6 | 5 | 11 | 21 |
| 43 | | | | 1 | 0 | 1 | 2 | 1 | 1 | 3 | 3 | 5 | 7 | 15 | 35 |
| $51^2$ | | | | | 1 | 0 | 0 | 0 | 3 | 1 | 0 | 6 | 3 | 10 | 21 |
| 421 | | | | | | 1 | 0 | 0 | 3 | 2 | 3 | 12 | 9 | 35 | 105 |
| $3^21$ | | | | | | | 1 | 0 | 0 | 2 | 0 | 4 | 6 | 20 | 70 |
| $32^2$ | | | | | | | | 1 | 0 | 1 | 3 | 3 | 7 | 25 | 105 |
| $41^3$ | | | | | | | | | 1 | 0 | 0 | 4 | 1 | 10 | 35 |
| $321^2$ | | | | | | | | | | 1 | 0 | 6 | 6 | 40 | 210 |
| $2^31$ | | | | | | | | | | | 1 | 0 | 3 | 15 | 105 |
| $31^4$ | | | | | | | | | | | | 1 | 0 | 5 | 35 |
| $2^21^3$ | | | | | | | | | | | | | 1 | 10 | 105 |
| $21^5$ | | | | | | | | | | | | | | 1 | 21 |
| $1^7$ | | | | | | | | | | | | | | | 1 |

| $M_7$ | 7 | 61 | 52 | 43 | $51^2$ | 421 | $3^21$ | $32^2$ | $41^3$ | $321^2$ | $2^31$ | $31^4$ | $2^21^3$ | $21^5$ | $1^7$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 7 | 1 | −1 | −1 | −1 | 2 | 2 | 2 | 2 | −6 | −6 | −6 | 24 | 24 | −120 | 720 |
| 61 | | 1 | 0 | 0 | −2 | −1 | −1 | 0 | 6 | 4 | 2 | −24 | −18 | 120 | −840 |
| 52 | | | 1 | 0 | −1 | −1 | 0 | −2 | 3 | 3 | 6 | −12 | −18 | 84 | −504 |
| 43 | | | | 1 | 0 | −1 | −2 | −1 | 2 | 4 | 3 | −14 | −14 | 70 | −420 |
| $51^2$ | | | | | 1 | 0 | 0 | 0 | −3 | −1 | 0 | 12 | 6 | −60 | 504 |
| 421 | | | | | | 1 | 0 | 0 | −3 | −2 | −3 | 12 | 15 | −90 | 630 |
| $3^21$ | | | | | | | 1 | 0 | 0 | −2 | 0 | 8 | 6 | −40 | 280 |
| $32^2$ | | | | | | | | 1 | 0 | −1 | −3 | 3 | 8 | −35 | 210 |
| $41^3$ | | | | | | | | | 1 | 0 | 0 | −4 | −1 | 20 | −210 |
| $321^2$ | | | | | | | | | | 1 | 0 | −6 | −6 | 50 | −420 |
| $2^31$ | | | | | | | | | | | 1 | 0 | −3 | 15 | −105 |
| $31^4$ | | | | | | | | | | | | 1 | 0 | −5 | 70 |
| $2^21^3$ | | | | | | | | | | | | | 1 | −10 | 105 |
| $21^5$ | | | | | | | | | | | | | | 1 | −21 |
| $1^7$ | | | | | | | | | | | | | | | 1 |

## Appendix 3. Partial generating functions for strong embeddings in the body-centred cubic lattice ($b = 1$)

$$F_1 = Y^8$$

$$F_2 = 4Y^{15} + 2Y^{14} - 3Y^{12} - 3Y^8$$

$$F_3 = 28Y^{22} + 16Y^{21} - 2Y^{20} - 40Y^{19} + 12Y^{18} - 15Y^{16} - 8Y^{15} - 24Y^{14} + 24Y^{13} - 6Y^{12} + 12Y^{10} + 3Y^8$$

$$F_4 = 204Y^{29} + 228Y^{28} - 120Y^{27} - 466Y^{26} + 216Y^{25} + 45Y^{24} - 262Y^{23} - 90Y^{22} - 186Y^{21} + 207Y^{20} + 304Y^{19} - 225Y^{18} + 144Y^{17} - 30Y^{16} + 12Y^{15} + 186Y^{14} - 104Y^{13} - 51Y^{12} - 12Y^8$$

$$F_5 = 1562Y^{36} + 2872Y^{35} - 1632Y^{34} - 5440Y^{33} + 1081Y^{32} + 3600Y^{31} - 2704Y^{30} - 4856Y^{29} - 834Y^{28} + 6016Y^{27} + 3096Y^{26} - 2968Y^{25} - 1411Y^{24} + 2568Y^{23} + 384Y^{22} + 1848Y^{21} - 2884Y^{20} - 760Y^{19} + 1476Y^{18} - 992Y^{17} - 405Y^{16} + 96Y^{15} + 200Y^{14} + 48Y^{13} - 96Y^{12} + 72Y^{11} + 60Y^{10} + 3Y^8$$

$$F_6 = 12\,544Y^{43} + 32\,882Y^{42} - 15\,656Y^{41} - 63\,697Y^{40} - 13\,116Y^{39} + 82\,316Y^{38} - 20\,568Y^{37} - 97\,568Y^{36} - 15\,068Y^{35} + 111\,046Y^{34} + 55\,628Y^{33} - 40\,276Y^{32} - 77\,792Y^{31} + 57\,180Y^{30} + 40\,212Y^{29} - 11\,127Y^{28}$$

$$-26\,492\,Y^{27}-27\,200\,Y^{26}+13\,848\,Y^{25}-2262\,Y^{24}+6892\,Y^{23}$$
$$-7758\,Y^{22}-812\,Y^{21}-2200\,Y^{20}+7956\,Y^{19}+8170\,Y^{18}-8952\,Y^{17}+144\,Y^{16}$$
$$+2460\,Y^{15}+342\,Y^{14}-444\,Y^{13}-827\,Y^{12}+264\,Y^{11}-36\,Y^{10}-33\,Y^{8}.$$

## References


Becker H W and Riordan J 1948 *Am. J. Math.* **70** 385-94
Bell E T 1934 *Ann. Math.* **35** 258-77
Bonferroni C E 1936 *Pubblic. Ist Sup. Sc. Ec. Comm. di Firenze* **8** 1-62
Broderick T S 1937 *Proc. Irish Acad.* **44** 19-28
Broggi U 1933 *Ist. Lombardo Rendi. II* **66** 196-202
Craig C C 1928 *Metron* **7** no 4 3-74
de Gennes P G 1976 *Recherche* **7** 919
Domb C 1960 *Adv. Phys.* **9** 149-361
Essam J W 1971 *Discrete Math.* **1** 83-112
—— 1972 *Phase Transitions and Critical Phenomena* vol 2, ed C Domb and M S Green (New York: Academic) ch 6
—— 1980 *Rep. Prog. Phys.* **43** 833-912
Essam J W and Fisher M E 1970 *Rev. Mod. Phys.* (*Suppl.*) **42** 271-88
Ettinghausen A 1826 *Die Combinatorische Analysis* (Vienna)
Fréchet M 1940 *Les probabilités associées à un système d'événements compatibles et dépendants: événements en nombre fini fixe* (Paris: Hermann et Cie)
—— 1943 *Les probabilités associées à un système d'événements compatibles et dépendants: cas particuliers et applications* (Paris: Hermann et Cie)
Geiringer H 1938 *Rev. Math. Union Interbalkanique* **2** 1-26
Ginsburg J 1929 *The Encyclopaedia Britannica* 14th edn *Stirling Numbers*
Golomb W S 1967 *Graph Theory and Theoretical Physics* ed F Harary (New York: Academic) pp 1-41
Good I J 1961 *Ann. Math. Stat.* **32** 535-48
Gumbel E J 1938 *Giorn. Dell'Ist. Ital. degli attuari* (*Rome*) **9** 1-33
Harary F 1967 *Graph Theory and Theoretical Physics* ed F Harary (London: Academic) pp 1-41
Heap B R 1963 *Proc. Phys. Soc.* **82** 252-63
Jordan C 1933 *Giorn. Dell'Ist. Ital. degli attuari* (*Rome*) **4** 505-13
Jordan C 1934 *Acta Sci. Math.* **7** 103-11
Kirkpatrick S 1973 *Rev. Mod. Phys.* **45** 574
Klarner D A 1967 *Can. J. Math.* **19** 851-63
Kubo R 1962 *J. Phys. Soc. Japan* **17** 1100-20
Levin J and Dalton R E 1962 *Math. Comput.* **16** 416-23
Lukacs E 1955 *Am. Math. Mon.* **62** 340-8
Lunnon W F 1971 *Computers in Number Theory* ed A O L Atkin and B J Birch (New York: Academic) pp 347-72
—— 1972 *Graph Theory and Computing* ed R Read (New York: Academic) pp 101-8
MacMahon P A 1915 *Combinatory Analysis I* (Cambridge: CUP)
—— 1916 *Combinatory Analysis II* (Cambridge: CUP)
Margolina A *et al* 1983 *Phys. Rev.* B **28** 1652-4
Martin J L 1974 *Phase Transitions and Critical Phenomena* vol 2 ed C Domb and M S Green (New York: Academic) pp 97-112
Meeron E 1957 *J. Chem. Phys.* **27** 1238-46
Redelmeier D H 1981 *Discrete Math.* **36** 191-203
Riordan J 1946 *Bull. Am. Math. Soc.* **52** 664-7
—— 1958 *An Introduction to Combinatorial Analysis* (New York: Wiley)
Shante V K S and Kirkpatrick S 1971 *Adv. Phys.* **20** 325-57
Sherman S 1964 *J. Math. Phys.* **5** 1137-9
Spitzer F 1956 *Trans. Am. Math. Soc.* **82** 323-39
Stauffer D 1979 *Phys. Rep.* **54** 1-74
Sykes M F 1979 *J. Phys. A: Math. Gen.* **12** 879-92

Sykes M F, Essam J W and Gaunt D S 1965 *J. Math. Phys.* **6** 283–98

Sykes M F, Gaunt D S, Essam J W and Elliott C J 1973a *J. Phys. A: Math. Gen.* **6** 1507–16

Sykes M F, Gaunt D S, Essam J W, Heap B R, Elliott C J and Mattingly S R 1973c *J. Phys. A: Math. 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 1976a *J. Phys. A: Math. Gen.* **9** 97–103

—— 1976b *J. Phys. A: Math. Gen.* **9** 715–24

—— 1976c *J. Phys. A: Math. Gen.* **9** 725–30

Sykes M F, Gaunt D S, Martin J C, Mattingly S R and Essam J W 1973d *J. Math. Phys.* **14** 1071–4

Sykes M F, Gaunt D S, Mattingly S R, Essam J W and Elliott C J 1973e *J. Math. Phys.* **14** 1066–70

Sykes M F and Glen M 1976 *J. Phys. A: Math. Gen.* **9** 87–95

Sykes M F, McKenzie S, Watts M G and Gaunt D S 1975a *J. Phys. A: Math. Gen.* **8** 1461–8

Sykes M F, Watts M G and Gaunt D S 1975b *J. Phys. A: Math. Gen.* **8** 1441–7

—— 1975c *J. Phys. A: Math. Gen.* **8** 1448–60

Teixeira 1880 *Giorn. di Matematica di Battaglini* **18** 301–7

Thiele T N 1903 *Theory of Observations* (London: C and E Layton) (reprinted in 1931 *Ann. Math. Stat.* **2** 165–307)

Uhlenbeck G E and Ford G W 1962 *Studies in Statistical Mechanics* vol 1, Part B, ed J de Boer and G E Uhlenbeck (Amsterdam: North-Holland)

Welsh D J A 1977 *Sci. Prog. Oxford* **64** 65

Whitney H 1932 *Bull. Am. Math. Soc.* **38** 572–9

Wu F Y 1978 *Studies in Foundations and Combinatorics* (*Adv. Math Suppl. Stud.*) vol 1 (New York: Academic) 151