could solve the structures. Clearly, the default settings are not optimal for each individual structure.

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The Enumeration and Symmetry-Significant Properties of Derivative Lattices. II. Classification by Colour Lattice Group

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(*Received* 3 *January* 1992; *accepted* 15 *July* 1992)

Abstract

Dirichlet-series generating functions may be constructed to enumerate the number of colour lattice groups of any order in the triclinic case. Appropriate factorization of the previously known lattice-enumerating functions gives the number of derivative lattices belonging to each of these lattice groups. These numbers are tabulated for all indices up to 20. Based on these Dirichlet functions, asymptotic estimates of the average values of the corresponding arithmetic functions may be made; these are 1.977 for the three-dimensional colour lattice groups of order n and $1.823gh^2$ for the derivative lattices having group structure $C_{fgh}\otimes C_{fg}\otimes C_f$. Such estimates can also be made for the relative abundance of groups with different numbers of cycles in their structure; a single-cycle structure occurs for roughly 92% of all derivative lattices. A similar argument shows that, in over 98% of cases, one properly chosen co-opted term suffices to ensure primitivity in direct methods.

Introduction

The rapidly expanding field of mathematical chemistry, that is the application of graph theory and combinatorics to chemistry, has had considerable impact on organic chemistry and even in inorganic chemistry has developed enough to warrant a recent major review (King, 1992). Despite this, there have been few attempts to apply such approaches to solid-state and crystal chemistry. This series of papers, together with some parallel work on graph-theory approaches to the bond-valence distribution in solids (Rutherford, 1990, 1992*a*), respresents an attempt to redress this situation and explore the potential that mathematical chemistry holds for the enrichment of crystallography.

One important concept of combinatorics is the generating function, where the number of distinct objects with a given property is simply the coefficient of one term in the expansion of that function. The application of power-series generating functions to isomer-counting problems in chemistry derives from Cayley (1874). Their advantages, besides elegance and compactness, lie in their usefulness in deriving statistical information on, and asymptotic estimates of, the number of isomers (or other geometric objects) involved in the enumeration.

Derivative lattices (Billiet & Bertaut, 1983) arise in practice both as real lattices (commensurate super-

0108-7673/93/020293-08$06.00

lattices) and as reciprocal lattices in the consideration of phase-determining techniques and, in particular, problems of rational dependence between large structure factors. In fact, it was originally to gain statistical information for a test of such rational dependence that Dirichlet generating functions were introduced to crystallography (Rutherford, 1992*b*). In that paper, the generating functions were derived to provide, for each Patterson symmetry of the basic lattice, the number of derivative lattices of equal index with the same point-group symmetry. The purpose of this second paper is to extend this approach of using Dirichlet functions to an enumeration of derivative lattices, now in the general case only, but in terms of their classification by colour lattice group (Harker, 1978), rather than just by index. Not only will this provide much more detailed statistical information on the probable occurrence of various group structures in practice, but the author intends in a future publication to show that it leads to a much improved method of attack on those enumeration problems recognized by McLarnan & Moore (1981) as colouring problems, where the N colours representing structural elements ($N<n$) may be arranged according to their full permutation group. It is this situation, rather than the more restricted case of the colour symmetry group for which $n=N$, that is relevant to most counting problems involving structural derivative lattices.

Colour lattice groups

The coloured symmetry groups have been the subject of research for a number of years. A detailed critical review of this area has been provided by Schwarzenberger (1984). However, the specific question of the possible forms taken by their translational subgroups in N colours was only resolved by Harker (1978). He recognized that in three dimensions they were the Abelian groups of stable form $C_{fgh}\otimes C_{fg}\otimes C_f$ of order $N=f^3g^2h$, f, g and h being positive integers. He further described these groups as being of three types, which he classified as follows.

Type I. Here there are no adjacent points of the same colour, $f>1$ and $g>1$, and the group structure comprises the product of three distinct cycles.

Type II. Points all of the same colour are adjacent in one set of parallel lines only, $f=1$ but $g>1$, and the group comprises the product of two distinct cycles.

Type III. Points of the same colour occur in nets in the structure, $f=g=1$, and the group structure comprises a single cycle.

Senechal (1979) placed these ideas within the general context of colour symmetry groups by recognizing that the order k of any colour group must have the form

$$k=\mu\Delta,$$

where μ arises from colour permutations by the symmetry of the basis lattice unit cell and Δ is the determinant of a sublattice of that basic reference lattice. Senechal also recognized that certain number-theoretical constraints applied to the indices of such sublattices, such as

$$\Delta=p^2+q^2 \quad \text{or} \quad \Delta=p^2-pq+q^2$$

for square and hexagonal lattices, respectively. This approach was extended by Jarratt & Schwarzenberger (1980) to provide a list of coloured plane groups for $k\leq 15$.

The colour lattice groups were applied to possible magnetic structures by Kucab (1981), who showed that the number of distinct groups of order n could be enumerated using the Euler generating function

$$\varphi(x)=\prod_{j=1}^{D}(1-x^j)^{-1}=\sum_{r=0}^{\infty}\gamma_D(r)x^r,$$

where $\gamma_D(r)$ is the number of D-nary partitions of r. Here D is the number of dimensions (usually three) and if

$$n=\prod_{i=1}^{l}p_i^{r_i}$$

then the total number of groups is

$$\prod_{i=1}^{l}\gamma_D(r_i).$$

Kucab gives a number of formulae for specific values of D.

Meanwhile, Rolley-Le Coz & Billiet (1980) had examined the triclinic-lattice preservation problem, *i.e.* the equivalence classes of rows and nets of the basic lattice with respect to the translation group of a derivative lattice. This led Rolley-Le Coz, Senechal & Billiet (1983) to consolidate much of this work by showing that the Abelian-group structure is an underlying property of the specific derivative lattice, for the general lattice-preservation problem, irrespective of whether the marks on the individual basis lattice points represent colour, spin or some other relevant property. More recently, Rutherford (1988) investigated similar relationships holding within the reciprocal lattice and found that the essentially identical algebraic structures could be applied, for example, to the symbolic addition phase-determining process.

On the question of the number of distinct derivative lattices of index n for a given basic lattice, the required relationships were established in general by Bertaut & Billiet (1979), and the triclinic case was studied in detail by Billiet & Rolley-Le Coz (1980). The latter expressed their results in terms of restrictions on the possible integral elements of standard triangular transformation matrices of determinant n. The number of such matrices may, in turn, be related to the arithmetic functions that are the coefficients in the Dirichlet series (Rutherford, 1992*b*).

Dirichlet-series generating functions

This paper will make considerable use of special Dirichlet series, *viz* series of the type

$$F(s)=\sum_{n=1}^{\infty} a_n n^{-s},$$

where $F(s)$ is called the generating function of a_n, the corresponding arithmetic function. We shall be interested in cases for which a_n simply enumerates some property associated with the natural number n and in such cases the variable s has no real significance.* The Dirichlet series used in the present work are 'multiplicative' in the number-theory sense, that is the a_n are multiplicative over the primes. In other words,

$$a_m a_n = a_{mn},$$

provided m and n have no common factor. They include the Riemann zeta function

$$\zeta(s)=\sum_{n=1}^{\infty} n^{-s},$$

where a_n takes the value 1 for all n, and its inverse

$$\zeta^{-1}(s)=\sum_{n=1}^{\infty} \mu(n)n^{-s},$$

which involves the Möbius function $\mu(n)$, defined as $\mu(a)=1$ if $a=1$, $\mu(a)=(-1)^r$ if a is the product of r distinct prime factors, *i.e.* if a is square-free, and $\mu(a)=0$ otherwise, *i.e.* if a is divisible by the square of a prime.

Each of these series can also be expressed as an infinite product over the prime numbers, for example

$$\zeta(s)=\prod_{p}(1-p^{-s})^{-1}.$$

We shall also use Dirichlet functions of the type

$$\zeta(s)/\zeta(ks)=\sum_{n=1}^{\infty} q_k(n)n^{-s},$$

which enumerates a function $q_k(n)$, the characteristic function of the set of k-free integers, that is $q_k(n)=0$ if n contains a repeated prime factor of the type p^k and $q_k(n)=1$ otherwise, that is if n is 'k-free'. In particular, $q_2(n)=1$ if n is square-free and $q_2(n)=|\mu(n)|$.

We shall also make use of a general formula to express, in terms of factors of the index n, the arithmetic function enumerated by a product of Dirichlet functions. This requires the introduction of another arithmetic function, $d_k(n)$, the generalized divisor function. This function represents the number of ways that n can be expressed as the product of k factors, any number of which may be unity, and where a different order of the factors is treated as distinct. If the jth such representation of n has the form

$$\prod_{i=1}^{k} c_{ij},$$

a product of Dirichlet functions F_i, which enumerate arithmetic functions f_i, has the expansion

$$\prod_{i=1}^{k} F_i(s)=\sum_{n=1}^{\infty}\sum_{j=1}^{d_k(n)}\left[\prod_{i=1}^{k} f_i(c_{ij})\right]n^{-s}.$$

The techniques of asymptotic estimation used to determine the numbers of the various objects of interest for large values of the lattice index (and colour lattice group order), n, have been taken from Knopfmacher (1990). Knopfmacher is interested in enumeration within algebraic structures known as arithmetic semigroups, which have the properties:

(1) each element has a unique factorization

$$a=p_1^{a_1}p_2^{a_2}p_3^{a_3}\ldots,$$

where the p's are the primes of the system and the a's are positive integers;

(2) there is a real norm such that $|1|=1$, $|p|>1$;

(3) $|ab|=|a||b|$;

(4) the total number of elements of norm $|p|$ is finite.

For an arithmetic semigroup there are many parallels with the prototype system of natural numbers and, in particular, the multiplicative properties of Dirichlet-type generating functions will still be appropriate because of property (3). Thus we shall be interested in establishing whether a particular arithmetic function has a 'zeta formula' that can be applied to derive asymptotic estimates, as it must if it represents the number of elements of an arithmetic semigroup.

The colour lattice groups, being the finite Abelian groups in another guise, do form such an arithmetic semigroup and they are enumerated by a zeta formula, which provides an asymptotic estimate of their number. In fact, the work of Erdös & Sykeres (1935) to resolve this particular problem was a major impetus to the development of this branch of number theory.

As an illustration of the approach, we begin by constructing a generating function that enumerates the isomorphism classes of Abelian groups of order n, given the restriction of there being no more than D overall cycles. This number derives from Kucab (1981), but this alternative way of expressing it is more convenient for the arguments presented below. The total number of such classes, given no dimension

* However, where $F^{-1}(s)$ represents a probability, as in Rutherford (1992*b*), s must take a value for which the Dirichlet series converges.

restriction, is $\prod_{i=1}^{l} \gamma(r_i)$, for

$$n = \prod_{i=1}^{l} p_i^{r_i}.$$

Here $\gamma(r)$ is the total number of partitions of the prime power r. However, since we are restricted to D dimensions, the partition of each prime power in the canonical form of n into at most D parts is allowed. The corresponding Euler generating function that enumerates such a partition of a number is

$$\varphi(x) = \prod_{j=1}^{D} (1-x^j)^{-1} = \sum_{r=0}^{\infty} \gamma_D(r) x^r,$$

where $\gamma_D(r)$ is the number of partitions of r into at most D parts. Now we may substitute p^{-s} for x, where p represents any prime number. This gives

$$[(1-p^{-s})(1-p^{-2s})\dots(1-p^{-Ds})]^{-1}$$
$$= 1 + \sum_{a=1}^{\infty} \gamma_D(a) p^{-as}.$$

We now use this expression to create the multiplicative function we require as a product over the primes:

$$\prod_p [(1-p^{-s})(1-p^{-2s})\dots(1-p^{-Ds})]^{-1}$$
$$= \prod_p \left[1 + \sum_{a_i=1}^{\infty} \gamma_D(a_i) p^{-a_i s}\right],$$

which gives, by application of the fundamental theorem of arithmetic,

$$1 + \sum_{n=2}^{\infty} \left\{\prod_{p_i|n} [\gamma_D(a_i)]\right\} n^{-s},$$

where $n = \prod_p p_i^{ai}$. This shows that this generating function does indeed enumerate the required arithmetic function. However, we can convert this product form to a simple product of zeta functions,

$$\prod_p [(1-p^{-s})(1-p^{-2s})\dots(1-p^{-Ds})]^{-1}$$
$$= \prod_p (1-p^{-s})^{-1} \prod_p (1-p^{-2s})^{-1} \dots \prod_p (1-p^{-Ds})^{-1}$$
$$= \zeta(s)\zeta(2s)\dots\zeta(Ds).$$

We next look at the lattices themselves. We can derive an arithmetic function based on the Billiet & Rolley-Le Coz (1980) matrix formulation and the factorization scheme introduced above, now limited to D terms. The required arithmetic function is

$$\sum_{j=1}^{d_D(n)} \left[\prod_{i=1}^{D} c_{ij}^{i-1}\right]$$

if the jth representation of n has the form

$$\prod_{i=1}^{D} c_{ij}.$$

The number of such lattices is enumerated by (Rutherford, 1992*b*)

$$\prod_{i=1}^{D} \zeta(s-i+1),$$

that is, $\zeta(s)\ \zeta(s-1)$ for $D=2$ and $\zeta(s)\ \zeta(s-1) \times \zeta(s-2)$ for $D=3$.

Since these systems of lattices are again enumerated by zeta formulae, we might ask the question whether they also each form an arithmetic semigroup. This is not the case, for although multiplicative in the primes, such a system does not exhibit unique factorization within the powers of one prime number. This is precisely where the difficulties in the application of the inclusion/exclusion principle arose in Rutherford (1992*b*).

Thus we have a system (the lattices) that is classified by another system (the colour lattice groups), both of which are enumerated by a zeta formula with D factors. It remains to derive such generating functions for the number of lattices in each class. Like Rutherford (1992*b*), we examine the very simple one-dimensional case first and subsequently the more complex cases.

One-dimensional case

The number of one-dimensional lattices of index n is one only for each n and is therefore enumerated by

$$\zeta(s) = \sum_{n=1}^{\infty} 1 \times n^{-s}.$$

Since there is only one lattice for each n, there can be only one structure, which is that of the cyclic group C_n. This is consistent with the number of such groups being enumerated by

$$\zeta(s)\zeta(2s)\dots\zeta(Ds) = \zeta(s) = \sum_{n=1}^{\infty} 1 \times n^{-s}$$

for $D=1$.

Two-dimensional case

The number of distinct algebraic structures in two dimensions is given by the expansion of $\zeta(s)\zeta(2s)$, which is

$$1+2^{-s}+3^{-s}+2\times 4^{-s}+\dots+6^{-s}+\dots+2\times 8^{-s}$$
$$+2\times 9^{-s}+\dots+2\times 12^{-s}+\dots+3\times 16^{-s}+\dots$$
$$+2\times 18^{-s}+\dots+2\times 24^{-s}+\dots+2\times 27^{-s}+\dots$$
$$+3\times 32^{-s}+\dots+4\times 36^{-s}+\dots.$$

Here only those leading terms that involve powers of the primes 2 and 3 only have been included to show the general nature of the terms. The structures comprise all possibilities of the type $C_{n/f}\otimes C_f;\ f^2|n$. For example, when n is 4, 32 and 36, the possible structures are, respectively,

$$C_4 \text{ and } C_2 \otimes C_2;$$

$$C_{32}, C_{16} \otimes C_2 \text{ and } C_8 \otimes C_4;$$

$$C_{36}, C_{18} \otimes C_2, C_{12} \otimes C_3 \text{ and } C_6 \otimes C_6.$$

Harker (1978) tabulates all the possibilities for $n \leq 50$.

As for the number of lattices, we note that the function $d_2(n)$, which denotes the range of the inner summation, is simply the number of divisors of n and therefore the arithmetic function corresponding to a product of two Dirichlet functions is of the form

$$\sum_{d|n} f_1(d) f_2(n/d) = \sum_{d|n} f_1(n/d) f_2(d).$$

Hence the function that enumerates the lattices of index n is

$$\zeta(s)\zeta(s-1) = \sum_{n=1}^{\infty} \left[\sum_{d|n} 1 \times (n/d) \right] n^{-s}$$

$$= \sum_{n=1}^{\infty} \sigma_1(n) n^{-s},$$

since the sum over divisors reduces to $\sigma_1(n)$, the sum of the divisors of n.

Now we have to identify how the overall $\sigma_1(n)$ lattices are distributed over the possible structures. This breakdown depends on the arithmetic function $q_2(n)$, which is generated by $\zeta(s)\zeta^{-1}(2s)$. If we write

$$\zeta(s)\zeta(s-1) = [\zeta(s)\zeta^{-1}(2s) \times \zeta(s-1)]\zeta(2s),$$

we can interpret the multiplication by $\zeta(2s)$ as representing an expansion in both directions by some factor f of a lattice of index n/f^2 and group structure C_{n/f^2}, to generate a structure $C_{n/f} \otimes C_f$.

The term in the square brackets above, taken alone, enumerates a function

$$\sum_{d|n} (n/d) q_2(d),$$

which is the number of distinct lattices belonging to a given colour lattice group. We shall call this number the class size and so we find that the various class sizes for a fixed n are given by the identity

$$\sigma_1(n) = \sum_{f^2|n} \sum_{d|(n/f^2)} (n/df^2) q_2(d).$$

For example, for $n = 12$, we find the corresponding values of f to be 1 and 2. For $f = 1$, corresponding to C_{12}, we have

$$\sum_{d|12} q_2(d)(12/d) = 0 \times 1 + 1 \times 2 + 0 \times 3 + 1 \times 4$$

$$+ 1 \times 6 + 1 \times 12 = 24$$

and, for $f = 2$ ($C_6 \otimes C_2$), we have

$$\sum_{d|3} q_2(d)(3/d) = 1 \times 1 + 1 \times 3 = 4,$$

which together make

$$\sigma_1(12) = 28.$$

The effect of the arithmetic function on the right-hand side is to partition the divisors of n, expressed in the form n/df^2, according to the value of f for which d is square-free. Some results are given in Table 1.

Table 1. *The number of derivative nets belonging to each two-dimensional colour-lattice group of structure $C_{n/f} \otimes C_f$, $f^2 | n$, and order $n \leq 20$*

n	f	Number of nets	Total
2	1	3	3
3	1	4	4
4	1	6	
	2	1	7
5	1	6	6
6	1	12	12
7	1	8	8
8	1	12	
	2	3	15
9	1	12	
	3	1	13
10	1	18	18
11	1	12	12
12	1	24	
	2	4	28
13	1	14	14
14	1	24	24
15	1	24	24
16	1	24	
	2	6	
	4	1	31
17	1	18	18
18	1	36	
	3	3	39
19	1	20	20
20	1	36	
	2	6	42

Three-dimensional case

Here the structures comprise all possibilities of the type

$$C_{n/f^2g} \otimes C_{fg} \otimes C_f;\ f^3 | n,\ g^2 | n/f^3,$$

while the function that enumerates the lattices of index n is

$$\zeta(s)\zeta(s-1)\zeta(s-2) = \sum_{n=1}^{\infty} \left[\sum_{d|n} (n/d)^2 \sigma_1(d) \right] n^{-s}.$$

The breakdown by colour lattice group now depends on both $q_2(n)$, as before, and a new arithmetic function, $q_3(n)$, which is generated by $\zeta(s)\zeta^{-1}(3s)$. We must now write

$$\zeta(s)\zeta(s-1)\zeta(s-2)$$
$$= \{[\zeta(s)/\zeta(3s)][\zeta(s-1)/\zeta(2s-2)]\zeta(s-2)\}$$
$$\times \zeta(2s-2)\zeta(3s).$$

We now have two types of expansion from a one-cycle structure to consider. These are the expansion in one net by a factor g in each direction, represented by

$\zeta(2s-2)$, and an expansion by a factor f in all three dimensions, given by $\zeta(3s)$. The term in the bracket above now enumerates a function,

$$\sum_{j=1}^{d_3(n)} q_3(c_{ij})q_2(c_{2j})c_{2j}c_{3j}^2,$$

by use of the formalism as before, and so we now have the enumerating identity

$$\sum_{d|n}(n/d)^2\sigma_1(d)=\sum_{f^3|n}\sum_{g^2|(n/f^3)} g^2\sum_{j=1}^{d_3(n/f^3g^2)} q_3(c_{ij})\times q_2(c_{2j})c_{2j}c_{3j}^2.$$

We may now write the class size as

$$S(n,f,g)=g^2\sum_{j=1}^{d_3(n/f^3g^2)} q_3(c_{ij})q_2(c_{2j})c_{2j}c_{3j}^2,$$

where the factor g^2 arises from the multiplication by the function $\zeta(2s-2)$, since

$$\zeta(2s-2)=1+4\times 2^{-2s}+9\times 3^{-2s}+16\times 4^{-2s}+\dots.$$

For example, we have three possible structures for $n=24$, C_{24}, $C_{12}\otimes C_2$ and $C_6\otimes C_2\otimes C_2$. In each case, we run through the factorization of $k=(n/f^3g^2)$ in the sequence $1\times 1\times k\dots 1\times k\times 1\dots k\times 1\times 1$.

C_{24}. Here, $f=g=1$ and

$$\begin{aligned}S(24,1,1)&=1^2\sum_{j=1}^{d_3(24)} q_3(c_{ij})q_2(c_{2j})c_{2j}c_{3j}^2\\&=1^2(576+288+192+0+96+0+0\\&\quad+0+144+72+48+0+24+0+64\\&\quad+32+0+0+36+18+12+6+16\\&\quad+8+0+0+0+4+2+0)\\&=1638.\end{aligned}$$

$C_{12}\otimes C_2$. Here, $f=1$ and $g=2$ and

$$\begin{aligned}S(24,1,2)&=2^2\sum_{j=1}^{d_3(6)} q_j(c_{ij})q_2(c_{2j})c_{2j}c_{3j}^2\\&=2^2(36+18+12+6+9+3+4+2+1)\\&=364.\end{aligned}$$

$C_6\otimes C_2\otimes C_2$. Here, $f=2$ and $g=1$ and

$$\begin{aligned}S(24,2,1)&=1^2\sum_{j=1}^{d_3(3)} q_3(c_{ij})q_2(c_{2j})c_{2j}c_{3j}^2\\&=1^2(9+3+1)\\&=13.\end{aligned}$$

The total number of lattices of index 24 is

$$\sum_{d|24}(24/d)^2\sigma_1(d)=2015=1638+364+13.$$

Some results are given in Table 2.

Table 2. *The number of derivative lattices belonging to each three-dimensional colour-lattice group of structure $C_{n/f^2g}\otimes C_{fg}\otimes C_f$, $f^3|n$, $g^2|(n/f^3)$, and order $n\le 20$*

n	f, g	Number of lattices	Total
2	1, 1	7	7
3	1, 1	13	13
4	1, 1	28	
	1, 2	7	35
5	1, 1	31	31
6	1, 1	91	91
7	1, 1	57	57
8	1, 1	126	
	1, 2	28	
	2, 1	1	155
9	1, 1	117	
	1, 3	13	130
10	1, 1	217	217
11	1, 1	133	133
12	1, 1	364	
	1, 2	91	455
13	1, 1	183	183
14	1, 1	399	399
15	1, 1	403	403
16	1, 1	504	
	1, 2	124	
	1, 4	16	
	2, 1	7	651
17	1, 1	307	307
18	1, 1	819	
	1, 3	91	910
19	1, 1	381	381
20	1, 1	868	
	1, 2	217	1085

Asymptotic estimation

Knopfmacher (1990) gives a number of formulae for the asymptotic estimation of arithmetic functions enumerated by Dirichlet series, which include error estimates. We shall ignore the error estimates. The formula we shall apply is that

$$F(s)=\zeta(s-w)\prod_i f_i(s)$$

enumerates an arithmetic function having asymptotic density

$$n^w\prod_i f_i(w+1),$$

provided each Dirichlet function f_i is absolutely convergent for the argument $(w+1)$. In fact, since the cases we are considering involve only zeta functions, they have the form

$$F(s)=\zeta(s-w)\prod_i \zeta[a_i(s-b_i)],$$

which corresponds to the asymptotic density

$$n^w\prod_i \zeta[a_i(w-b_i+1)]$$

provided $a_i\ge 1$ and $0\le b_i\le w$ for all i.

The first result we require is one that refers to the number of classes of Abelian groups. This result was derived by Erdös & Sykeres (1935),

$$\prod_{r=2}^{\infty} \zeta(r) = 2.29485\ldots$$

in the unrestricted case or

$$\prod_{r=2}^{D} \zeta(r)$$

when the group structure is restricted to at most D cycles. Specific values of interest are

$$\zeta(2) = \pi^2/6 = 1.64493\ldots; \qquad D = 2$$

and

$$\zeta(2)\zeta(3) = 1.97730\ldots; \qquad D = 3.$$

The number of lattices of given index involves a product of zeta functions for which the smallest argument is $s-D+1$ and therefore we expect the asymptotic density to be proportional to n^{D-1}. In fact, it is

$$n^{D-1} \prod_{r=2}^{D} \zeta(r).$$

These results show that the average class size is n^{D-1}.

However, we may refine this estimate considerably, for it is clear from Table 1 that, for given n, the class size decreases as f increases. This arises because each lattice having a structure with $f > 1$ derives from one with $f = 1$ by the expansion explicit in the function $\zeta(2s)$. Thus the class size is independent of the factor f and can be derived by consideration of the single-cycle ($f = 1$) structures only. As we saw above, the number of lattices of index n and structure C_n in the two-dimensional case is enumerated by

$$\zeta(s)\zeta^{-1}(2s)\zeta(s-1) = \sum_{n=1}^{\infty} \left[\sum_{d|n} (n/d) q_2(d) \right] n^{-s}.$$

The function on the left gives the asymptotic density

$$n\zeta(2)/\zeta(4) = (15/\pi^2)n = 1.51982\ldots \times n.$$

Now, to take all values of f into account, we simply replace n by its other factor h and find the asymptotic average of the class size to be

$$1.51982\ldots \times h.$$

However, the actual class size will vary considerably about this average, being a minimum when h is prime and relatively large when h has many factors.

We now examine the distribution of lattices among groups of one cycle, two cycles and so on. The results show that in two dimensions the proportion of lattices with a one-cycle colour lattice group structure is

$$\zeta^{-1}(4) = 90/\pi^4 = 0.92394\ldots.$$

Extension of this argument gives, for D dimensions, a number of one-cycle lattices

$$n^{D-1} \prod_{r=2}^{D} \zeta(r)/\zeta(r^2)$$

and the relative density of one-cycle colour lattice groups

$$\prod_{r=2}^{D} \zeta^{-1}(r^2).$$

This latter formula can be extended to the limit of large D,

$$\prod_{r=2}^{\infty} \zeta^{-1}(r^2) = 0.92207\ldots.$$

For $D = 3$, the values are $1.82324\ldots \times n^2$ and $0.92209\ldots$. Similarly, an investigation of the variation in class sizes in three dimensions gives, for the average, the formula

$$\{[\zeta(2)\zeta(3)]/[\zeta(4)\zeta(9)]\}gh^2 = 1.82324\ldots \times gh^2,$$

where the actual class size relative to this average depends on the number of factors of g and h.

In three dimensions, the above approach may be extended in another way. The lattices in three dimensions that do not have a colour lattice group of three distinct cycles is enumerated by

$$\{[\zeta(s)/\zeta(3s)][\zeta(s-1)/\zeta(2s-2)]\zeta(s-2)\}\zeta(2s-2)$$

or

$$[\zeta(s)/\zeta(3s)]\zeta(s-1)\zeta(s-2).$$

The arithmetic function has asymptotic density

$$n^2\zeta(2)\zeta(3)/\zeta(9)$$

and the proportion of lattices in this category is

$$\zeta^{-1}(9) = 0.99800\ldots.$$

This indicates that the three types of three-dimensional colour lattices occur in the ratio

$$\text{type I} : \text{type II} : \text{type III} = 0.00200 : 0.01447 : 0.92209.$$

An application to direct methods

The results for this general case can be applied equally readily to the reciprocal lattice, although the two may not be the same for specific higher symmetries that involve centrings. Rutherford (1988) has suggested that the process of origin determination in direct methods of phase determination can be considered as imposing a structure equivalent to the colour-lattice structure of a derivative lattice, in terms of which the symbolic addition process is modular. After origin determination (and enantiomorph selection where appropriate), it is necessary to introduce additional phased reflections, the 'co-opted terms', to ensure the primitivity of the starting set used.* It is generally

* See Rogers (1980) for a good explanation of this.

understood that more than one such term may be required, although typically examples used require only one. This section is intended to show the probabilities associated with the minimum necessary number of such terms in the triclinic case.

Since the same colour translation groups apply to the reciprocal lattice as to the direct lattice, their number and relative frequency will be given by the same formulae as above with the assumption that a typical data set is large enough for the asymptotic formulae to be closely approximated. We can also make the correlation that if a lattice belongs to a colour group comprising one cycle only it will require one co-opted term and if two cycles, two terms *etc.* However, the reciprocal sublattice imposed by the defining trio in the phase-determining process must be of odd index to resolve the origin ambiguity. In such a case we must eliminate the prime 2 from our formulae, by making use of the prime-product form

$$\zeta(s)=\prod_p (1-p^{-s})^{-1},$$

with any function $\zeta(s)$ replaced by

$$\prod_{p\neq 2} (1-p^{-s})^{-1} \quad \text{or} \quad (1-2^{-s})\zeta(s).$$

This is analogous to the handling of centred lattices by Rutherford (1992*b*). For example, while the proportion of all integers that are square-free is

$$\zeta^{-1}(2)=6/\pi^2=0.60792\ldots,$$

the proportion of odd integers that are square-free is

$$[(1-2^{-2})\zeta(2)]^{-1}=8/\pi^2=0.81057\ldots.$$

On this basis, the asymptotic average number of triclinic derivative lattices of odd index is

$$\tfrac{3}{4}\times\tfrac{7}{8}\zeta(2)\zeta(3)n^2$$

and, since the fraction of integers that are odd is $\frac{1}{2}$, the fraction of all lattices having odd index is

$$\tfrac{1}{2}\times\tfrac{3}{4}\times\tfrac{7}{8}\zeta(2)\zeta(3)n^2/\zeta(2)\zeta(3)n^2=\tfrac{1}{2}\times\tfrac{3}{4}\times\tfrac{7}{8}=0.328125.$$

Examination of the lower part of Table 2 shows that this ratio is approximated there.

To return to the co-opted terms, the expression $[\zeta(4)\zeta(9)]^{-1}$ becomes $(16/15)\times(512/511)$ $[\zeta(4)\zeta(9)]^{-1}$ and $\zeta^{-1}(9)$ becomes $(512/511)\zeta^{-1}(9)$. When evaluated, these modified expressions give the ratio for the cases of a minimum of one co-opted term, or of two or of three, to be

$$0.98548:0.01447:0.00005.$$

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Representations of Point Groups Spanned by Sets of Equivalent Bipoints or Multipoints

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(*Received* 16 *June* 1992; *accepted* 17 *July* 1992)

Abstract

The properties of the representations of the three-dimensional point groups spanned by sets of equivalent bipoints are studied (characters and reductions); these representations are either principal induced representations or monomial representations induced by the subgroups (stabilizer subgroups and

0108-7673/93/020300-06$06.00