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The Crystallographic Restriction in Higher Dimensions*

BY HOWARD HILLER†

Department of Mathematics, Columbia University, New York, NY 10027, USA

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Abstract

The crystallographic restriction in dimensions two and three is generalized to arbitrary dimensions. It is shown that m can occur as the order of an element of the point group of an n-dimensional space group if and only if $\Phi(m) \leq n$ where Φ is an additive version of Euler's totient function. A table of these allowable orders in dimensions ≤ 23 is provided.

Introduction

A fundamental theorem of mathematical crystallography limits the possible orders of elements in the point groups of two- and three-dimensional space groups to 2, 3, 4 or 6. Coxeter (1973) attributes the original geometric proof to Barlow. A trigonometric proof is given, for example, in Rees (1983). None of these techniques readily generalizes to higher dimensions and a more algebraic approach is required. The recent work of Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (1978) emprically extends the possible orders of rotations in dimension 4 to include orders 5, 8, 10 and 12.

Schwarzenberger (1980) attempted to extend the crystallographic restriction to higher dimensions. He claimed that the order m of an element of a point group of an n-dimensional space group must satisfy $\varphi(m) \leq n$, where $\varphi(.)$ denotes Euler's totient function (see below). In fact, this is true for irreducible elements (*i.e.* elements that do not leave invariant a sublattice of smaller dimension) and goes back to the work of Hermann (1949). Schwarzenberger failed to treat the reducible case. We show how to handle this situation and hence give a complete generalization of the crystallographic restriction.

The required change in the statement is the replacement of the standard Euler totient function by an 'additive' version of it. We describe the classical Euler function φ and this modification Φ in § 1. We also prove there the main result (theorem 1.5). The techniques involved are taken from elementary linear algebra and elementary number theory. In § 2 we give a table of these results for dimensions up to 23.

1. Euler functions

The classical totient function of Euler is defined by

(1.0) $\varphi(m)$ = the number of k, $0 < k < m$, which are relatively prime to m.

One can phrase this definition somewhat more abstractly. Let C_m denote the ring of integers modulo m. If R^* denotes the (multiplicatively) invertible elements of a ring R, then $\varphi(m)$ denotes the size of C_m^*. It is easy to check that $\varphi(.)$ is determined by the following two rules:

(1.1) (i) if p is a prime, then

$$\varphi(p^k) = p^k - p^{k-1} = p^k(1-1/p);$$

(ii) if m and m' are relatively prime, then

$$\varphi(mm') = \varphi(m)\varphi(m').$$

Hence if m has a prime decomposition $m = p_1^{k_1} \ldots p_s^{k_s}$ (we always assume that $p_1 < p_2 < \ldots < p_s$), then

$$\begin{aligned}\varphi(m) &= \varphi(p_1^{k_1}) \ldots \varphi(p_s^{k_s}) \\ &= p_1^{k_1}(1-1/p_1) \ldots p_s^{k_s}(1-1/p_s) \\ &= m \prod_{p|m} (1-1/p).\end{aligned}$$

We now define a new additive version $\Phi(.)$ of the Euler function. It agrees with the ordinary φ function for prime powers, *i.e.* satisfies (1.1i) but (1.1ii) is replaced by

(ii′) If m and m' are relatively prime then

$$\Phi(mm') = \Phi(m) + \Phi(m')$$

unless $m = 2$ and n is odd, in which case $\Phi(2n) = \Phi(n)$.

We let $GL(n, \mathbb{Z})$ denote the group of integral $n \times n$ matrices A whose inverses exist and are also integral. This last condition is equivalent to $\det(A) = \pm 1$. We recall that the order of a matrix A is the smallest integer m so that $A^m = I$, the identity matrix. We now consider the following function.

(1.2) $g(m)$ = the smallest n so that $GL(n, \mathbb{Z})$ contains a matrix of order m.

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Our first observation is that our problem reduces to computing $g(m)$.

(1.3) *Proposition.* $g(m)$ is the smallest dimension of a space group whose point group contains an element of order m.

Proof. Firstly suppose A is a square matrix of size $n=g(m)$ and order m given by the definition (1.2). Then A defines a faithful integral representation of C_m on a free Abelian group $\mathbb{Z}^n$. We can then let the space group G be simply the semidirect product $\mathbb{Z}^n \circ C_m$, with point group C_m. This is simply the symmorphic space group corresponding to the arithmetic crystal class $(C_m, \mathbb{Z}^n)$.

Conversely, if G is a space group whose point group H contains an element x of order m then the faithful representation $f: H \to \mathrm{Aut}(T)$ of H on the lattice T produces a matrix $A=f(x)$ that satisfies the requirements of (1.2).

We recall that a complex number ζ is an *mth root of unity* if $\zeta^m=1$ [for example, $\zeta=\exp(2\pi i/m)$]. If m is the smallest such number, then m is called the *period* of ζ and ζ is called a *primitive* mth root of unity. There are $\varphi(m)$ primitive mth roots of unity. We turn now to the calculation of $g(m)$. We have the following easy but important lemma:

(1.4) *Lemma.* If a primitive mth root of unity ζ is an eigenvalue of an integral $n \times n$ matrix A, then all the primitive mth roots of unity are eigenvalues of A. In particular, $n \geq \varphi(m)$.

Proof. The characteristic polynomial of $A=\det(xI-A)$ is integral and hence is invariant under permutation of the primitive roots of unity. As ζ is a root, the result follows.

The main result is:

(1.5) *Theorem.* $g(m)=\Phi(m)$.

Proof. It suffices to show that $g(m)$ satisfies the properties (1.1i) and (ii′) above. Clearly if m is odd $g(2m)=g(m)$, by considering the matrix $-A$.

Next we observe that $g(m) \leq \varphi(m)$ by considering the ring of integers in a cyclotomic field, *i.e.* the rational numbers extended by the mth roots of unity. This is a lattice that admits the primitive mth roots of unity as an integral basis and the matrix representing multiplication by $\exp(2\pi i/m)$ proves the observation.

Suppose that A in $GL(n, \mathbb{Z})$ has order m, where $n=g(m)$. Since every matrix of finite order is diagonalizable over the complex numbers, A is conjugate in $GL(n, \mathbb{C})$ to

$$\begin{pmatrix} \zeta_1 & & & \\ & \zeta_2 & & \\ & & \ddots & \\ & & & \zeta_n \end{pmatrix}.$$

Now if m is a prime power p^k one can demonstrate the statement of the theorem by observing that one eigenvalue ζ_i of the matrix must be a primitive p^kth root of unity and then invoking (1.4).

Hence we are reduced to considering the case where $m=p_1^{k_1}\ldots p_s^{k_s}$ where we can assume that if $p_1=2$, then $k_1>1$. We must show

$$n \geq \sum_{i=1}^{s} \varphi(p_i^{k_i}).$$

Suppose ζ_1 is a primitive m_1th root of unity and m_1 is divisible by some $p_i^{k_i}$, $1 \leq i \leq s$. (Otherwise move on to ζ_2.) Suppose

$$m_1 = \left(\prod_{i \in I_1} p_i^{k_i}\right) n_1.$$

Now remove all the primitive m_1th roots of unity from the multiset of eigenvalues $\zeta_1, \ldots, \zeta_n$ and repeat this procedure for the ζ_i remaining with lowest index. One generates a sequence $m_1, \ldots, m_t$ with, say,

$$m_j = \left(\prod_{i \in I_j} p_i^{k_i}\right) n_j$$

and no p_i, $i \in I_j$, dividing into n. Since A has order m,

$$I_1 \cup \ldots \cup I_t = \{1, 2, \ldots, s\}. \qquad (*)$$

Hence:

$$\begin{aligned} g(m) = n &\geq \varphi(m_1) + \ldots + \varphi(m_t) && \text{by (1.4)} \\ &\geq \varphi\left(\prod_{i \in I_1} p_i^{k_i}\right) + \ldots + \varphi\left(\prod_{i \in I_t} p_i^{k_i}\right) && \text{by (1.1ii)} \\ &= \prod_{i \in I_1} \varphi(p_i^{k_i}) + \ldots + \prod_{i \in I_t} \varphi(p_i^{k_i}) && \text{by (1.1ii)} \\ &\geq \sum_{i \in I_1} \varphi(p_i^{k_i}) + \ldots + \sum_{i \in I_t} \varphi(p_i^{k_i}) \\ &\geq \sum_{i=1}^{s} \varphi(p_i^{k_i}) && \text{by (*)}. \end{aligned}$$

The penultimate inequality follows from the fact that $\prod a_i \geq \sum a_i$, if all $a_i > 1$. This hypothesis is guaranteed by our assumption on n. This completes the proof.

Remarks. The following two comments were suggested by the referee.

1. An alternative proof of (1.6) can be constructed using well known properties of the *cyclotomic polynomials* $f_d(T)$. We recall that these polynomials can be defined in the following way (see Lang, 1971). Let

$$f_d(T) = \prod_{\mathrm{period}(\zeta)=d} (T-\zeta)$$

so that

$$T^m - 1 = \prod_{d \mid m} f_d(T).$$

Certainly $f_1(T)=T-1$ and the $f_m(T)$ can then be

defined recursively by

$$f_m(T) = (T^m - 1) \Big/ \prod_{\substack{d|n \\ d<n}} f_d(T).$$

For example, if p is a prime then $f_p(T) = 1 + T + T^2 + \ldots + T^{p-1}$. For prime powers p^k, $f_{p^k}(T) = f_p(T^{p^{k-1}})$. Each cyclotomic polynomial $f_d(T)$ has degree $\varphi(d)$ and is irreducible over the rational numbers.

Suppose A in $GL(n, \mathbb{Z})$ has order m. Then since the minimal polynomial $M_A(T)$ of A divides into the characteristic polynomial of A (Cayley-Hamilton theorem) of degree n: $\deg(M_A) \leq n$. Since $A^m = I$, M_A divides into $T^m - I = \prod_{d|m} f_d(T)$. Since the cyclotomic polynomials are irreducible:

$$M_A(T) = f_{d_1}(T) \ldots f_{d_r}(T)$$

for some divisors $d_1, \ldots, d_r$ of m. We claim now that m is the least common multiple of $d_1, \ldots, d_r$. If d divides into N, $1 \leq i \leq r$, then $M_A(T)$ divides into $\prod_{d|N} f_d(T) = X^N - 1$. But then $A^N = I$, so m divides into N, since m is the order of A. In particular m divides into the product $d_1 \ldots d_r$ and we get:

$$n \geq \deg(M_A) = \sum_{i=1} \varphi(d_i) = \Phi(d_1 \ldots d_r) \geq \Phi(m).$$

This completes the argument.

2. One can define a function $\bar{g}(.)$ by replacing $GL(n, \mathbb{Z})$ by $SL(n, \mathbb{Z})$ in the definition of $g(.)$. If one defines a function $\bar{\Phi}$ by deleting the clause 'unless ...' in the definition (ii') of $\Phi(m)$, then one also has $\bar{g}(m) = \bar{\Phi}(m)$.

2. Computations

Fix a dimension n and let Ord (n) denote the set of natural numbers that occur as orders of elements in the point groups of n-dimensional space groups. For example, we have Ord (2) = Ord $(3) = \{1, 2, 3, 4, 6\}$. According to (1.5)

$$\text{Ord}(n) = \{m: \Phi(m) \leq n\}, \tag{2.0}$$

where $\Phi(.)$ denotes the additive Euler function of § 1. In particular, Ord $(n) \subseteq$ Ord $(n+1)$ and we also have the following generalization of Ord (2) = Ord (3):

(2.1) *Proposition.* Ord $(2n)$ = Ord $(2n+1)$, for all $n \geq 1$.

Proof. It is an easy consequence of the definition of $\Phi(.)$ that $\Phi(k)$ is even, $k > 2$. Hence the result follows from (2.0).

Hence to enumerate the elements of Ord (n), it suffices to understand ord (n) = Ord (n) − Ord $(n-1) = \{m: \Phi(m) = n\}$, for even $n \geq 2$. Note that by (2.1) ord (n) is empty for odd n greater than one. In addition ord $(1) = \{2\}$ and for convenience we set ord $(0) = \{1\}$. The following result facilitates the computation of ord (n).

Table 1. *Computation of ord* (n)

(p, k) entry $= p^k - p^{k-1}$.

p \ k	1	2	3	4
3	2	6	18	54
5	4	20	100	
7	6	42		
11	10			
13	12			
17	16			
19	18			
23	22			
⋮	⋮			
101	100			

Table 2. *Generation of values of ord* (n) *from Table* 1

ord $(n) = \{m: \Phi(m) = n\}$.

n	ord (n)
0	1
1	2
2	3, 4, 6
4	5, 8, 10, 12
6	7, 9, 14, 15, 18, 20, 24, 30
8	16, 21, 28, 36, 40, 42, 60
10	11, 22, 35, 45, 48, 56, 70, 72, 84, 90, 120
12	13, 26, 33, 44, 63, 66, 80, 105, 126, 140, 168, 180, 210
14	39, 52, 55, 78, 88, 110, 112, 132, 144, 240, 252, 280, 360, 420
16	17, 32, 34, 65, 77, 99, 104, 130, 154, 156, 198, 220, 264, 315, 336, 504, 630, 840
18	19, 27, 38, 51, 54, 68, 91, 96, 102, 117, 176, 182, 195, 231, 234, 260, 312, 390, 396, 440, 462, 560, 660, 720, 1260
20	25, 50, 57, 76, 85, 108, 114, 136, 160, 170, 204, 273, 364, 385, 468, 495, 520, 528, 546, 616, 770, 780, 792, 924, 990, 1008, 1320, 1680, 2520
22	23, 46, 75, 95, 100, 119, 135, 143, 150, 152, 153, 190, 216, 224, 228, 238, 270, 286, 288, 306, 340, 408, 455, 480, 585, 624, 693, 728, 880, 910, 936, 1092, 1155, 1170, 1386, 1540, 1560, 1848, 1980, 2310

(2.2) *Proposition.* For all $n > 1$

$$\text{ord}^+(2n) = 2\,\text{ord}^-(2n) \cup \bigcup_k 2^{k+1}\,\text{ord}^-(2n - 2^k),$$

where k satisfies $k \geq 1$ and $2^k \leq 2n$.

Proof. If m is in ord$^+$ $(2n)$ but not in 2 ord$^-$ $(2n)$, then m contains a $(k+1)$th power of 2, $k \geq 1$, and $\Phi(m) = 2n$. Hence $m = 2^{k+1}s$, where s is odd, so clearly $\Phi(s) = \Phi(m) - \Phi(2^{k+1}) = 2n - 2^k$ and the result follows.

This result reduces the computation of ord (n) to its odd elements. Suppose we want to find the set ord (100). In order to exploit (2.2) we make a table with rows labelled by the prime numbers $p > 2$, columns labelled by the natural numbers $k \geq 1$ and whose (p, k) entry is $p^k - p^{k-1}$. To calculate ord$^-$ (100), we need only that part of the table containing values ≤ 100. This turns out to be quite small; see Table 1.

Starting with ord (2) = {3, 4, 6} and observing from Table 1 that ord$^-$ (4) = {5}, we get

$$\text{ord}^+(4) = 2\,\text{ord}^-(4) \cup 4\,\text{ord}^-(2) \cup 8\,\text{ord}^-(0) = \{8, 10, 12\}.$$

Hence

$$\text{ord}(4) = \text{ord}^+(4) \cup \text{ord}^-(4) = \{5, 8, 10, 12\}.$$

This result is consistent with the enumeration of the four-dimensional space groups given by Brown *et al.* (1978).

Continuing in this fashion one can generate the values for dimensions $n \leq 100$ using Table 1 alone. We have done this for $n \leq 23$ in Table 2.

It is interesting to observe that the first example where the maximum of the allowable new orders does not increase occurs in going from dimensions 20 to 22.

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Direct Methods and Superstructures. I. Effects of the Pseudotranslations on the Reciprocal Space

BY G. CASCARANO, C. GIACOVAZZO AND M. LUIĆ*

Dipartimento Geo-Mineralogico, Università, Piazza Umberto I, 70121 *Bari, Italy*

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Abstract

The effects on the reciprocal space of one or more pseudotranslations occurring in a crystal structure are studied. A quantitative theory is described, which gives full account of the subsets of pseudonormalized structure factors whose mean intensity significantly deviates from unity. Conversely, statistical criteria are suggested aiming at facilitating the recognition of the nature of the superstructure. The theory has been implemented into a computer program that, from 72 different pseudotranslational symmetries, chooses the most probable one, estimates the number of atoms suffering pseudosymmetry and renormalizes structure factors.

Symbols and abbreviations

$\mathbf{h} = (h, k, l)$: vectorial index of a reflection.
f: atomic scattering factor. The thermal factor is included; anomalous dispersion is not.
$F_\mathbf{h}$, $E_\mathbf{h}$: structure factor and normalized structure factor respectively with vectorial index $\mathbf{h}$.
$\mathbf{C}_s = (\mathbf{R}_s, \mathbf{T}_s)$: sth symmetry operator. $\mathbf{R}_s$ is the rotational part, $\mathbf{T}_s$ the translational part.
m: order of the space group (it coincides with the number of symmetry operators).
$\mathbf{u}_i$: ith pseudotranslation in the unit cell.
p: number of atoms (symmetry-equivalent included) whose positions are related by the pseudotranslations $\mathbf{u}$.
n_i: order of the pseudotranslation $\mathbf{u}_i$ (see § 2*a*).
F_p, E_p: structure factor and normalized structure factor relative to the p atoms.
q: number of atoms (symmetry-equivalent included) whose positions are not related by any pseudotranslation.
t_p: number of independent atoms that generate the p atoms when the pseudotranslations $\mathbf{u}_i$ and the symmetry operators C_s, $s = 1, \ldots, m$, are applied.
t_q: number of independent atoms that generate the q atoms by application of the symmetry operators $\mathbf{C}_s$, $s = 1, \ldots, m$.
$\rho(\mathbf{r})$: electron density function in the unit cell.
$\rho_p(\mathbf{r})$: electron density function corresponding to the p atoms.
$\sum_{t_p}$, $\sum_{t_q}$, $\sum_p$, $\sum_q$, $\sum_N \equiv \sum f_j^2$ (thermal factor included) where the summation is extended to the t_p, t_q, p, q, N atoms respectively.

* Present address: 'Rudjer Bošković' Institute, Bijenička 54, 41000 Zagreb, Yugoslavia.

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