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holds for negative values of i. The crystal ball for the f.c.c. is obtained if we always reduce b (say), and that for the h.c.p. if we alternately reduce a and b. In any case we have

$$
\begin{aligned}
S(n) &= P(a_{-n}, b_{-n}) + 3(a_{n+1} + b_{-n+1}) + \cdots + 3(a_0 + b_0) + \cdots \\
&\qquad + 3(a_{n-1} + b_{n-1}) + P(a_n, b_n) \\
&= 2T_{n+1} + 6n + 2\sum_{i=1}^{n-1} 3(2n - i) + a_{-n}b_{-n} + a_n b_n \\
&= S^{fcc}(n) + a_{-n}b_{-n} + a_n b_n \ , \qquad (60)
\end{aligned}
$$

and similarly

$$
G(n) = G^{fcc}(n) + \sum_{i=-n}^{n} a_i b_i \ . \qquad (61)
$$

The assertions of the theorem follow from (60), (61) after some elementary algebra which we omit. ■

5. Concluding remarks

Several open questions remain. Is there a well-placed lattice that is not well-coordinated? (See Remark following Theorem 6.) Can the reader find a general proof of the formulae for the coordination sequences of A_d^* (Eq. (30)), D_d ((34)) and the sodalite net ((56))?

The Voronoi graphs (defined at the beginning of Section 1) should also be investigated. It follows from the work of Rajan and Shende ([21]; [6] , p. xxviii) that, except for root lattices, the Voronoi graph always properly contains the contact graph. What are the analogues of the coordination sequences for the Voronoi graphs of A_d^*, D_d^*, E_6^*, E_7^*, for example?

Acknowledgements

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4. The Barlow packings

Let L denote any three-dimensional packing formed by stacking layers of the hexagonal lattice A_2. As in [9] we shall refer to these as the *Barlow packings*. Let $S(N)$, $G(n)$ denote the n-th terms in the coordination and crystal ball sequences with respect to an arbitrary point in any such L.

Theorem 16. *For any Barlow packing L,*

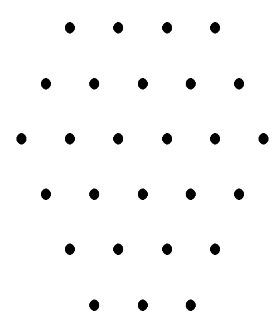
$$10n^2 + 2 \quad \leq \quad S(n) \leq \left\lfloor \frac{21n^2}{2} \right\rfloor + 2 \quad (n > 0) \; , \tag{58}$$

$$\frac{5}{6}\Delta_4(n) + \frac{1}{6}\Delta_2(n) \quad \leq \quad G(n) \leq \frac{7}{8}\Delta_4(n) + (-1)^n \frac{1}{8} \quad (n \geq 0) \; . \tag{59}$$

For any $n > 1$, the only Barlow packing that achieves either the left-hand value or the right-hand value for all choices of central sphere is the face-centered cubic lattice or hexagonal close-packing, respectively.

Remarks. This interesting result was conjectured by O'Keeffe [19]; it had in fact already been established [7]. The assertion on p. 801 of [17] that any Barlow packing has $G(2) = 57$ is plainly incorrect: as shown in [9] there are Barlow packings with $G(2) = 55$, 56 and 57.

Proof. Let $H(a, b)$ denote a hexagonal arrangement of points in which the edges of the hexagon contain respectively $a+1$, $b+1$, $a+1$, $b+1$, $a+1$, $b+1$ points. For example, $H(3, 2)$ is



The number of points in $H(a, b)$ is $P(a, b) = T_{a+b+1} + ab$, where $T_n = n(n+1)/2$ is a triangular number, and its perimeter is $3(a + b)$. The n-th crystal ball with respect to an arbitrary point of L consists of a stack of $2n + 1$ hexagons $\{H(a_i, b_i) : -n \leq i \leq n\}$, for some choice of integers $a_{-n} < a_{-n+1} < \cdots < a_n$, $b_{-n} < b_{-n+1} < \cdots < b_n$. Furthermore $a_0 = b_0 = n$, $a_1 + b_1 = a_{-1} + b_{-1} = 2n - 1, \ldots, a_n + b_n = a_{-n} + b_{-n} = n$. At each stage, as we proceed from $H(a_i, b_i)$ to $H(a_{i+1}, b_{i+1})$, for $0 \leq i < n$, just one of a_i and b_i drops by 1; a similar assertion

Root lattices in general

Looking back over this section, we observe several properties that hold for all root lattices.

Theorem 15. *Let* Λ *be one of* A_d*,* D_d *or* E_6*,* E_7*,* E_8*.*

(i) Consider the faces in which the contact polytope meets the fundamental simplex. These faces are in one-to-one correspondence with the nodes of the extended Coxeter-Dynkin diagram ([6], Figs. 21.1 to 21.3) that are not the extending node and whose removal does not make the diagram disconnected.

(ii) The fractional height of a lattice point in the cone above such a face is an integer if and only if the weight c_i *associated with that node is 1 (see [6], p. 483 and Fig. 23.1; [10], p. 194).*

(iii) Λ *is well-placed if and only if the vertices on any face of the contact polytope span* Λ*.*

The explanation for (ii) is that the c_i's give the index of the sublattice spanned by the vertices of the corresponding face.

We suspect that (iii) may hold for all lattices, but do not have a proof.

The d-dimensional sodalite net

O'Keeffe [18] defines the d-dimensional sodalite net to consist of the holes in the A_d^* lattice, with each point joined to its $d+1$ nearest neighbors. The case $d = 2$ gives the familiar 6^3 hexagonal net. From the coordination sequences of these nets for $d \le 6$ given in [18], Grosse-Kunstleve [16] observed that the coordinator polynomial appears to be $1 + x + x^2 + \cdots + x^d$. If this is true in general it implies

$$S(n) = \binom{n+d}{d} - \binom{n-1}{d} , \tag{56}$$

$$G(n) = \binom{n+d+1}{d+1} - \binom{n}{d+1} . \tag{57}$$

The expression on the right-hand side of (57) is the number of points in a d-dimensional centered simplex. It should therefore be possible to establish the validity of (56) and (57) by finding a bijection between the crystal balls in d-dimensional sodalite and the points of a d-dimensional centered simplex. This is easy to do for $d = 2$, but for higher d the expressions (56) and (57) are at present only conjectures. (Theorems 4 and 7 do not apply.)

h	#	$G'(h)$	$I'(h)$	$S(h)$
0	1	1	0	1
between 0 & 1	0			
1	240	241	1	240
between 1 & 2	0			
2	9120	9361	241	9120
between 2 & 3	17280			
3	657600	131041	26641	121680
between 3 & 4	1244160			
4	9773280	996001	338401	864960
between 4 & 5	16623360			
5	69467520	5109841	2240161	4113840
.	...	...	...	...

Table II: Numbers of points in E_8 lattice by fractional height. $G'(h)$ is the number with fractional height $\leq h$, and $I'(h)$ is the number with fractional height $< h$. The final column gives the coordination sequence.

Besides verifying that these polynomials matched the computer results for $n \leq 13$, we also checked that $G(-n) = I(n)$ for $n \leq 13$ (cf. Theorem 7). For $n \geq 4$ our values for the coordination sequence $S(n)$ do not agree with those given in [19]; we believe the latter are incorrect. Again, the fact that E_8 is not well-coordinated is responsible for the complicated formula in (54).

We display the coordinator triangle for $E_3 = A_1 \oplus A_2$, $E_4 = A_4$, $E_5 = D_5$, E_6, E_7 and E_8, followed by the coordinator polynomials for E_7^* and E_6^* (the row for E_2 is omitted since that lattice is not generated by its minimal vectors):

$$
\begin{array}{lccccccccc}
 & & & & & \cdots & & & & \\
E_3: & & & 1 & 5 & & 5 & 1 & & \\
E_4: & & 1 & 16 & & 36 & & 16 & 1 & \\
E_5: & & 1 & 35 & 180 & & 180 & 35 & 1 & \\
E_6: & 1 & 66 & 645 & & 1384 & & 645 & 66 & 1 \\
E_7: & 1 & 119 & 2037 & 8211 & & 8787 & 2037 & 119 & 1 \\
E_8: & 1 \;\; 232 & 7228 & 55384 & & 133510 & & 107224 & 24508 & 232 \;\; 1 \\
E_7^* & 1 & 49 & 567 & 2263 & & 3703 & 2583 & 625 & 1 \\
E_6^*: & 1 & 48 & 519 & & 1024 & & 519 & 48 & 1
\end{array}
$$

In contrast to the A_n and D_n cases, there is no apparent pattern to these coefficients.

Note that the last four lines of this table are not palindromic, displaying again the fact that these lattices are not well-coordinated.

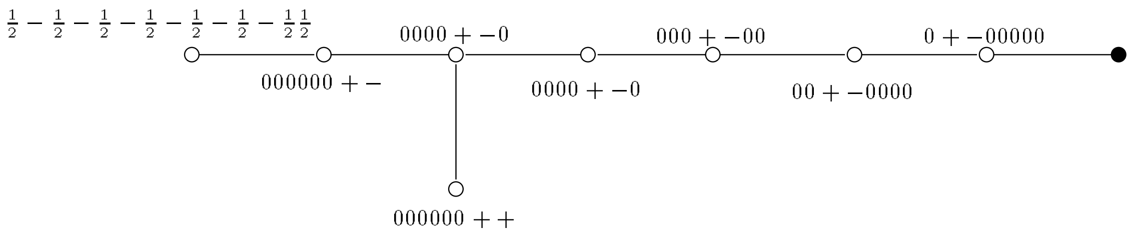


Figure 2: Extended Coxeter-Dynkin diagram for E_8, labeled to show walls of fundamental simplex.

The two faces in which the contact polytope meets this fundamental simplex correspond to the left and bottom nodes of Fig. 2, and have equations

$$\pi_1 \cdot x = 1, \qquad \pi_1 = (1,0,0,0,0,0,0,0) \ , \tag{52}$$

$$\pi_2 \cdot x = 1, \qquad \pi_2 = \left(\frac{5}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}\right) \ , \tag{53}$$

respectively. The face defined by (52) contains 14 points of E_8, forming an orthoplex, and spanning a sublattice D_8 of index 2 in E_8. The face defined by (53) contains eight points, forming a regular simplex and spanning a sublattice A_3 of index 3 in E_8. The fractional heights of points in the cones above these two faces are given by $\pi_1 \cdot x$ and $\pi_2 \cdot x$ respectively. The final result of this analysis is the following.

Theorem 14. *Any point of E_8 is equivalent under the Weyl group to one satisfying (51), for which the fractional height is*

$$fht(x) = \max\left\{x_1, \frac{5x_1 + x_2 + x_3 + \cdots x_8}{6}\right\} \ .$$

E_8 is well-rounded but not well-coordinated, and $G(n)$ and $S(n)$ $(n > 0)$ are polynomials of degrees 8 and 7 respectively.

With the help of a computer we determined the numbers of points of fractional height ≤ 13. In order to do this we precomputed a list of the 256 different types of stabilizers of points satisfying (51). The results of the enumeration are partially shown in Table II.

Using Theorem 14, these values suffice to determine $S(n)$ and $G(n)$. We have $G(n) = G'(n)$, $n \geq 0$, $n \in \mathbb{Z}$, and $S(n) = G(n) - G(n-1)$, $n \geq 1$, $n \in \mathbb{Z}$, from which it follows that

$$S(n) = \frac{456}{7}n^7 - 120n^6 + 312n^5 - 120n^4 - 48n^3 + 240n^2 - \frac{624}{7}n \ , \quad (n > 0) \ , \tag{54}$$

$$G(n) = \frac{57}{7}n^8 + \frac{108}{7}n^7 + 30n^6 + 72n^5 + 39n^4 + 36n^3 + \frac{300}{7}n^2 - \frac{24}{7}n + 1 \ . \tag{55}$$

Using Theorem 12, these computed values suffice to determine $S(n)$ and $G(n)$. From $S(n) = S'(n) + S'(n - 1/2)$, $(n \geq 1)$, $G(n) = G'(n)$ $(n \geq 0)$, $n \in \mathbb{Z}$, we find

$$\begin{aligned} S(n) &= \frac{148}{5}n^6 - \frac{12}{5}n^5 + 52n^4 + 12n^3 + \frac{212}{5}n^2 - \frac{48}{5}n + 2 \ , \quad (n > 0) \ , \qquad (47) \\ G(n) &= \frac{148}{35}n^7 + \frac{72}{5}n^6 + 24n^5 + 28n^4 + \frac{488}{15}n^3 + \frac{98}{5}n^2 + \frac{68}{21}n + 1 \ . \qquad (48) \end{aligned}$$

$\mathbf{E_7^*}$. The contact polytope for E_7^* is a Hesse polytope E_{21} ([4], p. 101). There are two types of faces, simplices, whose vertices span a sublattice of index 3 in E_7^*, and orthoplexes, whose vertices span a sublattice of index 2. We omit the details, and just summarize the result.

Theorem 13. . *The dual lattice E_7^* is well-rounded but not well-coordinated, the fractional heights are in $\frac{1}{6}\mathbb{Z}$, and $G(n)$, $S(n)$ $(n > 0)$ are polynomials in n of degrees 7 and 6 respectively.*

With the aid of a computer we found sufficiently many values to establish that

$$S(n) = \frac{68}{5}n^6 - \frac{216}{5}n^5 + 148n^4 - 192n^3 + \frac{902}{5}n^2 - \frac{264}{5}n + 2, \quad (n > 0) \ , \qquad (49)$$

$$G(n) = \frac{68}{35}n^7 - \frac{2}{5}n^6 + \frac{74}{5}n^5 + 8n^4 + \frac{56}{5}n^3 + \frac{97}{5}n^2 + \frac{37}{35}n + 1 \ . \qquad (50)$$

Notice that the formulae (47) and (49) for $S(n)$ for these lattices are much more complicated than the corresponding formula (38) and (40) for E_6 and E_6^*, reflecting the fact that E_7 and E_7^* are not well-coordinated.

$\mathbf{E_8}$. The "standard" E_8 consists of the points $x = (x_1, \ldots, x_8)$ whose coordinates are either all integers or all halves of odd integers and whose sum is even. The contact polytope is the Gosset polytope 4_{21} ([4, p. 94]). There are two types of faces, 2160 faces that are orthoplexes and 17280 simplicial faces. We use the extended Coxeter-Dynkin diagram shown in Fig. 2, where we have adopted the same conventions as in Fig. 1.

From the planes defined by the nodes in Fig. 2 we see that the points in the fundamental simplex satisfy

$$x_2 \geq x_3 \geq x_4 \geq x_5 \geq x_6 \geq x_7 \geq |x_8| \ ,$$

$$x_1 \geq x_2 + x_3 + x_4 + x_5 + x_6 + x_7 - x_8 \ .$$

However, these together imply $x_1 \geq x_2$, and so we can conclude that the fundamental simplex consists of the points satisfying

$$\begin{aligned} & x_1 \geq x_2 \geq \cdots \geq x_7 \geq |x_8| \ , \\ & x_1 + x_8 \geq x_2 + \cdots + x_7 \ . \end{aligned} \qquad (51)$$

the face only generate a sublattice A_7, of index 2 in E_7, and if $x \in E_7$ is in the cone above this face,

$$fht(x) = \pi_2 \cdot x = x_2 + \frac{x_3 + x_4 + x_5 + x_6 + x_7 - x_8}{4} \in \frac{1}{2}\mathbb{Z} ,$$

and $ht(x) = \lceil fht(x) \rceil$.

For a general point of E_7 satisfying (42), we have

$$fht(x) = \max \left\{ x_2 + x_3,\ x_2 + \frac{x_3 + x_4 + x_5 + x_6 + x_7 - x_8}{4} \right\} , \tag{45}$$

and

$$ht(x) = \lceil fht(x) \rceil . \tag{46}$$

By applying Theorem 7 we obtain:

Theorem 12. *Let E_7 consist of the points $x = (x_1, \ldots, x_8)$ of E_8 in which the first two coordinates are equal. Any such point of E_7 is equivalent under the Weyl group of E_7 to one satisfying (42), for which the fractional height is given by (45) and the height by (46). E_7 is well-rounded but not well-coordinated. $G(n)$ and $S(n)$ $(n > 0)$ are polynomials in n of degrees 7 and 6 respectively.*

A computer was now used to determine the numbers of points of fractional height up to 6.5, making use of knowledge of the subgroups of the Weyl group to calculate the number of lattice points equivalent to a given point. The results are partially shown in Table I.

h	$S'(h)$	$G'(h)$
0	1	1
0.5	0	1
1	126	127
1.5	0	127
2	2898	3025
2.5	0	3025
3	25886	28911
3.5	576	29487
4	132930	162417
4.5	4032	166449
5	485982	652431
...	...	...

Table I: Numbers of points of fractional height exactly h ($S'(h)$) and at most h ($G'(n)$) in E_7 lattice.

E₇. We define E_7 to consist of the points $x = (x_1, \ldots, x_8)$ in the standard E_8 for which the first two coordinates are equal. The contact polytope is the polytope 2_{31} ([4], p. 100). There are two types of faces, 56 faces that are Schläfli polytopes (also called 2_{21} polytopes), and 576 simplicial faces. We use the extended Coxeter-Dynkin diagram shown in Fig. 1.

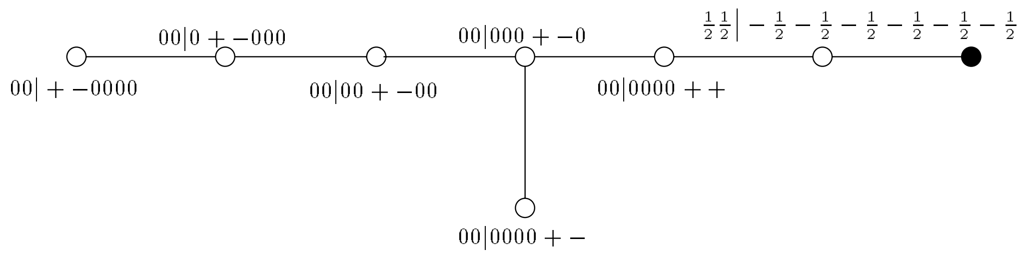


Figure 1: Extended Coxeter-Dynkin diagram for E_7, labeled to show walls of fundamental simplex.

The extending node in Fig. 1 is shaded, and the other nodes are labeled with the equations that define the walls of the fundamental simplex (compare [6], Fig. 21.3(b), where slightly different coordinates were used). In Fig. 1, $+1$ and -1 have been abbreviated to $+$ and $-$. The left-most node for example defines the wall $x_3 - x_4 \geq 0$.

The points in the fundamental simplex therefore satisfy

$$\begin{aligned} & x_1 = x_2, \ x_3 \geq x_4 \geq x_5 \geq x_6 \geq x_7 \geq |x_8| \ , \\ & x_1 + x_2 \geq x_3 + x_4 + x_5 + x_6 + x_7 + x_8 \ . \end{aligned} \tag{42}$$

The two faces in which the contact polytope meets this fundamental simplex correspond to the left and bottom nodes of Fig. 1, and have equations

$$\pi_1 \cdot x = 1, \qquad \pi_1 = \left(\frac{1}{2}, \frac{1}{2}, 1, 0, 0, 0, 0, 0\right) \ , \tag{43}$$

$$\pi_2 \cdot x = 1, \qquad \pi_2 = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}, -\frac{1}{4}, \right) \ , \tag{44}$$

respectively. The face defined by (43) contains 27 points of E_7, namely 110^6, $001(\pm 1, 0^5)$ and $\frac{1}{2}\frac{1}{2}\frac{1}{2}(\pm\frac{1}{2})^{5+}$, forming a Schläfli polytope. These 27 points span E_7. If x is a point of E_7 in the cone above this face,

$$fht(x) = \pi_1 \cdot x = x_2 + x_3 \in \mathbb{Z} \ ,$$

and $ht(x) = fht(x)$. On the other hand the face defined by (44) contains seven points of E_7, namely 110^6, $(\frac{1}{2})^6$ and $\frac{1}{2}\frac{1}{2}(-\frac{1}{2}\frac{1}{2}^4) - \frac{1}{2}$, forming a regular simplex. Now however the points on

The root lattices E_6, E_7, E_8 and their duals

The coordination sequences for E_6 and E_6^* were found experimentally by O'Keeffe [19], so for these lattices we give only enough information to justify his results.

$\mathbf{E_6}$. The contact polytope for the root lattice E_6 is the polytope called 1_{22} in Coxeter's notation ([4], p. 104; [10], p. 201). There are 54 faces, all 5-dimensional hemicubes. If we define E_6 to consist of the points in the standard E_8 (see below) in which the first three coordinates are equal, then the typical face has equation $\pi \cdot x = 1$, where $\pi = (2/3, 2/3, 2/3, 0, 0, 0, 0, 0)$. The vertices of E_6 on this face have coordinates $\left(\left(\frac{1}{2}\right)^3; \left(\pm\frac{1}{2}\right)^{5+}\right)$, the exponent $5+$ indicating that only even sign combinations are permitted. The fractional height of a point $x \in E_6$ in the cone above this face is $fht(x) = \pi \cdot x$. This is an integer, so E_6 is well-placed, and it is also easy to see that $\pi \cdot x = ht(x)$. Thus we have proved:

Theorem 10. *E_6 is well-coordinated.*

This establishes the coordination sequence

$$S(n) = \frac{117}{5}n^5 + 36n^3 + \frac{63}{5}n, \quad (n > 0) \tag{38}$$

found empirically in [19]. Also

$$G(n) = \frac{39}{10}n^6 + \frac{117}{10}n^5 + \frac{75}{4}n^4 + 18n^3 + \frac{267}{20}n^2 + \frac{63}{10}n + 1 \ . \tag{39}$$

$\mathbf{E_6^*}$. The contact polytope for the dual lattice E_6^* is a diplo-Schläfli polytope ([4], p. 104), and coincides with the Voronoi polytope for E_6. The contact polytope has 72 faces, one for each minimal vector of E_6. For example, the face defined by the minimal vector $\pi = (1/2, 1/2, 1/2, -1/2, -1/2, -1/2, -1/2, -1/2,) \in E_6$ has equation $\pi \cdot x = 1$. This face contains 12 points of E_6^*, forming a diplo-simplex. All faces are of this type. From this it is easy to obtain:

Theorem 11. *E_6^* is well-coordinated.*

This establishes the coordination sequence

$$S(n) = 18n^5 + 30n^3 + 6n \quad (n > 0) \tag{40}$$

found empirically in [19]. Also

$$G(n) = 3n^6 + 9n^5 + 15n^4 + 15n^3 + 9n^2 + 3n + 1 \ . \tag{41}$$

The remaining three lattices are not well-placed, although they are well-rounded.

The rows of this triangle suggest that[3]

$$P_d(x) = \frac{1}{2}\left\{(1+\sqrt{x})^{2d} + (1-\sqrt{x})^{2d}\right\} - 2dx(1+x)^{d-2} \ , \tag{33}$$

an expression which is certainly valid for $d \le 12$. Assuming (33) holds in general, we find from (9) that

$$S(n) = \sum_{k=0}^{d} \left\{ \binom{2d}{2k} - 2d\binom{d-2}{k-1} \right\} \binom{n-k+d-1}{d-1} \ . \tag{34}$$

Again an equivalent combinatorial identity could be written down using (32) (compare (23)).

The dual lattice D_d^* and the generalized b.c.c. net

As was pointed out in [19], the contact graph for D_d^*, for $d \ge 5$, is simply the union of two disjoint copies of the contact graph for $\mathbb{Z}^d$.

However, a more interesting graph is obtained if — using the standard coordinates for D_d^*, see [6], Section 7.4 of Chap. 4 — each point is joined to those points that differ from it by the vectors $(\pm\frac{1}{2}, \pm\frac{1}{2}, \ldots, \pm\frac{1}{2})$. This generalizes the contact graph for the b.c.c. lattice D_3^*, and we shall refer to it as the *generalized b.c.c. net.* The coordination number is 2^d, and the crystal balls are cubes, with

$$\begin{aligned} S(n) &= (n+1)^d - (n-1)^d, \quad n > 0 \ , && (35) \\ G(n) &= (n+1)^d + n^d, \quad n \ge 0 \ . && (36) \end{aligned}$$

The $G(n)$ are *centered cube numbers.* The coordinator triangle is

$$\begin{array}{ccccccccccc} & & & & & 1 & & & & & \\ & & & & 1 & & 1 & & & & \\ & & & 1 & & 2 & & 1 & & & \\ & & 1 & & 5 & & 5 & & 1 & & \\ & 1 & & 12 & & 22 & & 12 & & 1 & \\ 1 & & 27 & & 92 & & 92 & & 27 & & 1 \\ & & & & & \cdots & & & & & \end{array} ,$$

and

$$P_d(x) = (1+x) \sum_{k=0}^{d-1} \left\langle {d \atop k} \right\rangle x^k \ , \tag{37}$$

where the $\left\langle {d \atop k} \right\rangle$ are Eulerian numbers ([3], p. 243; [15], p. 254; [22], p. 215). In Comtet's notation ([3, p. 244]), $P_d(x) = (x+1)A_n(x)/x$, where $A_n(x)$ is an Eulerian polynomial.

[3]We are grateful to Colin Mallows for this formula.

The expressions x_1, $\frac{1}{2}(x_1 + \cdots + x_d)$, $\frac{1}{2}(x_1 + \cdots - x_d)$ then give the fractional heights of points in the cones above these three faces, and the fractional height of a general point in the fundamental simplex is the maximum of these three expressions, which is always an integer. Furthermore, it is easy to show that a point with fractional height n can actually be written as a sum of n minimal vectors, and so the lattice is well-coordinated.

Finally, the last two faces in (31) are equivalent under the full automorphism group of D_d, since this includes all sign changes of the coordinates.

We collect these results in the following theorem.

Theorem 9. *Any point $x = (x_1, \ldots, x_d) \in D_d$ is equivalent to one satisfying*

$$x_1 \geq x_2 \geq \cdots \geq x_d \ .$$

For such a point we have

$$fht(x) = ht(x) = \max \left\{ x_1, \frac{1}{2} \sum x_i \right\} \ .$$

The number of points in D_d equivalent to x is

$$2^{d-a_0} \frac{d!}{\prod\limits_{i=0}^{n} a_i!} \ , \tag{32}$$

where a_i is the number of components x_j that are equal to i, for $0 \leq i \leq n = ht(x)$. The lattice is well-coordinated, $G(n)$ and $S(n)$ $(n > 0)$ are polynomials of degrees d and $d-1$ respectively, and the crystal balls are ambo-orthoplexes.

We had already determined the coordination sequence for D_4 some years ago (see Sequence M5182 of [25][2], and also (1)), and it was given independently by O'Keeffe [19], who also found the coordination sequences for D_5 and D_6. We have extended this work to D_{12}, finding that the coordinator triangle is

$$\begin{array}{c}
1 \\
1 \quad 1 \\
1 \quad 2 \quad 1 \\
1 \quad 9 \quad 9 \quad 1 \\
1 \quad 20 \quad 54 \quad 20 \quad 1 \\
1 \quad 35 \quad 180 \quad 180 \quad 35 \quad 1 \\
1 \quad 54 \quad 447 \quad 852 \quad 447 \quad 54 \quad 1 \\
1 \quad 77 \quad 931 \quad 2863 \quad 2863 \quad 931 \quad 77 \quad 1 \\
\cdots
\end{array}$$

[2] We remark in passing that most of the sequences mentioned in the paper have been added to the electronically accessible version of this table [24].

triangle is

$$\begin{array}{ccccccccccccccccccc}
 & & & & & & & & & 1 & & & & & & & & & \\
 & & & & & & & & 1 & & 1 & & & & & & & & \\
 & & & & & & & 1 & & 4 & & 1 & & & & & & & \\
 & & & & & & 1 & & 5 & & 5 & & 1 & & & & & & \\
 & & & & & 1 & & 6 & & 16 & & 6 & & 1 & & & & & \\
 & & & & 1 & & 7 & & 22 & & 22 & & 7 & & 1 & & & & \\
 & & & 1 & & 8 & & 29 & & 64 & & 29 & & 8 & & 1 & & & \\
 & & 1 & & 9 & & 37 & & 93 & & 93 & & 37 & & 9 & & 1 & & \\
 & 1 & & 10 & & 46 & & 130 & & 256 & & 130 & & 46 & & 10 & & 1 & \\
1 & & 11 & & 56 & & 176 & & 386 & & 386 & & 176 & & 56 & & 11 & & 1 \\
 & & & & & & & & & \cdots & & & & & & & & &
\end{array}$$

The last two rows, corresponding to $d = 8$ and 9, were obtained by extrapolating the pattern of the earlier rows, which appears to be

$$P_{2m}(x) = \sum_{k=0}^{m} \binom{2k}{k} x^k (1+x)^{2m-2k} \,, \tag{28}$$

$$P_{2m+1}(x) = (1+x) P_{2m}(x) \,. \tag{29}$$

Assuming these expressions hold in general, then by expanding (9) we find that

$$S(n) = \sum_{k=0}^{d} \binom{n-k+d-1}{d-1} \sum_{i=0}^{k} \binom{2i}{i} \binom{d-2i}{k-i} \,. \tag{30}$$

This agrees with O'Keefe's empirical results for $d \leq 7$, and presumably for general d could be established in a similar manner to Eq. (23).

The root lattice D_n

We take D_d to consist of the points $x = (x_1, \ldots, x_d) \in \mathbb{Z}^d$ with $\sum x_i$ even. The contact polytope is an "ambo-orthoplex" ([4], p. 90), having $2d(d-1)$ vertices, all of the form $(\pm 1^2, 0^{d-2})$. The Weyl group $W(D_d)$ has order $2^{d-1}d!$ and contains all permutations and all even sign changes of the coordinates.

Any point $x \in D_d$ is equivalent under this group to one satisfying

$$x_1 \geq x_2 \geq \cdots \geq x_{d-1} \geq |x_d| \,,$$

these inequalities defining the fundamental simplex. As in the case of A_d, the intersection of this simplex with the contact polytope has a face for each nonzero glue vector of D_d. There are three faces, defined by

$$\begin{gathered} x_1 = 1 \,, \\ \tfrac{1}{2}(x_1 + \cdots + x_{d-1} + x_d) = 1 \,, \\ \tfrac{1}{2}(x_1 + \cdots + x_{d-1} - x_d) = 1 \,. \end{gathered} \tag{31}$$

The dual lattice A_d^*

The contact polytope for A_d^* is a diplo-simplex ([4], p. 88), with $2d+2$ vertices $\pm v_i$, $0 \le i \le d$, where

$$v_i = \left(\left(\frac{1}{d+1} \right)^d , \left(\frac{-d}{d+1} \right)^1 \right) ,$$

with the $-d/(d+1)$ entry in the i^{th} coordinate. A typical face of the contact polytope contains

$$\frac{d}{2} \ +v_i\text{'s} \quad \text{and} \quad \frac{d}{2} \ -v_i\text{'s} \ ,$$

if d is even, and either

$$\frac{d+1}{2} \ +v_i\text{'s} \quad \text{and} \quad \frac{d-1}{2} \ -v_i\text{'s} \ ,$$

or

$$\frac{d-1}{2} \ +v_i\text{'s} \quad \text{and} \quad \frac{d+1}{2} \ +v_i\text{'s}$$

if d is odd.

We will now show that A_d^* is well-coordinated. We use A_4^* as an illustration, the general case being precisely similar. The face defined by $\pi \cdot x = 1$, where $\pi = (1,1,0,-1,-1)$, contains the vertices v_0, v_1, $-v_3$ and $-v_4$. All faces of the contact polytope are of this type.

Consider a point $x = (x_0, x_1, x_2, x_3, x_4) \in A_4^*$ in the cone from the origin that contains this face. Let x have fractional height h, so that $\pi \cdot x = h$. We claim that $ht(x) = h$. By Theorem 1,

$$x = c_0 v_0 + c_1 v_1 - c_3 v_3 - c_4 v_4 \ , \tag{26}$$

where $c_i \in \mathbb{Q}$, $c_i \ge 0$, $\sum c_i = h$. Since $x \in A_4^*$ and v_0, v_1, v_3, v_4 span A_4^*, x can also be written as

$$x = m_0 v_0 + m_1 v_1 - m_3 v_3 - m_4 v_4 \ , \tag{27}$$

where the m_i are integers. Since v_0, v_1, v_3, v_4 are linearly independent, the representation of x is unique, and (26) and (27) agree. Therefore $h = \sum m_i$ is an integer, and since (27) displays x as a sum of h minimal vectors, $ht(x) = fht(x) = h$, showing that this lattice is well-coordinated.

O'Keeffe [19] gave polynomials for the coordination sequences for $d \le 7$, and the preceding argument now justifies these formulae. Using O'Keeffe's results, we find that the coordinator

The k-th entry in the d-th row is $\binom{d}{k}^2$ (for $k = 0, 1, \ldots$), so that

$$\mathcal{S}(x) = \frac{\sum_{k=0}^{d} \binom{d}{k}^2 x^k}{(1-x)^d} \ , \tag{21}$$

and hence

$$S(n) = \sum_{k=0}^{d} \binom{d}{k}^2 \binom{n-k+d-1}{d-1} \ , \tag{22}$$

with a similar expression for $G(n)$. The following elegant proof of (22) is due to C. L. Mallows. From Theorem 8, Eq. (22) is equivalent to the identity

$$\sum_a \frac{(d+1)!}{\prod_{i=-n}^{n} a_i!} = \sum_{k=0}^{d} \binom{d}{k}^2 \binom{n-k+d-1}{d-1} \ , \tag{23}$$

where the sum on the left extends over all $a = (a_{-n}, \ldots, a_n)$ satisfying

$$\sum_{i=-n}^{n} a_i = d+1, \quad \sum_{i>0} i a_i = \sum_{i<0} i a_{-i} = n \ .$$

If we multiply the left-hand side summand of (23) by

$$x^{a_0}(xy)^{a_1}(xz)^{a_{-1}}(xy^2)^{a_2}(xz^2)^{a_{-2}} \ldots \ ,$$

we see that the left-hand side of (23) is equal to the coefficient of $x^{d+1}y^n z^n$ in

$$(d+1)! \exp\left\{x + \frac{xy}{1-y} + \frac{xz}{1-z}\right\} = (d+1)! \exp\left\{x \frac{1-yz}{(1-y)(1-z)}\right\} \ ,$$

or in other words to

$$\text{coefficient of } \ y^n z^n \ \text{ in } \ \left\{\frac{1-yz}{(1-y)(1-z)}\right\}^{d+1} \ . \tag{24}$$

On the other hand the right-hand side of (23) is

$$\text{coefficient of } \ y^n z^n \ \text{ in } \ \left\{\frac{1-yz}{(1-y)(1-z)}\right\}^{-d} \ . \tag{25}$$

Call these two expressions $c_L(n,d)$ and $c_R(n,d)$. Contour integration now shows that

$$\begin{aligned} \sum_{n=0}^{\infty}\sum_{d=0}^{\infty} c_L(n,d) u^n v^d &= \sum_{n=0}^{\infty}\sum_{d=0}^{\infty} c_R(n,d) u^n v^d \\ &= \left\{1 - 2v\frac{1+u}{1-u} + v^2\right\}^{-1/2} \ , \end{aligned}$$

completing the proof.

It is curious[1] that Eq. (21) is the expansion of $L_d((1+x)/(1-x))$ in powers of x, where L_d is the d-th order Legendre polynomial (see [20], p. 86). We are not aware of any other connections between the root system A_d and the Legendre polynomial L_d.

[1] We are grateful to Herb Wilf for this remark.

for $1 \leq i \leq d$, has equation

$$\frac{1}{2}[i] \cdot x = \frac{i}{2(d+1)}(x_0 + \cdots + x_{d-i}) - \frac{(d+1-i)}{2(d+1)}(x_{d-i+1} + \cdots + x_d) = 1 \ . \qquad (20)$$

This face contains $i(d-i)$ vertices of the contact polytope, those with a single $+1$ in any of the first $d+1-i$ coordinates and a single -1 in any of the last i coordinates.

Consider a point $x \in A_d$ lying in the fundamental simplex, in the cone above the face defined by (20). The reflecting planes of the affine (infinite) Weyl group of type A_n partition the whole space into simplices. The height of x, and also its fractional height, is given by the number of reflecting planes between x and the origin, which is $\frac{1}{2}[i] \cdot x$.

For an arbitrary point $x \in A_d$ in the fundamental simplex (19), the height is

$$\max_{i=1,\ldots,d} \frac{1}{2}[i] \cdot x \ ,$$

which is simply $\frac{1}{2}\sum |x_i|$. Thus a point such as $(7,3,0,-5,-5) \in A_4$ can be written as the sum of $\frac{1}{2}\sum |x_i| = 10$ minimal vectors, and no fewer. From collecting these results and applying Theorem 7, we obtain:

Theorem 8. *Any point $x = (x_0, \ldots, x_d) \in A_d$ is equivalent under the Weyl group to one with coordinates satisfying (19). For such a point we have*

$$fht(x) = ht(x) = \frac{1}{2}\sum |x_i| \ .$$

The number of points in A_d equivalent to this point is $(d+1)!/\prod_{i=-n}^{n} a_i!$, where a_i is the number of components x_j that are equal to i, for $-n \leq i \leq n$, $n = ht(x)$. The lattice is well-coordinated, and $G(n)$, $S(n)$ $(n > 0)$ are polynomials in n of degrees d, $d-1$ respectively. The crystal balls are shorter ambo-diplo-simplices.

O'Keeffe [19] empirically determined the coordination sequences for A_d for $d \leq 7$, in each case finding that $S(n)$ is a polynomial in n of degree $d-1$. The correctness of these expressions is now justified. Using Theorem 8, we have extended O'Keeffe's results to $d = 10$, and find that the coordinator triangle is

$$\begin{array}{ccccccccccc}
 & & & & & 1 & & & & & \\
 & & & & 1 & & 1 & & & & \\
 & & & 1 & & 4 & & 1 & & & \\
 & & 1 & & 9 & & 9 & & 1 & & \\
 & 1 & & 16 & & 36 & & 16 & & 1 & \\
1 & & 25 & & 100 & & 100 & & 25 & & 1 \\
 & & & & & \cdots & & & & &
\end{array}$$

The structure of the coordinator polynomials both here and in subsequent examples becomes clearer if the coefficients of the successive polynomials $P_d(x)$ for $d = 0, 1, 2, \ldots$ are displayed in a triangular array (with coefficients of highest powers on the right). We call this the *coordinator triangle*:

$$\begin{array}{ccccccccc} & & & & 1 & & & & \\ & & & 1 & & 1 & & & \\ & & 1 & & 2 & & 1 & & \\ & 1 & & 3 & & 3 & & 1 & \\ 1 & & 4 & & 6 & & 4 & & 1 \\ & & & & \cdots & & & & \end{array}$$

In this case of course the coordinator triangle is simply Pascal's triangle of binomial coefficients $\binom{d}{k}$. O'Keeffe [18], Table 6, gave the coordination sequences for $d \le 10$, but the present description is both simpler and holds for all d. It follows from (16) that the coefficient of n^{d-1} in $S(n)$ is $2^d/(d-1)!$, as conjectured in [18].

The root lattice A_d

The contact polytopes of the lattices A_n, D_n, E_6, E_7, E_8 and their duals were described in [4].

We define A_d to consist of the points $x = (x_0, x_1, \ldots, x_d) \in \mathbb{Z}^{d+1}$ with $\sum x_i = 0$. The contact polytope has $d(d+1)$ vertices, of the form $(1, -1, 0^{d-1})$. These are at the midpoints of the shorter edges of the diplo-simplex formed by the vectors (from coset [1] of A_d in A_d^*)

$$\pm \left(\left(\frac{1}{d+1} \right)^d, \ \left(\frac{-d}{d+1} \right)^1 \right) .$$

The contact polytope was incorrectly described as an "ambo-diplo-simplex" in [4]; a better name would be "shorter ambo-diplo-simplex".

A fundamental simplex for the Weyl group $W(A_n)$ of order $(n+1)!$ is described in Figs. 21.1 and 21.6 of [6]. It consists of the points satisfying

$$x_0 \ge x_1 \ge \cdots \ge x_d, \quad \sum x_i = 0 . \tag{19}$$

This simplex is an infinite cone which meets the contact polytope in d faces, one for each nonzero glue vector of A_d (cf. [6], Chapters 4 and 21). The face corresponding to the glue vector

$$[i] = \left(\underbrace{\frac{i}{d+1}, \ldots, \frac{i}{d+1}}_{d+1-i}, \quad \underbrace{-\frac{d+1-i}{d+1}, \ldots, -\frac{d+1-i}{d+1}}_{i} \right) ,$$

integral $n \geq 0$, $G(n)$ and $I(n)$ are respectively given by polynomials $g(n)$ and $i(n)$ of degree d, satisfying

$$g(-n) = (-1)^d i(n) \quad n \in \mathbb{Z} \ .$$

Furthermore, $S(0) = 1$, while for $n > 0$, $S(n)$ is a polynomial $s(n)$ of degree $d-1$ satisfying $s(0) = 1 - (-1)^d$.

Proof. The hypothesis implies that the set of points of height $\leq n$ is convex, and the other assertions follow from Ehrhart's reciprocity law (cf. Theorem 4). ∎

In particular, Theorem 7 applies if the lattice is well-coordinated.

3. Root lattices and their duals

In this section we discuss the coordination sequences of the root lattices, their duals and some related nets.

The cubic lattice $\mathbb{Z}^d$

The contact polytope for $\mathbb{Z}^d$ is a d-dimensional cube, and a typical point $x = (x_1, \ldots, x_d) \in \mathbb{Z}^d$ has

$$fht(x) = ht(x) = \sum_{i=1}^{d} |x_i| \ . \tag{15}$$

The coordination sequence for the 1-dimensional integer lattice $\mathbb{Z}$ is $\{1, 2, 2, 2, \ldots\}$, with generating function $\mathcal{S}(x) = (1+x)/(1-x)$. Therefore, for $\mathbb{Z}^d$, the direct product of d copies of $\mathbb{Z}$, we have $\mathcal{S}(x) = (1+x)^d/(1-x)^d$,

$$S(n) = \sum_{k=0}^{d} \binom{d}{k} \binom{n-k+d-1}{d-1} \ , \tag{16}$$

$$G(n) = \sum_{k=0}^{d} \binom{d}{k} \binom{n-k+d}{d} \ , \tag{17}$$

and $P_d(x) = (1+x)^d$. From (15), (16) we have the identity

$$\sum_{(a_0, a_1, \ldots)} \frac{d! 2^{d-a_0}}{\prod_{i=0}^{n} a_i!} = \sum_{k=0}^{d} \binom{d}{k} \binom{n-k+d-1}{d-1} \tag{18}$$

the sum being over all $(a_0, a_1, \ldots, a_n) \in \mathbb{Z}^{n+1}$ satisfying $\sum a_i = d$, $\sum i a_i = n$.

The crystal balls are orthoplexes (cf. [4]), and the $G(n)$ are *centered orthoplex numbers.*

that the lattice is not well-placed. Further investigation shows that this lattice *is* well-rounded, with

$$G'(n) = G(n) = \frac{2}{3}n^5 + \frac{5}{4}n^4 + \frac{5}{2}n^3 + \frac{15}{2}n^2 + \frac{23}{6}n + 1 \ ,$$

which is indeed not symmetric about $-1/2$, and that

$$S'(n) = S(n) = \frac{10}{3}n^4 - \frac{5}{3}n^3 + \frac{20}{3}n^2 + \frac{5}{3}n + 1 \ \ (n > 0) \ .$$

Thus lattices that are not well-placed (hence not well-coordinated) exist in all dimensions above 4. As we will see, the lattices E_7, E_7^* and E_8 are also not well-placed.

Remark. Well-coordinated lattices are well-rounded, and it is at first tempting to conjecture that the converse is also true. However, we believe that a counterexample (a well-placed lattice that is not well-rounded) will be found in perhaps as low as five dimensions. The next example shows that in general the set of lattice points of height $\le n$ need not even be *lattice-convex*, i.e. need not have the property that every lattice point in the convex hull of the points of height n has height $\le n$.

Definition. A d-dimensional lattice Λ is *anabasic* if it has the property that although it is generated by its minimal vectors, no subset of d of the minimal vectors generates it. A particular 11-dimensional lattice, which we call "the" anabasic lattice B, was described in [8].

The anabasic lattice B has precisely 24 minimal vectors $\pm u_1, \ldots, \pm u_7$, $\pm v_1, \ldots, \pm v_5$, satisfying $2 \sum_{i=1}^{7} u_i = 3 \sum_{i=1}^{5} v_i = 6w$ (say). Then $2w = \sum v_i \in B$, $3w = \sum u_i \in B$, so $w \in B$. The heights of the multiples of w are:

vector:	w	$2w$	$3w$	$4w$	$5w$	$6w$	$7w$	$8w$	$9w$	$\cdots$
height:	12	5	7	10	12	14	17	19	21	$\cdots$

and $fht(w) = 7/3$. The set of points of height ≤ 5 is not lattice-convex, since it contains $2w$ but not w.

In this example, $fht(w) = 7/3$ while $ht(w) = 12$, so the anabasic lattice is neither well-placed nor well-rounded. However, most of the lattices Λ we consider in this paper are well-rounded.

Theorem 7. *If a d-dimensional lattice Λ is well-rounded, then the set of $u \in \Lambda$ with $ht(u) \le n$ is lattice-convex, and the crystal balls are magnified versions of the contact polytope. For* from the symmetry property of Bernoulli polynomials ([1, Eq. (23.1.8)]). Thus (13) implies (12), and (12) and (8) imply (10), showing that $\mathcal{G}$ is well-placed. ∎

For example, the f.c.c. lattice is well-coordinated, since $G'(n) = G(n) = {}^1\!/_3(2n+1)(5n^2+5n+3)$ satisfies $G'(-n) = -G'(n-1)$: its values at

$$\cdots \quad -3 \quad -2 \quad -1 \quad 0 \quad 1 \quad 2 \quad 3 \quad \cdots$$

being respectively

$$\cdots \quad -55 \quad -13 \quad -1 \quad 1 \quad 13 \quad 55 \quad 147 \quad \cdots .$$

Also

$$S'(n) = G'(n) - G'(n-1) = 10n^2 + 2 = S(n) ,$$

for $n \ge 1$, an even polynomial.

Theorem 6. *Every lattice of dimension d at most 4 is well-coordinated.*

The cases $d = 1$ and 2 are easy. The case $d = 3$ follows from Theorem 5 and the fact (cf. [19]) that for a three-dimensional lattice, $S(n) = (S(1)-2)n^2 + 2$, $n > 0$. The proof for $d = 4$ is longer and will be given elsewhere. ∎

It follows from Theorem 4 that the coordination sequence for any four-dimensional lattice is given by

$$S(n) = \left(\frac{S(2)}{6} - \frac{S(1)}{3} \right) n^3 - \left(\frac{S(2)}{6} - \frac{2S(1)}{3} \right) n , \tag{14}$$

for $n > 0$ (compare [19], p. 906).

On the other hand, the following five-dimensional lattice is not well-placed, and so not well-coordinated. We start from the lattice D_5^*, generated by the vectors $v_1 = (1,0,0,0,0)$, $\ldots$, $v_5 = (0,0,0,0,1)$ and $v_6 = ({}^1\!/_2, {}^1\!/_2, {}^1\!/_2, {}^1\!/_2, {}^1\!/_2)$, and "squash" it in the v_6 direction until $v_1, \ldots, v_6$ all have the same length. The resulting lattice has Gram matrix

$$\frac{1}{21} \begin{bmatrix} 20 & -1 & -1 & -1 & 8 \\ -1 & 20 & -1 & -1 & 8 \\ -1 & -1 & 20 & -1 & 8 \\ -1 & -1 & -1 & 20 & 8 \\ 8 & 8 & 8 & 8 & 20 \end{bmatrix} ,$$

the entries in which are the inner products of the new vectors v_1, v_2, v_3, v_4, v_6. It is easy to check that $w = v_6 - v_1 - v_2$ has height 3 but fractional height 2.5 (in fact $ht(2w) = 5$), showing generating function for the crystal ball numbers $G(n)$ is

$$\sum_{n=0}^{\infty} G(n)x^n = \frac{\mathcal{S}(x)}{1-x} = \frac{P_d(x)}{(1-x)^{d+1}} \ .$$

Note that if a lattice Λ is the direct product of lattices M and N, then the corresponding generating functions satisfy $\mathcal{S}_\Lambda(x) = \mathcal{S}_M(x)\mathcal{S}_N(x)$, and the coordinator polynomial for Λ is the product of those for M and N.

It follows from the definition that $\mathcal{G}$ is well-placed if any one of these three equivalent conditions holds:

$$\text{(a)} \qquad fht(u) \in \mathbb{Z}, \quad \text{for all } u \in \mathcal{G} \ ;$$

$$\text{(b)} \qquad I'(n) = G'(n-1), \quad \text{for} \ \ n = 1, 2, \ldots \ ; \tag{10}$$

$$\text{(c)} \qquad S'(n) = G'(n) - G'(n-1), \quad \text{for} \ \ n = 1, 2, \ldots \ . \tag{11}$$

These conditions amount to saying that every point lies on the boundary of $n\mathcal{P}$, for some integral $n \ge 0$.

The polynomials $g'(n)$, $s'(n)$ and $i'(n)$ that give the values of $G'(n)$, $S'(n)$ and $I'(n)$ for integral $n > 0$ are also interesting for negative n:

Theorem 5. *$\mathcal{G}$ is well-placed if and only if either*

$$(d) \ \ g'(-n) = (-1)^d g'(n-1), \quad \textit{for all} \ \ n \in \mathbb{Z} \ , \tag{12}$$

or

$$(e) \ \ s'(-n) = (-1)^{d-1} s'(n), \quad \textit{for all} \ \ n \in \mathbb{Z}, \quad n \neq 0 \tag{13}$$

holds.

Equation (12) asserts that the values of $|g'(n)|$ are symmetric about $n = -1/2$, and (13) that $s'(n)$ is an even polynomial in n if d is odd, and an odd polynomial in n if d is even.

Proof. If $\mathcal{G}$ is well-placed then $g'(-n) = (-1)^d i'(n)$ (from Theorem 4), $= (-1)^d g'(n-1)$ (from (10)). Let $\sigma(x) = g'(x) - g'(x-1)$, so that $s'(n) = \sigma(n)$ for $n = 1, 2, \ldots$. Then $\sigma(x) = (-1)^d\{g'(-x-1) - g'(-x)\} = (-1)^{d-1}\sigma(-x)$, so $s'(-n) = (-1)^{d-1}s'(n)$, $n \neq 0$. Conversely, if (13) holds, then there is an even (if d is odd) or odd (if d is even) polynomial $\sigma(x)$ of degree $d-1$ such that $s'(h) = \sigma(h)$ for $h > 0$. Then $g'(h) = \sum_{t<h} \sigma(t)$ is a sum of linear combinations of Bernoulli polynomials of degrees d, $d-2$, $d-4, \ldots$, and (12) follows

Theorem 3. *There is a constant C depending only on the lattice Λ such that*

$$ht(u) - fht(u) \le C, \quad \textit{for all} \quad u \in \Lambda \ . \tag{6}$$

Furthermore,

$$fht(u) = \lim_{n \to \infty} \frac{ht(nu)}{n} \ . \tag{7}$$

Proof. Consider a vector $u \in \Lambda$ with fractional height n. From Theorem 1 we can write $u = \sum_{i=1}^{d} c_i v_i$ with $c_i \ge 0$, $\sum c_i = n$. If $u' = \sum \lfloor c_i \rfloor v_i$, then $ht(u') \le \sum \lfloor c_i \rfloor \le fht(u)$. However, u and u' differ only by a lattice vector in $\mathcal{P}$, of which there are only finitely many. (6) follows, and (7) is an immediate consequence. Note that the limit in (7) exists, since height is a subadditive function. ∎

Theorem 3 can be interpreted as saying that for large n the clusters of points of fractional height $\le n$ and of height $\le n$ look roughly the same, except that the faces of the latter may be somewhat "pitted". For well-rounded lattices they are exactly the same.

We shall make frequent use of the following result, which is a immediate consequence of Ehrhart's reciprocity law [11], [12], [13], [14] (see also Stanley [27], [28]).

Theorem 4. *For integral $n \ge 0$, $G'(n)$ and $I'(n)$ are respectively given by polynomials $g'(n)$ and $i'(n)$ in n of degree d, satisfying*

$$g'(-n) = (-1)^d i'(n), \quad n \in \mathbb{Z} \ . \tag{8}$$

Furthermore, $S'(0) = 1$, while for $n > 0$, $S'(n)$ is a polynomial $s'(n)$ of degree $d-1$ satisfying $s'(0) = 1 - (-1)^d$.

Since obviously $S(n) = G(n) - G(n-1)$ for $n > 0$, it follows from Theorem 4 that for well-rounded lattices (for which $G(n) = G'(n)$) $S(n)$ for $n > 0$ is also a polynomial $s(n)$ in n of degree $d-1$. If this is so then the generating function

$$\mathcal{S}(x) = \sum_{n=0}^{\infty} S(n) x^n$$

can be written as

$$\mathcal{S}(x) = \frac{P_d(x)}{(1-x)^d} \ , \tag{9}$$

for some polynomial $P_d(x)$ which we call the *coordinator polynomial.* These polynomials usually provide the most concise specification of the coordination sequences. (9) implies that the and so

$$fht(u) \le ht(u) \ . \tag{4}$$

A lattice for which equality holds in (2) is called *well-placed*, because each point appears on the boundary of some $n\mathcal{P}$, for $n \ge 0$, $n \in \mathbb{Z}$. A lattice for which equality holds in (3) is called *well-rounded*, because its heights are obtained just by the appropriate rounding of the fractional heights. Finally, if equality holds in (4), or equivalently if equality holds in both (2) and (3), we call the lattice *well-coordinated.*

Theorem 1. *A point $u \in \Lambda$ has fractional height h if and only if it can be written in the form*

$$u = \sum_{i=1}^{d} c_i v_i \ , \tag{5}$$

where $c_i \in \mathbb{Q}$, $c_i \ge 0$, $\sum c_i = h$, and $v_1, \ldots, v_d$ are distinct minimal vectors of Λ belonging to a face of the contact polytope.

Proof. If $fht(u) = h$, then as we magnify the contact polytope, forming $a\mathcal{P}$ for increasing a, u first belongs to $a\mathcal{P}$ when $a = h$, at which point u is on the boundary of $h\mathcal{P}$. Since the faces of $h\mathcal{P}$ are convex $(d-1)$-dimensional polytopes, by Carathéodory's theorem ([29], Theorem 2.2.12) we can write u as a linear combination of at most d of the vertices of that face:

$$u = \sum_{i=1}^{d} \lambda_i (hv_i) \ ,$$

with $\lambda_i \ge 0$, $\sum \lambda_i = 1$, from which (5) follows. The converse is immediate. ∎

On the other hand, the points of height n ($n \in \mathbb{Z}, n \ge 0$) are exactly the points that can be written as a linear combination of minimal vectors of Λ with nonnegative coefficients that sum to n. If instead we allowed real coefficients with sum at most n, we would obtain all of $n\mathcal{P}$. Of course the vertices of $n\mathcal{P}$ have height n. Thus we have established:

Theorem 2. *The points of fractional height at most h ($h \ge 0$) are all the lattice points in or on $h\mathcal{P}$. The points of height at most n ($n \in \mathbb{Z}, n \ge 0$) are a subset — which necessarily includes the vertices — of the lattice points in or on $n\mathcal{P}$. Furthermore, $fht(u) \le ht(u)$ for all $u \in \Lambda$, $G'(n) \ge G(n)$ for integers $n \ge 0$, and the lattice is well-rounded if and only if $G'(n) = G(n)$ for all integers $n \ge 0$.*

as follows:

$$\begin{array}{lll} d=1: & \text{for } \mathbb{Z}, & G(n)=\Delta_2(n)=2n+1\ , \\ d=2: & \text{for } A_2, & G(n)=\Delta_3(n)=3n^2+3n+1\ , \\ d=3: & \text{for h.c.p.}, & G(n)=\frac{7}{8}\Delta_4(n)+(-1)^n\frac{1}{8}= \text{ nearest integer to } \frac{7}{8}\Delta_4(n)\ , \\ d=4: & \text{for } D_4, & G(n)=\frac{4}{5}\Delta_5(n)+\frac{1}{5}= \text{ nearest integer to } \frac{4}{5}\Delta_5(n)\ . \end{array} \tag{1}$$

However, in higher dimensions this notation is not especially useful. The formula (55) for E_8, for example, does not simplify when expressed in terms of $\Delta_k(n)$.

The following symbols will be used: $\lfloor\ \rfloor$ for integer part or floor, $\lceil\ \rceil$ for ceiling, $\mathbb{Z}$ for the integers, $\mathbb{Q}$ for the rationals, $\mathbb{R}$ for the reals. For undefined terms from lattice theory see [6], and for the definition of less familiar polytopes (see as the "ambo-simplex") see [4]. This paper is part of series dealing with the properties of low-dimensional lattices from various points of view, the previous part being [5].

2. Contact graphs of lattices

Most of this paper will be concerned with the case when $\mathcal{G}$ is the contact graph of a d-dimensional lattice Λ that is spanned by its minimal vectors. Let $\mathcal{P}$ denote the contact polytope of the lattice, that is, the convex hull of the minimal vectors [4].

We define the *fractional height* of a vector $u \in \Lambda$ (or of the corresponding node of $\mathcal{G}$) to be

$$fht(u) = \min_{h \ge 0} \{u \in h\mathcal{P}\}\ ,$$

where $h\mathcal{P} = \{hx : x \in \mathcal{P}\}$, $h \ge 0$. Let $G'(h) = \#\{u \in \Lambda : fht(u) \le h\}$, $I'(h) = \#\{u \in \Lambda : fht(u) < h\}$, and $S'(h) = \#\{u \in \Lambda : fht(u) = h\} = G'(h) - I'(h)$.

In fact it seems that there are three reasonable ways of measuring height:

- the fractional height, $fht(u)$,
- the fractional height rounded up, $\lceil fht(u) \rceil$, and
- the height, $ht(u)$.

Obviously we have

$$fht(u) \le \lceil fht(u) \rceil\ , \tag{2}$$

and we shall prove in a moment that

$$\lceil fht(u) \rceil \le ht(u)\ , \tag{3}$$

u to the origin. Also, for $n = 0, 1, 2, \ldots$, we set

$$\begin{aligned} G(n) &= \#\{u \in \mathcal{G} : ht(u) \le n\} \ , \\ I(n) &= \#\{u \in \mathcal{G} : ht(u) < n\} \ , \\ S(n) &= \#\{u \in \mathcal{G} : ht(u) = n\} = G(n) - I(n) \ . \end{aligned}$$

Then $S(0)$, $S(1), \ldots$ is the *coordination sequence* of $\mathcal{G}$.

The paper is arranged as follows. In Section 2 we study the contact graphs of lattices, and introduce the notion of the fractional height of a lattice point u. This measures by how much the contact polytope of the lattice must be magnified before it contains u. The fractional height never exceeds the height (Theorem 2) and differs from it by a bounded amount (Theorem 3).

A lattice is called *well-coordinated* if the fractional heights are the same as the heights. Well-coordinated lattices have many desirable properties that make them easier to analyze. Although the root lattices A_d and D_d are well-coordinated (Theorems 8 and 9), lattices that are not well-coordinated exist in all dimensions above 4 (Theorem 6 and subsequent paragraphs). In particular, the lattices E_7, E_7^* and E_8 are not well-coordinated (Theorems 12–14).

An extreme example of a lattice that is not well-coordinated is the 11-dimensional "anabasic" lattice described in Section 2: this contains vectors u with the property that $ht(2u) < ht(u)$!

Section 3 studies the coordination sequences of the lattices A_d, D_d, E_6, E_7, E_8, their duals and some related nets. It is worth remarking that in this section we will see graphs in which the crystal ball numbers $G(n)$ are equinumerous with centered simplices (the sodalite net), centered cubes (the generalized b.c.c. net), and centered orthoplexes ($\mathbb{Z}^d$), representing all the regular polytopes in high dimensions (cf. [10]).

In Section 4 it is shown that among all Barlow packings, that is, those formed from layers of the hexagonal lattice, the hexagonal close packing (or h.c.p.) has both the highest coordination sequence and the highest crystal ball sequence, while the face-centered cubic (or f.c.c.) lattice has the lowest. This establishes a conjecture made in [19].

The highest crystal ball numbers for packings in dimensions $d \le 4$ have a concise description in terms of the function

$$\Delta_k(n) = (n+1)^k - n^k \ ,$$

1. Introduction

The *coordination sequence* of an infinite vertex-transitive graph $\mathcal{G}$ is the sequence $\{S(0), S(1), S(2), \ldots\}$, where $S(n)$ is the number of vertices at distance n from some fixed vertex of $\mathcal{G}$. The partial sums $G(n) = S(0) + S(1) + \cdots + S(n)$ are called the *crystal ball* numbers. As in the work of Brunner and Laves [2], O'Keeffe [18], [19], Grosse-Kunstleve [16] and others, in our examples $\mathcal{G}$ will usually be the *contact graph* of a d-dimensional lattice packing [6] or net [30], formed by taking the vertices to be the points of the lattice or net and joining each point to its closest neighbors.

Although we will not study it here, there is another way to construct a graph from a lattice that has some advantages over the contact graph. This is the *Voronoi graph*: again the vertices represent lattice points, but now two vertices are joined if the corresponding Voronoi cells [6, p. 33] are adjacent. The contact graph is always a subgraph. The chief advantage of the Voronoi graph is that it is meaningful for any lattice, whereas the contact graph is of little use for general lattices (consider for instance a two-dimensional lattice in which the generating vectors have different lengths). The Voronoi graph may also provide a better model for crystal growth. Consider the body-centered cubic (b.c.c.) lattice D_3^*, for example, in which the Voronoi cells are truncated octahedra. The vertices within distance n of a given vertex in the Voronoi graph are the lattice points that can be reached by stacking truncated octahedra to depth n around a fixed truncated octahedron. These points form a roughly spherical cluster, whereas as we shall see in Section 3 the vertices at distance n from a given vertex in the contact graph form a cluster with the shape of a cube.

The contact graph has been used by the authors cited above as a way of defining the density of a lattice or net. It is worth mentioning that the *theta series* [26], [23], [6] may be more appropriate for that purpose, since it exactly gives the numbers of points in ever-increasing spheres about a particular point.

Nevertheless, for lattices and nets that are related to the root lattices A_d, D_d, E_d, the contact graphs and the associated coordination sequences are of considerable interest in their own right, and we shall investigate their properties in this paper, extending the work of O'Keeffe [18], [19].

Throughout this paper, if $\mathcal{G}$ is a distance-transitive graph with some fixed choice of origin, and u is a vertex of $\mathcal{G}$, the *height* of u, $ht(u)$, is the number of edges in the shortest path from

Low-Dimensional Lattices VII: Coordination Sequences

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ABSTRACT

The coordination sequence $\{S(n)\}$ of a lattice or net gives the number of nodes that are n bonds away from a given node. $S(1)$ is the familiar coordination number. Extending work of O'Keeffe and others, we give explicit formulae for the coordination sequences of the root lattices A_d, D_d, E_6, E_7, E_8 and their duals. Proofs are given for many of the formulae, and for the fact that in every case $S(n)$ *is* a polynomial in n, although some of the individual formulae are conjectural. In the majority of cases the set of nodes that are at most n bonds away from a given node form a polytopal cluster whose shape is the same as that of the contact polytope for the lattice. It is also shown that among all the Barlow packings in three dimensions the hexagonal close packing has the greatest coordination sequence, and the face-centered cubic lattice the smallest, as conjectured by O'Keeffe.