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Coordination sequences for lattices

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Abstract. Coordination sequences for five 3-dimensional, ten 4-dimensional and eleven higher-dimensional lattices have been determined and all but one can be expressed as simple polynomials. Some regularities in these polynomials are observed. The correlation between topological and geometric density is demonstrated for 4-dimensional lattices. It is conjectured that hexagonal closest packing is topologically the densest packing in three dimensions.

Introduction

Considerable attention has been devoted to the geometrical properties of lattice sphere packings (Conway, Sloane, 1988). Here I discuss a topological property of these structures – their coordination sequences. If we consider the centers of spheres in a sphere packing to be vertices, and contact between two spheres to correspond to an edge joining the two vertices, a sphere packing can be considered as an infinite net. A kth topological neighbor of a given vertex in a net is one for which the shortest path to the reference vertex consists of k edges. The coordination sequence (CS) associated with a vertex is the sequence of numbers n_k of kth neighbors of that vertex (Brunner, 1979 and references therein). Obviously for lattices the coordination sequence is the same for every point. The coordination sequence is in a sense analogous to the theta series (Conway, Sloane, 1988) of a lattice which provides information about numbers of geometrical neighbors. Just as for theta series, the lattice defines the CS but not vice versa.

Coordination sequences for the primitive hypercubic lattices, Z^N, were reported (O'Keeffe, 1991a) for N (the dimension of the space) ≤ 10. In that work it was shown that the coordination sequence could be expressed as a simple polynomial in k. I have now determined coordination sequences for lattice sphere packings in two to four dimensions and a few higher-dimensional lattices and find the same behavior which is reported here. It should be emphasized that the coordination sequences were found simply by counting neighbors using a computer, but that large numbers (about 10^6) of neighbors were enumerated and the polynomials found by inspection of the results. The algorithm used is an adaptation of one designed for three dimensions and rapidly becomes inefficient for large N. Counting neighbors proceeds rapidly on a microcomputer, but because (as implemented) one needs to keep track of vertices counted, the amount of memory available restricts the number of shells counted and precludes investigation of high-dimensional structures. It would possibly be rewarding to derive the polynomials directly (analytically) as this might lead to deeper insights into the nature of lattices and related structures.

Two dimensions

In two dimensions there are just two lattice sphere (circle) packings: the square and hexagonal lattices with coordination numbers $z = 4$ and 6 respectively and $n_k = zk$. In two dimensions, one already learns that coordination sequences do not uniquely determine a structure, thus $n_k = 4k$ for the Archimedian tesselation 3.4.6.4 as well as for 4^4. For the tesselation 6^3, which may be considered as the net formed by the holes of 3^6, $n_k = 3k$.

Three dimensions

Three dimensional lattice sphere packings (Table 1) are cF = face-centered cubic ($z = 12$), tI = body-centered tetragonal, with $c/a = \sqrt{(2/3)}$ ($z = 10$), hP = hexagonal, with $c/a = 1$ and cI = body-centered cubic (both with

Table 1. Properties of three-dimensional lattices. The g_{ij} are the components of the (symmetric) metric matrix of the primitive cell with $g_{ii} = 1$ (appropriate for packings of unit spheres), z is the coordination number, and r is the number of points per unit volume. The polynomial under n_k is the expression for the coordination sequence.

lattice	g_{12}	g_{13}	g_{23}	z	r	n_k	
cF	1/2	1/2	1/2	12	$\sqrt{2} = 1.414$	$10k^2 + 2$	
tI	−1/2	−1/4	−1/4	10	$4/3 = 1.333$	$8k^2 + 2$	– 8527
cI BCC	−1/3	−1/3	−1/3	8	$\sqrt{27/4} = 1.299$	$6k^2 + 2$	5897
hP	−1/2	0	0	8	$2/\sqrt{3} = 1.154$	$6k^2 + 2$	〃
cP	0	0	0	6	1	$4k^2 + 2$	〃

Table 2. Properties of four-dimensional lattice sphere packings. Entries for each lattice are on two rows. The lattice is identified by the name and number of Wondratschek, Bülow and Neubüser (1971). The g_{ij} are the components of the (symmetric) metric matrix of the primitive cell with $g_{ii} = 1$ (appropriate for packings of unit diameter spheres), z is the coordination number, and r is the number of points per unit cell volume. The polynomial under n_k is the expression for the coordination sequence.

	lattice						z	r	
	g_{12}	g_{13}	g_{14}	g_{23}	g_{24}	g_{24}		n_k	
	64. Z-centered hypercubic						24	2	D_4
A7900	1/2	0	1/2	1/2	0	−1/2		$16k^3 + 8k$	
	62. SN-centered icosahedral						20	$4/\sqrt{5} = 1.789$	A_4
A8383	1/2	1/2	1/2	1/2	1/2	1/2		$(35k^3 + 25k)/3$	
	59. RR-centered di-isohexagonal orthogonal						18	$16/9 = 1.778$	
8528	1/4	−1/2	−1/2	−1/2	−1/2	1/4		$11k^3 + 7k$	
	54*. F-centered cubic orthogonal						14	$\sqrt{2} = 1.414$	
8529	0	0	0	1/2	1/2	1/2		$(20k^3 + 22k)/3$	
	60. Primitive di-isohexagonal orthogonal						12	$4/3 = 1.333$	
8530	−1/2	0	0	0	0	−1/2		$6k^3 + 6k$	
	31*. I-centered tetragonal orthogonal						12	$4/3 = 1.333$	
1386	0	0	0	−1/4	−1/4	−1/2		$(16k^3 + 20k)/3$	
	61. Primitive icosahedral						10	$16/5\sqrt{5} = 1.431$	
8531	−1/4	−1/4	−1/4	−1/4	−1/4	−1/4		$5k^3 + 5k$	A_4^*
	52*. I-centered cubic orthogonal						10	$\sqrt{27/4} = 1.299$	
8532	0	0	0	−1/3	−1/3	−1/3		$4k^3 + 6k$	
	46*. Primitive hexagonal tetragonal						10	$2/\sqrt{3} = 1.155$	
	−1/2	0	0	0	0	0		$4k^3 + 6k$	
	63. Primitive hypercubic						8	1	
8412	0	0	0	0	0	0		$(8k^3 + 16k)/3$	

* lattice parameters not all determined by symmetry

$z = 8$) and cP = primitive cubic ($z = 6$). For all these lattices, $n_k = (z - 2)k^2 + 2$ (cf. Brunner, 1979); a result that is easy to derive in each case (cf. Williams, 1972). It is interesting that the same expression also holds for the body-centered cubic lattice if connections to both first and second geometric neighbors are counted as edges ($z = 8 + 6 = 14$, $n_k = 12k^2 + 2$). This last result has been known for a long time (Marvin, 1939).

The expression $n_k = (z - 2)k^2 + 2$ also holds (O'Keeffe, 1991b) for the sodalite net (lattice complex W*) for which $z = 4$. The vertices of the net are in the (tetrahedral) holes of the cI lattice. The same expression holds again for the net with vertices in the centers of the trigonal prismatic holes of the hP lattice with $c/a = 1/\sqrt{3}$. This arrangement of prismatically stacked 6^3 nets (lattice complex G with specialized metric) corresponds to a sphere packing with $z = 5$. Unfortunately higher dimensions are not quite so simple.

It should be remarked that cF appears to be the least dense twelve-coordinate structure in the topological sense. For hexagonal closest packing (hcp) the CS is given by:

$$hcp: \quad n_k = \lfloor 21k^2/2 \rfloor + 2 .$$

Here $\lfloor\ \rfloor$ indicates rounding down to the nearest integer. For all of the many intermediate packings (such as hc, hcc, etc.) that I have investigated n_k is intermediate between that for cF and hcp and in fact the sequence provides an easy way for computer recognition of such packings, and is so used.

Four dimensions

Ten four-dimensional lattice sphere packings have been identified and investigated. These are listed in Table 2 using the names and numbering of Wondratschek, Bülow and Neubüser (1971). In the same way as, in three dimensions, the body-centered tetragonal lattice becomes a ten-coordinated sphere packing and the primitive hexagonal lattice becomes an eight-coordinated sphere packing for a special value of c/a, so some of these lattice packings correspond to special values of the lattice parameters not determined by symmetry. These are identified by an asterisk in the table. The coordination sequences given in the table can all be expressed as $n_k = ak^3 + (z - a)k$, but a does not depend only on z.

A simple 16-coordinated sphere packing in four dimensions is derived by placing sphere centers in the holes of D_4. Referred to a hypercubic cell (with lattice points at 0, 0, 0, 0 and 1/2, 1/2, 1/2, 1/2) vertices are at the six distinct permutations of 1/2, 1/2, 0, 0. This is in fact the regular honeycomb {3, 4, 3, 3} (Coxeter, 1963). After the experience with two and three dimensions, it was thought that this structure might also have a simple CS. In fact it is slightly more complicated: after $n_1 = 16$ one has for k even, $n_k = 12k^3 + 8k - 8$ and for k odd, $n_k = 12k^3 + 4k + 8$.

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Higher dimensions

Polynomials for n_k for the primitive hypercubic lattices for N dimensions ($N \leq 10$) and for a generalization of the sodalite net (the net formed by the holes of the lattice A_n^*) for $N \leq 6$ have been given earlier (O'Keeffe, 1991a). Here some other well known lattices (Conway, Sloane, 1988) are considered.

The family of lattices A_N^* are simply defined in terms of the metric matrix of the primitive cell, which has (for unit lattice vectors) all diagonal terms equal to 1 and all off-diagonal terms equal to $-1/N$. The coordination number is $z = 2N + 2$. The three-dimensional example is cI (Table 1) and the four-dimensional example is number 61 (Table 2). For dimensions five to seven one has:

$$A_5^*: \quad n_k = 5k^4/2 + 15k^2/2 + 2 .$$ A8533

$$A_6^*: \quad n_k = 7k^5/6 + 35k^3/6 + 7k .$$ A8534

$$A_7^*: \quad n_k = 7k^6/18 + 35k^4/9 + 175k^2/18 + 2 .$$ A8535

Another simple family consists of the lattices A_N (reciprocal to A_N^*) with coordination number $N(N+1)$. For these lattices the off-diagonal terms in the metric matrix of the primitive cell are all equal to 1/2. The three-dimensional example is *cF* (Table 1) and the four-dimensional example is number 62 (Table 2). For dimensions five to seven I find:

$$A_5: \quad n_k = 21k^4/2 + 35k^2/2 + 2\,.$$

$$A_6: \quad n_k = 77k^5/10 + 49k^3/2 + 49k/5\,.$$

$$A_7: \quad n_k = 143k^6/30 + 77k^4/3 + 707k^2/30 + 2\,.$$

Another family studied is that of the "checkerboard" lattices D_n. D_3 is again *cF* and D_4 is number 64 in Table 2. D_5 is the densest five-dimensional sphere packing (40-coordinated). For D_5 and D_6 the CS are:

$$D_5: \quad n_k = 18k^4 + 20k^2 + 2\,.$$

$$D_6: \quad n_k = 232k^5/15 + 104k^3/3 + 148k/15\,.$$

The lattices reciprocal to D_N are not new topologically. D_4^* is the same as D_4 and for $N \geq 5$, D_N^* is $2N$ coordinated and hence topologically equivalent to Z^N.

In six-dimensions the densest lattice sphere packing corresponds to the 72-coordinated lattice E_6 (Conway and Sloane 1988). For this lattice:

$$E_6: \quad n_k = 117k^5/5 + 36k^3 + 63k/5\,.$$

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The reciprocal lattice of E_6 is 54-coordinated. It has a particularly simple CS:

$$E_6^*: \quad n_k = 18k^5 + 30k^3 + 6k\,.$$

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The example of E_6 can serve to illustrate why I have not explored higher dimensions. For this lattice there are 5276898 points in the first ten topological coordination shells of a given lattice point compared with only 3870 for *cF* (the densest three-dimensional lattice). The "obvious" general algorithms for enumerating CS's either are quick but require a lot of memory, or have modest demands on memory but are slow. Six dimensions appears to be the practical limit for small computers unless one exploits the symmetry of the lattice.

E_8, which is important in many different contexts, is an example of a high-symmetry lattice. Referred to a centered hypercubic cell with $a = \sqrt{2}$ (appropriate for a packing of unit diameter spheres), lattice points are at (a) all combinations of even numbers of 0 and 1/2, (b) all combinations of even numbers of 1/4 and 3/4 (a total of 256 per cell). The nearest neighbors of the point at 0,0,0,0,0,0,0,0 are (a) all 112 combinations of ±1/2, ±1/2, 0,0,0,0,0,0 and (b) all 128 combinations with an even number of plus signs of ±1/4, ±1/4, ±1/4, ±1/4, ±1/4, ±1/4, ±1/4, ±1/4. Coordinates of points in the next three shells and my results for the CS out to n_8 are given in Table 3. No simple pattern has been discerned in the CS in this instance.

Table 3. Coordination sequence for E_8. For the first four shells, coordinates of neighbors of $(0^8) = 0,0,0,0,0,0,0,0$ are given in multiples of 1/4, and all permutations and sign combinations are to be taken except a prefix "e" (or "o") means only even (or odd) numbers of positive and negative signs are to be used.

k	n_k	coordinates of topological neighbors
1	240	$(2^2 0^6)$ e(1^8)
2	9120	$(4^2 0^6)$ $(4 2^2 0^5)$ $(4 0^7)$ e(2^8) $(2^6 0^2)$ $(2^4 0^4)$ o$(3 1^7)$ e$(3^2 1^6)$
3	121680	$(6^2 0^6)$ $(6 4 2 0^5)$ $(6 2^3 0^4)$ $(6 2 0^6)$ $(4^3 0^5)$ e$(4^2 2^6)$ $(4^2 2^4 0^2)$ $(4 2^6 0)$ $(4 2^4 0^3)$ $(4^2 2^2 0^4)$ o(2^8) e$(5^2 1^6)$ e$(5 3^2 1^5)$ o$(5 3 1^6)$ e$(5 1^7)$ e(3^8) e$(3^6 1^2)$ o$(3^5 1^3)$ e$(3^4 1^4)$ o$(3^3 1^5)$
4	863168	$(8^2 0^6)$ $(8 6 2 0^5)$ $(8 4^2 0^5)$ $(8 4 2^2 0^4)$ $(8 4 0^6)$ $(8 2^4 0^3)$ $(2^2 0)$ $(8 0^7)$ $(6^2 4 0^5)$ e$(6^2 2^6)$ $(6^2 2^4 0)$ $(6^2 2^2 0^4)$ e$(6 4^2 2^5)$ $(6 4^2 2^3 0)$ $(6 4^2 2 0^4)$ $(6 4 2^5 0)$ $(6 4 2^3 0^3)$ $(6 2^7)$ $(6 2^5 0)$ e(4^8) e$(4^6 2^2)$ e$(4^6 0^2)$ $(4^5 2^2 0)$ o$(4^5 0^3)$ $(4^4 2^4)$ $(4^4 2^2 0^2)$ $(4^4 0^4)$ $(4^3 2^4 0)$ $(4^3 2^2 0^3)$ o$(4^2 2^6)$ e$(7^2 1^6)$ e$(7 5 3 1^5)$ o$(7 5 1^6)$ e$(7 3^3 1^4)$ o$(7 3^2 1^5)$ e$(7 3 1^6)$ o$(7 1^7)$ e$(5^3 1^5)$ e$(5^2 3^6)$ e$(5^2 3^4 1^2)$ o$(5^2 3^3 1^3)$ e$(5^2 3^2 1^4)$ o$(5^2 3 1^5)$ e$(5 3^6 1)$ o$(5 3^5 1^2)$ e$(5 3^4 1^3)$ e$(5 3^3 1^4)$ o$(3^7 1)$
5	4093232	
6	14823904	
7	44288656	
8	114514688	

Topological and geometrical density

The topological density has been defined (cf. O'Keeffe, 1991b) as

$$\varrho_k = \left(\sum_{i=1}^{k} n_i \right) \Big/ k^3\,.$$

The limit as k goes to infinity is ϱ_∞. For an N-dimensional net with a CS given by a power series, $n_k = ak^{N-1} + \ldots$, one simply has $\varrho_\infty = a/N$.

There is some interest in the correlation of topological and geometrical density (Stixrude, Bukowinski, 1990; O'Keeffe, 1991b). Fig. 1 shows the correlation for the four-dimensional lattices of Table 2. Clearly the correlation, while not perfect, is very strong.

Remarks

For all lattice sphere packings studied other than E_8 (two for $N = 2$, five for $n = 3$, ten for $N = 4$, and eleven for $N > 4$, a total of 28), the coordination sequence, n_k, is

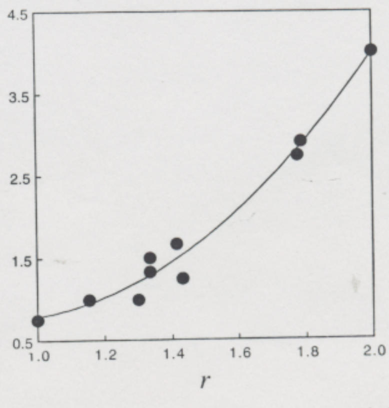

Fig. 1. The topological density $\varrho_\infty = a/4$, for the four-dimensional lattice sphere packings discussed in the text, plotted against the geometrical density, r, expressed as the number of unit diameter spheres per unit volume. The line is a quadratic fit to guide the eye.

given by a polynomial in k. Furthermore, only odd powers of k are involved for even N and only even powers of k for odd N. The coefficient of k^0 is always 2. The CS for the five generalized sodalite nets behave similarly. These observations suggest that it should be possible, at least in some cases, to derive the polynomials analytically rather than empirically (as here).

Other structures (compare the four-dimensional honeycomb $\{3,4,3,3\}$ discussed above) generally do not have a CS that is a simple polynomial although use of the round-down function (as for *hcp* given above) allows expression of CS's for some apparently complex structures. For example, the topologically very different four-connected three-dimensional nets of the zeolites type A and rho (Wells, 1984) with 24 vertices in the repeat unit both have the CS: $n_k = \lfloor 8k^2 + 14)/5 \rfloor$.

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References

Brunner, G. O.: The properties of coordination sequences and conclusions regarding the lowest possible density of zeolites. J. Solid State Chem. **29** (1979) 41–45.

Conway, J. H.; Sloane, N. J. H.: Sphere Packings, Lattices and Groups. Springer-Verlag, New York 1988.

Coxeter, H. S. M.: Regular Polytypes. Second edition. MacMillan, New York 1963.

Marvin, J. W.: The aggregation of orthic tetrakaidecahedra. Science **83** (1939) 188.

O'Keeffe, M.: *N*-dimensional diamond, sodalite and rare sphere packings. Acta Crystallogr. A **47** (1991 a) 748–753.

O'Keeffe, M.: Dense and rare four-connected nets. Z. Kristallogr. **196** (1991 b) 21–37.

Stixrude, L.; Bukowinski, M. S. T.: Rings, topology, and the density of tectosilicates. Am. Mineral. **75** (1990) 1159–1169.

Wells, A. F.: Structural Inorganic Chemistry. 5th Ed. Clarendon Press, Oxford 1984.

Williams, R.: Natural Structure. Eudaemon Press, Moorpark, CA 1972. Reprinted as The Geometrical Foundation of Natural Structure. Dover, New York 1977.

Wondratschek, H.; Bülow, R.; Neubüser, J.: On crystallography in higher dimensions. III. Results in R_4. Acta Crystallogr. A **27** (1971) 523–535.