Coordination sequences for root lattices and related graphs

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Dedicated to Ted Janssen on the occasion of his 60th birthday

The coordination sequence $s_\Lambda(k)$ of a graph Λ counts the number of its vertices which have distance k from a given vertex, where the distance between two vertices is defined as the minimal number of bonds in any path connecting them. For a large class of graphs, including in particular the classical root lattices, we present the coordination sequences and their generating functions, summarizing and extending recent results of Conway and Sloane [1].

Introduction

Discrete versions of physical models are usually based on graphs, particularly on periodic lattices. For instance, a lattice may serve as an abstraction of the regular arrangement of atoms in a crystalline solid, and the physical model introduces suitable degrees of freedom associated to the vertices or the edges of the graph, depending on the type of physical property one intends to study. Conversely, for a given lattice model describing some interesting physical situation, one might be interested to understand the influence of the underlying graph on the physical properties of the system.

For example, an important class of lattice models are classical and quantum spin models intended to describe magnetic ordering, the famous Ising model being the simplest and most thoroughly studied member of this group. For these models, one is mainly interested in their critical properties, i.e., the behaviour of physical quantities at and in the vicinity of the phase transition point where magnetic ordering occurs. In many cases, these critical properties are "universal" in the sense that they do not depend on the details of the particular model under consideration, but only on a number of rather general features such as the space dimension, the symmetries and the range of the interactions.

In contrast, the precise location of the critical point (the critical temperature) depends sensitively on the underlying graph. It has been demonstrated recently [2, 3] that the location of the critical points for Ising and percolation models on several lattices can be well approximated by empirical functions involving the dimension and the coordination number of the lattice. On the other hand, these quantities alone cannot completely determine the critical point as can be seen from data obtained for different graphs with identical dimension and (mean) coordination number [4, 5, 6]. This poses the question how to include more detail of the lattice in order to improve the approximation. In our view, it is the natural approach to investigate higher coordination numbers (i.e., the number of next-nearest neighbours and so on) of the lattice and their influence on the physical properties of the model.

With this in mind, we started to analyze the coordination sequences of various graphs, and, in particular, the classical root lattices [7, 8]. Apart from some numerical investigation [9, 10], this did not seem to have attracted a lot of research. However, when we finished our calculations and started to work on the proofs, we became aware of recent results of Conway and Sloane [1] where the problem is solved for the root lattices A_n ($n \geq 1$), D_n ($n \geq 4$), E_6, E_7, and E_8, together with proofs for most of the results. (The corresponding sequences are not contained in [11], but have been added to [12].) Not treated, however, are the periodic graphs obtained from the root systems B_n ($n \geq 2$), C_n ($n \geq 2$), F_4, and G_2. They do not result in new *lattices* (seen as the set of points reached by integer linear combinations of the root vectors), but they do result in different *graphs*, because they have rather different connectivity patterns. We thus call them *root graphs* from now on.

In what follows, we present the results on the coordination sequences and their generating functions in a concise way, including some of the material of [1], but omitting proofs. The latter, in many cases, follow directly from [1] or can be traced back to it — with two exceptions mentioned explicitly later on.

Preliminaries and general setup

The calculation of the coordination sequence of a lattice first means to specify the corresponding graph, i.e., to specify who is neighbour of whom in the lattice. In the simplest example of all, the lattice $\mathbb{Z}$, each lattice point has precisely two neighbours, one to the left and one to the right. Consequently, the number $s_{\mathbb{Z}}(k)$

of kth neighbours is $s_{\mathbb{Z}}(0) = 1$ and $s_{\mathbb{Z}}(k) = 2$ for $k \geq 1$, with generating function

$$S_{\mathbb{Z}}(x) \;=\; \sum_{k=0}^{\infty} s_{\mathbb{Z}}(k)\, x^k \;=\; \frac{1+x}{1-x}\,, \tag{1}$$

compare [13] for elementary background material on this type of approach. If we combine two lattices Λ_1, Λ_2 in Euclidean spaces $\mathbb{E}_1, \mathbb{E}_2$, respectively, to the direct sum $\Lambda_1 \oplus \Lambda_2$ in $\mathbb{E}_1 \oplus \mathbb{E}_2$, together with the rule that $x = (x_1, x_2)$ is neighbour of $y = (y_1, y_2)$ in $\Lambda_1 \oplus \Lambda_2$ if and only if x_1 is neighbour of y_1 in Λ_1 *and* x_2 is neighbour of y_2 in Λ_2, the new generating function is a product:

$$\begin{aligned} S_{\Lambda_1 \oplus \Lambda_2}(x) &= \sum_{k=0}^{\infty} s_{\Lambda_1 \oplus \Lambda_2}(k)\, x^k \\ &= \sum_{m=0}^{\infty} \sum_{\ell=0}^{m} s_{\Lambda_1}(\ell)\, s_{\Lambda_2}(m-\ell)\, x^m \\ &= S_{\Lambda_1}(x) \cdot S_{\Lambda_2}(x)\,. \end{aligned} \tag{2}$$

A direct application to the situation of the cubic lattice $\mathbb{Z}^n$ immediately gives its generating function

$$S_{\mathbb{Z}^n}(x) \;=\; \left(\frac{1+x}{1-x}\right)^n \;=\; \frac{1}{(1-x)^n} \sum_{k=0}^{n} \binom{n}{k} x^k \tag{3}$$

which (accidentally) coincides with its θ-function [7]. Similarly, if we know the generating functions for certain lattices, we can extend them to all direct sums of this type. It is thus reasonable to take a closer look at the root lattices (see [7] for definition and background material and [8] for details on the underlying root systems and their classification). In view of the previous remark, it is sufficient to restrict to the simple root lattices which are characterized by connected Dynkin diagrams [8, 7]. The corresponding graphs are obtained by the rule that a lattice point x has all other lattice points as neighbours that can be reached by a root vector. Note that, due to this rule, *all* root systems will appear. As an example, consider A_2 and G_2: they define the same root lattice, but different graphs and hence different coordination sequences, see Figure 1. Also, F_4 defines the same lattice as D_4^*, the dual of D_4 and equivalent to it as a lattice, but not the same graph. Similarly, B_n (for which the root lattice is just $\mathbb{Z}^n$) and C_n (whose root lattice coincides with that of D_n) define different graphs for $n \geq 3$, while those of B_2 and C_2 are equivalent (they yield a square lattice with points connected along the edges and the diagonals of the squares).

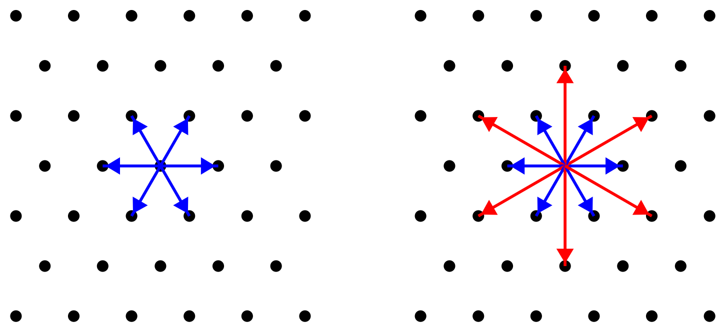

Figure 1: The vector stars of the root systems A_2 (left) and G_2 (right). They define neighbouring points in the corresponding root graphs.

In all examples to be discussed below, the generating function is of the form

$$S_\Lambda(x) \;=\; \frac{P_\Lambda(x)}{(1-x)^n} \tag{4}$$

where Λ is a lattice in n-dimensional Euclidean space and $P_\Lambda(x)$ is an integral polynomial of degree n (for a proof of this statement for the root lattices, see [1]; the remaining cases rest upon the proper generalization of the concept of well-roundedness to root graphs). It is therefore sufficient to list the polynomials in the numerator of (4) for the lattices and graphs under consideration.

Results

Although we shall give the generating functions below, the explicit values of the coordination numbers $s_\Lambda(k)$ of root graphs Λ in dimension $n \leq 8$ are, for convenience, shown in Table 1 for $1 \leq k \leq 10$. Note that, by definition, we set $s_\Lambda(0) = 1$ in all cases.

The coordinator polynomials $P_\Lambda(x)$ of the root graphs belonging to the four infinite series turn out to be given by

$$P_{A_n}(x) \;=\; \sum_{k=0}^{n} \binom{n}{k}^2 x^k \tag{5}$$

$$\begin{aligned} P_{B_n}(x) \;&=\; \frac{1}{2}\left[(1+\sqrt{x})^{2n+1} + (1-\sqrt{x})^{2n+1}\right] \;-\; 2nx(1+x)^{n-1} \\ &=\; \sum_{k=0}^{n} \left[\binom{2n+1}{2k} \;-\; 2k\binom{n}{k}\right] x^k \end{aligned} \tag{6}$$

$$P_{C_n}(x) \;=\; \frac{1}{2}\left[(1+\sqrt{x})^{2n} + (1-\sqrt{x})^{2n}\right] \;=\; \sum_{k=0}^{n} \binom{2n}{2k} x^k \tag{7}$$

$$
\begin{aligned}
P_{D_n}(x) &= \frac{1}{2}\left[(1+\sqrt{x})^{2n} + (1-\sqrt{x})^{2n}\right] \;-\; 2nx(1+x)^{n-2} \\
&= \sum_{k=0}^{n} \left[\binom{2n}{2k} - \frac{2k(n-k)}{n-1} \binom{n}{k} \right] x^k \, . \qquad (8)
\end{aligned}
$$

In all cases, the coefficients of the polynomials are rather simple expressions in terms of binomial coefficients

$$
\binom{n}{k} = \frac{n!}{k!\,(n-k)!} \, . \qquad (9)
$$

The results for the graphs A_n ($n \geq 1$) and D_n ($n \geq 4$) are just those contained in [1], and the polynomials for C_n ($n \geq 2$) can be derived by the methods outlined there, if one observes that the *longer* roots of C_n generate a sublattice that is equivalent to $\mathbb{Z}^n$. However, the expressions for B_n ($n \geq 2$), as those for D_n ($n \geq 4$) here and in [1], are conjectures based on enumeration of coordination sequences for a large number of examples. The striking similarity between B_n and D_n might actually help to find a proof. The connection is rather intimate: while all roots of B_n generate $\mathbb{Z}^n$, the long roots alone generate D_n, and each point of B_n can be reached from 0 by using a path with at most one short root.

For the three root graphs related to the exceptional (simply laced) Lie algebras E_6, E_7, and E_8, the coordinator polynomials read

$$
\begin{aligned}
P_{E_6}(x) &= 1 + 66\,x + 645\,x^2 + 1384\,x^3 + 645\,x^4 + 66\,x^5 + x^6 \qquad (10) \\
P_{E_7}(x) &= 1 + 119\,x + 2037\,x^2 + 8211\,x^3 + 8787\,x^4 + 2037\,x^5 \\
&\quad + 119\,x^6 + x^7 \qquad (11) \\
P_{E_8}(x) &= 1 + 232\,x + 7228\,x^2 + 55384\,x^3 + 133510\,x^4 + 107224\,x^5 \\
&\quad + 24508\,x^6 + 232\,x^7 + x^8 \qquad (12)
\end{aligned}
$$

as has been proved in [1]. Finally, for the two remaining root graphs we find

$$
\begin{aligned}
P_{F_4}(x) &= 1 + 44\,x + 198\,x^2 + 140\,x^3 + x^4 \qquad (13) \\
P_{G_2}(x) &= 1 + 10\,x + 7\,x^2 \, . \qquad (14)
\end{aligned}
$$

Let us give an explicit proof for the last example. Clearly, $s_{G_2}(0) = 1$ and $s_{G_2}(1) = 12$. Then, for $n \geq 2$, one can explicitly show that the graph G_2, in comparison to A_2 (which also happens to be equivalent to the lattice generated by the long roots of G_2, see Figure 1), has a shell structure with $s_{G_2}(n) = 2s_{A_2}(n) + s_{A_2}(n-1) = 18n - 6$, from which the above statement follows. By similar arguments, the other examples with short and long root vectors can be traced back to the lattice case; the corresponding shell structure of the root graph

Table 1: First coordination numbers of root graphs of dimension $n \leq 8$

Λ	$s_\Lambda(1)$	$s_\Lambda(2)$	$s_\Lambda(3)$	$s_\Lambda(4)$	$s_\Lambda(5)$	$s_\Lambda(6)$	$s_\Lambda(7)$	$s_\Lambda(8)$	$s_\Lambda(9)$	$s_\Lambda(10)$
A_1	2	2	2	2	2	2	2	2	2	2
A_2	6	12	18	24	30	36	42	48	54	60
A_3	12	42	92	162	252	362	492	642	812	1002
A_4	20	110	340	780	1500	2570	4060	6040	8580	11750
A_5	30	240	1010	2970	7002	14240	26070	44130	70310	106752
A_6	42	462	2562	9492	27174	65226	137886	264936	472626	794598
A_7	56	812	5768	26474	91112	256508	623576	1356194	2703512	5025692
A_8	72	1332	11832	66222	271224	889716	2476296	6077196	13507416	27717948
B_2	8	16	24	32	40	48	56	64	72	80
B_3	18	74	170	306	482	698	954	1250	1586	1962
B_4	32	224	768	1856	3680	6432	10304	15488	22176	30560
B_5	50	530	2562	8130	20082	42130	78850	135682	218930	335762
B_6	72	1072	6968	28320	85992	214864	467544	918080	1665672	2838384
B_7	98	1946	16394	83442	307314	907018	2282394	5095650	10368386	19594106
B_8	128	3264	34624	216448	954880	3301952	9556160	24165120	54993792	115021760
C_2	8	16	24	32	40	48	56	64	72	80
C_3	18	66	146	258	402	578	786	1026	1298	1602
C_4	32	192	608	1408	2720	4672	7392	11008	15648	21440
C_5	50	450	1970	5890	14002	28610	52530	89090	142130	216002
C_6	72	912	5336	20256	58728	142000	301560	581184	1038984	1749456
C_7	98	1666	12642	59906	209762	596610	1459810	3188738	6376034	11879042
C_8	128	2816	27008	157184	658048	2187520	6140800	15158272	33830016	69629696
D_4	24	144	456	1056	2040	3504	5544	8256	11736	16080
D_5	40	370	1640	4930	11752	24050	44200	75010	119720	182002
D_6	60	792	4724	18096	52716	127816	271908	524640	938652	1581432
D_7	84	1498	11620	55650	195972	559258	1371316	2999682	6003956	11193882
D_8	112	2592	25424	149568	629808	2100832	5910288	14610560	32641008	67232416
E_6	72	1062	6696	26316	77688	189810	405720	785304	1408104	2376126
E_7	126	2898	25886	133506	490014	1433810	3573054	7902594	15942206	29896146
E_8	240	9120	121680	864960	4113840	14905440	44480400	114879360	265422960	561403680
F_4	48	384	1392	3456	6960	12288	19824	29952	43056	59520
G_2	12	30	48	66	84	102	120	138	156	174

is defined by the coordination spheres of its sublattice generated by the set of long root vectors.

Finally, it is interesting to note that the coordination sequences for root graphs Λ of type A_n, C_n, D_n, and E_6 result in self-reciprocal polynomials $P_\Lambda(x)$, i.e.,

$$P_\Lambda(x) \;=\; x^n \cdot P_\Lambda(1/x) \tag{15}$$

while the others do not; for a geometric meaning of this property we refer to [1].

Outlook

We presented the coordination sequences and their generating functions for root lattices and, more generally, graphs based upon the root systems, namely for the series A_n $(n \geq 1)$, B_n $(n \geq 2)$, C_n $(n \geq 2)$, and D_n $(n \geq 4)$, and for the exceptional cases E_6, E_7, E_8, F_4, and G_2. Proofs of various cases can be found in Conway and Sloane [1] or directly based on their results, but the generating functions for B_n and D_n are still conjectural at the moment.

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