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 \( \Lambda \) 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 \cite{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 \cite{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 \cite{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 \cite{7,8}. Apart from some numerical investigation \cite{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 \cite{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 \cite{11}, but have been added to \cite{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 \cite{1}, but omitting proofs. The latter, in many cases, follow directly from \cite{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 \( k \)th 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 \cite{13} for elementary background material on this type of approach. If we combine two lattices \( \Lambda_1, \Lambda_2 \) 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 \( \Lambda_1 \) and \( x_2 \) is neighbour of \( y_2 \) in \( \Lambda_2 \), the new generating function is a product:

\[
S_{\Lambda_1 \oplus \Lambda_2}(x) = \sum_{k=0}^{\infty} s_{\Lambda_1 \oplus \Lambda_2}(k) x^k
= \sum_{m=0}^{\infty} \sum_{\ell=0}^{m} s_{\Lambda_1}(\ell) s_{\Lambda_2}(m - \ell) x^m
= S_{\Lambda_1}(x) \cdot S_{\Lambda_2}(x). \tag{2}
\]

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 \( \theta \)-function \cite{4}. 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 \cite{7} for definition and background material and \cite{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 \cite{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).
In all examples to be discussed below, the generating function is of the form

\[ S_\Lambda(x) = \frac{P_\Lambda(x)}{(1-x)^n} \]  (4)

where \( \Lambda \) 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 \( \Lambda \) in dimension \( n \leq 8 \) are, for convenience, shown in Table I 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

\[ P_{A_n}(x) = \sum_{k=0}^{n} \binom{n}{k}^2 x^k \]  (5)

\[ P_{B_n}(x) = \frac{1}{2} \left[ (1 + \sqrt{x})^{2n+1} + (1 - \sqrt{x})^{2n+1} \right] - 2nx(1 + x)^{n-1} \]

\[ = \sum_{k=0}^{n} \left[ \binom{2n+1}{2k} - 2k \binom{n}{k} \right] x^k \]  (6)

\[ P_{C_n}(x) = \frac{1}{2} \left[ (1 + \sqrt{x})^{2n} + (1 - \sqrt{x})^{2n} \right] = \sum_{k=0}^{n} \binom{2n}{2k} x^k \]  (7)
\[ P_{D_n}(x) = \frac{1}{2} \left[ (1 + \sqrt{x})^{2n} + (1 - \sqrt{x})^{2n} \right] - 2nx(1+x)^{n-2} \]
\[ = \sum_{k=0}^{n} \left[ \frac{(2n)}{2k} - \frac{2k(n-k)}{n-1} \left( \frac{n}{k} \right) \right] x^k. \quad (8) \]

In all cases, the coefficients of the polynomials are rather simple expressions in terms of binomial coefficients
\[ \binom{n}{k} = \frac{n!}{k!(n-k)!}. \quad (9) \]

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
\[
\begin{align*}
P_{E_6}(x) &= 1 + 66x + 645x^2 + 1384x^3 + 645x^4 + 66x^5 + x^6 \quad (10) \\
P_{E_7}(x) &= 1 + 119x + 2037x^2 + 8211x^3 + 8787x^4 + 2037x^5 + 119x^6 + x^7 \quad (11) \\
P_{E_8}(x) &= 1 + 232x + 7228x^2 + 55384x^3 + 133510x^4 + 107224x^5 + 24508x^6 + 232x^7 + x^8 \quad (12)
\end{align*}
\]
as has been proved in [1]. Finally, for the two remaining root graphs we find
\[
\begin{align*}
P_{F_4}(x) &= 1 + 44x + 198x^2 + 140x^3 + x^4 \quad (13) \\
P_{G_2}(x) &= 1 + 10x + 7x^2. \quad (14)
\end{align*}
\]
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 \( n \leq 8 \)

| \( A \) | \( s_\Lambda(1) \) | \( s_\Lambda(2) \) | \( s_\Lambda(3) \) | \( s_\Lambda(4) \) | \( s_\Lambda(5) \) | \( s_\Lambda(6) \) | \( s_\Lambda(7) \) | \( s_\Lambda(8) \) | \( s_\Lambda(9) \) | \( s_\Lambda(10) \) |
|------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| \( A_1 \) | 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 | 78580 | 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 | 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 $\Lambda$ of type $A_n$, $C_n$, $D_n$, and $E_6$ result in self-reciprocal polynomials $P_{\Lambda}(x)$, i.e.,

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

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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