On the Contact Numbers of Ball Packings on Various Hexagonal Grids

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Abstract
We describe the structure of the different hexagonal grids in dimension \(d = 3\), propose short notation for them, investigate the contact numbers of ball packings in these grids and share some computational results up to 200 balls, using mainly the greedy algorithm. We consider the octahedral grid, too.

1 Introduction
Considering \(n\) balls of the same radius in the \(d\)-dimensional Euclidean space for any but fixed number \(n \in \mathbb{N}\) such that each pair of balls have at most one common ("tangential", "touching" or "kissing") point, the total number of such points is called the contact number of this ball-configuration. For any \(n\) we may ask for configurations which have maximal contact numbers. These maximal contact numbers are denoted by \(c(n,d)\), we shorten \(c(n,3)\) simply by \(c(n)\). Many recent contributions deal with the maximal contact number of balls, using theoretical and empirical approaches as well (see eg. [AMB11], [B12], [B13], [BR13], [BK16], [R15], [R16] and [Sz16a]), [BSzSz15] and [H15] deal with related questions. The possible configurations have many applications e.g. in material science and other fields of applied physics and chemistry, see e.g. [BSM11], [HHH12] or [N12].

When packing balls of the same (e.g. unit) radius, it is quite natural to investigate regular packings, eg. on regular grids. In the case \(d = 2\) (plane) Harborth [H74] proved that the (unique) hexagonal grid (lattice) is the optimal configuration for congruent circles, see the blue circles on Figure 1. This means that the centers of the circles fit on the grid (a lattice in fact)

\[
\left\{ i \cdot [2,0]^T + j \cdot [1,\sqrt{3}]^T : i,j \in \mathbb{Z} \right\}.
\]

In dimension \(d = 3\) the hexagonal grids can be obtained as follows. First, place some balls in planes in the above planar method, we call these sets layers. Second, put such layers onto each other: the layers are translated with a
vector like $\ell_1 := \left[ 1, \sqrt{1/3}, \sqrt{8/3} \right]^T$ to get the neighbour layer (like in the usual placement of melons), as the blue and red circles show in Figure 1 (top view).

However, when considering three or more layers, we have several different possibilities. Think the blue layer in the middle and the red one above it. Then, for the layer below the blue circles we have two different possibilities. Either just put the balls "exactly below" the red ones, i.e. translating the red layer with the vector $t := \left[ 0, 0, -2 \cdot \sqrt{8/3} \right]^T$, in which case both the layers above and below the blue one are red. The other possibility is to move the blue layer with the vector $-\ell_1$ resulting the green circles. Equivalently, rotating the red layer by $60^\circ$ and translate it with the vector $t$ we get the green layer.

![Figure 1: Possible neighbouring layers (top view)](image)

We propose to choose and fix a middle (blue) layer for forthcoming constructions, since when packing the next ball (step by step) we can place it both above and below the configuration we already have.

In general, when placing several layers above each other, for each next layer we can choose the vector either $\ell_1 = L_v + L_h$ or $\ell_2 = L_v - L_h$ to move the previous layer to get the next one above it, where

$$L_v := \left[ 0, 0, \sqrt{8/3} \right]^T, \quad L_h := \left[ 1, \sqrt{1/3}, 0 \right]^T$$

are the vertical and horizontal translating vectors. Similarly, if we plan a next layer below the bottom layer we may choose either $-\ell_1 = -L_v - L_h$ or $-\ell_2 = -L_v + L_h$ to move the bottom layer to get the next one below it. A general notation for all the obtainable grids is discussed in Section 2. The usual
hexagonal lattice can be obtained when taking always the same vector, e.g. $\ell_1$ between all consecutive layers.

Though the contacts of balls depend only on neighbouring layers, but when we have to place fixed number $(n)$ of balls, different grids often provide different configurations and different maximal contact numbers. Examples in [Sz16b] show even 30\% differences in different grids! This problem and examples are discussed in Section 4 and in [Sz16b].

An important question is whether $c(n)$ can be achieved for all $n \in \mathbb{N}$ in one of the hexagonal grids. Since all the grids are 12-regular (each ball has 12 touching neighbours) we suspect that the answer is yes: $c_{\text{grids}}(n) = 6n - o(n)$ might hold for $n \to \infty$. For example, none of the constructions shown in [AMB11, p.35] and in [BK16] for $c(6) = 12$ do exist in any grid, but the configuration shown in Figure 2 (top and perspective view) yield the same contact number.

![Figure 2: $c(6) = 12$ on a grid](image)

Exact values of $c(n)$ for $n \leq 20$ can be found e.g. in [AMB11, p.38] and [BK16, p.5] and some lower bounds for $n \leq 27$ in [Sz16a]. Our present computations (see Section 4 and [Sz16b]) show that for all these $n$ the (maximal) value of $c(n)$ can be achieved in some appropriate grid, possibly not by the greedy algorithm. Examples for this phenomenon are the cases $n = 14$ and $n = 15$ : the greedy algorithm (see Table 2) found less contacts, but other algorithm (see Section 4) found the exact values:

![Figure 3: $c(14) = 40$ and $c(15) = 44$ on a grid](image)
Conjecture 1 The exact (maximal) value for each \( n \in \mathbb{N} \) can be achieved in some hexagonal grid. □

We have to emphasize that different \( n \) numbers often require different grids for achieving the maximal contact number. Our computational results for \( n \leq 200 \) are explained in Section 4; the details can be found in [Sz16b].

We consider also the octahedral lattice at the end of the forthcoming Sections and in [Sz16b], comparing to [B12] and [R16].

2 Notations

Notation 2 For any geometrical point \( P \in \mathbb{R}^3 \) we denote the usual Cartesian coordinates of \( P \) by \([x, y, z]_D\) or \([P]_D\), we often leave the subscript \( D \) (and \( T \) is for transposing the vector).

If \( P \in \mathcal{G}_\mathbb{Z} \) is an element of a hexagonal grid \( \mathcal{G}_\mathbb{Z} \), determined by the vector \( \varepsilon \) (see Definition 3), the inner hexagonal coordinates are denoted by \([P]_G\) or \([P]_{-\varepsilon}\), or simply by \([P]_H\) when \( \varepsilon \) is clear from the context.

In each grid we have \([0, 0, 0]_G = [0, 0, 0]_D\). □

Definition 3 For any infinite (or finite) sequence \( \varepsilon = (\ldots, \varepsilon_{-m}, \ldots, \varepsilon_0, \varepsilon_1, \ldots) \) such that \( \varepsilon_0 = 0 \) and \( \varepsilon_k \in \{-1, +1\} \) for \( k \in \mathbb{Z} \setminus \{0\} \) we define the hexagonal grid \( \mathcal{G}_\mathbb{Z} \subset \mathbb{R}^3 \) as follows.

The 0-th layer (as in \([1]\)) is

\[
\mathcal{L}_0 := \left\{ i \cdot \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}_D + j \cdot \begin{bmatrix} 1 \\ \sqrt{3} \\ 0 \end{bmatrix}_D : i, j \in \mathbb{Z} \right\}
\]

and for \( P \in \mathcal{L}_0 \) the hexagonal coordinates are \([P]_G := [i, j, 0]_T\).

For \( k > 0 \) (\( k \in \mathbb{Z} \)) we define the \( k \)-th layer

\[
\mathcal{L}_k := \{ R + L_v + \varepsilon_k L_h : R \in \mathcal{L}_{k-1} \}
\]

(see \([2]\) for \( L_v \) and \( L_h \)), the hexagonal coordinates for \( P = R + L_v + \varepsilon_k L_h \) and \([R]_G := [i, j, k-1]_T \) are \([P]_G := [i, j, k]_T\).

For \( k < 0 \) (\( k \in \mathbb{Z} \)) we let the \( k \)-th layer

\[
\mathcal{L}_k := \{ R - L_v + \varepsilon_k L_h : R \in \mathcal{L}_{k+1} \}
\]

and the hexagonal coordinates for \( P = R - L_v + \varepsilon_k L_h \) and \([R]_G := [i, j, k+1]_T \) are \([P]_G := [i, j, k]_T\).

Finally we put

\[
\mathcal{G}_\mathbb{Z} := \bigcup_{k \in \mathbb{Z}} \mathcal{L}_k . \quad \square
\]

Clearly in \([i, j, k]_G\) \( k \) denotes the layer number, i.e., "vertical" coordinate, while \( i, j \) are "horizontal" ones as in \([1]\). The relation whether "any two balls with centers in hexagonal coordinates \([i_1, j_1, k_1]_G\) and \([i_2, j_2, k_2]_G\) contact each other or not" can be easily decided.
The usual **hexagonal lattice** can be obtained when taking always the same direction, e.g. for $\vec{\mathbb{e}}_{HL} = (...,-1,0,+1,...)$. This lattice is

$$G_{HEX} = \{ x \cdot \overrightarrow{i} + y \cdot \overrightarrow{j} + z \cdot \ell_1 : x, y, z \in \mathbb{Z} \} \quad (7)$$

where

$$\overrightarrow{i} = \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}_D, \quad \overrightarrow{j} = \begin{bmatrix} 1/\sqrt{3} \\ 0 \\ 0 \end{bmatrix}_D, \quad \ell_1 = \begin{bmatrix} 1/\sqrt{1/3} \\ \sqrt{8/3} \end{bmatrix}. \quad (8)$$

In the case our balls all are contained in $\bigcup_{k=t_1}^{t_2} \mathcal{L}_k$ for some fixed $t_1, t_2 \in \mathbb{Z}$, then only the values $\varepsilon_{t_1},...,\varepsilon_{t_2}$ are interesting for us, so $\vec{\mathbb{e}}$ can be chosen a finite sequence and can be shortened in a single (rational) number.

**Notation 4** For finite sequences $\vec{\mathbb{e}} = (\varepsilon_{t_1},...,\varepsilon_{t_2})$ for which $\varepsilon_k \in \{-1,+1\}$, for any $t_1, t_2 \in \mathbb{Z}$ we write

$$\text{type} (\vec{\mathbb{e}}) := \sum_{k=t_1}^{t_2} 2^s(\varepsilon_k) \quad \text{where} \quad s(\varepsilon_k) = \begin{cases} 0 & \text{if } \varepsilon_k = -1 \\ 1 & \text{if } \varepsilon_k = +1 \end{cases}. \quad \Box \quad (9)$$

**Proposition 5** For any $k \in \mathbb{Z}$ and $P \in G$, $P = [i,j,k]^T \in \mathcal{L}_k$ we have

(i) the Hexagonal coordinates of $P$ are: for $k \geq 0$

$$P [i,j,k]^T = P [i,j,0]^T + kL_v + L_h \sum_{t=1}^{k} \varepsilon_t \quad (10)$$

(where $\sum_{t=1}^{k} \varepsilon_t = 0$), and for $k < 0$

$$P [i,j,k]^T = P [i,j,0]^T + kL_v + L_h \sum_{t=k}^{-1} \varepsilon_t \quad . \quad (11)$$

(ii) the Cartesian coordinates of the point $P$ are for each $k \in \mathbb{Z}$

$$[P]_D = i \cdot \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}_D + j \cdot \begin{bmatrix} 1/\sqrt{3} \\ 0 \\ 0 \end{bmatrix}_D + k \cdot \begin{bmatrix} 0 \\ 0 \\ \sqrt{8/3} \end{bmatrix}_D + S_k \cdot \begin{bmatrix} 1/\sqrt{1/3} \\ 0 \end{bmatrix}_D \quad (12)$$

where

$$S_k = \begin{cases} \sum_{t=1}^{k} \varepsilon_t & \text{for } k > 0 \\ 0 & \text{for } k = 0 \\ \sum_{t=k}^{-1} \varepsilon_t & \text{for } k < 0 \end{cases}. \quad \Box \quad (13)$$

Similar (also triangular) **barycentric** coordinate system is also used in chemistry, see e.g. [Sz99].

The **octahedral** grid is, in fact, a lattice and is unique. Any layer is a lattice of squares of side 2, the vector $[1, 1, \sqrt{2}]^T$ moves layers to the next one, i.e. we have:
Definition 6  The octahedral lattice is
\[ G_{OCT} := \left\{ x \cdot \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix} + y \cdot \begin{bmatrix} 0 \\ 2 \\ 0 \end{bmatrix} + z \cdot \begin{bmatrix} 1 \\ 1 \sqrt{2} \end{bmatrix} : x, y, z \in \mathbb{Z} \right\}. \]

(14)

3 Former results

Exact values of \( c(n) \) for \( n \leq 19 \) can be found e.g. in [AMB11, p.38] and [BK16, p.5], some lower bounds for \( 20 \leq n \leq 27 \) in [Sz16a]:

\[
\begin{array}{c|cccccccc}
 n & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\
 \hline
 0 & - & 0 & 1 & 3 & 6 & 9 & 12 & 15 & 18 & 21 \\
 10 & 25 & 29 & 33 & 36 & 40 & 44 & 48 & 52 & 56 & 60 \\
 20 & 64 & 67 & 72 & 76 & 80 & 84 & 87 & 90 & - & - \\
\end{array}
\]

Table 1 Results from [BK16] (1 \( \leq n \leq 19 \)) and from [Sz16a] (20 \( \leq n \leq 27 \))

Using a construction in the octahedral lattice [B12], [BR13] and [BK16] states
\[
 c(n) \geq 4k^3 - 6k^2 + 2k = d(k) \approx 6n - o\left(n^{2/3}\right)
\]

for \( n = \frac{2k^3+k}{3} \) (\( k \in \mathbb{N} \)), that is

\[
\begin{array}{c|cccccccc}
 k & 1 & 2 & 3 & 4 & 5 & 6 & \ldots \\
 \hline
 n & 1 & 6 & 19 & 44 & 85 & 146 & \ldots \\
 c(n) \geq & 0 & 12 & 60 & 168 & 360 & 660 & \ldots \\
\end{array}
\]

Table 2 Summary of [B12]

[R16] contains a figure for \( k = 4 \) and some values for these \( n \) and their \( c(n) \) are shown in Table 2.

Summary[\ref{summary}]
gives a comparison of the results obtained by different methods.

4 Computational results

In [Sz16a] we forced the computer to check all the cases in a \( 3 \times 3 \times 3 \) grid, i.e. 3 layers and \(-1 \leq i, j \leq +1\) for all \( n \leq 27 \), running time varied from some seconds to 1 - 2 hours. Since this kind of total checkings in \( 4 \times 4 \times 4 \) required several days running time, we turned to the greedy algorithm, which terminated in some seconds even for \( n > 200 \).

In our recent computations we investigated \( n \) many balls up to \( n \leq 200 \) in the grids \( G_i \) listed in [Sz16b] in file GNMOHOH3e-160626-0050,* and defined in Section[\ref{section}]. Our algorithm had the possibility to use 31 layers, starting at layer 0, but all the balls which have been finally chosen plus their neighbours (possible further ones for larger \( n \) configurations) occupied only the layers \( L_{-4}, \ldots, L_4 \). In other words, we had to investigate the sequences \( \epsilon_0 = (\epsilon_{-4}, \ldots, \epsilon_{-1}, 0, \epsilon_1, \ldots, \epsilon_4) \) only, which means \( 2^{8-1} = 128 \) cases, since, by symmetry we assumed \( \epsilon_1 = +1 \).
Greedy algorithm means, that we started with an arbitrary ball, and in each step we chose the next one which has the most neighbour (touching ball) among the old ones (we have chosen in previous steps). The greedy method implies that from the configuration for 200 balls we can reconstruct each configurations for each \( n \leq 200 \) - we have to consider the balls \( B_1, \ldots, B_n \) only. So, one can easily read out each configuration in each grid for each \( n \leq 200 \) from the files in [Sz16b]. Table 3 contains the maximum contact number for each \( n \), we have investigated all the 128 grids.

| \( n \) | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|-------|---|---|---|---|---|---|---|---|---|---|
| 0     | - | 0 | 1 | 3 | 6 | 9 | 11| 15| 18| 21|
| 10    | 25| 29| 33| 36| 39| 43| 48| 52| 56| 60|
| 20    | 64| 68| 72| 75| 79| 84| 89| 93| 97|102|
| 30    |106|110|114|119|123|126|130|135|140|145|
| 40    |150|153|157|162|167|172|177|183|187|191|
| 50    |195|200|205|210|214|218|222|227|232|236|
| 60    |242|247|251|257|261|265|271|275|280|284|
| 70    |288|293|298|303|308|312|317|322|328|332|
| 80    |337|342|348|352|356|360|365|369|375|380|
| 90    |385|389|394|398|403|408|414|419|424|428|
| 100   |433|438|444|448|453|458|463|468|473|477|
| 110   |481|487|491|496|501|505|510|514|519|524|
| 120   |530|535|541|546|551|555|559|563|568|573|
| 130   |578|583|589|594|600|605|610|615|620|625|
| 140   |630|633|638|643|648|652|658|663|669|674|
| 150   |679|684|690|695|701|706|712|717|723|727|
| 160   |711|715|721|724|730|734|738|742|747|751|
| 170   |782|788|793|798|802|806|810|815|820|825|
| 180   |830|834|839|844|849|855|860|865|871|877|
| 190   |882|888|894|899|905|909|914|920|925|931|
| 200   |935|     |     |     |     |     |     |     |     |     |

**Table 3** Hexagonal lower bounds by greedy algorithm

We also made a run in the octahedral lattice, details can be found in [Sz16b] in files MH5b-200b-en.*. txt Table 4 shows the cases when octahedral greedy algorithm resulted better bound than the hexagonal one in Table 3:

| \( n \) | 14 | 15 | 57 | 58 | 59 | 176 | 177 | 178 | 179 | 180 | 181 | 182 |
|-------|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|
| Hexa  | 39 | 43 | 227| 232| 236| 810 | 815 | 820 | 825 | 830 | 834 | 839 |
| Octa  | 40 | 44 | 228| 233| 237| 811 | 817 | 822 | 828 | 833 | 837 | 841 |

**Table 4** The cases when octahedral is better than hexagonal

We can shortly summarize our experiments as:
Summary 7 Based on Table 3 (i.e. the greedy algorithm in hexagonal grids), we can state the followings.

(i) for \( n \leq 19 \) Table 3 gives the so far known results except for \( n = 6 \), but this case is cured in Figure 2,
(ii) for \( n \leq 200 \) Table 3 gives the best lower bounds with the following exceptions:
- for \( n = 6 \) see Figure 2 (so \( 12 \leq c(6) \)),
- for \( n = 14, 15 \) see Figure 3 and Table 4 (so \( 40 \leq c(14) \) and \( 44 \leq c(15) \)),
- for \( n = 23, 24 \) see Table 1 and [Sz16a] (so \( 76 \leq c(23) \) and \( 80 \leq c(24) \)),
- for \( n = 44 \) see Table 2 (so \( 168 \leq c(44) \)),
- for \( n = 57 - 59 \) see Table 4 (so \( 228 \leq c(57) \), \( 233 \leq c(58) \) and \( 237 \leq c(59) \)),
- for \( n = 146 \) see Table 2 (so \( 660 \leq c(146) \)),
- for \( n = 176 - 182 \) see Table 4
  (so \( 811 \leq c(176) \), \( 817 \leq c(177) \), \( 822 \leq c(178) \), \( 828 \leq c(179) \), \( 833 \leq c(180) \),
  \( 837 \leq c(181) \) and \( 841 \leq c(182) \)). □

Though for the exceptional cases \( n \geq 44 \) we do not have constructions in hexagonal grids at this moment, as good as in Tables 2 and 4, we still believe in Conjecture [1].

Further experiments are in progress.

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