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Letter to Arthur Baragar on a “Crystallographic Sphere Packing”

from Alex Kontorovich

Dear Arthur,

As mentioned when we discussed, the “Structure Theorem for Crystallographic Packings” (see Theorem 31 in the paper [KN17] with Kei Nakamura) allows one to just “look” at a Coxeter diagram and immediately see the corresponding sphere packing. Let me carry out the calculation explicitly (and post the corresponding Mathematica file) for the case of the integer orthogonal group $O_F(\mathbb{Z})$ preserving the quadratic form $F$, where

$$F(x_1, \ldots, x_5) := x_1^2 + \cdots + x_4^2 - 3x_5^2.$$ 

This orthogonal group $O_F(\mathbb{Z})$ is reflective, meaning that the group generated by all reflections in $O_F(\mathbb{Z})$ is itself a lattice (i.e. is of finite index in $O_F(\mathbb{Z})$). One proves this by running Vinberg’s algorithm [Vin72], as carried out in Mcleod [Mcl11] (see the case $n = 4$ in Mcleod’s Figure 1). The resulting reflection group has Coxeter diagram given by:

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1 2 3 4 5 6
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The meaning of this diagram is that “walls” (spheres/planes) labelled (1) and (2) meet at infinity (tangentially), (2) and (3) meet at dihedral angle $\pi/4$, (3) and (4) meet at dihedral angle $\pi/3$, as do (4) and (5), and lastly, (5) and (6) meet at dihedral angle $\pi/6$, with all other dihedral angles being $\pi/2$ (that is, orthogonal). To build a packing based on this diagram, we will need to realize the walls of a configuration explicitly. Instead of running Vinberg’s algorithm (the knowledge of which is not necessary for what follows), since we are already given the diagram, we will reverse-engineer the configuration, as follows.

We will use inversive coordinates (see [Kon17]), attaching to a sphere $S$ of radius $r$ and center $(x, y, z)$ (oriented internally) the vector

$$v_S := \left( \frac{1}{r}, \frac{1}{r}, \frac{x}{r}, \frac{y}{r}, \frac{z}{r} \right),$$

where the “co-radius” $\hat{r}$ is the radius of the sphere after inversion through the unit sphere; one calculates that

$$\hat{r} = \frac{r}{x^2 + y^2 + z^2 - r^2}.$$ 

For a sphere with external orientation, $r$ is negative. If $S$ is a plane, the inversive coordinates are obtained by taking limits of appropriate spheres as $r \to \infty$, so the second entry in $v_S$ becomes 0, and it turns out the last three coordinates become the unit normal vector to the plane in the direction of its interior.
From (♠), it is immediate that \( Q(v_S) = -1 \), where \( Q \) is the quadratic form with half-Hessian

\[
Q = \begin{pmatrix}
\frac{1}{2} & 1 & 0 & 0 & 0 \\
1 & -1 & \frac{1}{\sqrt{2}} & 0 & 0 \\
0 & \frac{1}{\sqrt{2}} & -1 & \frac{1}{2} & 0 \\
0 & 0 & \frac{1}{2} & -1 & \frac{1}{2} & 0 \\
0 & 0 & 0 & \frac{1}{2} & -1 & \frac{\sqrt{3}}{2} \\
0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} & -1
\end{pmatrix}.
\]

(Here \( I_3 \) is the \( 3 \times 3 \) identity matrix.) The dihedral angle \( \theta \) between spheres given by inversive coordinates \( v_1, v_2 \) is computed by the “inversive product”

\[ v_1 \ast v_2 = \cos \theta, \quad \text{where} \quad v_1 \ast v_2 := v_1 \cdot Q \cdot v_2^\dagger, \]

and “\( \dagger \)” denotes transpose. If the spheres do not meet but instead are separated by a hyperbolic distance \( d \), then \( v_1 \ast v_2 = \cosh d \). Hence to realize the above Coxeter diagram explicitly as walls, we will need to find inversive coordinates \( v_1, \ldots, v_6 \) of the six walls in the diagram, so that the “Gram matrix” \( G = [v_1 \ast v_j] \) of all inversive products becomes:

\[
G = \begin{pmatrix}
-1 & 1 & 0 & 0 & 0 & 0 \\
1 & -1 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\
0 & \frac{1}{\sqrt{2}} & -1 & \frac{1}{2} & 0 & 0 \\
0 & 0 & \frac{1}{2} & -1 & \frac{1}{2} & 0 \\
0 & 0 & 0 & \frac{1}{2} & -1 & \frac{\sqrt{3}}{2} \\
0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} & -1
\end{pmatrix}.
\]

To do this, may take (1) and (2) to be horizontal planes (tangent at infinity), and since (4), (5), and (6) are orthogonal to (1) and (2), they must then be vertical planes; moreover these three form a 30-60-90 triangle. So we may already assign (1) to have inversive coordinates, say,

\[ v_1 = (0, 0, 0, 0, -1), \]

which means that (1) is the \( xy \)-plane with normal vector pointing down (i.e., its interior is the lower half-space). The wall (2) will similarly have coordinates

\[ v_2 = (?, 0, 0, 0, 1), \]

that is, a plane with upwards pointing normal vector, but we’re not sure yet where in space it will be positioned. Let us choose (4) to be the \( xz \)-plane with normal pointing in the positive-\( y \) direction:

\[ v_4 = (0, 0, 0, 1, 0). \]

Then (5) can also be a vertical plane through the origin, and in order to meet (4) at angle \( \pi/3 \), we set

\[ v_5 = (0, 0, \frac{\sqrt{3}}{2}, -\frac{1}{2}, 0). \]

This determines that wall (6) has coordinates

\[ v_6 = (?, 0, -1, 0, 0), \]

and “\( ? \)” here can be chosen arbitrarily, say, 2, so that (6) becomes the plane \( x = 1 \). Having determined \( v_1, v_4, v_5, \) and \( v_6 \), we may compute the coordinates, \( v_3 \), of (3) by using knowledge of its inversive products with \( v_1, v_4, v_5, \) and \( v_6 \). We find (see the Mathematica file) that

\[
v_3 = \left( -\frac{4}{\sqrt{3}} + \frac{1}{2\sqrt{3}}, -\frac{1}{2\sqrt{3}}, -\frac{1}{2}, 0 \right).
\]
Now the “?” in $v_2$ may be determined by solving $v_2 \star v_3 = \cos \pi/4 = \sqrt{2}/2$; we compute that

$$v_2 = \left(2\sqrt{6}, 0, 0, 1\right).$$

Collecting these vectors into a matrix $V = \{v_i\}$ whose rows are the coordinates,

$$V = \begin{pmatrix}
0 & 0 & 0 & 0 & -1 \\
2\sqrt{6} & 0 & 0 & 0 & 1 \\
-\frac{4}{\sqrt{3}} & \frac{1}{2\sqrt{3}} & -\frac{1}{2\sqrt{3}} & -\frac{1}{2} & 0 \\
0 & 0 & 0 & 1 & 0 \\
0 & 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\
2 & 0 & -1 & 0 & 0
\end{pmatrix},$$

we may check that indeed

$$V \cdot Q \cdot V^\dagger = G.$$ 

Thus we have the desired Gramian (what you would call “intersection pairing”). Here’s the configuration in space:

Now our Structure Theorem says that one obtains a packing by taking the “cluster” to be just the wall (1), and letting reflections through to rest (the “cocluster”) act on (1). The reflection $R_v$ through a sphere $S$ given by inversive coordinates $v$ is a Mobius transformation, that is, $R_v \in O_Q(\mathbb{R})$, and is given by the standard formula

$$R_v: x \mapsto x - 2\frac{x \star v}{v \star v}v,$$

that is, 

$$R_v = I + 2Q \cdot v^\dagger \cdot v.$$ 

(This is because $v$ is actually the normal vector in “Lorentz space” to the plane corresponding to $S$ — see again [Kon17].) Thus our “thin” group $\Gamma < O_Q(\mathbb{R})$ acts on the right on $v_1$ and is
generated by the reflections:

\[ R_2 = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
24 & 1 & 0 & 0 & 2\sqrt{6} \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
-4\sqrt{6} & 0 & 0 & 0 & -1
\end{pmatrix}, \quad R_3 = \begin{pmatrix}
\frac{1}{3} & \frac{12}{3} & -\frac{1}{12} & -\frac{1}{4\sqrt{3}} & 0 \\
\frac{16}{3} & \frac{1}{3} & \frac{2}{3} & -\sqrt{\frac{2}{3}} & 0 \\
-\frac{4}{3} & \frac{6}{3} & \frac{5}{6} & -\frac{1}{2\sqrt{3}} & 0 \\
-\frac{4}{\sqrt{3}} & \frac{1}{2\sqrt{3}} & -\frac{1}{2\sqrt{3}} & \frac{5}{3} & 0 \\
0 & 0 & 0 & 0 & 1
\end{pmatrix}, \quad R_4 = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 1
\end{pmatrix}, \quad R_5 = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
0 & 0 & \frac{1}{\sqrt{243}} & \frac{1}{\sqrt{243}} & 0 \\
0 & 0 & \frac{1}{\sqrt{243}} & \frac{1}{\sqrt{243}} & 0 \\
0 & 0 & 0 & 0 & 1
\end{pmatrix}, \quad R_6 = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
4 & 1 & -2 & 0 & 0 \\
4 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1
\end{pmatrix}.

Now we can look at the orbit \( O = v_1 \cdot \Gamma: \)

And that’s all there is to it! Now, this is all just to construct the packing; issues of (super)integrality, etc, are discussed in [KN17]. Note that, though we started with a nice integral form \( F \), the vectors \( v_j \) and reflection matrices \( R_j \) can have arbitrary (not even algebraic, should we choose to apply some random Mobius transformation to the whole picture) entries. But because the “supergroup” (see [KN17]) of \( \Gamma \) is arithmetic (in particular, it is commensurate to \( O_F(\mathbb{Z}) \)), we know that there exist configurations of this packing in which all bends (reciprocals of radii) are integers.

Best wishes,

Alex
REFERENCES


