Dec 2017

Letter to Arthur Baragar on a "Crystallographic Sphere Packing"

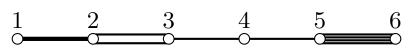
from Alex Kontorovich

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

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

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:



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 $\mathcal{S}$ of radius r and center (x, y, z) (oriented internally) the vector

$$v_{\mathcal{S}} := (\frac{1}{\widehat{r}}, \frac{1}{r}, \frac{x}{r}, \frac{y}{r}, \frac{z}{r}),$$

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

$$\widehat{r} = \frac{r}{x^2 + y^2 + z^2 - r^2}. \qquad (\spadesuit)$$

For a sphere with external orientation, r is negative. If $\mathcal{S}$ is a plane, the inversive coordinates are obtained by taking limits of appropriate spheres as $r \to \infty$, so the second entry in $v_{\mathcal{S}}$ 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 $Q(v_{\mathcal{S}}) = -1$, where Q is the quadratic form with half-Hessian

$$Q = \begin{pmatrix} & \frac{1}{2} & \\ \frac{1}{2} & & \\ & & -I_3 \end{pmatrix}.$$

(Here I_3 is the 3×3 identity matrix.) The dihedral angle θ between spheres given by inversive coordinates v_1, v_2 is computed by the "inversive product"

$$v_1 \star v_2 = \cos\theta, \qquad \text{where} \qquad v_1 \star v_2 := v_1 \cdot Q \cdot v_2^{\dagger},$$

and "†" denotes transpose. If the spheres do not meet but instead are separated by a hyperbolic distance d, then $v_1 \star v_2 = \cosh d$. 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" $G = [v_i \star v_j]$ 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

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

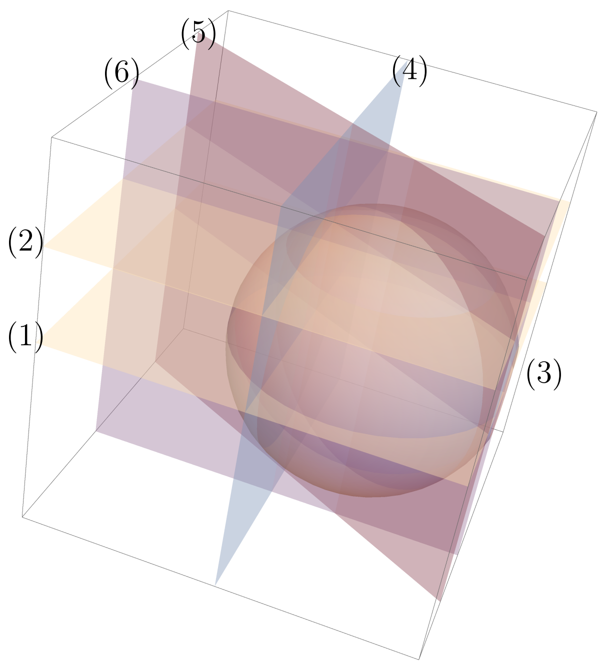
Collecting these vectors into a matrix $V = \{v_i\}$ whose rows are the coordinates,

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

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 $\mathcal{S}$ 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

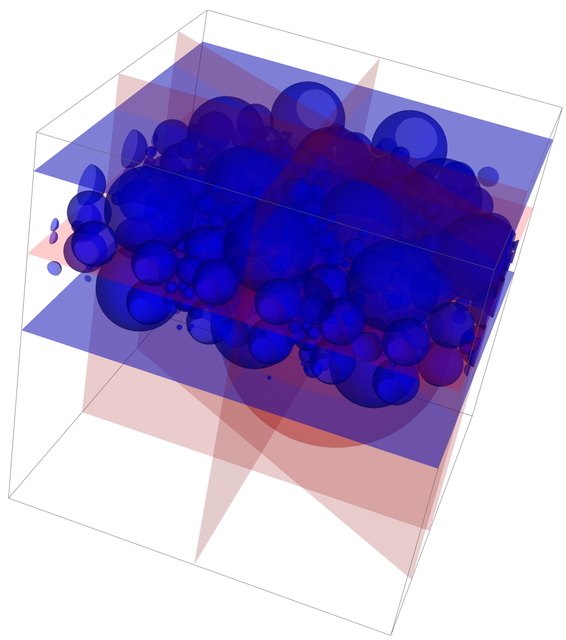
$$R_v : x \mapsto x - 2\frac{x \star v}{v \star v}v, \qquad \text{that is,} \qquad R_v \ = \ I + 2Q \cdot v^{\dagger} \cdot v.$$

(This is because v is actually the normal vector in "Lorentz space" to the plane corresponding to $\mathcal{S}$ – 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:

$$R_2 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 24 & 1 & 0 & 0 & 2\sqrt{6} \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ -4\sqrt{6} & 0 & 0 & 0 & -1 \end{pmatrix}, \quad R_3 = \begin{pmatrix} \frac{1}{3} & \frac{1}{12} & -\frac{1}{12} & -\frac{1}{4\sqrt{3}} & 0 \\ \frac{16}{3} & \frac{1}{3} & \frac{2}{3} & \frac{2}{\sqrt{3}} & 0 \\ -\frac{4}{3} & \frac{1}{6} & \frac{5}{6} & -\frac{1}{2\sqrt{3}} & 0 \\ -\frac{4}{\sqrt{3}} & \frac{1}{2\sqrt{3}} & -\frac{1}{2\sqrt{3}} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$R_4 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad R_5 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad R_6 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 4 & 1 & -2 & 0 & 0 \\ 4 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Now we can look at the orbit $\mathcal{O} = v_1 \cdot \Gamma$:



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 Γ 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

[KN17] A. Kontorovich and K. Nakamura. Geometry and arithmetic of crystallographic packings, 2017. https://arxiv.org/abs/1712.00147.

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[Mcl11] John Mcleod. Hyperbolic reflection groups associated to the quadratic forms $-3x_0^2 + x_1^2 + \cdots + x_n^2$. *Geom. Dedicata*, 152:1–16, 2011.

[Vin72] È. B. Vinberg. The groups of units of certain quadratic forms. *Mat. Sb. (N.S.)*, 87(129):18–36, 1972.