

# Quantizing, packing, covering and Isoperimetric properties of the 12-16 partition of 3-space

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## Abstract

There are several open questions in mathematics about which partition of  $R^3$  into polytopes is the best at: packing, covering, quantizing or has the lowest surface energy. This paper concentrates on a particular partition, the 12-16 partition, and determines how well it performs with respect to these four characteristics, with emphasis on the quantizing properties.

## 1 Introduction

When transmitting information in the form of real numbers, whether they be weights, wavelengths, durations, etc. we do not want to be sending them with arbitrary precision, as this uses up too much bandwidth. For example, it is much ‘easier’ to send 0.667 than it is to send 0.6666666666666666... So, if we have a piece of information  $x \in R^n$ , that is our piece of information consists of  $n$  real numbers, we instead send  $a$ , the closest point to  $x$  in  $(\frac{1}{1000}Z)^n$ . This is equivalent to rounding each of the real numbers to the 3rd decimal place, and this rounding will induce an averaged squared error per bit of information.

The question arises; is this the best way to approximate  $x$ ? or can we find partitions of  $R^n$  into cells with centres (of the same volume but with different shape to  $(\frac{1}{1000}Z)^n$ ) that gives rise to less average squared error per bit of information when all information in a cell gets quantized (rounded) to the centre. This leads us to the quantizer problem.

The quantizer problem in  $R^n$  is to find the partition of  $R^n$  which has the lowest *normalized second moment*. The normalized second moment is a scaleless representation of the averaged squared error per bit of information as mentioned above, scaleless here meaning it does not depend on volume

or even dimension. This quantizer problem remains unsolved in  $R^3$ , with the Voronoi partition <sup>1</sup> of the BCC (body centred cubic) lattice - which is represented by points  $Z^3 \cup (Z^3 + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}))$  - having the lowest normalized second moment of all partitions tested. It is however known that if the problem is restricted to Voronoi partitions of lattices then BCC lattice is the best. [3, pg 60] [1]

There are several other open questions regarding partitions of  $R^3$ . The Kelvin Problem is the question of finding which partition of  $R^3$  into volume 1 cells gives the lowest average surface area per cell. As dealing with volume 1 cells can be inconvenient, the problem can be generalized to ask which partition of  $R^3$  into equal volume cells gives the highest *Isoperimetric quotient*, a scaleless quality that is inversely proportional to the average surface area of the cells. The *Kelvin Conjecture* was that the solution to the Kelvin Problem was a slight distortion of the Voronoi partition of the BCC lattice, so as to satisfy Plateaus rules for a structure of minimal surface area, that the surfaces which bound the cells must meet at 120°. [11, pg 47] This conjecture was believed to be true for over 100 years, but was disproven recently when D. Weaire and R. Phelan created what is now known as the *Phelan-Weaire Partition* which has a higher Isoperimetric quotient than Kelvins BCC partition. [11, pg 49]

The *packing problem* asks what partition of  $R^3$  (or more generally  $R^n$ ) has the greatest packing density with equal sized spheres. It was conjectured by J. Kepler in 1611 [8, pg. 3] that no partition of  $R^3$  has greater packing density than the Voronoi partition of the FCC (face centered cubic) lattice - which is also known as  $D_3$  and is represented by the points:

$$D_3 = \{z \in Z^3 : z.(1, 1, 1) \in 2Z\}$$

although the problem is still open. There have been proofs offered of the Kepler conjecture, although most, including Hsiang's in [8], have been declared incomplete, as there are holes in the arguments used. However, Thomas Hales, who has done much work on this problem, [6], [7], claims to have a proof, [4] which is generally accepted by the mathematical community to be correct. However, since it is a 500 page proof by exhaustion, there is not yet final consensus on whether the proof is complete and the problem officially remains open.

Finally, the covering problem asks what partition of  $R^3$  (or more generally  $R^n$ ) has the lowest covering thickness with equal sized spheres. In

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<sup>1</sup>We call a partition of  $R^n$  into the Voronoi regions of the points  $a \in \mathcal{A}$  the Voronoi partition of  $\mathcal{A}$

other words, what arrangement of overlapping spheres (of equal size) will cover all of space most efficiently (minimum overlapping). If this problem is restricted to lattice partitions, the solution is known to be the BCC lattice, however the general problem in  $R^3$  is still open, with the BCC lattice being the best known covering. [2]

As two of these problems are settled for lattice partitions, pursuing other lattices seems pointless. However, there are other periodic partitions (with more than one congruent cell) that may improve the best known results for these problems. Most notably the PW partition, which uses two different cells, has been shown to be superior isoperimetrically to the best known lattice Voronoi partition for the Kelvin Problem. Let us define a few necessary terms.

Consider a cell  $S$  in  $R^n$  with ‘centre’  $c \in S$ . We define  $V$ , the volume of  $S$ ;  $U$ , the *unnormalized second moment* of  $S$  about  $c$ ; and  $G$ , the *normalized second moment* of  $S$  about  $c$ , by

$$\begin{aligned} V(S) &= \int_S dx \\ U(S, c) &= \int_S \|x - c\|^2 dx \\ G(S, c) &= \frac{1}{n} \frac{U(S, c)}{V(S)^{1+\frac{2}{n}}} \end{aligned}$$

We call  $c$  the *baricentre* of  $S$

A useful aspect of  $G$  is that it does not depend on the size of  $S$ , only the shape. For example, consider a cube  $C_a$  of side length  $2a$  in  $R^3$ , centered at the origin. Then

$$\begin{aligned} V(C_a) &= \int_{-a}^a \int_{-a}^a \int_{-a}^a dx dy dz = 8a^3 \\ U(C_a) &= \int_{-a}^a \int_{-a}^a \int_{-a}^a (x^2 + y^2 + z^2) dx dy dz = \frac{16a^5}{3} \\ G(C_a) &= \frac{1}{3} \frac{16a^5}{3} \frac{1}{(8a^3)^{5/3}} = \frac{1}{12} \end{aligned}$$

Note that  $G(C_a)$  has no dependence on  $a$ . In fact, similar computations will show that any cube in  $R^3$  has a normalized second moment of  $\frac{1}{12}$  about its centre, regardless of its position or size (however, a cube may have normalized second moment  $\neq \frac{1}{12}$  about a point that is not its centre). This means

that the normalized second moment of a partition in  $R^n$  is invariant under any rotation or translation of the partition in  $R^n$ , as well as scaling by any real number.

We say a partition of  $R^n$  is *periodic* if it is composed of translates of a fundamental unit  $F$  consisting of  $L$  cells  $S_1, S_2, \dots, S_L$  with centres  $c_1, c_2, \dots, c_L$ . The normalized second moment of this partition is

$$G(F) = \frac{1}{n} \frac{\frac{1}{L} \sum_{i=1}^L U(S_i, c_i)}{\left(\frac{1}{L} \sum_{i=1}^L V(S_i)\right)^{1+\frac{2}{n}}}$$

We will take this as the definition of the normalized second moment of a periodic partition in  $R^n$ . [5]

For a set of points  $\mathcal{A}$  in  $R^n$  we define the *Voronoi region of  $a \in \mathcal{A}$* ,  $V_a$  by:

$$V_a = \{x \in R^n : \|x - a\| \leq \|x - a'\| \forall a' \in \mathcal{A}\}$$

We can also define the *packing density* and *covering thickness* for such a periodic partition. Let  $r_{pack}$  be the largest possible radius such that were we to place an  $n$ -ball  $B_i$  of radius  $r_{pack}$  at each of the points  $c_i$  in  $F$ , then each  $B_i$  would lie entirely inside  $S_i$ . Then the packing density for this periodic partition will be the percentage of the fundamental unit that lies inside  $\cup B_i$ , or written another way

$$Packing\ Density\ (PD) = \frac{\sum_{i=1}^L V(B_i)}{\sum_{i=1}^L V(S_i)} = L \frac{V(B_1)}{V(F)}$$

Where  $V(B_1) = \frac{4}{3}\pi r_{pack}^3$  is the volume of each  $B_i$  (since they all have radius  $r_{pack}$ ) and  $V(F) = \sum_{i=1}^L V(S_i)$  is the volume of the fundamental unit. The packing density is always less than or equal to 1, with the more efficient packings having a higher packing density. The classical sphere packing problem, which partition of  $R^3$  has the highest packing density, is an unsolved problem. It is conjectured to be the Voronoi partition of the FCC lattice, which has packing density  $\frac{\pi}{\sqrt{18}} \approx .7405$ . [3, pg. 2] The best known upper bound was for many years Rogers' 1958 result that no partition of  $R^3$  can have packing density greater than 0.7796... [10] Recently Rogers' upper bound has been improved, with Lindsay finding a new upper bound of 0.7784... [9] It is widely believed that the known FCC result is the best result possible, with Rogers remarking "many mathematicians believe, and all physicists know..." (that the correct answer is the FCC lattice).

Now, let  $r_{cover}$  be the smallest possible radius such that were we to place an  $n$ -ball  $D_i$  of radius  $r_{cover}$  at each of the points  $c_i$ , then every point in  $S_i$  would lie in  $D_i$ . Then similarly to the packing density,

$$Covering\ Thickness\ (CT) = \frac{\sum_{i=1}^L V(D_i)}{\sum_{i=1}^L V(S_i)} = L \frac{V(D_1)}{V(F)}$$

The covering thickness is always greater than or equal to one, with the more efficient coverings having a lower covering thickness. The best known covering partition of  $R^3$  is the Voronoi partition of the BCC lattice, with a covering thickness of  $1.4635\dots$ , and this is known to be the best lattice covering of  $R^3$  [2]

If we want the packing density or covering thickness of a single cell we have to alter the definition slightly:

$$PD(cell) = \frac{V(inside)}{V(Cell)}$$

$$CT(cell) = \frac{V(outside)}{V(Cell)}$$

Where the insphere of a cell is the largest possible sphere that can be completely contained in the cell, and the outsphere is the smallest possible sphere that can completely contain the cell.

As the packing density and covering thickness are simply ratios of volume, they are, like the normalized second moment, scaleless.

We define the scaleless quality  $I$ , the *Isoperimetric quotient* of a partition

$$I = \frac{36\pi V^2}{A^3}$$

Where  $V$  is the cell volume and  $A$  the *average* cell surface area. So, a partition of equal volume cells with Isoperimetric quotient  $I$  scaled down to volume one cells, (as required for the Kelvin Problem) would have average surface area:

$$A = \sqrt[3]{\frac{36\pi}{I}}$$

The better a partition is in respect to the Kelvin problem, the higher its Isoperimetric quotient. The constants are chosen so that  $I(sphere) = 1$ , and all other shapes will have  $I < 1$ .

As mentioned earlier, the Phelan-Weaire partition was able to out perform the perturbed BCC lattice (call the Plat(BCC) lattice, since it obeys

Plateau’s restraints) in the Kelvin Problem. Where  $I(\text{Plat}(BCC)) = 0.757$ ,  $I(PW) = 0.764$ , [11, pg 49] an increase of 0.3%.

The Phelan-Weaire partition is made up of a collection of dodecahedra and 14-hedra, and since the normalized second moment is in a sense a measure of the “roundness” of a cell, it was thought that perhaps the Phelan-Weaire may also be able to out perform the BCC in terms of the normalized second moment as well as the Kelvin Problem. However N Kashyap and D Newhoff showed that this was not the case. [5] Curiously, and at the moment inexplicably, the PW partition with equal volume cells has exactly the same normalized second moment as the FCC lattice.

If we consider individual cells rather than partitions of space, it is quite clear from the definitions that a sphere  $S^3$  is the optimal cell for all four of normalized second moment, Isoperimetric quotient, Packing density and Covering thickness.

$$\begin{aligned} G(S^3) &\approx 0.077 & I(S^3) &= 1 \\ PD(S^3) &= 1 & CT(S^3) &= 1 \end{aligned}$$

This is of no immediate use for partitions, since clearly spheres can not fill  $R^3$ , however from this it seems natural to assume that increasing the number of sides in the cells of a partition of  $R^3$  will make the cells more “sphere-like”, resulting in better performed partitions in these four characteristics.

There is a partition of  $R^3$  into dodecahedra and 16-hedra, called for lack of a better name the 12-16 Partition, and that will be the main subject of this paper. We primarily investigate this with respect to the normalized second moment, and give an estimate for the Isoperimetric quotient (‘estimate’ as the base shape could be perturbed to Plat(12-16) to satisfy Plateau’s constraint and the Isoperimetric quotient would improve). However, as the four characteristics mentioned are all in a sense measuring the same thing (the “roundness” of the partition), we also find the packing density and covering thickness of the 12-16 partition.

The next chapter focuses on calculating the quantizing properties of the 12-16 partition

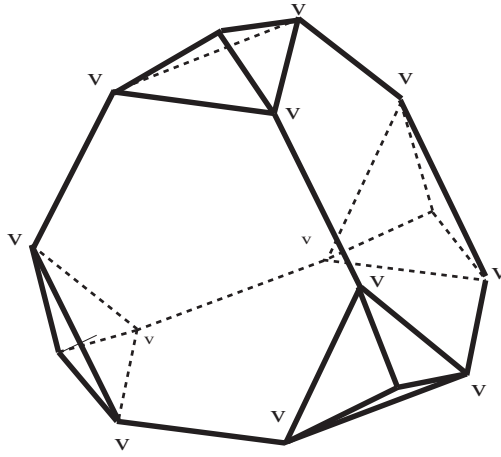
## 2 The 12-16 Partition

We now consider a new class of partitions of  $R^3$ , the 12-16 partitions, based on the Voronoi partition of a set of centres  $\mathcal{C}$  and a scale value  $\alpha$ . To define the set  $\mathcal{C}$  we begin with the *diamond packing*  $\mathcal{D} = D_3 \cup (D_3 + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}))$ .

[3, pg 113] Each point in this packing has a Voronoi region with 16 vertices and 16 faces. Let the set of all points  $u$  that make up a vertex of a Voronoi region of a point  $d \in \mathcal{D}$  be called  $\mathcal{U}$ . If we define  $\mathcal{V} \subset \mathcal{U}$  as

$$\mathcal{V} = \left\{ v \in \mathcal{U} : \|v - d\| = \frac{\sqrt{11}}{4} \right\}$$

where  $d$  is the centre of the voronoi cell that  $v$  is a part of; then  $\mathcal{C} = \mathcal{D} \cup \mathcal{V}$ . The following diagram shows a typical Voronoi region of a point in  $\mathcal{D}$ .



The unlabeled vertices belong to  $\mathcal{U} \setminus \mathcal{V}$  and have no relevance to the 12-16 partition.

The points  $c \in \mathcal{D} \subset \mathcal{C}$  labeled  $c_{16}$  have 16 near vertices (they form the centres of 16 sided polygons) and the points  $c \in \mathcal{V} \subset \mathcal{C}$  labeled  $c_{12}$  have 12 near vertices (they form the centres of dodecagons).

(2 centres  $c$  and  $c'$  said to be near if the Voronoi cell around  $c$  and the Voronoi cell around  $c'$  share a boundary face)

For example, the origin  $(0, 0, 0)$  has 16 near vertices:

$$\mathcal{N} = \left\{ \begin{array}{cccc} \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right), & \left(\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\right), & \left(-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right), & \left(-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right), \\ \left(-\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right), & \left(-\frac{3}{4}, -\frac{1}{4}, -\frac{1}{4}\right), & \left(\frac{3}{4}, -\frac{1}{4}, \frac{1}{4}\right), & \left(\frac{3}{4}, \frac{1}{4}, -\frac{1}{4}\right), \\ \left(\frac{1}{4}, -\frac{3}{4}, \frac{1}{4}\right), & \left(-\frac{1}{4}, -\frac{3}{4}, -\frac{1}{4}\right), & \left(\frac{1}{4}, \frac{3}{4}, -\frac{1}{4}\right), & \left(-\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right), \\ \left(\frac{1}{4}, \frac{1}{4}, -\frac{3}{4}\right), & \left(-\frac{1}{4}, -\frac{1}{4}, -\frac{3}{4}\right), & \left(-\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right), & \left(\frac{1}{4}, -\frac{1}{4}, \frac{3}{4}\right) \end{array} \right\}$$

In fact, if we call the set of these 16 vertices and the origin  $\mathcal{S}$ , (ie  $\mathcal{S} = \mathcal{N} \cup \{(0, 0, 0)\}$ ) then for  $c = (a, b, c) + (x, y, z)$ ,  $a, b, c \in Z$

$$c \in \mathcal{C} \Leftrightarrow (x, y, z) \in \mathcal{S} \text{ and } (a + b + c) \in 2Z$$

Since we are interested in the normalized second moment, as well as other scaleless qualities, we can scale this partition by any real number without consequence, so we scale by 4 to remove fractions. This gives us a new set of vectors

$$\mathcal{C}' = \{x \in R^3 : \frac{x}{4} \in \mathcal{C}\}$$

(we define  $\mathcal{D}'$  and  $\mathcal{V}'$  in the same way)

For the remainder of this paper we will be referring to this scaled partition whenever we mention 12-16 partition, as it is easier to deal with and all the attributes we are looking for are scaleless.

Each member of this class of 12-16 partitions is parameterized by a real number  $\frac{4}{11} \leq \alpha \leq \frac{16}{11}$  which defines the cells (the dodecahedra and 16-hedra) as follows:

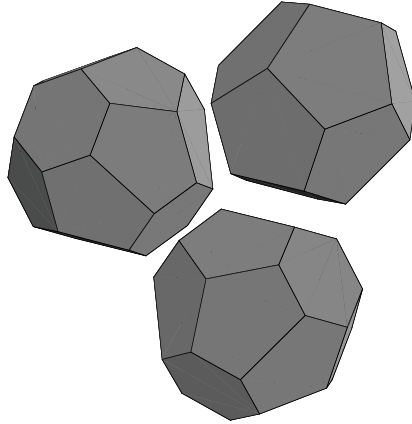
- For any point  $d \in \mathcal{D}$  call the cell around  $d$ ,  $S_d$ . Then:

$$x \in S_d \Leftrightarrow \begin{cases} \|x - d\| \leq \|x - d'\| & \forall d' \in \mathcal{D}' \\ \|x - d\| \leq (\frac{2-\alpha}{\alpha})\|x - v'\| & \forall v' \in \mathcal{V}' \end{cases}$$

- For any point  $v \in \mathcal{V}$  call the cell around  $v$ ,  $S_v$ . Then:

$$y \in S_v \Leftrightarrow \begin{cases} \|y - v\| \leq \|y - v'\| & \forall v' \in \mathcal{V}' \\ \|y - v\| \leq (\frac{\alpha}{2-\alpha})\|y - d'\| & \forall d' \in \mathcal{D}' \end{cases}$$

The cells end up looking something like this for  $\alpha \approx 1$



The top right cell is a dodecahedron, while the other two are 16-hedra.

We note that for  $\alpha = 1$ , the cells are Voronoi regions. The reason for the restriction on  $\alpha$  is that if  $\alpha$  were to be less than  $\frac{4}{11}$  or greater than  $\frac{16}{11}$

the combinatorics of the partition would change. For example, the 3 faces meeting at an edge for  $\frac{4}{11} \leq \alpha \leq \frac{16}{11}$  would fail to meet simultaneously for  $\alpha < \frac{4}{11}$ . This can be seen later by the fact that some edge lengths would become negative if  $\frac{4}{11} \leq \alpha \leq \frac{16}{11}$  was not true.

A face of  $S_d$  or  $S_v$  corresponds to points  $x$  where the above inequality is in fact an equality for *one* other vertex in  $\mathcal{C}'$ , an edge of  $S_d/S_v$  points  $x$  where it is an equality for *two* other vertices in  $\mathcal{C}'$  and a vertex of  $S_d/S_v$  where it is an equality for *three* other vertices in  $\mathcal{C}'$ .

All the 16-hedra in these partitions are congruent to the 16-hedron  $C_{16}$  centered at the origin. This 16-hedron has vertices:

$$\begin{aligned}
& \text{cyc } \frac{1}{12} \{(4 - 11\alpha), (4 - 11\alpha), (44 - 22\alpha)\} \\
& \text{cyc } \frac{-1}{12} \{-(4 - 11\alpha), (4 - 11\alpha), (44 - 22\alpha)\} \\
& \text{cyc } \frac{-1}{12} \{(4 - 11\alpha), -(4 - 11\alpha), (44 - 22\alpha)\} \\
& \text{cyc } \frac{-1}{12} \{(4 - 11\alpha), (4 - 11\alpha), -(44 - 22\alpha)\} \\
& \text{cyc } \frac{1}{12} \{(20 - 22\alpha), (28 - 11\alpha), -(28 - 11\alpha)\} \\
& \text{cyc } \frac{1}{12} \{(20 - 22\alpha), -(28 - 11\alpha), (28 - 11\alpha)\} \\
& \text{cyc } \frac{1}{12} \{-(20 - 22\alpha), (28 - 11\alpha), (28 - 11\alpha)\} \\
& \text{cyc } \frac{-1}{12} \{(20 - 22\alpha), (28 - 11\alpha), (28 - 11\alpha)\} \\
& \text{cyc } \frac{11}{10} \{(2 - \alpha), (2 - \alpha), -(2 - \alpha)\} \\
& \quad \frac{-11}{10} \{(2 - \alpha), (2 - \alpha), (2 - \alpha)\}
\end{aligned}$$

Where  $\text{cyc}\{x, y, z\} = \{x, y, z\} \cup \{y, z, x\} \cup \{z, x, y\}$

Similarly, all the dodecahedrons in these partitions are congruent to a dodecahedron  $C_{12}$  centered at the origin (note that this dodecahedron is not

a part of the partition). We take this  $C_{12}$  to be the dodecagon centred at  $\{3, -1, 1\}$  translated by  $\{-3, 1, -1\}$ . This dodecahedron has vertices:

$$\begin{aligned}
& \pm \frac{1}{12} \{(8 - 22\alpha), (8 + 11\alpha), -(16 - 11\alpha)\} \\
& \pm \frac{1}{12} \{(8 - 22\alpha), (16 - 11\alpha), -(8 + 11\alpha)\} \\
& \pm \frac{1}{12} \{(16 - 11\alpha), (8 - 22\alpha), -(8 + 11\alpha)\} \\
& \pm \frac{1}{12} \{(16 - 11\alpha), (8 + 11\alpha), -(8 - 22\alpha)\} \\
& \pm \frac{1}{12} \{(8 + 11\alpha), (16 - 11\alpha), -(8 - 22\alpha)\} \\
& \pm \frac{1}{12} \{(8 + 11\alpha), (8 - 22\alpha), -(16 - 11\alpha)\} \\
& \pm \frac{1}{10} \{(8 + 11\alpha), (12 - 11\alpha), -(12 - 11\alpha)\} \\
& \pm \frac{1}{10} \{(12 - 11\alpha), (12 - 11\alpha), -(8 + 11\alpha)\} \\
& \pm \frac{1}{10} \{(12 - 11\alpha), (8 + 11\alpha), -(12 - 11\alpha)\} \\
& \pm \{1, 1, -1\}
\end{aligned}$$

To better describe these shapes, we make use of a formula which formulates volume and second moment recursively from [3, pg 455] which we summarize here:

**Theorem 1** *Suppose  $P$  is an  $n$ -dimensional polytope with  $N_1$  congruent faces  $F_1, F_1' \dots$ ;  $N_2$  congruent faces  $F_2, F_2' \dots$  etc. and with baricentre  $c$ . Let  $a_i \in F_i$  be the foot of the perpendicular from  $c$  to  $F_i$  and let  $h_i = \|ca_1\|$ . Then:*

$$\begin{aligned}
V(P) &= \sum_i \frac{N_i h_i}{n} V(F_i) \\
U(P, c) &= \sum_i \frac{N_i h_i}{n+2} (h_i^2 V(F_i) + U(F_i, a_i))
\end{aligned}$$

In our partition there are 3 types of faces:

- those that divide 2 16-hedrons (type 1)

- those that divide 2 dodecahedrons (type 2)
- those that divide a dodecahedron and a 16-hedron (type 3)

All faces are of one of these types, and all faces of the same type are congruent.

Our typical 16-hedron  $C_{16}$  has 4 near centres that form centres of other 16-hedrons, and 12 near centres that form centres of dodecahedrons. Hence it will have 4 faces of type 1 and 12 faces of type 3.

A typical face  $F_1$  of type 1 is the face between  $C_{16}$  and the 16-hedron centered at  $\{2, 2, 2\}$ , which has vertices:

$$\begin{aligned} & \frac{1}{12}\{(28 - 11\alpha), (28 - 11\alpha), -(20 - 22\alpha)\} \\ & \frac{-1}{12}\{(4 - 11\alpha), -(44 - 22\alpha), (4 - 11\alpha)\} \\ & \frac{1}{12}\{-(20 - 22\alpha), (28 - 11\alpha), (28 - 11\alpha)\} \\ & \frac{-1}{12}\{(4 - 11\alpha), (4 - 11\alpha), -(44 - 22\alpha)\} \\ & \frac{1}{12}\{(28 - 11\alpha), -(20 - 22\alpha), (28 - 11\alpha)\} \\ & \frac{-1}{12}\{-(44 - 22\alpha), (4 - 11\alpha), (4 - 11\alpha)\} \end{aligned}$$

Thus a face of type 1 is a regular hexagon of side length:

$$\frac{1}{12}\| \{-(32 - 22\alpha), (16 - 11\alpha), (16 - 11\alpha)\} \| = \frac{16 - 11\alpha}{2\sqrt{6}}$$

Which has area:

$$V(F_1) = \frac{6}{2} \frac{(16 - 11\alpha)}{4\sqrt{2}} \frac{(16 - 11\alpha)}{2\sqrt{6}} = \frac{\sqrt{3}}{16} (16 - 11\alpha)^2$$

(since the perpendicular distance from the baricentre of the face to the edge is  $h_{F_1}(e) = \frac{1}{4\sqrt{2}}(16 - 11\alpha)$ )

A typical face  $F_3$  of type 3 is the face between  $C_{16}$  and the dodecahedron centered at  $\{-3, -1, -1\}$ , which has vertices:

$$\frac{-11}{10}\{(2 - \alpha), (2 - \alpha), (2 - \alpha)\}$$

$$\begin{aligned} & \frac{-1}{12} \{(28 - 11\alpha), (28 - 11\alpha), (20 - 22\alpha)\} \\ & \frac{-1}{12} \{(44 - 22\alpha), -(4 - 11\alpha), (4 - 11\alpha)\} \\ & \frac{-1}{12} \{(44 - 22\alpha), (4 - 11\alpha), -(4 - 11\alpha)\} \\ & \frac{-1}{12} \{(28 - 11\alpha), (20 - 22\alpha), (28 - 11\alpha)\} \end{aligned}$$

Thus a face of type 3 is an irregular pentagon with:

- 2 edges of length:  $\frac{1}{60} \|(8+11\alpha), (8+11\alpha), -4(8+11\alpha)\| = \frac{\sqrt{2}}{20}(8+11\alpha)$
- 2 edges of length:  $\frac{1}{12}(16 - 11\alpha) \|-1, 2, 1\| = \frac{\sqrt{6}}{12}(16 - 11\alpha)$
- 1 edge of length:  $\frac{\sqrt{2}}{6}(4 - 11\alpha)$

with respective distances from the centre of the face  $h_{F_3}(e_1) = \frac{\sqrt{22}}{6}(2 - \alpha)$ ,  $h_{F_3}(e_2) = \frac{\sqrt{66}}{8}\alpha$  and  $h_{F_3}(e_3) = \frac{\sqrt{22}}{6}(2 - \alpha)$ , and so has area:

$$\begin{aligned} V(F_3) &= \frac{1}{n} [2V(e_1)h_{F_3}(e_1) + 2V(e_2)h_{F_3}(e_2) + V(e_3)h_{F_3}(e_3)] \\ &= \frac{1}{2} [2 \frac{\sqrt{2}}{20}(8 + 11\alpha) \frac{\sqrt{22}}{6}(2 - \alpha) + 2 \frac{\sqrt{6}}{12}(16 - 11\alpha) \frac{\sqrt{66}}{8}\alpha + \\ & \quad \frac{\sqrt{2}}{6}(4 - 11\alpha) \frac{\sqrt{22}}{6}(2 - \alpha)] \\ &= \frac{\sqrt{11}}{60}(8 + 11\alpha)(2 - \alpha) + \frac{\sqrt{11}}{16}\alpha(16 - 11\alpha) + \frac{\sqrt{11}}{36}(4 - 11\alpha)(2 - \alpha) \\ &= \frac{\sqrt{11}}{720}(32 + 1408\alpha - 847\alpha^2) \end{aligned}$$

From the definition of  $\alpha$ , the distance from the centre of  $C_{16}$  to the centre of an  $F_3$  face is  $h_{16}(F_3) = \frac{\sqrt{11}}{2}(2 - \alpha)$ , and clearly the distance to the centre of an  $F_1$  face is  $h_{16}(F_1) = \sqrt{3}$  (half the distance between the centres of two adjacent 16-hedra), so the volume of  $C_{16}$  is:

$$\begin{aligned} V(C_{16}) &= \frac{1}{n} [4V(F_1)h_{16}(F_1) + 12V(F_3)h_{16}(F_3)] \\ &= \frac{1}{3} [4\sqrt{3} \frac{\sqrt{3}}{16}(16 - 11\alpha)^2 + 12 \frac{\sqrt{11}}{720}(32 + 1408\alpha - 847\alpha^2) \frac{\sqrt{11}}{2}(2 - \alpha)] \\ &= \frac{1}{4}(16 - 11\alpha)^2 + \frac{11}{120}(32 + 1408\alpha - 847\alpha^2) \\ &= \frac{1}{360}(9317\alpha^3 - 23232\alpha^2 - 1056\alpha + 23744) \end{aligned}$$

Our typical dodecahedron  $C_{12}$  has 6 faces of type 2 and 6 faces of type 3. We have already found the area of the type 3 faces, so all that remains is to find the area of a type 2 face.

A typical face  $F_2$  of type 2 is the face between the dodecahedron at  $\{3, -1, 1\}$  and the dodecahedron at  $\{5, 1, 1\}$ , which after translating by  $\{-3, 1, -1\}$  is the face between  $C_{12}$  and the dodecahedron at  $\{2, 2, 0\}$ , which has vertices:

$$\{1, 1, -1\}$$

$$\frac{1}{10}\{(12 - 11\alpha), (8 + 11\alpha), -(12 - 11\alpha)\}$$

$$\frac{1}{12}\{(16 - 11\alpha), (8 + 11\alpha), -(8 - 22\alpha)\}$$

$$\frac{1}{12}\{(8 + 11\alpha), (16 - 11\alpha), -(8 - 22\alpha)\}$$

$$\frac{1}{10}\{(8 + 11\alpha), (12 - 11\alpha), -(12 - 11\alpha)\}$$

Thus a face of type 2 is an irregular pentagon with:

- 2 edges of length:  $\frac{1}{10}\| \{-(2 - 11\alpha), (2 - 11\alpha), (2 - 11\alpha)\} \| = \frac{\sqrt{3}}{10}(11\alpha - 2)$
- 2 edges of length:  $\frac{1}{60}\| \{(8 + 11\alpha), -(8 + 11\alpha), 4(8 + 11\alpha)\} \| = \frac{\sqrt{2}}{20}(8 + 11\alpha)$
- 1 edge of length:  $\frac{1}{6}\| \{-(4 - 11\alpha), (4 - 11\alpha), 0\} \| = \frac{\sqrt{2}}{6}(11\alpha - 4)$

with respective distances from the centre of the face  $h_{F_2}(e_1) = \frac{\sqrt{2}}{\sqrt{3}}$  and  $h_{F_2}(e_2) = h_{F_2}(e_3) = \frac{1}{6}(11\alpha - 4)$ , and so has area:

$$\begin{aligned} V(F_2) &= \frac{1}{n}[2V(e_1)h_{F_2}(e_1) + 2V(e_2)h_{F_2}(e_2) + V(e_3)h_{F_2}(e_3)] \\ &= \frac{1}{2}\left[2\frac{\sqrt{3}}{10}(11\alpha - 2)\frac{\sqrt{2}}{\sqrt{3}} + 2\frac{\sqrt{2}}{20}(8 + 11\alpha)\frac{1}{6}(11\alpha - 4) + \right. \\ &\quad \left. \frac{\sqrt{2}}{6}(11\alpha - 4)\frac{1}{6}(11\alpha - 4)\right] \\ &= \frac{\sqrt{2}}{10}(11\alpha - 2) + \frac{\sqrt{2}}{120}(8 + 11\alpha)(11\alpha - 4) + \frac{\sqrt{2}}{36}(4 - 11\alpha)^2 \\ &= \frac{11\sqrt{2}}{45}(11\alpha^2 + \alpha - 1) \end{aligned}$$

From the definition of  $\alpha$ , the distance from the centre of  $C_{12}$  to the centre of an  $F_3$  face is  $h_{12}(F_3) = \frac{\sqrt{11}\alpha}{2}$ , and clearly the distance to the centre of an

$F_2$  face is  $h_{12}(F_2) = \sqrt{2}$  (half the distance between the centres of 2 adjacent dodecahedra), so the volume of  $C_{12}$  is:

$$\begin{aligned}
V(C_{12}) &= \frac{1}{n}[6V(F_2)h_{12}(F_2) + 6V(F_3)h_{12}(F_3)] \\
&= 2\frac{11\sqrt{2}}{45}(11\alpha^2 + \alpha - 1)2\sqrt{2} + 2\frac{\sqrt{11}}{720}(32 + 1408\alpha - 847\alpha^2)\frac{\sqrt{11}\alpha}{2} \\
&= \frac{88}{45}(11\alpha^2 + \alpha - 1) + \frac{11}{720}(32 + 1408\alpha - 847\alpha^2) \\
&= \frac{-11}{720}(847\alpha^3 - 2112\alpha^2 - 96\alpha + 64)
\end{aligned}$$

Since each dodecahedron is in contact with 6 other dodecahedrons and 6 16-hedrons, and each 16-hedron is in contact with 12 dodecahedrons and 4 16-hedrons, the ratio of 16-hedrons to dodecahedrons is 1:2. Thus our fundamental unit is some multiple of  $(2C_{12} + C_{16})$ . But then:

$$\begin{aligned}
G(F) &= \frac{1}{n} \frac{\frac{1}{L} \sum_{i=1}^L U(S_i, c_i)}{\left(\frac{1}{L} \sum_{i=1}^L V(S_i)\right)^{1+\frac{2}{n}}} \\
&= \frac{1}{n} \frac{\frac{1}{L} \sum_{i=1}^{\frac{L}{3}} 2U(C_{12}, 0) + U(C_{16}, 0)}{\left(\frac{1}{L} \sum_{i=1}^{\frac{L}{3}} 2V(C_{12}) + V(C_{16})\right)^{1+\frac{2}{n}}} \\
&= \frac{1}{n} \frac{\frac{1}{3}(2U(C_{12}, 0) + U(C_{16}, 0))}{\left(\frac{1}{3}(2V(C_{12}) + V(C_{16}))\right)^{1+\frac{2}{n}}}
\end{aligned}$$

Thus we can treat the fundamental unit as being  $2C_{12}$ s and a  $C_{16}$ , and then (since  $n = 3$ ) we have:

$$G(F) = \frac{3^{\frac{2}{3}}}{3} \frac{U(F')}{V(F')^{\frac{5}{3}}}$$

where

$$U(F') = 2U(C_{12}, 0) + U(C_{16}, 0)$$

and

$$V(F') = 2V(C_{12}) + V(C_{16})$$

But we have already found  $V(C_{12})$  and  $V(C_{16})$ , so we have:

$$\begin{aligned}
V(F') &= 2V(C_{12}) + V(C_{16}) \\
&= 2 \left( \frac{-11}{720} (847\alpha^3 - 2112\alpha^2 - 96\alpha + 64) \right) + \\
&\quad \frac{1}{360} (9317\alpha^3 - 23232\alpha^2 - 1056\alpha + 23744) \\
&= 64
\end{aligned}$$

As we would like, since we want  $F'$  to act like our fundamental unit,  $V(F')$  has no dependence on  $\alpha$ .

Now to find the  $U$  values.

### 3 Finding the Unnormalized Second Moments of $C_{16}$ and $C_{12}$

Our job to begin with is to find  $U(F_i, c_i)$ , where  $c_i$  is the point on  $F_i$  that also lies on the line segment joining the centres of the 2 hedrons that the face is a part of (we need to use this baricentre since we want to use equation (2)). This is the baricentre we used in finding the volumes, so we already know our  $h_{F_i}(e_j)$  values. All that remains is to find the different  $U_{F_i}(e_j, d_j)$ , where the point  $d_j$  on edge  $e_j$  is such that the line  $d_j c_i$  is perpendicular to  $e_j$ .

$F_1$  is a regular hexagon, so all the edges are congruent. Also the baricentres  $d$  of these edges  $e$  are just the midpoints, so for both vertices on  $e$ ,  $h(v_i)$  is just  $\frac{V(e)}{2}$ . Using the convention that  $V(v) = 1$  and  $U(v) = 0$  for any vertice  $v$  (required for Theorem 1 to work in 1-dimension), we have:

$$\begin{aligned}
U_{F_1}(e, d) &= \frac{2\frac{V(e)}{2}}{1+2} \left( \left( \frac{V(e)}{2} \right)^2 V(v) + U(v) \right) \\
&= \frac{\left( \frac{16-11\alpha}{2\sqrt{6}} \right)^3}{12} \\
&= \frac{\sqrt{6}(16-11\alpha)^3}{3456}
\end{aligned}$$

Then

$$\begin{aligned}
U(F_1, c_1) &= \frac{6h_{F_1}(e)}{2+2} ((h_{F_1}(e))^2V(e) + U_{F_1}(e, d)) \\
&= \frac{3}{2} \left( \left( \frac{(16-11\alpha)}{4\sqrt{2}} \right)^3 \left( \frac{16-11\alpha}{2\sqrt{6}} \right) + \frac{1}{4\sqrt{2}}(16-11\alpha) \left( \frac{\sqrt{6}(16-11\alpha)^3}{3456} \right) \right) \\
&= \frac{5\sqrt{3}(16-11\alpha)^4}{4608}
\end{aligned}$$

$F_2$  and  $F_3$  require more work, since they are irregular pentagons and each have 3 different types of edge. Also these edges do not all have 2 congruent vertices (ie their baricenters  $d$  are not the midpoints of the edges) so the working to find the different  $U(e, d)$  for these faces becomes rather longwinded and messy. We skip most of that and just give the results:

$$\begin{aligned}
U_{F_2}(e_1, d_1) &= \frac{\sqrt{3}}{3000}(11\alpha - 2)(363\alpha^2 - 462\alpha + 172) \\
U_{F_2}(e_2, d_2) &= \frac{\sqrt{2}}{36000}(11\alpha + 8)(1573\alpha^2 - 2332\alpha + 1072) \\
U_{F_2}(e_3, d_3) &= \frac{\sqrt{2}(11\alpha - 4)^3}{1296}
\end{aligned}$$

$$\begin{aligned}
U(F_2, c_2) &= \frac{2h_{F_2}(e_1)}{2+2} ((h_{F_2}(e_1))^2V_{F_2}(e_1) + U_{F_2}(e_1, d_1)) + \\
&\quad \frac{2h_{F_2}(e_2)}{2+2} ((h_{F_2}(e_2))^2V_{F_2}(e_2) + U_{F_2}(e_2, d_2)) + \\
&\quad \frac{h_{F_2}(e_3)}{2+2} ((h_{F_2}(e_3))^2V_{F_2}(e_3) + U_{F_2}(e_3, d_3)) \\
&= \frac{\sqrt{2}}{1944000}(10556161\alpha^4 - 10179488\alpha^3 + 1788864\alpha^2 + \\
&\quad 1733248\alpha - 398624)
\end{aligned}$$

$$\begin{aligned}
U_{F_3}(e_1, d_1) &= \frac{\sqrt{2}}{36000}(11\alpha + 8)(1573\alpha^2 - 2332\alpha + 1072) \\
U_{F_3}(e_2, d_2) &= \frac{\sqrt{6}(16-11\alpha)^3}{3456} \\
U_{F_3}(e_3, d_3) &= \frac{\sqrt{2}(11\alpha - 4)^3}{1296}
\end{aligned}$$

$$\begin{aligned}
U(F_3, c_3) &= \frac{2h_{F_3}(e_1)}{2+2} ((h_{F_3}(e_1))^2 V_{F_3}(e_1) + U_{F_3}(e_1, d_1)) + \\
&\quad \frac{2h_{F_3}(e_2)}{2+2} ((h_{F_3}(e_2))^2 V_{F_3}(e_2) + U_{F_3}(e_2, d_2)) + \\
&\quad \frac{h_{F_3}(e_3)}{2+2} ((h_{F_3}(e_3))^2 V_{F_3}(e_3) + U_{F_3}(e_3, d_3)) \\
&= \frac{-\sqrt{11}}{15552000} (12659141\alpha^4 - 39200128\alpha^3 + 46320384\alpha^2 - \\
&\quad 23744512\alpha - 1951744)
\end{aligned}$$

$$\begin{aligned}
U(C_{16}, 0) &= \frac{4h(F_1)}{3+2} ((h(F_1))^2 V(F_1) + U(F_1)) + \\
&\quad \frac{12h(F_3)}{3+2} ((h(F_3))^2 V(F_3) + U(F_3)) \\
&= \frac{1}{12960000} (692680351\alpha^5 - 4456134760\alpha^4 + 10637139040\alpha^3 - \\
&\quad 9643758080\alpha^2 - 525521920\alpha + 3915040768)
\end{aligned}$$

$$\begin{aligned}
U(C_{12}, 0) &= \frac{6h(F_2)}{3+2} ((h(F_2))^2 V(F_2) + U(F_2)) + \\
&\quad \frac{6h(F_3)}{3+2} ((h(F_3))^2 V(F_3) + U(F_3)) \\
&= \frac{-1}{25920000} (692680351\alpha^5 - 1688985760\alpha^4 + 814359040\alpha^3 - \\
&\quad 652974080\alpha^2 - 107345920\alpha + 43168768)
\end{aligned}$$

$$\begin{aligned}
U(F') &= U(C_{16}, 0) + 2U(C_{12}, 0) \\
&= \frac{-307461\alpha^4 + 1091420\alpha^3 - 998976\alpha^2 - 46464\alpha + 430208}{1440}
\end{aligned}$$

Similarly to with the volume, the highest power of  $\alpha$  cancels from the sum when considering the fundamental unit, leaving us with a quartic rather than a quintic. Now we put it all together to find the result we've been looking for:

$$\begin{aligned}
G(F) &= \frac{3^{\frac{2}{3}} U(F')}{3 V(F')^{\frac{5}{3}}} \\
&= 3^{-\frac{1}{3}} \frac{-307461\alpha^4 + 1091420\alpha^3 - 998976\alpha^2 - 46464\alpha + 430208}{1474560}
\end{aligned}$$

## 4 Varying $\alpha$

To find the  $\alpha$  that gives the lowest value of  $G$ , we need to know  $\frac{dG}{d\alpha}$  and solve for  $\frac{dG}{d\alpha} = 0$  to find critical points.

$$\frac{dG}{d\alpha} = 3^{-\frac{1}{3}} \frac{-1229844\alpha^3 + 3274260\alpha^2 - 1997952\alpha - 46464}{1474560}$$

So  $\frac{dG}{d\alpha} = 0$  at  $\alpha = 1$  or  $\alpha = \frac{4}{11} (16 \pm 3\sqrt{30})$  and of these, only  $\alpha = 1$  lies in our allowed range  $\frac{4}{11} \leq \alpha \leq \frac{16}{11}$

So, since the only critical point of  $G$  in the range  $\frac{4}{11} \leq \alpha \leq \frac{16}{11}$  is at  $\alpha = 1$  the minimum value of  $G$  will be at one of  $\alpha = \frac{4}{11}, \frac{16}{11}$  or 1

$$G(F) = \begin{cases} \frac{19}{256} 3^{\frac{2}{3}} \approx 0.1544 & \text{at } \alpha = \frac{4}{11} \\ \frac{168727}{4423680} 3^{\frac{2}{3}} \approx 0.0793 & \text{at } \alpha = 1 \\ \frac{67}{1280} 3^{\frac{2}{3}} \approx 0.1089 & \text{at } \alpha = \frac{16}{11} \end{cases}$$

The lowest value of  $G(F)$  occurs at  $\alpha = 1$  and is roughly 0.0793, greater than both the truncated octahedron of the BCC ( $G \approx 0.0785$  [3, pg60]) and the Phelan Weaire partition ( $G \approx 0.0787$  [5]).

However, if we look at the 2 different type of cells individually at  $\alpha = 1$ :

$$\begin{aligned}
V(C_{12}) &= \frac{14267}{720} \\
U(C_{12}, 0) &= \frac{899097601}{25920000} \\
G(C_{12}) &= \frac{899097601}{4280100 \sqrt[3]{10} (42801)^{2/3}} \\
&\approx 0.0797 \\
V(C_{16}) &= \frac{8773}{360} \\
U(C_{16}, 0) &= \frac{619445399}{12960000} \\
G(C_{16}) &= \frac{2188853}{18600 \sqrt[3]{5} (26319)^{2/3}} \\
&\approx 0.0778
\end{aligned}$$

So the 16-hedra by themselves have a lower normalized second moment than both the BCC and the Phelan Weaire. Our reasoning that the higher number of faces resulting in a lower normalized second moment wasnt far off, it is just that the dodecahedra offset the 16-hedra by too much.

Although the 12-16 partition does not out perform the BCC with respect to normalized second moment, we can still check how it fares in the Kelvin problem, as well as its packing density and covering thickness. We have from earlier that:

$$V(C_{16}) = \frac{1}{360}(9317\alpha^3 - 23232\alpha^2 - 1056\alpha + 23744)$$

$$V(C_{12}) = \frac{-11}{720}(847\alpha^3 - 2112\alpha^2 - 96\alpha + 64)$$

So  $V(C_{16}) = V(C_{12}) = \frac{64}{3}$  when  $\alpha = \alpha_c \approx 1.05672$

The surfaces areas for  $C_{16}$  and  $C_{12}$  are:

$$SA(C_{16}) = 4V(F_1) + 12V(F_3)$$

$$SA(C_{12}) = 6V(F_2) + 6V(F_3)$$

So, at  $\alpha_c$ :

$$V(F_1) = \frac{\sqrt{3}}{16}(16 - 11\alpha_c)^2 \approx 2.07309$$

$$V(F_2) = \frac{11\sqrt{2}}{45}(11\alpha_c^2 + \alpha_c - 1) \approx 4.26585$$

$$V(F_3) = \frac{\sqrt{11}}{720}(32 + 1408\alpha_c - 847\alpha_c^2) \approx 2.64434$$

and

$$SA(C_{16}) \approx 40.0244$$

$$SA(C_{12}) \approx 41.4611$$

giving a mean surface area per cell of

$$MSA = \frac{1}{3}(2SA(C_{12}) + SA(C_{16})) \approx 40.982$$

and now we can calculate the isoperimetric quotient:

$$\begin{aligned} I(12-16) &\approx 36\pi \frac{(\frac{64}{3})^2}{40.982^3} \\ &\approx 0.7478 \end{aligned}$$

less than both the Kelvin BCC and the PW packing. However considering the cells themselves:

$$\begin{aligned} I(C_{12}) &\approx 36\pi \frac{(\frac{64}{3})^2}{41.4611^3} \\ &\approx 0.7222 \\ I(C_{16}) &\approx 36\pi \frac{(\frac{64}{3})^2}{40.0244^3} \\ &\approx 0.8028 \end{aligned}$$

Again, the 16-hedron out-performs both the Kelvin BCC and the PW partition when considered on its own, but is let down by the dodecahedra. In fact it also out performs both the individual cells of the PW partition, since:

$$\begin{aligned} G(C_{12}(PW)) &\approx 0.0783 & I(C_{12}(PW)) &\approx 0.749 \\ G(C_{14}(PW)) &\approx 0.0789 & I(C_{14}(PW)) &\approx 0.765 \quad [5] \end{aligned}$$

We now work out the packing density and covering density. Packing density is easy, as the packing radius  $r_{pack}$  is just the lowest of the 4 values  $h_{16}(F_1), h_{16}(F_3), h_{12}(F_2), h_{12}(F_3)$ , since these are the perpendicular distances from the centres of the cells to the faces, if  $r_{pack}$  was larger than any of these the ball  $B_i$  would not lie entirely inside that cell. So

$$r_{pack} = \begin{cases} h_{12}(F_3) = \frac{\sqrt{11}}{2}\alpha & \frac{4}{11} \leq \alpha \leq \sqrt{\frac{8}{11}} \\ h_{12}(F_2) = \sqrt{2} & \sqrt{\frac{8}{11}} < \alpha < (2 - \sqrt{\frac{8}{11}}) \\ h_{16}(F_3) = \frac{\sqrt{11}}{2}(2 - \alpha) & (2 - \sqrt{\frac{8}{11}}) \leq \alpha \leq \frac{16}{11} \end{cases}$$

And the packing density is:

$$L \frac{V(B_1)}{V(F)} = 3 \frac{\frac{4}{3}\pi r_{pack}^3}{64} = \frac{\pi r_{pack}^3}{16}$$

The most efficient packing occurs at the maximum value of  $r_{pack}$ , which is  $\sqrt{2}$ , so the most efficient packing density for the 12-16 partition is:

$$\frac{\pi\sqrt{2}^3}{16} = \frac{\pi\sqrt{2}}{8} \approx 0.555$$

Covering thickness is slightly more difficult, as the covering radius  $r_{cover}$  is equal to the maximum of  $\|v - c\|$  where  $c$  is a centre of a cell and  $v$  is any vertex of that same cell. Since all the cells are congruent to either  $C_{16}$  or  $C_{12}$  it is enough to consider the vertices of these cells. Conveniently, in both these cases we take  $c = (0, 0, 0)$  and so only have to consider  $\|v\|$ .

Clearly when looking at vertices of  $C_{16}$  there are only 3 distinct values of  $\|v\|$  since all vertices of  $C_{16}$  are one of 3 “starting” vertices:

- $\frac{1}{12}\{(4 - 11\alpha), (4 - 11\alpha), (44 - 22\alpha)\}$
- $\frac{1}{12}\{(20 - 22\alpha), (28 - 11\alpha), -(28 - 11\alpha)\}$
- $\frac{-11}{10}\{(2 - \alpha), (2 - \alpha), (2 - \alpha)\}$

acted on by some combination of central automorphisms

$$(x, y, z) \longrightarrow (z, x, y) \quad \text{and} \quad (x, y, z) \longrightarrow (x, -y, -z)$$

Similarly for  $C_{12}$  there are only 3 distinct values of  $\|v\|$  so we have as possible values:

$$\begin{aligned} \left\| \frac{1}{12}\{(4 - 11\alpha), (4 - 11\alpha), (44 - 22\alpha)\} \right\| &= \sqrt{\frac{1}{24}(121\alpha^2 - 352\alpha + 328)} \\ \left\| \frac{1}{12}\{(20 - 22\alpha), (28 - 11\alpha), -(28 - 11\alpha)\} \right\| &= \sqrt{\frac{1}{24}(121\alpha^2 - 352\alpha + 328)} \\ \left\| \frac{-11}{10}\{(2 - \alpha), (2 - \alpha), (2 - \alpha)\} \right\| &= \frac{11\sqrt{3}}{10}(2 - \alpha) \\ \left\| \frac{1}{12}\{(8 - 22\alpha), (8 + 11\alpha), -(16 - 11\alpha)\} \right\| &= \sqrt{\frac{1}{24}(121\alpha^2 - 88\alpha + 64)} \\ \left\| \frac{1}{10}\{(8 + 11\alpha), (12 - 11\alpha), -(12 - 11\alpha)\} \right\| &= \sqrt{\frac{11}{100}(33\alpha^2 - 32\alpha + 32)} \\ \left\| \{1, 1, -1\} \right\| &= \sqrt{3} \end{aligned}$$

Thus:

$$r_{cover} = \begin{cases} \frac{11\sqrt{3}}{10}(2 - \alpha) & \frac{4}{11} \leq \alpha \leq \frac{64}{77} \\ \sqrt{\frac{1}{24}(121\alpha^2 - 352\alpha + 328)} & \frac{64}{77} < \alpha < 1 \\ \sqrt{\frac{1}{24}(121\alpha^2 - 88\alpha + 64)} & 1 \leq \alpha \leq \frac{16}{11} \end{cases}$$

and as with packing, the covering thickness is  $\frac{1}{16}\pi r_{cover}^3$ . The most efficient covering occurs at the minimum value of  $r_{cover}$ , which is  $\frac{1}{2}\sqrt{\frac{97}{6}}$ , so the most efficient covering thickness for the 12-16 partition is:

$$\frac{\pi}{16} \left( \frac{1}{2} \sqrt{\frac{97}{6}} \right)^3 \approx 1.595$$

The best packing partition, the FCC lattice, has a packing density of  $\approx 0.74$  [3, pg 15] and the best covering partition, the BCC lattice, has a covering thickness of  $\approx 1.46$  [3, pg 24], so the 12-16 Partition is far from optimal in either of these respects. In comparison, the Phelan Weaire Partition has a packing density of  $\frac{5\sqrt{5}\pi}{48} \approx 0.73$  and covering thickness  $\frac{125\sqrt{3}\pi}{432} \approx 1.57$  [5]

However, as has been the case with the normalized second moment and the isoperimetric quotient, perhaps one of the individual cells will offer a better solution in the cases of packing and covering aswell.

Taking the definition of a packing radius of a cell  $(S, c)$  to be the largest value  $r$  for which a sphere of radius  $r$  centred at  $c$  would lie entirely within the cell, we have:

$$r_{pack}(C_{12}) = \begin{cases} h_{12}(F_3) = \frac{\sqrt{11}}{2}\alpha & \frac{4}{11} \leq \alpha < \sqrt{\frac{8}{11}} \\ h_{12}(F_2) = \sqrt{2} & \sqrt{\frac{8}{11}} \leq \alpha \leq \frac{16}{11} \end{cases}$$

$$r_{pack}(C_{16}) = \begin{cases} h_{16}(F_1) = \sqrt{3} & \frac{4}{11} \leq \alpha \leq 2(1 - \sqrt{\frac{3}{11}}) \\ h_{16}(F_3) = \frac{\sqrt{11}}{2}(2 - \alpha) & 2(1 - \sqrt{\frac{3}{11}}) < \alpha \leq \frac{16}{11} \end{cases}$$

The packing density of  $C_{12}$ ,  $\frac{4}{3} \frac{\pi}{V(C_{12})} r_{pack}^3(C_{12})$  has a maximum value of

$$\frac{120\sqrt{2}\pi}{1012 - 65\sqrt{22}} \approx 0.754 \text{ at } \alpha = \sqrt{\frac{8}{11}}$$

The packing density of  $C_{16}$ ,  $\frac{4}{3} \frac{\pi}{V(C_{16})} r_{pack}^3(C_{16})$  has a maximum value of

$$\frac{15\sqrt{3}\pi}{405 - 53\sqrt{33}} \approx 0.812 \text{ at } \alpha = 2(1 - \sqrt{\frac{3}{11}})$$

Similarly, taking the definition of a covering radius of a cell  $(S, c)$  to be the smallest value  $r$  for which all points  $x \in S$  lie within the sphere of radius  $r$  centered at  $c$ , we have:

$$r_{cover}(C_{12}) = \begin{cases} \sqrt{3} & \frac{4}{11} \leq \alpha \leq \frac{26}{33} \\ \frac{\sqrt{\frac{11}{100}(33\alpha^2 - 32\alpha + 32)}}{\sqrt{\frac{1}{24}(121\alpha^2 - 88\alpha + 64)}} & \frac{26}{33} < \alpha < \frac{64}{77} \\ \sqrt{\frac{1}{24}(121\alpha^2 - 88\alpha + 64)} & \frac{64}{77} \leq \alpha \leq \frac{16}{11} \end{cases}$$

$$r_{cover}(C_{16}) = \begin{cases} \frac{11\sqrt{3}}{10}(2 - \alpha) & \frac{4}{11} \leq \alpha \leq \frac{64}{77} \\ \sqrt{\frac{1}{24}(121\alpha^2 - 352\alpha + 328)} & \frac{64}{77} < \alpha \leq \frac{16}{11} \end{cases}$$

The covering thickness of  $C_{12}$ ,  $\frac{4}{3} \frac{\pi}{V(C_{12})} r_{cover}^3(C_{12})$  has a maximum value of

$$\frac{304\sqrt{38}\pi}{3885} \approx 1.515 \text{ at } \alpha = \frac{64}{77}$$

The covering thickness of  $C_{16}$ ,  $\frac{4}{3} \frac{\pi}{V(C_{16})} r_{cover}^3(C_{16})$  has a maximum value of

$$\frac{81\sqrt{3}\pi}{322} \approx 1.369 \text{ at } \alpha = \frac{64}{77}$$

It is interesting to note that both  $C_{12}$  and  $C_{16}$  have their most efficient covering at  $\alpha = \frac{64}{77}$ , yet the 12-16 partition has its most efficient covering at  $\alpha = 1$ . This is possible because when looking at the covering of the whole partition, only one value of  $r_{cover}$  is allowed, and  $r_{cover}(C_{12}) \neq r_{cover}(C_{16})$  at  $\alpha = \frac{64}{77}$ .

The following table compares the packing density and covering thickness of the various partitions mentioned in this paper:

	Packing Density	Covering Thickness
<i>BCC</i>	0.68 [3, pg. 16]	1.46 [3, pg. 38]
<i>FCC</i>	0.74 [3, pg. 2]	2.09 [3, pg. 38]
<i>PW</i>	0.73 [5]	1.57 [5]
12-16	0.56	1.60
$C_{12}$	0.75	1.52
$C_{16}$	0.81	1.37

**Table 1**

Again we see the  $C_{16}$  performs the best when considered by itself.

## 5 Quantizing Algorithm

To make any use of the 12-16 partition, it is useful to have an algorithm to determine the coordinates of centre of the cell that  $x$  lies in for any point  $x$ .

We recall that every centre in  $c \in \mathcal{C}$  is of the form  $c = (a, b, c) + (x, y, z)$  where  $a, b, c \in \mathbb{Z}$ ,  $(a + b + c) \in 2\mathbb{Z}$  and  $(x, y, z) \in \mathcal{S}$ . So, taking into account scaling by 4, every centre  $c' \in \mathcal{C}'$  is of the form

$$c' = (a, b, c) + (x, y, z)$$

where  $a, b, c \in 8Z$  and  $(x, y, z) \in \mathcal{T}$ . Here  $\mathcal{T} = \mathcal{T}_1 \cup \mathcal{T}_2$  where:

$$\begin{aligned}\mathcal{T}_1 &= \{\text{cyc}(2, -2, -2), \text{cyc}(4, 4, 0) \\ &\quad (0, 0, 0), (2, 2, 2)\} \\ \mathcal{T}_2 &= \{\text{cyc}(3, 1, -1), \text{cyc}(3, -1, 1), \text{cyc}(-3, 3, 3) \\ &\quad \text{cyc}(-3, 1, 1), \text{cyc}(-3, -1, -1), (-3, -3, -3)\}\end{aligned}$$

Consider any point  $x = (x_1, x_2, x_3)$  in  $R^3$ .

A centre of a dodecahedron  $c_{12} = a + t_v, a \in 8Z^3, t_v \in \mathcal{T}_2$ , is the closest centre of a dodecahedron to  $x$  (ie minimizes  $d(x, v), v \in \mathcal{V}$ ) if and only if

$$\min_{t \in \mathcal{T}_2} [d(x - t, a)] = d(x - t_v, a)$$

So, for each  $t_i \in \mathcal{T}_2$ , let  $v_i = t_i + a_i$ , where

$$a_i \in 8Z^3 \text{ and satisfies } \min_{a \in 8Z^3} [d(x - t_i, a)] = d(x - t_i, a_i)$$

Then  $c_{12} = v_j$ , where  $v_j$  is the closest of all the  $v_i$ s to  $x$

$$\left( \text{ie } d(v_j, x) = \min_{1 \leq i \leq 16} [d(v_i, x)] \right)$$

Similarly, a centre of a 16-hedron  $c_{16} = b + t_d, b \in 8Z^3, t_d \in \mathcal{T}_1$  is the closest centre of a 16-hedron to  $x$  (ie minimizes  $d(x, d), d \in \mathcal{D}$ ) if and only if

$$\min_{t \in \mathcal{T}_1} [d(x - t, b)] = d(x - t_d, b)$$

So, for each  $t_i \in \mathcal{T}_1$ , let  $d_i = t_i + b_i$ , where

$$b_i \in 8Z^3 \text{ and satisfies } \min_{b \in 8Z^3} [d(x - t_i, b)] = d(x - t_i, b_i)$$

Then  $c_{16} = d_j$  where  $d_j$  is the closest of all the  $d_i$ s to  $x$

$$\left( \text{ie } d(d_j, x) = \min_{1 \leq i \leq 8} [d(d_i, x)] \right)$$

Then  $x$  lies in the cell centred at:

$$\begin{cases} c_{12} & \text{if, } (2 - \alpha)d(x, c_{12}) < \alpha d(x, c_{16}) \\ c_{16} & \text{otherwise} \end{cases}$$

Using this method of determining which cell arbitrary  $x \in R^3$  lies in, and therefore which centre it gets 'rounded' to if we used the 12-16 partition

to transmit information as mentioned at the beginning of this paper, this quantising algorithm was coded in Mathematica<sup>2</sup>, and subsequently used to verify  $G(12 - 16)$  experimentally (see later)

```

Drep = {{3, 1, -1},
        {1, -1, 3}, {-1, 3, 1}, {3, -1, 1}, {-1, 1, 3}, {1, 3, -1},
        {-3, 1, 1}, {1, -3, 1}, {1, 1, -3}, {-3, -1, -1}, {-1, -3, -1},
        {-1, -1, -3}, {-3, 3, 3}, {3, -3, 3}, {3, 3, -3}, {-3, -3, -3}};
sixrep = {{0, 0, 0}, {2, -2, -2}, {-2, 2, -2}, {-2, -2, 2}, {4, 4, 0},
          {4, 0, 4}, {0, 4, 4}, {2, 2, 2}};

closeDcen[pt_] := Module[{rep, i, curr cand, this cand, curr dis, this dis},

    rep = Drep[[1]];
    curr cand = rep + 8*(Round[1/8*(pt - rep)]);
    curr dis = N[(curr cand - pt).(curr cand - pt)];
    For[i = 2, i Length[Drep], i++,
        rep = Drep[[i]];
        this cand = rep + 8*(Round[1/8*(pt - rep)]);
        this dis = N[(this cand - pt).(this cand - pt)];
        If[this dis < curr dis,
            curr dis = this dis;
            curr cand = this cand,
        ]
    ];

    Return[curr cand];

] (* end of closeDcen *)

```

```

closesixcen[pt_] := Module[{rep, i, curr cand, this cand, curr dis, this dis},

    rep = sixrep[[1]];
    curr cand = rep + 8*(Round[1/8*(pt - rep)]);
    curr dis = N[(curr cand - pt).(curr cand - pt)];
    For[i = 2, i Length[sixrep], i++,
        rep = sixrep[[i]];
        this cand = rep + 8*(Round[1/8*(pt - rep)]);

```

---

<sup>2</sup>My supervisor wrote this code for mathematica, using my quantizing algorithm.

```

    thisdis = N[(thiscand - pt).(thiscand - pt)];
    If[thisdis < currdis,
      currdis = thisdis;
      currcand = thiscand,
    ]
  ];

Return[curr cand];

] (* end of closesixcen *)

quansixtwelv[pt_] := Module[{both, closD, clossix},

  both = {};
  closD = closeDcen[pt];
  clossix = closesixcen[pt];
  If[(2 - alpha)^2*((
    closD - pt).(closD - pt)) < alpha^2*((clossix - pt).(clossix - pt)),
    both = closD,
    both = clossix];

  Return[both];

]; (* end of quansixtwelv *)

```

The quantising algorithm  $Q(x)$  was used to experimentally verify  $G$  by estimating  $G$  1000 times by finding the average squared error  $(Q(x) - x)^2$  of 1000 random points  $x$ . The mean of these experimentally generated  $G_i$  – the experimental estimate of  $G$  is 0.0793264 and the  $G_i$  had a standard deviation of 0.001223 putting the calculated ‘theoretical’ value of  $G$  0.0793381 within 0.0095415 standard deviations of the experimental  $G$ , very close. Thus we have our value of  $G$ , as well as our quantizing algorithm, supported empirically.

## 6 Conclusion

The main goal of this thesis was to calculate the quantizing properties of the 12-16 partition for any given  $\alpha$  in order to determine whether a 12-16 partition of  $R^3$  could obtain a lower normalized second moment than the

BCC lattice. We have shown that it can't, with the lowest value obtained higher than both the best PW quantizer and the BCC lattice, nor can it outperform the most efficient known partitions in any terms of Isoperimetric quotient, packing density or covering thickness. However, our reasoning that it was worth testing the 12-16 because of its high number of sides per cell had merit, as Tables 1 and Table 2 show that the 16-hedron  $C_{16}$  is the most efficient cell in all 4 attributes tested, (of all cells looked at in this paper).

Cell	G(Cell)	I(Cell)
$BCC$	0.0785	0.753
$C_{12}(PW)$	0.0783	0.749
$C_{14}(PW)$	0.0789	0.765
$C_{12}(12-16)$	0.0797	0.722
$C_{16}(12-16)$	0.0778	0.803

**Table 2**

This gives evidence that “rounder” objects do indeed have lower normalized second moment, higher isoperimetric quotient, higher packing density and lower covering thickness. The problem for the 12-16 partition was that it had twice as many dodecahedra as 16-hedra, and the dodecahedron is not sufficiently regular to be very well performed in any of the categories tested.

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