MANUAL TO THE COMPUTER PROOF THAT D_3 GIVES THE UNIQUE MINIMUM OF $h(L)$ FOR $n = 3$

PETER SARNAK AND ANDREAS STRÖMBERGSSON

The present text can be viewed as an appendix to our paper "Minima of Epstein's Zeta Function and Heights of Flat Tori". Our purpose here is to give a description of some more technical aspects regarding the computer programs which we use to prove that the face-centered cubic lattice is the unique minimum for the height function. We will use the same notation as in our paper.

Note that comments of an even more technical nature are given in the source codes themselves.

1. RATIONALS.PARI

The PARI file rationals.pari contains routines for rigorous interval arithmetic, using only operations on integers and rational numbers.

Throughout the code, D denotes a large positive integer which is kept fixed. The basic elements on which the routines operate are *intervals of the form* $\big[a/D, b/D\big]$ *with* $a, b \in \mathbb{Z}$, $a \leqq b$. The routines in rationals.pari perform multiplication, division, exponentiation and some linear algebra on such intervals, as well as computation of power functions and the complementary incomplete Gamma function $\Gamma(s, x)$. Here, if f is any function from $\mathbb{R}^n$ to $\mathbb{R}$ and $\big[a_1^{(j)}/D, a_2^{(j)}/D\big]$ $(j = 1, 2, ..., n)$ are intervals as above, we regard an interval $\big[e_1/D, e_2/D\big]$ as a correct output from

$$\text{“}f\Big(\big[a_1^{(1)}/D, a_2^{(1)}/D\big], ..., \big[a_1^{(n)}/D, a_2^{(n)}/D\big]\Big)\text{”}$$

if and only if

$$f(x_1, ..., x_n) \in \big[e_1/D, e_2/D\big], \qquad \forall (x_1, ..., x_n) \in \prod_{j=1}^{n} \big[a_1^{(j)}/D, a_2^{(j)}/D\big].$$

Naturally, we here always try to make the interval $\big[e_1/D, e_2/D\big]$ as small as we can.

Most of the arithmetic operations which we need are easy to carry out and we refer to the source code itself for individual comments. Here we will only discuss briefly the computation of $\Gamma(s, y)$. We only need this for a few specific (exact!) values of $s \in \mathbb{Q}$ (in particular for $s = \frac{3}{2}$) and positive y (bounded from below). We do this computation using Taylor expansions in a rather naive way.

First we fix a reasonably large y_0 (such as $y_0 = 30$). We compute good upper and lower bounds on $\Gamma(s, y_0)$ as follows. Note that for each $N \in \mathbb{Z}^+$ we have

$$\begin{aligned}(1) \qquad \Gamma(s, y_0) = & e^{-y_0} y_0^{s-1} \left(1 + \sum_{j=1}^{N} (s-1)(s-2)\cdots(s-j) y_0^{-j} \right) \\ & + (s-1)(s-2)\cdots(s-(N+1)) \cdot \Gamma\Big(s-(N+1), y_0\Big).\end{aligned}$$

as follows by using the recursion formula $\Gamma(s, y_0) = e^{-y_0} y_0^{s-1} + (s-1) \cdot \Gamma(s-1, y_0)$ repeatedly. Choosing N such that $(s-1)(s-2)\cdots(s-(N+1)) \leqq 0$ we obtain from (1) combined with $\Gamma(s-(N+1), y_0) > 0$ an upper bound on $\Gamma(s, y_0)$, and similarly by taking N such that $(s-1)(s-2)\cdots(s-(N+1)) \geqq 0$ we obtain a lower bound on $\Gamma(s, y_0)$. These bounds are quite precise when y_0 is large and N is chosen appropriately.

Having thus computed $\Gamma(s, y_0)$ to good precision, we can also compute the higher Taylor coefficients of the function $y \mapsto \Gamma(s, y)$ at $y = y_0$, since, directly from the definition of $\Gamma(s, y)$ we have, for each $n \geqq 0$,

$$\frac{\partial^{n+1}}{\partial y^{n+1}} \Gamma(s, y) = e^{-y} \sum_{m=0}^{n} (-1)^{n+m+1} \binom{n}{m} (s-1)(s-2)\cdots(s-m) y^{s-m-1}.$$

Given some small number a_0 ($0 < a_0 < y_0$) we can also use the above formula to compute an upper bound on $\left| \frac{\partial^{n+1}}{\partial y^{n+1}} \Gamma(s, y) \right|$ valid throughout the interval $[y_0 - a_0, y_0 + a_0]$, by simply inserting absolute signs throughout in the sum. Hence we can use Taylor's formula to compute rigorous upper and lower bounds for $\Gamma(s, y)$ for arbitrary $y \in [y_0 - a_0, y_0 + a_0]$. In particular, we are able to compute $\Gamma(s, y_0 - a_0)$ to good precision. This procedure can now be repeated, replacing y_0 by $y_0 - a_0$, etc.

In this way we compute Taylor expansions (with rigorous bounds) of $y \mapsto \Gamma(s, y)$ valid for $y \in [y_0 - (m+1)a_0, y_0 - (m-1)a_0]$, successively for $m = 0, 1, 2, ..., M$ (where $y_0 - (M+1)a_0 > 0$). The coefficients of these expansions are computed and stored once and for all, and once this is done they can be used to compute $\Gamma(s, y)$ for any $y \in \big[y_0 - (M+1)a_0, y_0 + a_0\big]$ quite efficiently.

For example, as a preparation for the program global.c (cf. below) we use the routine "printtaylorcoeffs()" in rationals.pari to compute such Taylor expansions for the four cases $s = 0, 1, \frac{3}{2}, \frac{5}{2}$ (of course, $\Gamma(1, y) = e^{-y}$, but we opted not to use this fact, i.e. not to treat $s = 1$ differently than the less simple values $s = 0, \frac{3}{2}, \frac{5}{2}$). We used $y_0 = 35$, $a_0 = \frac{1}{16}$, $M = 551$, so that we cover the interval $y \in [\frac{1}{2}, 35 + \frac{1}{16}]$. We have stored the Taylor coefficients for this in the file "taylorcoeffs", which is used by global.c. (More precisely, we store the Taylor coefficients of the products $G(s, y) = y^{-s}\Gamma(s, y)$. In the same file we have also stored Taylor coefficients for the computation of the power functions $y \mapsto y^{1/3}$ and $y \mapsto y^{-1}$.)

2. INITBOXES.PARI

This PARI program covers our particular fundamental domain for $\mathcal{P}_3^\circ/\mathrm{GL}(3,\mathbb{Z})$ with Iwasawa boxes. Its result is to be stored in the file boxes.dat, which is used by the program global.f, cf. next section. The file boxes.dat is also directly available on our web-page.

The algorithm for producing this covering is described in detail in our paper.

3. GLOBAL.C

This C program proves that $F_{(2)}(Y) > 0.11336$ holds for all $Y \in B_j$, for each Iwasawa box $B_j \neq B_{fcc}$. It requires 64 bits integer arithmetic (for the type "long long int") to run correctly.

The 11427 boxes B_j are read from the file boxes.dat. As explained in our paper, the main task in our approach is to compute rigorous bounds on the first-order partial derivatives of $F_{(2)}(Y)$ in any given box B, i.e. positive numbers $C_1, ..., C_5$ such that

$$\left|\frac{\partial}{\partial y_1} F_{(2)}(Y)\right| \leqq C_1, ..., \left|\frac{\partial}{\partial t_{23}} F_{(2)}(Y)\right| \leqq C_5, \qquad \forall Y \in B.$$

Once this has been achieved the rest of the method, including the recursive subdivision of the boxes B_j whenever necessary, has been described in the paper.

Recall that we have defined $F_{(N)}(Y)$ as the truncated sum

$$F_{(N)}(Y) = \sum_{\substack{a \in \mathbb{Z}^3 - \{0\} \\ |a_1|,|a_2|,|a_3| \leqq N}} \Big(G(0, \pi \cdot Y^{-1}[a]) + G(\tfrac{3}{2}, \pi \cdot Y[a])\Big),$$

(cf. our paper; equation (25) and the text below (29)), and that we use Iwasawa coordinates $(y_1, y_2, t_{12}, t_{13}, t_{23})$ to parametrize $Y \in \mathcal{P}_3^\circ$;

$$Y = \begin{pmatrix} 1 & t_{12} & t_{13} \\ 0 & 1 & t_{23} \\ 0 & 0 & 1 \end{pmatrix}^t \begin{pmatrix} d_1 & 0 & 0 \\ 0 & d_2 & 0 \\ 0 & 0 & d_3 \end{pmatrix} \begin{pmatrix} 1 & t_{12} & t_{13} \\ 0 & 1 & t_{23} \\ 0 & 0 & 1 \end{pmatrix}; \qquad \begin{cases} d_1 = y_1^{\frac{2}{3}} y_2^{\frac{1}{3}} \\ d_2 = y_1^{-\frac{1}{3}} y_2^{\frac{1}{3}} \\ d_3 = y_1^{-\frac{1}{3}} y_2^{-\frac{2}{3}}. \end{cases}$$

Write $y_3 = t_{12}$, $y_4 = t_{13}$, $y_5 = t_{23}$, so that $F_{(2)}(Y)$ is now a function of $(y_1, y_2, y_3, y_4, y_5)$. Using $\frac{\partial}{\partial x} G(s, \pi x) = -\pi G(s+1, \pi x)$ and the formulae

$$\begin{aligned} Y &= \begin{pmatrix} d_1 & d_1 t_{12} & d_1 t_{13} \\ d_1 t_{12} & d_1 t_{12}^2 + d_2 & d_1 t_{12} t_{13} + d_2 t_{23} \\ d_1 t_{13} & d_1 t_{12} t_{13} + d_2 t_{23} & d_1 t_{13}^2 + d_2 t_{23}^2 + d_3 \end{pmatrix} \\ &= \begin{pmatrix} y_1^{\frac{2}{3}} y_2^{\frac{1}{3}} & y_1^{\frac{2}{3}} y_2^{\frac{1}{3}} y_3 & y_1^{\frac{2}{3}} y_2^{\frac{1}{3}} y_4 \\ y_1^{\frac{2}{3}} y_2^{\frac{1}{3}} y_3 & y_1^{\frac{2}{3}} y_2^{\frac{1}{3}} y_3^2 + y_1^{-\frac{1}{3}} y_2^{\frac{1}{3}} & y_1^{\frac{2}{3}} y_2^{\frac{1}{3}} y_3 y_4 + y_1^{-\frac{1}{3}} y_2^{\frac{1}{3}} y_5 \\ y_1^{\frac{2}{3}} y_2^{\frac{1}{3}} y_4 & y_1^{\frac{2}{3}} y_2^{\frac{1}{3}} y_3 y_4 + y_1^{-\frac{1}{3}} y_2^{\frac{1}{3}} y_5 & y_1^{\frac{2}{3}} y_2^{\frac{1}{3}} y_4^2 + y_1^{-\frac{1}{3}} y_2^{\frac{1}{3}} y_5^2 + y_1^{-\frac{1}{3}} y_2^{-\frac{2}{3}} \end{pmatrix} \end{aligned}$$

and

$$\begin{aligned} Y^{-1} &= \begin{pmatrix} d_1^{-1} + d_2^{-1} t_{12}^2 + d_3^{-1}(t_{13} - t_{12} t_{23})^2 & -d_2^{-1} t_{12} + d_3^{-1} t_{13} t_{23} - d_3^{-1} t_{12} t_{23}^2 & -d_3^{-1} t_{13} + d_3^{-1} t_{12} t_{23} \\ -d_2^{-1} t_{12} + d_3^{-1} t_{13} t_{23} - d_3^{-1} t_{12} t_{23}^2 & d_2^{-1} + d_3^{-1} t_{23}^2 & -d_3^{-1} t_{23} \\ -d_3^{-1} t_{13} + d_3^{-1} t_{12} t_{23} & -d_3^{-1} t_{23} & d_3^{-1} \end{pmatrix} \\ &= \begin{pmatrix} \dots & \dots & -y_1^{\frac{1}{3}} y_2^{\frac{2}{3}} (y_4 - y_3 y_5) \\ \dots & y_1^{\frac{1}{3}} y_2^{-\frac{1}{3}} + y_1^{\frac{1}{3}} y_2^{\frac{2}{3}} y_5^2 & -y_1^{\frac{1}{3}} y_2^{\frac{2}{3}} y_5 \\ -y_1^{\frac{1}{3}} y_2^{\frac{2}{3}} (y_4 - y_3 y_5) & -y_1^{\frac{1}{3}} y_2^{\frac{2}{3}} y_5 & y_1^{\frac{1}{3}} y_2^{\frac{2}{3}} \end{pmatrix}, \end{aligned}$$

we can compute explicit functions $P_{k\ell}^{(j)} = P_{k\ell}^{(j)}(y_1, y_2, y_3, y_4, y_5)$ and $R_{k\ell}^{(j)} = R_{k\ell}^{(j)}(y_1, y_2, y_3, y_4, y_5)$ (more precisely these are rational functions of $y_1^{\frac{1}{3}}, y_2^{\frac{1}{3}}, y_3, y_4, y_5$ with coefficients in $\mathbb{Q}$) such that, for each $j = 1, 2, 3, 4, 5$,

$$\begin{aligned} \frac{\partial}{\partial y_j} F_{(N)}(Y) = \sum_{\substack{a \in \mathbb{Z}^3 - \{0\} \\ |a_1|, |a_2|, |a_3| \leqq N}} \Big(&\big(\sum_{1 \leqq k \leqq \ell \leqq 3} P_{k\ell}^{(j)} \, a_k a_\ell \big) \cdot G(1, \pi \cdot Y^{-1}[a]) \\ &+ \big(\sum_{1 \leqq k \leqq \ell \leqq 3} R_{k\ell}^{(j)} \, a_k a_\ell \big) \cdot G(\tfrac{5}{2}, \pi \cdot Y[a]) \Big). \end{aligned} \tag{2}$$

We use this formula to evaluate $\frac{\partial}{\partial y_j} F_Q^{(N)}(0)$. To make certain that we made no typo when entering the expressions for all functions $P_{k\ell}^{(j)}$ and $R_{k\ell}^{(j)}$ into the program we made several tests comparing the values obtained with difference quotients $\big(F_{(N)}(Y_1) - F_{(N)}(Y)\big)/h$, where Y_1 corresponds to replacing y_j by $y_j + h$. (We did this both in C and in PARI; in the letter case using eg. $h = 10^{-15}$ and computations with 40 digits precision, and the derivative and the difference quotient agreed typically to the first ~ 15 digits.)

To evaluate *upper and lower bounds* on $\frac{\partial}{\partial y_j} F_Q^{(N)}(0)$ in a given box $B = [y_1^{(\ell)}, y_1^{(h)}] \times [y_2^{(\ell)}, y_2^{(h)}] \times \ldots \times [y_5^{(\ell)}, y_5^{(h)}]$ in the $(y_1, y_2, y_3, y_4, y_5)$-space we did the obvious thing: Use "interval arithmetic" to obtain upper and lower bounds on each of the functions $P_{k\ell}^{(j)}(y_1, y_2, y_3, y_4, y_5)$ and $R_{k\ell}^{(j)}(y_1, y_2, y_3, y_4, y_5)$ in B. (Thus every multiplication, addition, subtraction etc. is carried out with interval arithmetic; if the computer stores the real values $a^{(\ell)}, a^{(h)}, b^{(\ell)}, b^{(h)}$, such that we have $a \in [a^{(\ell)}, a^{(h)}]$ and $b \in [b^{(\ell)}, b^{(h)}]$, then we compute

"$[\min(a^{(\ell)}b^{(\ell)}, a^{(\ell)}b^{(h)}, a^{(h)}b^{(\ell)}, a^{(h)}b^{(h)}), \max(a^{(\ell)}b^{(\ell)}, a^{(\ell)}b^{(h)}, a^{(h)}b^{(\ell)}, a^{(h)}b^{(h)})]$" for the product $a \cdot b$, meaning that we know with certainty that $a \cdot b$ belongs to this interval.) Also use interval arithmetic to obtain upper and lower bounds on all elements in the matrices Y and Y^{-1}, and then to evaluate the desired sum (2).

(In particular, note that interval arithmetic is easy to do for the necessary special functions $G(1,x)$ and $G(\frac{5}{2},x)$, since we know that both these are decreasing in x. To gain speed, the program starts by tabulating, once and for all, a lot of values for $G(1,x)$ and $G(\frac{5}{2},x)$. Then in the computation, given $x \in [x^{(\ell)}, x^{(h)}]$ we then round $x^{(\ell)}$ *downwards* to a tabulated value, and $x^{(h)}$ *upwards* to a tabulated value, to obtain upper and a lower bounds on $G(1,x)$ and $G(\frac{5}{2},x)$.)

4. SPHERE.PARI

This PARI program is used to verify relation (32) in our paper, i.e.

$$B_{fcc} \subset B(g_0, 0.18),$$

which says that the fcc-box is completely contained in the ball of radius 0.18 about the fcc-point in $\mathcal{P}_3^\circ$. We recall that B_{fcc} is defined as the following box in Iwasawa parameters

$$B_{fcc} := [1.29, 1.34] \times [1.1, 1.15] \times [0.45, 0.5] \times [\tfrac{5}{11}, \tfrac{6}{11}] \times [0.3, 0.4],$$

and the fcc-point is $Y_3 = 2^{1/3}\begin{pmatrix} 1 & 1/2 & 1/2 \\ 1/2 & 1 & 1/2 \\ 1/2 & 1/2 & 1 \end{pmatrix}$ which has Iwasawa coordinates $(y_1, y_2, t_{12}, t_{13}, t_{23}) = (\frac{4}{3}, \frac{9}{8}, \frac{1}{2}, \frac{1}{2}, \frac{1}{3})$ (and we use the representative $g_0 = 2^{-1/3}\begin{pmatrix} 1 & 0 & 1 \\ -1 & -1 & 0 \\ 0 & 1 & 1 \end{pmatrix}$).

We will work below in the setting of an arbitrary, given box

$$B = [y_1^{(\ell)}, y_1^{(h)}] \times [y_2^{(\ell)}, y_2^{(h)}] \times [t_{12}^{(\ell)}, t_{12}^{(h)}] \times [t_{13}^{(\ell)}, t_{13}^{(h)}] \times [t_{23}^{(\ell)}, t_{23}^{(h)}] \tag{3}$$

and an arbitrary given point $Y_0 = I[g_0]$ with Iwasawa coordinates $(y_1, y_2, t_{12}, t_{13}, t_{23}) = (y_1^0, y_2^0, t_{12}^0, t_{13}^0, t_{23}^0)$ and representative $g_0 \in \mathrm{SL}_3(\mathbb{R})$. Clearly, our task is to prove a bound on the supremum distance

$$\sup\{\rho(Y_0, Y) \mid Y \in B\}.$$

At the end of the section we describe the numerical results we get in our particular case.

Using spherical coordinates (cf. [Ter2, p. 16]), an arbitrary geodesic from $Y_0 = g_0^t g_0$ in $\mathcal{P}_3^\circ$ can be written

$$t \mapsto Y = Y(t) = (\exp tA)[U g_0],$$

for some $A \in \mathfrak{a}$ and $U \in SO(3)$. We can here take A to belong to the space

$$\begin{aligned}\mathfrak{a}_1 &:= \Big\{ A = \begin{pmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{pmatrix} \mid a_1 + a_2 + a_3 = 0,\ a_1^2 + a_2^2 + a_3^2 = 1 \Big\} \\ &= \big\{ A \in \mathfrak{a} \mid \operatorname{tr} A^t A = 1 \big\}.\end{aligned}$$

Then the geodesic $t \mapsto Y(t)$ is parametrized by arc length. In other words the distance from Y_0 to $Y \in \mathcal{P}_3^\circ$ is given by

$$\rho = \rho(Y_0, Y) = ((\log \lambda_1)^2 + (\log \lambda_2)^2 + (\log \lambda_3)^2)^{1/2} \tag{4}$$

where λ_j are the three eigenvalues of $Y[g_0^{-1}]$. Using this we may now compute the Taylor expansion of ρ in terms of the Iwasawa coordinates for Y.

Let us write c_1, c_2 ($c_3 = 1$) for the usual symmetric functions associated with $\lambda_1, \lambda_2, \lambda_3$, i.e.

$$X^3 - c_1 X^2 + c_2 X - 1 = (X - \lambda_1)(X - \lambda_2)(X - \lambda_3) = \det(XI - Y[g_0^{-1}]).$$

We write s_j for the power sums $s_j = \lambda_1^j + \lambda_2^j + \lambda_3^j$ for $j = 0, 1, 2, 3, ...$, and we introduce the variables γ, δ by

$$3 + \gamma := s_1 = c_1 = \lambda_1 + \lambda_2 + \lambda_3; \qquad 3 + \delta := s_2 = \lambda_1^2 + \lambda_2^2 + \lambda_3^2. \tag{5}$$

Then since $c_2 = \frac{1}{2}(s_1^2 - s_2)$ the numbers $\lambda_1, \lambda_2, \lambda_3$ can be uniquely determined (up to permutation of the indices) from γ, δ, and so can the distance function ρ; and when Y is close to $I[g_0]$ then the pair (γ, δ) is close to $(0, 0)$ in $\mathbb{R}^2$. Using the relations $s_j = \text{trace } (Y[g_0^{-1}])^j$ for $j = 1, 2$ and the Iwasawa coordinates (cf. (27) in our paper), we see that γ and δ are explicit rational functions in $y_1^{\frac{1}{3}}, y_2^{\frac{1}{3}}, t_{12}, t_{13}, t_{23}$ of the form

$$\gamma = \frac{P_1(y_1^{\frac{1}{3}}, y_2^{\frac{1}{3}}, t_{12}, t_{13}, t_{23})}{y_1^{\frac{1}{3}} y_2^{\frac{2}{3}}}; \qquad \delta = \frac{P_2(y_1^{\frac{1}{3}}, y_2^{\frac{1}{3}}, t_{12}, t_{13}, t_{23})}{y_1^{\frac{2}{3}} y_2^{\frac{4}{3}}}, \tag{6}$$

where P_1, P_2 are explicit polynomials which we compute in [S-St, sphere.pari ("gmq3,dtq3")]. We change variables to

$$e_1 = y_1^{\frac{1}{3}} - (y_1^0)^{\frac{1}{3}},\ e_2 = y_2^{\frac{1}{3}} - (y_2^0)^{\frac{1}{3}},\ e_3 = t_{12} - t_{12}^0,\ e_4 = t_{13} - t_{13}^0,\ e_5 = t_{23} - t_{23}^0;$$

then $(e_1, e_2, e_3, e_4, e_5)$ is close to 0 in $\mathbb{R}^5$ whenever Y is close to $I[g_0]$, and the box B in (3) is given by

$$(e_1, ..., e_5) \in [E_1^{(\ell)}, E_1^{(h)}] \times [E_2^{(\ell)}, E_2^{(h)}] \times [E_3^{(\ell)}, E_3^{(h)}] \times [E_4^{(\ell)}, E_4^{(h)}] \times [E_5^{(\ell)}, E_5^{(h)}],$$

where

$$\begin{gathered} E_1^{(\ell)} = (y_1^{(\ell)})^{\frac{1}{3}} - (y_1^0)^{\frac{1}{3}},\ E_1^{(h)} = (y_1^{(h)})^{\frac{1}{3}} - (y_1^0)^{\frac{1}{3}},\ \ldots, \\ E_3^{(\ell)} = t_{12}^{(\ell)} - t_{12}^0,\ \ldots,\ E_5^{(h)} = t_{23}^{(h)} - t_{23}^0. \end{gathered}$$

We will actually work with the (possibly) larger box

$$B' := \big\{ (e_1, e_2, e_3, e_4, e_5) \mid |e_j| \leqq E_j,\ \forall j \big\},$$

where we have defined

$$E_j = \max\big(|E_j^{(\ell)}|, |E_j^{(h)}|\big), \qquad \text{for } j = 1,2,3,4,5.$$

We impose the condition that $E_j < (y_j^0)^{\frac{1}{3}}$ for $j = 1,2$. We then have the Taylor expansion, for $m, N_1 \in \mathbb{Z}^+$,

$$y_j^{-\frac{m}{3}} = (y_j^0)^{-\frac{m}{3}} + \sum_{n=1}^{N_1} \frac{(-1)^n m(m+1)...(m+n-1)(y_j^0)^{-\frac{m+n}{3}}}{n!} e_j^n + \varepsilon,$$

where the error ε is

$$|\varepsilon| \leqq \frac{m(m+1)...(m+N_1)}{(N_1+1)!}(y_j^0 - E_j)^{-\frac{m+N_1+1}{3}}|e_j|^{N_1+1}$$

Substituting these expansions (for $\langle j,m\rangle = \langle 1,1\rangle$, $\langle 2,2\rangle$, $\langle 1,2\rangle$, $\langle 2,4\rangle$) into (6), and using the bounds $|e_j| \leqq E_j$ for all terms of degree $> N_1$, we compute the Taylor expansion of degree N_1 for γ and δ,

$$\gamma = Q_1(e_1,e_2,e_3,e_4,e_5) + \varepsilon_1, \quad \delta = Q_2(e_1,e_2,e_3,e_4,e_5) + \varepsilon_2, \tag{7}$$

where Q_1, Q_2 are explicit polynomials of degree N_1, and we obtain explicit numerical upper bounds on $|\varepsilon_1|$, $|\varepsilon_2|$, cf. [S-St, sphere.pari ("gg, dd")]. We note that the constant and linear parts of Q_1 and Q_2 necessarily vanish, since $\gamma, \delta \geqq 0$ for all (e_1,e_2,e_3,e_4,e_5) (as follows from (5) together with $\lambda_1\lambda_2\lambda_3 = 1$ and the AG-inequality). Furthermore, using the bounds $|e_j| \leqq E_j$ in *all* terms, we obtain explicit numbers Γ, Δ such that

$$|\gamma| \leqq \Gamma, \qquad |\delta| \leqq \Delta, \tag{8}$$

for all $(e_1,e_2,e_3,e_4,e_5) \in B'$.

Note that the method actually gives explicit bounds on $\varepsilon_1, \varepsilon_2$ in (7) in the form of a sum of terms of the form $C \cdot \prod_j |e_j|^{n_j}$, with $\sum_j n_j = N_1 + 1$ and C an explicit constant. However, since we will eventually be mainly interested in the boundary of the Iwasawa box B, we have opted to work in [S-St, sphere.pari] with explicit *constants* bounding the errors, although these results are of course way off if we let $(e_1,e_2,e_3,e_4,e_5) \to 0$. Below we will use same symbol ε to denote the various (different!) errors obtained in our polynomial approximation formulae.

Recall the formula for ρ, cf. (4). The power expansion of $(\log x)^2$ in $|x-1| < 1$ is

$$(\log x)^2 = \sum_{n=1}^{\infty} \frac{2(-1)^n}{n}\left(\sum_{k=1}^{n-1}\frac{1}{k}\right)(x-1)^n.$$

Hence for each $N_2 \geqq 1$,

$$(\log x)^2 = \sum_{n=1}^{N_2} \frac{2(-1)^n}{n}\left(\sum_{k=1}^{n-1}\frac{1}{k}\right)(x-1)^n + \varepsilon,$$

where, using the fact that $\frac{2}{n}\left(\sum_{k=1}^{n-1}\frac{1}{k}\right)$ is decreasing for $n \geqq 1$,

$$\text{If } 0 < x \leqq 1: \qquad |\varepsilon| \leqq \sum_{n=N_2+1}^{\infty} \frac{2}{n}\left(\sum_{k=1}^{n-1}\frac{1}{k}\right)(1-x)^n \leqq \frac{2}{N_2+1}\left(\sum_{k=1}^{N_2}\frac{1}{k}\right)(1-x)^{N_2+1}x^{-1}$$

$$\text{If } 1 \leqq x < 2: \qquad |\varepsilon| \leqq \frac{2}{N_2+1}\left(\sum_{k=1}^{N_2}\frac{1}{k}\right)(x-1)^{N_2+1}$$

In particular, by (4), if $0 < C_3 < 1$ is a constant such that $|\lambda_j - 1| \leqq C_3$ for $j = 1, 2, 3$ (such a constant will be computed below, cf. (17)), we have

$$\rho^2 = \sum_{n=2}^{N_2} \frac{2(-1)^n}{n}\left(\sum_{k=1}^{n-1}\frac{1}{k}\right)\Big((\lambda_1-1)^n + (\lambda_2-1)^n + (\lambda_3-1)^n\Big) + \varepsilon, \tag{9}$$

where now

$$|\varepsilon| \leqq \frac{6}{N_2+1}\left(\sum_{k=1}^{N_2}\frac{1}{k}\right)C_3^{N_2+1}(1-C_3)^{-1}.$$

We define

$$\alpha_n = (\lambda_1-1)^n + (\lambda_2-1)^n + (\lambda_3-1)^n$$

and $\beta_1 = \alpha_1$, $\beta_2 = \sum_{j<k}(\lambda_j-1)(\lambda_k-1)$, $\beta_3 = \prod_j(\lambda_j-1)$, so that by Newton's formulae

$$\alpha_2 = \beta_1\alpha_1 - 2\beta_2, \qquad \alpha_3 = \beta_1\alpha_2 - \beta_2\alpha_1 + 3\beta_3,$$
$$\alpha_n = \beta_1\alpha_{n-1} - \beta_2\alpha_{n-2} + \beta_3\alpha_{n-3}, \qquad \text{for } n \geqq 4. \tag{10}$$

Using $X^3 - c_1X^2 + c_2X - 1 = (X-\lambda_1)(X-\lambda_2)(X-\lambda_3)$ and $c_1 = 3+\gamma$, $c_2 = \frac{1}{2}(s_1^2 - s_2) = 3 + 3\gamma + \gamma^2 - \delta/2$ we also find that

$$\beta_1 = \gamma, \qquad \beta_2 = \frac{\gamma^2}{2} + \gamma - \frac{\delta}{2}, \qquad \beta_3 = -\frac{\gamma^2}{2} - 2\gamma + \frac{\delta}{2}. \tag{11}$$

From (11) and (10) we see that each α_n is a polynomial in γ, δ, in which all terms $c\gamma^j\delta^k$ of degree $j + k < n/3$ vanish. In [S-St, sphere.pari ("lsum3")] we compute these polynomials for $1 \leqq n \leqq N_2$ and then substitute into (9), and in the resulting γ, δ-polynomial we use the bounds (8) on all terms of degree $> N_1$, thus obtaining

$$\rho^2 = P(\gamma, \delta) + \varepsilon, \tag{12}$$

where P is an explicit polynomial of degree N_1 and we have an explicit numerical bound on ε. Finally, we substitute (7) into (12), and use the bounds $|e_j| \leqq E_j$ on all terms containing any ε or being of degree $> N_1$, and obtain

$$\rho^2 = Q(e_1, e_2, e_3, e_4, e_5) + \varepsilon, \tag{13}$$

where Q is a polynomial of degree N_1 (with vanishing constant and linear terms), and we have an explicit numerical bound on the constant ε. This is the desired Taylor expansion formula. From this we obtain an explicit bound on ρ^2 valid throughout the box B' by simply using $|e_j| \leqq E_j$ in each term in (13). (For our cases, the resulting upper bound turns out to be off by less than 5% compared with the true upper bound on ρ in B'. If the box is larger the overshoot will generally be worse, but as long as the box is not *too* large it will still be easy to obtain a good upper bound on ρ, by making a more careful analysis of the second and third degree parts of $Q(e_1, e_2, e_3, e_4, e_5)$.)

To complete the argument we need to describe how to obtain an explicit upper bound C_3 on $\max_j |\lambda_j - 1|$ valid throughout the Iwasawa box B (this was used above). Wlog we may assume

$$|\lambda_1 - 1| \leqq |\lambda_2 - 1| \leqq |\lambda_3 - 1|. \tag{14}$$

Fix two positive constants C_1, C_2 satisfying

$$0 < C_1, C_2 < 1, \qquad C_2^2 < 2C_1 - C_1^2, \qquad C_1 + C_2 < \sqrt{2}. \tag{15}$$

We split the analysis into three cases:

Case 1: $|\lambda_1 - 1| > C_2|\lambda_3 - 1|$. In this case we have by (14),

$$|\beta_3| = \prod_{j=1}^{3} |\lambda_j - 1| > C_2^2|\lambda_3 - 1|^3.$$

Case 2: $|\lambda_1 - 1| \leqq C_2|\lambda_3 - 1|$ and $|(\lambda_3 - 1) \pm i(\lambda_2 - 1)| \geqq C_1|\lambda_3 - 1|$ (for both choices of the sign). In this case we have

$$|\alpha_2| = \left|\sum_{j=1}^{3} (\lambda_j - 1)^2\right| = \left|s_+ s_- + (\lambda_1 - 1)^2\right|,$$

where $s_\pm := (\lambda_3 - 1) \pm i(\lambda_2 - 1)$. Let $s_m = \min(|s_-|, |s_+|)$, $s_M = \max(|s_-|, |s_+|)$, and $D = \lambda_3 - 1$; then $s_+ + s_- = 2D$, and thus $s_m + s_M \geqq |s_+ + s_-| = 2|D|$. If $s_m \geqq |D|$ then $|s_+ s_-| = s_M s_m \geqq |D|^2$. Otherwise we have by our assumption $C_1|D| \leqq s_m < |D|$, and thus $|s_+ s_-| = s_M s_m \geqq (2|D| - s_m)s_m \geqq (2 - C_1)C_1|D|^2$, since the function $(2|D| - x)x$ is increasing in the interval $0 < x < |D|$. Hence

$$|\alpha_2| \geqq (2 - C_1)C_1|D|^2 - |\lambda_1 - 1|^2 \geqq ((2 - C_1)C_1 - C_2^2)|\lambda_3 - 1|^2.$$

(For note $(2 - C_1)C_1 < 1$.)

Case 3: Neither Case 1 or Case 2 hold. Then $|\lambda_1 - 1| \leqq C_2|\lambda_3 - 1|$, and there is some $\varepsilon \in \{1, -1\}$ such that $|(\lambda_3 - 1) + \varepsilon i(\lambda_2 - 1)| < C_1|\lambda_3 - 1|$. We then have

$$|\gamma| = \left|\sum_{j=1}^{3} (\lambda_j - 1)\right| \geqq \left|(\lambda_3 - 1) + \varepsilon i(\lambda_3 - 1) - \varepsilon i\big((\lambda_3 - 1) + \varepsilon i(\lambda_2 - 1)\big)\right| - |\lambda_1 - 1|$$

$$\geqq |1 + \varepsilon i| \cdot |\lambda_3 - 1| - C_1|\lambda_3 - 1| - C_2|\lambda_3 - 1| = \big(\sqrt{2} - C_1 - C_2\big) \cdot |\lambda_3 - 1|.$$

In view of our analysis in the three cases, we obtain in general, using (14) and (15),

$$\max_j |\lambda_j - 1| \leqq \max\left(\frac{|\beta_3|^{1/3}}{C_2^{2/3}}, \sqrt{\frac{|\alpha_2|}{2C_1 - C_1^2 - C_2^2}}, \frac{|\gamma|}{\sqrt{2} - C_1 - C_2} \right).$$

Using here $\beta_3 = -\frac{\gamma^2}{2} - 2\gamma + \frac{\delta}{2}$ and $\alpha_2 = \delta - 2\gamma$ (cf. (10), (11)), substituting (7) into these formulae, and finally using the bounds $|e_j| \leqq E_j$ in all terms, we compute explicit numbers $B_3, A_2 > 0$ such that

$$(16) \qquad |\beta_3| \leqq B_3, \qquad |\alpha_2| \leqq A_2, \qquad \forall (e_1, e_2, e_3, e_4, e_5) \in B'.$$

(Also recall $|\gamma| \leqq \Gamma$.) Using this (and playing some with the choice of the numbers C_1, C_2 satisfying (15), so as not to be unnecessarily wasteful), we finally obtain an explicit number C_3 such that

$$(17) \qquad \max_j |\lambda_j - 1| \leqq C_3, \qquad \forall (e_1, e_2, e_3, e_4, e_5) \in B'.$$

To conclude this section, we show the explicit numerical data obtained in our case of main interest, the fcc-point $Y_3 = 2^{1/3}\begin{pmatrix} 1 & 1/2 & 1/2 \\ 1/2 & 1 & 1/2 \\ 1/2 & 1/2 & 1 \end{pmatrix}$ with representative $g_0 = 2^{-1/3}\begin{pmatrix} 1 & 0 & 1 \\ -1 & -1 & 0 \\ 0 & 1 & 1 \end{pmatrix}$, and the box

$$B_{fcc} := [1.29, 1.34] \times [1.1, 1.15] \times [0.45, 0.5] \times [\tfrac{5}{11}, \tfrac{6}{11}] \times [0.3, 0.4].$$

We worked with cutoffs $N_1 = 6$, $N_2 = 20$ in the Taylor expansions, and then obtained (7) with

$$|\varepsilon_1| \leqq 8.5 \cdot 10^{-12}, \qquad |\varepsilon_2| \leqq 4.0 \cdot 10^{-8};$$

and in (8) we found,

$$|\gamma| \leqq \Gamma < 0.016, \qquad |\delta| \leqq \Delta < 0.063,$$

and in (16):

$$|\beta_3| \leqq B_3 < 0.0011, \qquad |\alpha_2| \leqq A_2 < 0.033.$$

Using $C_1 = 0.9$ and $C_2 = 0.4$ we then get

$$\max_j |\lambda_j - 1| \leqq C_3 < 0.2,$$

and we finally obtain in the Taylor formula for the point ρ^2, (13):

$$\rho^2 = Q(e_1, e_2, e_3, e_4, e_5) + \varepsilon, \qquad \text{with } |\varepsilon| \leqq 2.4 \cdot 10^{-7},$$

where Q is an explicit polynomial of degree $N_1 = 6$, with vanishing constant and linear parts, and with the quadratic part equal to:

$$3^{\frac{5}{3}}2^{-\frac{1}{3}}e_1^2 + 2^{\frac{4}{3}}3^{\frac{2}{3}}e_1e_2 + 8 \cdot 3^{-\frac{1}{3}}e_2^2 + 3e_3^2 - 2e_3e_4 + 3e_4^2 + \frac{9}{4}e_5^2.$$

Using the bounds $|e_j| \leqq E_j$ throughout we finally obtain:

$$\rho \leqq 0.17614 < 0.18.$$

(And on the other hand, one easily checks that for $(y_1, y_2, t_{12}, t_{13}, t_{23}) = (1.29, 1.1, 0.45, \frac{6}{11}, 0.4) \in B_{fcc}$ we have $\rho = 0.17277...$; hence the bound is not too bad.)

To sum up, we have proved that B_{fcc} is contained in the ball $B(g_0, 0.18)$ of radius 0.18 about the point $I[g_0]$, i.e.

$$B_{fcc} \subset B(g_0, 0.18), \qquad \text{where}$$
$$B(g_0, t_0) = \big\{ (\exp tA)[Ug_0] \mid 0 \leqq t \leqq t_0,\ A \in \mathfrak{a}_1,\ U \in SO(3) \big\} \subset \mathcal{P}_3^\circ.$$

5. LOCAL.PARI

This PARI program is used to prove relation (33) in our paper, i.e.

$$\mathfrak{F}(t\mathbf{x}) > \mathfrak{F}(0) \qquad \text{for all } \mathbf{x} \in S^4,\ 0 < t \leqq t_0 = 0.18.$$

Recall that we have defined

$$\mathfrak{F}(\mathbf{x}) := F_0\Big(\exp\big(x_1\mathbf{b}_1 + ... + x_5\mathbf{b}_5\big)[g_0]\Big) \qquad \text{for } \mathbf{x} = (x_1, ..., x_5) \in \mathbb{R}^5,$$

where $g_0 = 2^{-1/3}\begin{pmatrix} 1 & 0 & 1 \\ -1 & -1 & 0 \\ 0 & 1 & 1 \end{pmatrix}$ is our representative for the fcc-point.

Important parts of the algorithm for proving relation (33) has been described in our paper, and it will here suffice to add some more details on how to prove the partial result (37), viz. (with $t_0 = 0.18$)

$$(18) \quad q_2(\mathbf{x})t_0^2 + \min(q_3(\mathbf{x}), 0)t_0^3 + \min(q_4(\mathbf{x}), 0)t_0^4 \geqq 0.0002, \qquad \forall \mathbf{x} \in S^4.$$

We will use the fact that each q_d is $\mathrm{Aut}(D_3)$-invariant. $\mathrm{Aut}(D_3)$ is known to consist of all 48 coordinate permutations composed with sign changes in $\mathbb{R}^3$, i.e. $\mathrm{Aut}(D_3)$ is generated by the elements

$$\sigma_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

(Since $D_3 = \{2^{-\frac{1}{3}}(x_1, x_2, x_3) \mid \text{all } x_i \in \mathbb{Z},\ x_1 + x_2 + x_3 + x_4 \equiv 0 \pmod 2\}$, it is obvious that $\sigma_1, \sigma_2, \sigma_3$ belong to $\mathrm{Aut}(D_3)$, and this is all we need; i.e. we will never need the fact that $\mathrm{Aut}(D_3)$ contains *no other* than the above mentioned 48 elements.)

Recall that the action of $\sigma \in \mathrm{Aut}(D_3)$ on S^4 comes from the imbedding $S^4 \ni \mathbf{x} = (x_1, ..., x_5) \hookrightarrow x_1\mathbf{b}_1 + ... + x_5\mathbf{b}_5 \in \mathfrak{p}$ and the Ad-action of σ on $\mathfrak{p}$, i.e. $Y \mapsto \sigma^{-1} Y \sigma$. Now one checks by a direct computation, using our basis $\mathbf{b}1, ..., \mathbf{b}_5$ from p.12 (bottom) in our paper, that

$$\begin{aligned}
Y \mapsto \sigma_1^{-1} Y \sigma_1 : &\qquad \mathbf{b}_3 \mapsto \mathbf{b}_3, \quad \mathbf{b}_4 \mapsto \mathbf{b}_5, \quad \mathbf{b}_5 \mapsto \mathbf{b}_4. \\
Y \mapsto \sigma_2^{-1} Y \sigma_2 : &\qquad \mathbf{b}_3 \mapsto \mathbf{b}_4, \quad \mathbf{b}_4 \mapsto \mathbf{b}_3, \quad \mathbf{b}_5 \mapsto \mathbf{b}_5. \\
Y \mapsto \sigma_3^{-1} Y \sigma_3 : &\qquad \mathbf{b}_3 \mapsto -\mathbf{b}_3, \quad \mathbf{b}_4 \mapsto -\mathbf{b}_4, \quad \mathbf{b}_5 \mapsto \mathbf{b}_5.
\end{aligned}$$

Note also that the two subspaces $\mathbb{R}\mathbf{b}_1 + \mathbb{R}\mathbf{b}_2$ and $\mathbb{R}\mathbf{b}_3 + \mathbb{R}\mathbf{b}_4 + \mathbb{R}\mathbf{b}_5$ are both preserved by the action. It follows that $\mathrm{Aut}(D_3)$ contains all permutations and *even* sign changes of $\{\mathbf{b}_3, \mathbf{b}_4, \mathbf{b}_5\}$, viz., for every permutation τ of the set $\{3, 4, 5\}$ and every choice of $\langle \varepsilon_3, \varepsilon_4, \varepsilon_5 \rangle \in \{-1, 1\}^3$ with $\varepsilon_3 \varepsilon_4 \varepsilon_5 = 1$ there exists some $\sigma \in \mathrm{Aut}(D_3)$ such that $\sigma(x_1, x_2, x_3, x_4, x_5) = (*, *, \varepsilon_3 x_{\tau(3)}, \varepsilon_4 x_{\tau(4)}, \varepsilon_5 x_{\tau(5)}) \in S^4$ for all $\mathbf{x} = (x_1, ..., x_5) \in S^4$ (and this $\sigma \in \mathrm{Aut}(D_3)$ is actually unique up to sign change, $\sigma \longleftrightarrow -\sigma$).

Hence for each point $\mathbf{x} = (x_1, ..., x_5) \in S^4$ there is some $\sigma \in \mathrm{Aut}(D_3)$ such that $\sigma(x_1, ..., x_5)$ belongs to the set

(19)
$$\mathcal{F} = \mathcal{F}_1 \cup (-\mathcal{F}_1), \qquad \text{where } \mathcal{F}_1 = \Big\{ \mathbf{x} = (x_1, ..., x_5) \in S^4 \mid 0 \leqq x_3 \leqq x_4 \leqq x_5 \Big\}.$$

(This set $\mathcal{F}$ is in fact a fundamental domain for $S^4 / \mathrm{Aut}(D_3)$.) Hence, since each q_d is $\mathrm{Aut}(D_3)$-invariant we may restrict attention to points $\mathbf{x} \in \mathcal{F}$ when proving (18).

When it comes to the actual covering of $\mathcal{F}$ (or all of S^4) with boxes, it turns out that a lot of efficiency is gained by not making a too naive choice of boxes; for example the approach to simply divide $[-1, 1]^5$ into smaller congruent cubes and select for investigation those cubes which have non-empty intersection with S^4 was found to be quite wasteful (in terms of the bound obtained in (18) versus the number of selected boxes). An obvious improvement would be to try to shrink each selected box as much as is possible without loosing any points in its intersection with S^4; however, this task seems to be slightly complicated as there are quite a lot of possibilities for the "shape" of the intersection of a box and a sphere in several dimensions.

The precise method we used was as follows. We fix a positive integer N. For each $4-$dimensional box

$$B_{\mathbf{k}}^{(4)} = \left[\frac{k_1}{N}, \frac{k_1 + 1}{N} \right] \times \left[\frac{k_2}{N}, \frac{k_2 + 1}{N} \right] \times \left[\frac{k_3}{N}, \frac{k_3 + 1}{N} \right] \times \left[\frac{k_4}{N}, \frac{k_4 + 1}{N} \right] \subset \mathbb{R}^4$$

with $\mathbf{k} = (k_1, k_2, k_3, k_4) \in \{-N, -N+1, ..., N-1\}^4$, we set

$$\begin{aligned}
s_{\min} &= \inf\{ w_1^2 + w_2^2 + w_3^2 + w_4^2 \mid (w_1, w_2, w_3, w_4) \in B_{\mathbf{k}}^{(4)} \}, \\
s_{\max} &= \sup\{ w_1^2 + w_2^2 + w_3^2 + w_4^2 \mid (w_1, w_2, w_3, w_4) \in B_{\mathbf{k}}^{(4)} \}, \\
t &= \max_j \inf\{ w_j^2 \mid (w_1, w_2, w_3, w_4) \in B_{\mathbf{k}}^{(4)} \};
\end{aligned}$$

these numbers are of course simple functions of $\mathbf{k}$. We dispose of $B^{(4)}_{\mathbf{k}}$ if $s_{\min} + t > 1$; otherwise, if $s_{\min} + t \leqq 1$, we set

$$B_{\mathbf{k}} := B^{(4)}_{\mathbf{k}} \times \left[\sqrt{\max(t, 1 - s_{\max})}, \sqrt{1 - s_{\min}}\right] \subset \mathbb{R}^5, \tag{20}$$

We then claim that

(21) Every point $(x_1, ..., x_5) \in S^4$ with $|x_1|, |x_2|, |x_3|, |x_4| \leqq x_5$ lies in some box $B_{\mathbf{k}}$ as above.

Indeed, given such a point $(x_1, ..., x_5) \in S^4$, there is some $\mathbf{k} \in \{-N, -N + 1, ..., N - 1\}^4$ such that $(x_1, ..., x_4) \in B^{(4)}_{\mathbf{k}}$. For this $\mathbf{k}$ we have $s_{\min} \leqq x_1^2 + ... + x_4^2 \leqq s_{\max}$, i.e. $s_{\min} \leqq 1 - x_5^2 \leqq s_{\max}$, and $t \leqq \max(x_1^2, x_2^2, x_3^2, x_4^2)$. Hence $s_{\min} + t \leqq 1 - x_5^2 + \max(x_1^2, x_2^2, x_3^2, x_4^2) \leqq 1$, by our assumption on $(x_1, ..., x_5)$, so that the box $B^{(4)}_{\mathbf{k}}$ is not discarded. Our inequalities also show $\max(t, 1 - s_{\max}) \leqq x_5^2 \leqq 1 - s_{\min}$ so that $(x_1, ..., x_5) \in B_{\mathbf{k}}$, and (21) is proved.

Next let $d : \mathbb{R}^5 \to \mathbb{R}^5$ be the map $d(x_1, x_2, x_3, x_4, x_5) = (x_1, x_2, x_3, x_4, -x_5)$, and let $c_0, c_1, ..., c_4$ be the cyclic coordinate permutation maps $\mathbb{R}^5 \to \mathbb{R}^5$;

$$c_j(x_1, x_2, ..., x_5) = (x_{1+j}, x_{2+j}, ..., x_{5+j}),$$

where we define $x_6 := x_1$, $x_7 := x_2$, $x_8 := x_3$, $x_9 := x_4$. It then follows from (21) that

(22) Every point $(x_1, ..., x_5) \in S^4$ lies in some box $c_j(B_{\mathbf{k}})$ or $c_j(d(B_{\mathbf{k}}))$, with $\mathbf{k}$ as above and $j \in \{0, 1, 2, 3, 4\}$.

It is also clear from the construction that if N is not too small then the portion of S^4 which is covered by more than one such box is fairly small, i.e. the covering is not wasteful.

We obtain a box covering of our domain $\mathcal{F} \subset S^4$ (recall (19)) by discarding those boxes among $c_j(B_{\mathbf{k}})$, $c_j(d(B_{\mathbf{k}}))$ which have empty intersection with $\{(x_1, ..., x_5) \in \mathbb{R}^5 \mid 0 \leqq x_3 \leqq x_4 \leqq x_5\}$, and for each remaining box B we select both the boxes B and $-B$. It is now sufficient to show that (18) holds in each selected box B. We use straightforward interval arithmetic to obtain lower bounds on $q_3(\mathbf{x})$ and $q_4(\mathbf{x})$ for $\mathbf{x} \in B$. There is an advantage in treating the pairs B and $-B$ simultaneously, for the interval arithmetic operations also provides an upper bound for $q_3(\mathbf{x})$ on B, and the negative of this will be a lower bound for $q_3(\mathbf{x})$ on $-B$; and for $q_4(\mathbf{x})$ the lower bound obtained on B is also a lower bound on $-B$ (the same goes for $q_2(\mathbf{x})$).

For $q_2(\mathbf{x})$ we can do (much) better than using interval arithmetic in the box B, since we actually only need a lower bound for $\mathbf{x}$ in $B \cap S^4$, and $q_2(\mathbf{x})$ has the following special form (cf. our paper);

$$q_2(\mathbf{x}) = c_1(x_1^2 + x_2^2) + c_2(x_3^2 + x_4^2 + x_5^2) \qquad \text{with } \begin{cases} c_1 = 0.0236110815... \\ c_2 = 0.1509259456... \end{cases}$$

We claim

$$\inf_{\mathbf{x} \in B \cap S^4} q_2(\mathbf{x}) = \max((c_1 - c_2)s_1 + c_2, (c_2 - c_1)s_2 + c_1), \tag{23}$$

where

$$s_1 = \sup\{x_1^2 \mid \mathbf{x} \in B\} + \sup\{x_2^2 \mid \mathbf{x} \in B\},$$
$$s_2 = \inf\{x_3^2 \mid \mathbf{x} \in B\} + \inf\{x_4^2 \mid \mathbf{x} \in B\} + \inf\{x_5^2 \mid \mathbf{x} \in B\}.$$

Indeed, note that $0 < c_1 < c_2$ and that for $\mathbf{x} \in S^4$ we have

$$q_2(\mathbf{x}) = (c_1 - c_2)(x_1^2 + x_2^2) + c_2 = (c_2 - c_1)(x_3^2 + x_4^2 + x_5^2) + c_1.$$

Hence $\inf_{\mathbf{x}\in B\cap S^4} q_2(\mathbf{x}) \geqq (c_1 - c_2)s_1 + c_2$ follows from $x_1^2 + x_2^2 \leqq s_1$ in B, and $\inf_{\mathbf{x}\in B\cap S^4} q_2(\mathbf{x}) \geqq (c_2 - c_1)s_2 + c_1$ follows from $x_3^2 + x_4^2 + x_5^2 \geqq s_2$ in B. We also see that to prove the opposite inequality[1], $\inf_{\mathbf{x}\in B\cap S^4} q_2(\mathbf{x}) \leqq \max(c_1 s_1 + c_2(1 - s_1), c_1(1 - s_2) + c_2 s_2)$, it suffices to show that there is some point $\mathbf{x} \in B \cap S^4$ such that either $x_1^2 + x_2^2 = s_1$ or $x_3^2 + x_4^2 + x_5^2 = s_2$ holds. For each $j = 1, ..., 5$ we take x_j' and x_j'' such that $B \cap \{x_j = x_j'\} \neq \emptyset$, $B \cap \{x_j = x_j''\} \neq \emptyset$ and ${x_j'}^2 = \inf\{x_j^2 \mid \mathbf{x} \in B\}$, ${x_j''}^2 = \sup\{x_j^2 \mid \mathbf{x} \in B\}$. The intersection $B \cap S^4$ is easily seen to be nonempty by construction (for take $x_5 = \sqrt{1 - s_{\min}}$ in (20) above); hence ${x_1'}^2 + {x_2'}^2 + {x_3'}^2 + {x_4'}^2 + {x_5'}^2 \leqq 1$ and ${x_1''}^2 + {x_2''}^2 + {x_3''}^2 + {x_4''}^2 + {x_5''}^2 \geqq 1$. Furthermore, the union of the 3- and 2-dimensional boxes $B_1 = \{\mathbf{x} \in B \mid x_1 = x_1'',\ x_2 = x_2''\}$ and $B_2 = \{\mathbf{x} \in B \mid x_3 = x_3',\ x_4 = x_4',\ x_5 = x_5'\}$ is connected; in particular there is a curve from $(x_1', ..., x_5')$ to $(x_1'', ..., x_5'')$ lying entirely inside $B_1 \cup B_2$. This curve must intersect S^4 in some point $\mathbf{x}$, and by construction we have $\mathbf{x} \in B \cap S^4$, and either $x_1^2 + x_2^2 = s_1$ or $x_3^2 + x_4^2 + x_5^2 = s_2$. Hence (23) is proved.

Note that s_1, s_2 are easy to compute for a given box B; hence the right hand side of (23) is easily evaluated, and this gives us a sharp lower bound on $q_2(\mathbf{x})$ in the intersection $B \cap S^4$. Combining this with our lower bounds on $\min(q_3(\mathbf{x}), 0)$ and $\min(q_4(\mathbf{x}), 0)$ over all of B, obtained by interval arithmetic, we obtain a lower bound on the left hand side of (18), valid in $B \cap S^4$. We then take the infimum over all boxes B selected in the way described above, to obtain a lower bound valid throughout S^4. To obtain 0.0002 as in (18) (and even slightly better), we used $N = 8$; this leads to 7252 pairs of boxes $B, -B$ being analysed with (23) and interval arithmetic.

References

[S-St] P. Sarnak, A. Strömbergsson, www.math.uu.se/∼astrombe/height/height.html

[Ter2] A. Terras, *Harmonic Analysis on Symmetric Spaces and Applications, II*, Springer-Verlag, 1988.

[1]Note that we only need the “easy part”, $\inf_{\mathbf{x}\in B\cap S^4} q_2(\mathbf{x}) \geqq \max((c_1 - c_2)s_1 + c_2, (c_2 - c_1)s_2 + c_1)$, to prove the correctness of our computer verification of (18); however, the opposite inequality is of interest as it shows that we cannot improve our treatment of $q_2(\mathbf{x})$.