A Minimum Property for Cuboidal Lattice Sums

Shaun COOPER [a] and Peter SCHWERDTFEGER [b]

a) *School of Mathematical and Computational Sciences, Massey University Albany,*
   Private Bag 102904, North Shore Mail Centre, Auckland 0745, New Zealand
   E-mail: *s.cooper@massey.ac.nz*

b) *Centre for Theoretical Chemistry and Physics, The New Zealand Institute for Advanced Study*
   (NZIAS), Massey University Albany, Private Bag 102904, North Shore Mail Centre,
   Auckland 0745, New Zealand
   E-mail: *peter.schwerdtfeger@gmail.com*

Abstract. We analyse a family of lattices considered by Conway and Sloane and show that the corresponding Epstein zeta function attains a local minimum for the body-centred cubic lattice.

Key words: body-centred cubic; face-centred cubic; Epstein zeta function; lattice sum

2020 Mathematics Subject Classification: 11E45; 11H31

To Stephen Milne on the occasion
of his 75th birthday

1 Introduction

A lattice sum is an expression of the form

$$\sum_{\mathbf{x}} F(\mathbf{x}),$$

where the vector $\mathbf{x}$ ranges over a d dimensional lattice. In the case when

$$F(\mathbf{x}) = \begin{cases} \dfrac{1}{|\mathbf{x}|^s} & \text{if } \mathbf{x} \neq \mathbf{0}, \\ 0 & \text{if } \mathbf{x} = \mathbf{0}, \end{cases}$$

the lattice sum is a special case of Epstein's zeta function and has applications in number theory and theoretical chemistry, e.g., see [2] for comprehensive information or [3] for some recent applications in chemistry.

Rankin [15] showed that among two-dimensional lattice sums with discriminant 1, the Epstein zeta function is minimised by the hexagonal lattice. Further results on minimising lattice sums have been given in [1, 4, 7, 8, 9, 11, 13, 16].

In this work, we consider a one-parameter continuous family of lattices in three dimensions that includes the face-centred and body-centred cubic lattices, and show that the Epstein zeta function for the family has a local minimum that is attained by the body-centred cubic lattice.

2   Cuboidal lattices

Following Conway and Sloane [5], assume u and v are positive real numbers, let $A = u^2/v^2$, and consider the cuboidal lattice $\Lambda(u, v)$ generated by

$$\mathbf{r}_1 = (u, v, 0), \qquad \mathbf{r}_2(u, 0, v) \qquad \text{and} \qquad \mathbf{r}_3 = (0, v, v), \tag{2.1}$$

that is,

$$\Lambda(u, v) = \{c_1\mathbf{r}_1 + c_2\mathbf{r}_2 + c_3\mathbf{r}_3 \mid c_1, c_2, c_3 \in \mathbb{Z}\}. \tag{2.2}$$

The most important cases, ordered by decreasing value of A, are

(1) $A = 1$: the face-centred cubic (fcc) lattice,

(2) $A = 1/\sqrt{2}$: the mean centred-cuboidal (mcc) lattice,

(3) $A = 1/2$: the body-centred cubic (bcc) lattice, and

(4) $A = 1/3$: the axial centred-cuboidal (acc) lattice.

Thus, $\Lambda(u, v)$ is a continuous family that includes the fcc and bcc lattices which are well known to chemistry students. The other two lattices are less well known. The mcc lattice is the unique densest three-dimensional isodual lattice [5, Theorem 2], while the acc lattice is the least dense lattice with kissing number[1] 10, e.g., see [5, 10, 14].

In the remainder of this section, we do some standard calculations to find the minimum norm and packing density for the lattice $\Lambda(u, v)$, and use them to define the normalised lattice and associated Epstein zeta function. If

$$\mathbf{x} = c_1\mathbf{r}_1 + c_2\mathbf{r}_2 + c_3\mathbf{r}_3 \in \Lambda(u, v),$$

then

$$\|\mathbf{x}\|^2 = (c_1\mathbf{r}_1 + c_2\mathbf{r}_2 + c_3\mathbf{r}_3) \cdot (c_1\mathbf{r}_1 + c_2\mathbf{r}_2 + c_3\mathbf{r}_3) = (c_1, c_2, c_3)G(c_1, c_2, c_3)^{\mathsf{T}},$$

where G is the Gram matrix whose (i, j) entry is the dot product $\mathbf{r}_i \cdot \mathbf{r}_j$, that is,

$$G = \begin{bmatrix} u^2 + v^2 & u^2 & v^2 \\ u^2 & u^2 + v^2 & v^2 \\ v^2 & v^2 & 2v^2 \end{bmatrix} = v^2 \begin{bmatrix} A + 1 & A & 1 \\ A & A + 1 & 1 \\ 1 & 1 & 2 \end{bmatrix}. \tag{2.3}$$

The minimum norm of a lattice Λ is [6, p. 42]

$$\mu = \min\{\|\mathbf{x} - \mathbf{y}\|^2 \mid \mathbf{x}, \mathbf{y} \in \Lambda, \ \mathbf{x} \neq \mathbf{y}\} = \min\{\|\mathbf{x}\|^2 \mid \mathbf{x} \in \Lambda, \ \mathbf{x} \neq \mathbf{0}\}.$$

For the lattice $\Lambda(u, v)$, we have

$$\begin{aligned}
\mu &= \min\{\|\mathbf{x}\|^2 \mid \mathbf{x} \in \Lambda(u, v), \ \mathbf{x} \neq \mathbf{0}\} \\
&= \min\{(c_1, c_2, c_3)G(c_1, c_2, c_3)^{\mathsf{T}} \mid c_1, c_2, c_3 \in \mathbb{Z}, \ (c_1, c_2, c_3) \neq (0, 0, 0)\} \\
&= \min_{\substack{(c_1, c_2, c_3) \in \mathbb{Z}^3 \\ (c_1, c_2, c_3) \neq \mathbf{0}}} v^2\big((A + 1)c_1^2 + (A + 1)c_2^2 + 2c_3^2 + 2Ac_1c_2 + 2c_1c_3 + 2c_2c_3\big) \\
&= \min_{\substack{(c_1, c_2, c_3) \in \mathbb{Z}^3 \\ (c_1, c_2, c_3) \neq \mathbf{0}}} v^2\big(A(c_1 + c_2)^2 + (c_2 + c_3)^2 + (c_1 + c_3)^2\big)
\end{aligned}$$

---

[1] See [6, p. 21].

and it follows that

$$\mu = \begin{cases} 4Av^2 & \text{if } 0 < A < 1/3, \\ (A+1)v^2 & \text{if } 1/3 \le A \le 1, \\ 2v^2 & \text{if } A > 1. \end{cases} \tag{2.4}$$

The packing radius of a lattice is defined by $p = \frac{1}{2}\sqrt{\mu}$ and the packing density is [6, pp. 1–7]

$$\Delta = \frac{\text{volume of one sphere of radius } p}{(\det G)^{1/2}}.$$

From (2.3), we have $\det G = 4Av^6$, hence the packing density of $\Lambda(u,v)$ is given by

$$\Delta = \begin{cases} \dfrac{2\pi A}{3} & \text{if } 0 < A < 1/3, \\ \dfrac{\pi}{12}\sqrt{\dfrac{(A+1)^3}{A}} & \text{if } 1/3 \le A \le 1, \\ \dfrac{\pi}{6}\sqrt{\dfrac{2}{A}} & \text{if } A > 1. \end{cases} \tag{2.5}$$

The maximum packing density for this family of lattices is $\frac{\pi\sqrt{2}}{6} \approx 74\%$ for the fcc lattice at $A = 1$. This was conjectured by Kepler and proved by Hales [12] to be maximal among all packings in three dimensions. Since

$$\frac{\mathrm{d}}{\mathrm{d}A}\left(\frac{\pi}{12}\sqrt{\frac{(A+1)^3}{A}}\right) = \frac{\pi}{24}\left(\frac{A+1}{A^3}\right)^{1/2}(2A-1),$$

the packing density has a local minimum at $A = 1/2$, corresponding to bcc. Some special values of the density, together with the kissing numbers, are given in Table 1. A graph of the packing density as a function of A is shown in Figure 1.

Table 1. Packing density and kissing number as functions of A. Here (a,b) means $\{A \mid a < A < b\}$.

A	$(0,\frac{1}{3})$	$\frac{1}{3}$	$(\frac{1}{3},\frac{1}{2})$	$\frac{1}{2}$	$(\frac{1}{2},\frac{1}{\sqrt{2}})$	$\frac{1}{\sqrt{2}}$	$(\frac{1}{\sqrt{2}},1)$	1	$(1,\infty)$
name		acc		bcc		mcc		fcc	
density	$\frac{2\pi A}{3}$	$\frac{2\pi}{9}$	$\frac{\pi}{12}\sqrt{\frac{(A+1)^3}{A}}$	$\frac{\pi\sqrt{3}}{8}$	$\frac{\pi}{12}\sqrt{\frac{(A+1)^3}{A}}$			$\frac{\pi\sqrt{2}}{6}$	$\frac{\pi}{6}\sqrt{\frac{2}{A}}$
kiss. no.	2	10	8					12	4

In order to study physical properties of the lattice, we normalise so that the minimum distance is $\mu = 1$. Accordingly, from (2.4) let

$$v = \begin{cases} \dfrac{1}{2\sqrt{A}} & \text{if } 0 < A < 1/3, \\ \dfrac{1}{\sqrt{A+1}} & \text{if } 1/3 \le A \le 1, \\ \dfrac{1}{\sqrt{2}} & \text{if } A > 1. \end{cases} \tag{2.6}$$

The cases $0 < A < 1/3$ and $A > 1$ are of less interest because the normalised lattice degenerates to a lattice congruent to $\mathbb{Z}$ or $\mathbb{Z}^2$ in the limits $A \to 0$ and $A \to \infty$, respectively. From now
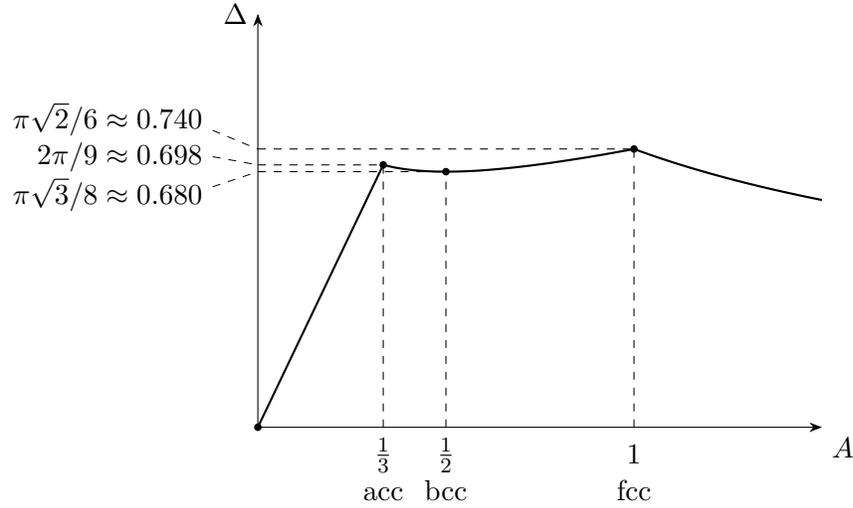
Figure 1. Graph of Δ as a function of A given by (2.5).

on, we assume $1/3 \leq A \leq 1$. From (2.3) and (2.6), the Gram matrix for the normalised lattice is

$$G = \frac{1}{A+1} \begin{bmatrix} A+1 & A & 1 \\ A & A+1 & 1 \\ 1 & 1 & 2 \end{bmatrix}.$$

The associated quadratic form is

$$\begin{aligned}
g(A; i, j, k) &= (i, j, k)G(i, j, k)^{\mathsf{T}} \\
&= \frac{1}{A+1}\big((A+1)i^2 + (A+1)j^2 + 2k^2 + 2Aij + 2ik + 2jk\big) \\
&= \frac{1}{A+1}\big(A(i+j)^2 + (j+k)^2 + (i+k)^2\big)
\end{aligned}$$

and the corresponding Epstein zeta function is

$$L(A; s) = {\sum_{i,j,k\in\mathbb{Z}}}' \left(\frac{1}{g(A; i, j, k)}\right)^s = {\sum_{i,j,k\in\mathbb{Z}}}' \left(\frac{A+1}{A(i+j)^2 + (j+k)^2 + (i+k)^2}\right)^s, \qquad (2.7)$$

where the primes indicate that the term corresponding to $(i, j, k) = (0, 0, 0)$ is omitted from the summations. The series (2.7) converges for $s > 3/2$ and we further assume $1/3 \leq A \leq 1$.

3 A minimum property

Numerical calculations in [3] suggest that for a fixed value of $s > 3/2$, the Epstein zeta function (2.7) appears to have a local minimum value at $A = 1/2$. This is confirmed by the following result.

Theorem 1. *Suppose $s > 3/2$. The Epstein zeta function $L(A; s)$ defined by (2.7) satisfies*

$$\left.\frac{\partial}{\partial A}L(A; s)\right|_{A=1/2} = 0 \qquad and \qquad \left.\frac{\partial^2}{\partial A^2}L(A; s)\right|_{A=1/2} > 0.$$

Proof. By definition, we have

$$L(A; s) = {\sum_{I,J,K\in\mathbb{Z}}}' \left(\frac{1}{g(A; I, J, K)}\right)^s,$$

where

$$g(A; I, J, K) = \frac{1}{A+1}\left(A(I + J)^2 + (J + K)^2 + (I + K)^2\right).$$

Now make the change of variables $(I, J, K) = (i - j, -k, j)$. This is a bijection since $(i, j, k) = (I + K, K, -J)$, and it follows that

$$L(A; s) = {\sum_{i,j,k\in\mathbb{Z}}}' \left(\frac{1}{g(A; i - j, -k, j)}\right)^s$$

$$= {\sum_{i,j,k\in\mathbb{Z}}}' \frac{1}{\left(i^2 + j^2 + k^2 - 2(ij + ik)\left(\frac{A}{A+1}\right) + 2jk\left(\frac{A-1}{A+1}\right)\right)^s}.$$

By direct calculation, the derivative is given by

$$\frac{\partial}{\partial A}L(A; s) = \frac{2s}{(A+1)^2}{\sum_{i,j,k\in\mathbb{Z}}}' \frac{ij + ik - 2jk}{\left(i^2 + j^2 + k^2 - 2(ij + ik)\left(\frac{A}{A+1}\right) + 2jk\left(\frac{A-1}{A+1}\right)\right)^{s+1}}. \tag{3.1}$$

Setting $A = 1/2$ gives

$$\left.\frac{\partial}{\partial A}L(A; s)\right|_{A=1/2} = \frac{8s}{9}{\sum_{i,j,k\in\mathbb{Z}}}' \frac{ij + ik - 2jk}{\left(i^2 + j^2 + k^2 - \frac{2}{3}(ij + ik + jk)\right)^{s+1}}. \tag{3.2}$$

Switching i and j gives

$$\left.\frac{\partial}{\partial A}L(A; s)\right|_{A=1/2} = \frac{8s}{9}{\sum_{i,j,k\in\mathbb{Z}}}' \frac{ij + jk - 2ik}{\left(i^2 + j^2 + k^2 - \frac{2}{3}(ij + ik + jk)\right)^{s+1}}, \tag{3.3}$$

while switching i and k in (3.2) gives

$$\left.\frac{\partial}{\partial A}L(A; s)\right|_{A=1/2} = \frac{8s}{9}{\sum_{i,j,k\in\mathbb{Z}}}' \frac{jk + ik - 2ij}{\left(i^2 + j^2 + k^2 - \frac{2}{3}(ij + ik + jk)\right)^{s+1}}. \tag{3.4}$$

On adding (3.2)–(3.4) and noting that

$$(ij + ik - 2jk) + (ij + jk - 2ik) + (jk + ik - 2ij) = 0,$$

it follows that

$$\left.\frac{\partial}{\partial A}L(A; s)\right|_{A=1/2} = 0.$$

Next, taking the derivative of (3.1) gives

$$\frac{\partial^2}{\partial A^2}L(A; s) = \frac{-4s}{(A+1)^3}{\sum_{i,j,k\in\mathbb{Z}}}' \frac{ij + ik - 2jk}{\left(i^2 + j^2 + k^2 - 2(ij + ik)\left(\frac{A}{A+1}\right) + 2jk\left(\frac{A-1}{A+1}\right)\right)^{s+1}}$$

$$+ \frac{4s(s+1)}{(A+1)^4}{\sum_{i,j,k\in\mathbb{Z}}}' \frac{(ij + ik - 2jk)^2}{\left(i^2 + j^2 + k^2 - 2(ij + ik)\left(\frac{A}{A+1}\right) + 2jk\left(\frac{A-1}{A+1}\right)\right)^{s+2}}.$$
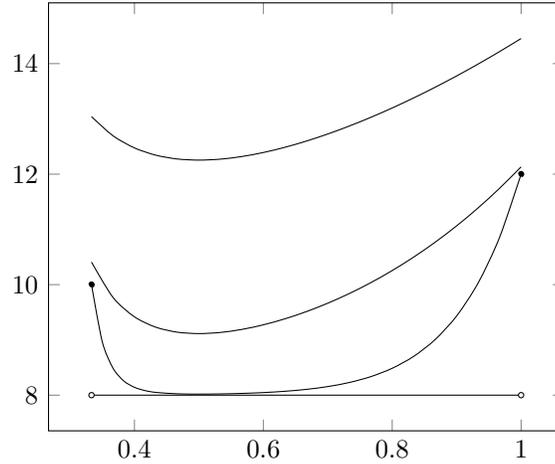
Figure 2. Graphs of $y = L(A; s)$ for $1/3 \leq A \leq 1$ given by (2.7) for (from top to bottom) $s = 3$, $s = 6$, $s = 20$ and $s = \infty$. In the limiting case $s \to \infty$ we have $L(A; \infty) = \text{kiss}(A)$ where $\text{kiss}(A)$ is the kissing number as a function of A as given in Table 1.

When $A = 1/2$ the first sum is zero by the calculations in the first part of the proof. Therefore,

$$\frac{\partial^2}{\partial A^2} L(A; s) \bigg|_{A=1/2} = \frac{64s(s+1)}{81} \sideset{}{'}\sum_{i,j,k \in \mathbb{Z}} \frac{(jk + ik - 2ij)^2}{\left(i^2 + j^2 + k^2 - \frac{2}{3}(ij + ik + jk)\right)^{s+2}}.$$

The term $(jk + ik - 2ij)^2$ in the numerator is non-negative and not always zero. The denominator is always positive because the quadratic form is positive definite. It follows that

$$\frac{\partial^2}{\partial A^2} L(A; s) \bigg|_{A=1/2} > 0$$

as required.

The calculations above are valid provided term-by-term differentiation of the series is allowed. All of the series encountered above converge absolutely and uniformly on compact subsets of the region $\text{Re}(s) > 3/2$. On restricting s to real values, the conclusion about positivity is valid for $s > 3/2$. ∎

A consequence of Theorem 1 is that for any fixed value $s > 3/2$, the lattice sum $L(A; s)$ attains a local minimum when $A = 1/2$. The values $s = 6$ and $s = 3$ are used in the classical Lennard–Jones 12-6 potential, so the values $s > 3/2$ are sufficient for physical applications. Some graphs of $y = L(A; s)$ for $1/3 \leq A \leq 1$ for various values of s are given in Figure 2.

A The limiting cases $A \to 0$ and $A \to \infty$

In Section 2, it was stated that the normalised lattices are congruent to $\mathbb{Z}$ or $\mathbb{Z}^2$ in the limits $A \to 0$ and $A \to \infty$, respectively. Here we provide an analysis for the case $A \to \infty$. When $A > 1$, by (2.1), (2.2) and (2.6) the normalised lattice is

$$\Lambda = \left\{ c_1 \left(\sqrt{\frac{A}{2}}, \frac{1}{\sqrt{2}}, 0 \right) + c_2 \left(\sqrt{\frac{A}{2}}, 0, \frac{1}{\sqrt{2}} \right) + c_3 \left(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}} \right) \mid c_1, c_2, c_3 \in \mathbb{Z} \right\}.$$

In the limit $A \to \infty$, the only vectors that remain finite are those with $c_2 = -c_1$, hence the limiting set is given by

$$\Lambda_\infty := \lim_{A \to \infty} \Lambda = \left\{ c_1 \left(0, \frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}} \right) + c_3 \left(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}} \right) \mid c_1, c_3 \in \mathbb{Z} \right\}.$$

The function $\phi \colon \Lambda_\infty \to \mathbb{Z}^2$ given by

$$\phi\left(c_1\left(0, \frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}}\right) + c_3\left(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right)\right) = (c_1, c_3)$$

is an isometry, i.e., it preserves distance, hence the normalised lattice in the limiting case $A \to \infty$ is congruent to $\mathbb{Z}^2$. The other limiting case $A \to 0$ may be analysed in a similar way by considering the normalised lattice in the case $0 < A < 1/3$. We omit the details as they are similar.

References

[1] Bétermin L., Optimality of the triangular lattice for Lennard–Jones type lattice energies: a computer-assisted method, *J. Phys. A* **56** (2023), 145204, 19 pages, arXiv:2104.09795.

[2] Borwein J.M., Glasser M.L., McPhedran R.C., Wan J.G., Zucker I.J., Lattice sums then and now, *Encyclopedia Math. Appl.*, Vol. 150, Cambridge University Press, Cambridge, 2013.

[3] Burrows A., Cooper S., Schwerdtfeger P., Instability of the body-centered cubic lattice within the sticky hard sphere and Lennard–Jones model obtained from exact lattice summations, *Phys. Rev. E* **104** (2021), 035306, 10 pages, arXiv:2107.11380.

[4] Cohn H., Kumar A., Miller S.D., Radchenko D., Viazovska M., Universal optimality of the E_8 and Leech lattices and interpolation formulas, *Ann. of Math.* **196** (2022), 983–1082, arXiv:1902.05438.

[5] Conway J.H., Sloane N.J.A., On lattices equivalent to their duals, *J. Number Theory* **48** (1994), 373–382.

[6] Conway J.H., Sloane N.J.A., Sphere packings, lattices and groups, 3rd ed., *Grundlehren Math. Wiss.*, Vol. 290, Springer, New York, 1999.

[7] Edelsbrunner H., Kerber M., Covering and packing with spheres by diagonal distortion in $\mathbb{R}^n$, in Rainbow of Computer Science, *Lecture Notes in Comput. Sci.*, Vol. 6570, Springer, Heidelberg, 2011, 20–35.

[8] Ennola V., On a problem about the Epstein zeta-function, *Proc. Cambridge Philos. Soc.* **60** (1964), 855–875.

[9] Faulhuber M., Steinerberger S., An extremal property of the hexagonal lattice, *J. Stat. Phys.* **177** (2019), 285–298, arXiv:1903.06856.

[10] Fields K.L., The fragile lattice packings of spheres in three-dimensional space, *Acta Cryst. Sect. A* **36** (1980), 194–197.

[11] Fields K.L., Locally minimal Epstein zeta functions, *Mathematika* **27** (1980), 17–24.

[12] Hales T.C., A proof of the Kepler conjecture, *Ann. of Math.* **162** (2005), 1065–1185.

[13] Montgomery H.L., Minimal theta functions, *Glasgow Math. J.* **30** (1988), 75–85.

[14] Patterson A., Crystal lattice models based on the close packing of spheres, *Rev. Sci. Instrum.* **12** (1941), 206–211.

[15] Rankin R.A., A minimum problem for the Epstein zeta-function, *Proc. Glasgow Math. Assoc.* **1** (1953), 149–158.

[16] Sarnak P., Strömbergsson A., Minima of Epstein's zeta function and heights of flat tori, *Invent. Math.* **165** (2006), 115–151.