

The BCC lattice in a long range interaction system

Xiaofeng Ren^{*†}

Department of Mathematics
The George Washington University
Washington, DC 20052, USA

Juncheng Wei[‡]

Department of Mathematics
University of British Columbia
Vancouver, BC, Canada V6T 1Z2

May 2, 2023

Abstract

While the hexagonal lattice is ubiquitous in two dimensions, the body centered cubic lattice and the face centered cubic lattice are both commonly observed in three dimensions. A geometric variational problem motivated by the diblock copolymer theory consists of a short range interaction energy and a long range interaction energy. In three dimensions, and when the long range interaction is given by the nonlocal operator $(-\Delta)^{-3/2}$, it is proved that the body centered cubic lattice is the preferred structure.

1 Introduction

In two dimensions the most familiar lattice is the hexagonal lattice, seen in many places like honeycomb, chicken wire fence, graphene, and carbon nanotube. In three dimensions, however, there are two common lattices: the body centered cubic lattice (BCC lattice) and the face centered cubic lattice (FCC lattice). In crystallography of metals the BCC lattice is found in iron, chromium, tungsten, and niobium, while the FCC lattice appears in aluminum, copper, gold, and silver. In the sphere packing problem the maximal packing density is attained by the hexagonal lattice in two dimensions [22, 16th], the FCC lattice in three dimensions [9, Hales], the E_8 lattice in eight dimensions [23, Viazovska], and the Leech lattice in 24 dimensions [5, Cohn, Kumar, Miller, Radchenko, and Viazovska].

Lattices studied in this paper arise from a geometric variational problem. Consider the free energy functional

$$J_{\Lambda,s}(\Omega) = P_{\Lambda}(\Omega) + \frac{\gamma}{2} \int_{\Omega} (-\Delta)^{-s} (\chi_{\Omega} - \omega)(x) dx \quad (1.1)$$

where

$$\omega \in (0, 1), \gamma > 0, s > 0 \quad (1.2)$$

are parameters. The functional is defined on subsets Ω of a sample space which we take to be $\mathbb{R}^d/\Lambda$, the flat torus of $\mathbb{R}^d$ modulo a lattice Λ , and the volume of Ω is fixed at ω times the volume of $\mathbb{R}^d/\Lambda$.

This problem is motivated by the Ohta-Kawasaki density functional theory for diblock copolymers [13]. A diblock copolymer molecule consists of a linear subchain of A-monomers grafted covalently to another subchain of B-monomers [1, Bates and Fredrickson]. Because of the repulsion between the unlike monomers, the different type sub-chains tend to segregate, but as they are chemically bonded in chain molecules,

^{*} Corresponding author. Phone: 1 202 994-6791; Fax: 1 202 994-6760; E-mail: ren@gwu.edu

[†]Supported in part by Simons Foundation Collaboration Grant for Mathematicians #709260, and NSF grant DMS-2307068

[‡]Supported in part by NSERC RGPIN-2018-03773

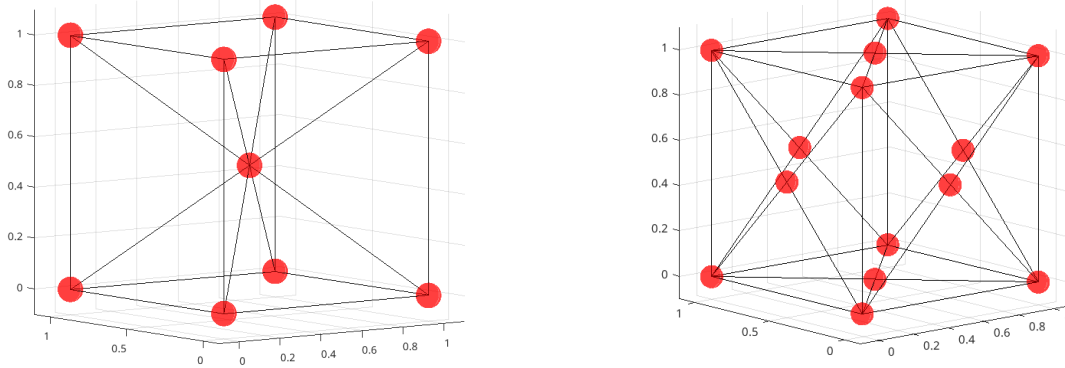


Figure 1: Making a BCC lattice and an FCC lattice out of a cubic lattice.

segregation of subchains lead to local micro-phase separation micro-domains rich in either A-monomers or B-monomers emerge to form a particular pattern called a morphological phase.

Many morphological phases have been observed in diblock copolymers. Of relevance to this work is the spherical phase. It occurs when the number of A-monomers is significantly smaller than the number of B-monomers in chain molecules. More precisely let N_A and N_B be the numbers of A-monomers and B-monomers respectively in a chain molecule. The composition parameter of a diblock copolymer is $\omega = N_A/(N_A + N_B) \in (0, 1)$, the same ω as in (1.2). Then a diblock copolymer exists in the spherical phase if ω is sufficiently small. In this phase the A-monomers form micro-domains of small balls and the B-monomers make up the rest of the system; [10, Helfand and Wasserman]. A diblock copolymer with larger ω -value exists in the cylindrical phase where A-monomers form cylinders; a diblock copolymer with ω -value close to $1/2$ exists in the lamellar phase where A- and B-monomers form planar layers; see [1]

It is known that the small balls in the spherical phase have approximately the same radius [17]. What is not clear is how these balls arrange themselves in space, the question we investigate in this paper.

The Ohta-Kawasaki theory treats monomer density fields as the main order parameters. In the strong segregation regime, the A-monomers occupy a subset Ω of the system sample, and the B-monomers occupy the complement of Ω . The authors of this paper showed that in this regime the Ohta-Kawasaki functional converges to a geometric variational problem like (1.1) in the sense of the Gamma limit theory [14].

We studied problem (1.1) on two and three dimensional bounded domains with zero Neumann boundary condition [16, 15, 17]. The exponent s there was taken to be 1, so the operator in the second term was $(-\Delta)^{-1}$ instead of $(-\Delta)^{-s}$ as in (1.1). It was proved in [17] that given a bounded domain in $\mathbb{R}^3$ and a positive integer N , if ω is sufficiently small and γ is suitably large, the variational problem (1.1) admits a stable stationary point which is the union of N perturbed balls. This result gave a mathematical confirmation of the existence of the spherical morphological phase in diblock copolymers.

The perturbed balls in the stationary point found in [17] have asymptotically the same radius; however the exact locations of the balls are not known. Generally one cannot expect a perfect periodic structure if the sample domain has boundary: there are always defects near the boundary. To circumvent this problem, in this paper we take the sample domain to be a flat torus, namely $\mathbb{R}^d/\Lambda$ where Λ is an d -dimensional lattice in $\mathbb{R}^d$. Obviously functions on $\mathbb{R}^d/\Lambda$ (or subsets of $\mathbb{R}^d/\Lambda$) can be viewed as Λ -periodic functions on $\mathbb{R}^d$ (or Λ -periodic subsets of $\mathbb{R}^d$). Our goal is to find a lattice which is optimal for problem (1.1).

The functional $J_{\Lambda, \omega}$ in (1.1) is defined on Lebesgue measurable subsets Ω of $\mathbb{R}^d/\Lambda$ of the prescribed volume:

$$|\Omega| = \omega |\mathbb{R}^d/\Lambda| \quad (1.3)$$

where $\omega \in (0, 1)$ is given in (1.2). Here $|\cdot|$ denotes the d -dimensional Lebesgue measure on $\mathbb{R}^d/\Lambda$. The number ω is the first parameter of this problem; it fixes the volume of Ω . The measure of the flat torus,

denoted $|R^d/\Lambda|$ or simply $|\Lambda|$, is the measure of a fundamental parallelepiped of Λ in R^d . It is also called the volume of the lattice Λ ; see (2.25).

The first term $P_\Lambda(\Omega)$ is the perimeter of Ω in R^d/Λ . If Ω is a subset with C^1 boundary, then the perimeter is simply the area of $\partial\Omega$. The second term in (1.1) is an integral over Ω multiplied by $y/2$ where

$$y \in (0, \infty) \quad (1.4)$$

is the second parameter of the problem. The integrand in the second term is the outcome of the operator $(-\Delta)^{-s}$ on $\chi_\Omega - \omega$ where χ_Ω is the characteristic function of Ω , i.e. $\chi_\Omega(x) = 1$ if $x \in \Omega$ and $= 0$ if $x \notin \Omega$. The constant s

$$s \in (0, \infty) \quad (1.5)$$

in the exponent of $-\Delta$ is the last parameter.

In the Ohta-Kawasaki theory, $(-\Delta)^{-1}$ is chosen for convenience; see [4, Choksi and Ren]. In this paper we mainly study the case $d = 3$ and $s = 3/2$ and show how this case is connected to the three dimensional analogy of Kronecker's limit formulas, and to the height problem for flat tori.

Denote Green's function of the operator $(-\Delta)^{-s}$ by $G_{\Lambda,s}$ so that

$$(-\Delta)^{-s} G_{\Lambda,s} = \delta - \frac{1}{|R^d/\Lambda|} \quad (1.6)$$

where δ is the delta measure centered at $0 \in R^d/\Lambda$. One decomposes $G_{\Lambda,s}$ into

$$G_{\Lambda,s}(x) = K_{d,s}(x) + R_{\Lambda,s}(x) \quad (1.7)$$

where $K_{d,s}$ is the fundamental solution of the operator $(-\Delta)^{-s}$ on R^d and $R_{\Lambda,s}$ is the regular part of $G_{\Lambda,s}$. While $K_{d,s}$ does not depend on Λ , the regular part of Green's function evaluated at 0, i.e. $R_{\Lambda,s}(0)$, contains much information about the lattice Λ . If $d = 3$ and $s = 3/2$, to find the optimal lattice, one should minimize $R_{\Lambda,3/2}(0)$ with respect to lattice Λ of unit volume; see Proposition 2.2.

We take the configuration Ω to be the simplest set: a ball of radius r , i.e. $\Omega = B_r$. By the constraint (1.3), r is related to ω via

$$\frac{\pi^{d/2} r^d}{\Gamma(\frac{d}{2} + 1)} = \omega |R^d/\Lambda|. \quad (1.8)$$

Then one compares the free energy per volume,

$$\frac{1}{|R^d/\Lambda|} J_{\Lambda,s}(B_r) \quad (1.9)$$

of the ball on different flat tori R^d/Λ . It turns out that to minimize (1.9) it suffices to consider lattices of unit volume; see Proposition 2.1. Then (1.8) becomes

$$\frac{\pi^{d/2} r^d}{\Gamma(\frac{d}{2} + 1)} = \omega \quad (1.10)$$

and r replaces ω as a main parameter. Since the spherical phase of a diblock copolymer exists when ω is small, we are interested in the scenario that r is small. Asymptotically, as $r \rightarrow 0$, the quantity (1.9) is determined by $R_{\Lambda,s}(0)$; see Proposition 2.2. Therefore $R_{\Lambda,s}(0)$ serves as a quantity that measures the optimality of lattice Λ in problem (1.1). We raise this question:

Question 1.1. Which lattice Λ of unit volume minimizes $R_{\Lambda,s}(0)$?

When s is in $(0, d/2)$, $K_{d,s}$ in (1.7) is given by the Riesz potential

$$K_{d,s}(x) = \frac{K_{d,s}}{|x|^{d-2s}}, \quad K_{d,s} = \frac{\Gamma(\frac{d-2s}{2})}{2^{2s} \pi^{d/2} \Gamma(s)} \quad (1.11)$$

where $\Gamma(\cdot)$ is the gamma function. When $d = 3$ and $s = 1$, the Riesz potential is $\frac{1}{4\pi|x|}$ which is known as the Coulomb potential.

The borderline case $s = d/2$ turns out to be very interesting, when it comes to $R_{\Lambda, d/2}(0)$. If $d = 2$, then $s = 1$ and $(-\Delta)^{-s}$ is the usual Laplacian $-\Delta$. The fundamental solution $K_{2,1}$ is not a Riesz potential but a logarithmic function

$$K_{2,1}(x) = \frac{1}{2\pi} \log \frac{1}{|x|}. \quad (1.12)$$

One can write Green's function $G_{\Lambda,1}$ of $-\Delta$ on a two dimensional flat torus in terms of a Jacobi's theta function and relate $R_{\Lambda,1}(0)$ to Dedekind's eta function. Chen and Oshita proved that among two dimensional lattices of unit area, $R_{\Lambda,1}(0)$ is minimized uniquely by the hexagonal lattice [2]. Sandier and Serfaty noted that one can also connect $R_{\Lambda,1}(0)$ to Dedekind's eta function via Kronecker's second limit formula. They gave another proof of Chen and Oshita's result in [19].

In this paper, we consider the case $s = d/2$ in three dimensions, i.e. $d = 3$ and $s = 3/2$. It will be shown in Lemma 3.3 that the fundamental solution $K_{3,3/2}$ is

$$K_{3,3/2}(x) = \frac{1}{2\pi^2} \log \frac{1}{|x|}. \quad (1.13)$$

We will prove the following theorem.

Theorem 1.2. *Let $d = 3$ and $s = 3/2$. Among three dimensional lattices Λ of unit volume, $R_{\Lambda,3/2}(0)$ is uniquely minimized by the BCC lattice.*

Two lattices are equivalent if we can transform one to the other by a dilation and an orthogonal transform. Equivalent lattices are indistinguishable. By a lattice, we often mean the equivalent class of a lattice. The uniqueness assertion in Theorem 1.2 means uniqueness up to this equivalence.

When $d = 2$ and $s = d/2 = 1$, the corresponding $R_{\Lambda,1}(0)$ can be expressed in terms of Dedekind's eta function; see [2, 12, 18] for this point and its applications. Here for $d = 3$ and $s = d/2 = 3/2$, we derive a key result, Lemma 3.3, that expresses $R_{\Lambda,3/2}(0)$ in terms of the variables in the Iwasawa decomposition of Λ^* . Here Λ^* is the dual lattice of Λ ; see (2.34) for the definition of a dual lattice.

The proof of the theorem uses the notion of the height of a manifold. Let M be a closed Riemannian manifold and

$$0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \dots \quad (1.14)$$

be the eigenvalues of $-\Delta$ on M , counting multiplicity. Define the zeta-regularization

$$Z(M, s) = \sum_{j=1}^{\infty} \frac{1}{\lambda_j^s}. \quad (1.15)$$

Then the height of M is

$$h(M) = Z'(M, 0). \quad (1.16)$$

Here $Z'(M, s)$ is the derivative of Z with respect to s .

We relate $R_{\Lambda,3/2}(0)$ to $h(\mathbb{R}^3/\Lambda^*)$, the height of $\mathbb{R}^3/\Lambda^*$. Here $\mathbb{R}^3/\Lambda^*$ is a flat torus viewed as a Riemannian manifold. We show in Lemma 4.5 that

$$h(\mathbb{R}^3/\Lambda^*) = (2\pi)^2 R_{\Lambda,3/2}(0) + 2 \log(2\pi). \quad (1.17)$$

Then we apply a theorem by Sarnak and Strömbergsson among lattices in $\mathbb{R}^3$ of unit volume, the height of the corresponding flat tori is minimized uniquely by the FCC lattice [20]. Since the BCC lattice is the dual lattice of the FCC lattice, Theorem 1.2 follows from (1.17).

Acknowledgments. We would like to thank Rustum Choksi for valuable discussions.

2 Preliminaries

The long range interaction term in (1.1) is denoted

$$I_{\Lambda,S}(\Omega) = \int_{\Omega} (-\Delta)^{-s} (\chi_{\Omega} - \omega)(x) dx \quad (2.1)$$

so that

$$J_{\Lambda,S}(\Omega) = P_{\Lambda}(\Omega) + \frac{Y}{2} I_{\Lambda,S}(\Omega). \quad (2.2)$$

Instead of $J_{\Lambda,S}(\Omega)$, it is more appropriate to consider

$$\mathcal{J}_{\Lambda,S}(\Omega) = \frac{1}{|R^d/\Lambda|} J_{\Lambda,S}(\Omega) \quad (2.3)$$

the energy of the configuration Ω per volume, when one studies the impact of the lattice Λ .

The size and the shape of a configuration play different roles in $\mathcal{J}_{\Lambda,S}(\Omega)$. To separate the two factors write the lattice as $t\Lambda$ where $t \in (0, \infty)$ and Λ is a lattice of unit volume, $|\Lambda| = 1$. Then $|t\Lambda| = t^d$. The size of the lattice $t\Lambda$ is given by t ; the shape of $t\Lambda$ by Λ . The configuration is also written as $t\Omega \subset R^d/t\Lambda$ with $\Omega \subset R^d/\Lambda$.

Proposition 2.1. 1. For fixed Λ and fixed Ω , $\mathcal{J}_{t\Lambda,S}(t\Omega)$ is minimized, with respect to t , at

$$t = t_{\Lambda,S,\Omega} = \frac{P_{\Lambda}(\Omega)^{1/(2s+1)}}{\text{sy}l_{\Lambda,S}(\Omega)}$$

and the minimum value is

$$\mathcal{J}_{t_{\Lambda,S,\Omega}\Lambda,S}(t_{\Lambda,S,\Omega}\Omega) = 1 + \frac{1}{2s} P_{\Lambda}(\Omega)^{2s/(2s+1)} \text{sy}l_{\Lambda,S}(\Omega)^{1/(2s+1)}.$$

2. If $\Omega = B_r$ and Λ is fixed, then $\mathcal{J}_{t\Lambda,S}(tB_r)$ is minimized, with respect to t , at

$$t = t_{\Lambda,S,B_r} = \frac{2\pi^{d/2} r^{d-1}}{\text{sy}l_{\Lambda,S}(B_r)\Gamma(d/2)}^{1/(2s+1)}$$

and the minimum value is

$$\mathcal{J}_{t_{\Lambda,S,B_r}\Lambda,S}(t_{\Lambda,S,B_r}B_r) = 1 + \frac{1}{2s} \frac{2\pi^{d/2} r^{d-1}}{\Gamma(d/2)}^{2s/(2s+1)} (\text{sy}l_{\Lambda,S}(B_r))^{1/(2s+1)}.$$

Proof. We show that

$$P_{t\Lambda}(t\Omega) = t^{d-1} P_{\Lambda}(\Omega), \quad (2.4)$$

$$I_{t\Lambda,S}(t\Omega) = t^{d+2s} I_{\Lambda,S}(\Omega). \quad (2.5)$$

The first scaling relation (2.4) follows from the definition of perimeter:

$$P_{\Lambda}(\Omega) = \sup_{\Omega} \int_{\Omega} \text{div } g(x) dx : g \in C^1(R^d/\Lambda, R^d), |g(x)| \leq 1 \ \forall x \in R^d/\Lambda. \quad (2.6)$$

To see (2.5), let λ_j , ($j = 0, 1, 2, \dots$ and $\lambda_0 = 0 < \lambda_1 \leq \lambda_2 < \dots$), be the eigenvalues of $-\Delta$ on R^d/Λ counting multiplicity, and φ_j be the corresponding eigenfunctions. Let $v = (-\Delta)^{-s} (\chi_{\Omega} - \omega)$ and assume

$$v(x) = \sum_{j=1}^{\infty} c_j \varphi_j(x), \quad x \in R^d/\Lambda. \quad (2.7)$$

Note that j starts from 1 here. Then

$$\chi_{\Omega}(x) - \omega = (-\Delta)^{-s} v(x) = \sum_{j=1}^{\infty} c_j \lambda_j^s \varphi_j(x). \quad (2.8)$$

On $\mathbb{R}^d/t\Lambda$, the eigenvalues of $-\Delta$ are $\frac{\lambda_j}{t^2}$, $j = 0, 1, 2, \dots$, and the corresponding eigenfunctions are $\varphi_j(\frac{\cdot}{t})$. Then, with $y \in \mathbb{R}^d/t\Lambda$,

$$\begin{aligned} (-\Delta)^{-s} v \left(\frac{y}{t} \right) &= (-\Delta)^{-s} \sum_{j=1}^{\infty} c_j \varphi_j \left(\frac{y}{t} \right) \\ &= \sum_{j=1}^{\infty} c_j \frac{\lambda_j}{t^2}^s \varphi_j \left(\frac{y}{t} \right) \\ &= t^{-2s} \chi_{\Omega} \left(\frac{y}{t} \right) - \omega \\ &= t^{-2s} (\chi_{t\Omega}(y) - \omega). \end{aligned}$$

Hence

$$(-\Delta)^{-s} (\chi_{t\Omega} - \omega)(y) = t^{2s} v \left(\frac{y}{t} \right), \quad (2.9)$$

and

$$I_{t\Lambda, s}(t\Omega) = \int_{t\Omega} t^{2s} v \left(\frac{y}{t} \right) dy = t^{d+2s} \int_{\Omega} v(x) dx = t^{d+2s} I_{\Lambda, s}(\Omega) \quad (2.10)$$

which proves (2.5).

The energy per cell area of $t\Omega$ is

$$\mathcal{E}_{t\Lambda, s}(t\Omega) = \frac{1}{t^d} J_{t\Lambda, s}(t\Omega) = \frac{1}{t} P_{\Lambda}(\Omega) + \frac{t^{2s}}{2} I_{\Lambda, s}(\Omega).$$

With respect to t , the last quantity is minimized at

$$t = t_{\Lambda, s, \Omega} = \frac{P_{\Lambda}(\Omega)}{s y I_{\Lambda, s}(\Omega)}^{1/(2s+1)} \quad (2.11)$$

and the minimum value is

$$\mathcal{E}_{t_{\Lambda, s, \Omega} \Lambda, s}(t_{\Lambda, s, \Omega} \Omega) = 1 + \frac{1}{2s} P_{\Lambda}(\Omega)^{2s/(2s+1)} s y I_{\Lambda, s}(\Omega)^{1/(2s+1)}. \quad (2.12)$$

This proves the first part of the proposition.

To see the second part, note that the area of a $(d-1)$ -sphere is

$$P_{\Lambda}(B_r) = \frac{2\pi^{d/2} r^{d-1}}{\Gamma(d/2)} \quad (2.13)$$

which does not depend on Λ . □

This proposition shows that to determine the optimal lattice when the configuration set is a ball, one only needs to minimize $I_{\Lambda, s}(B_r)$ with respect to lattice Λ of unit volume.

When $d = 2$ or 3 and $s = 1$, $I_{\Lambda, 1}(B_r)$ is essentially $R_{\Lambda, 1}(0)$, the regular part of Green's function at 0 , up to some additive and multiplicative constants [16, 17]. When $d = 3$ and $s = 3/2$, the next proposition provides an approximation of $I_{\Lambda, 3/2}(B_r)$; it asserts that as $r \rightarrow 0$, $I_{\Lambda, 3/2}(B_r)$ is asymptotically determined by $R_{\Lambda, 3/2}(0)$.

Proposition 2.2. When $d = 3$ and $s = 3/2$, there exist $c_1(r)$ and $c_2(r) > 0$ depending on r but not on Λ such that

$$\lim_{r \rightarrow 0} \frac{I_{\Lambda, 3/2}(B_r) - c_1(r)}{c_2(r)} = R_{\Lambda, 3/2}(0)$$

for each lattice Λ

Proof. In terms of Green's function $G_{\Lambda, s}$

$$(-\Delta)^{-s} (\chi_{B_r} - \omega)(w) = \int_{B_r} \int_{B_r} G_{\Lambda, s}(w - v) dv \quad (2.14)$$

$$I_{\Lambda, s}(B_r) = \int_{B_r} \int_{B_r} G_{\Lambda, s}(w - v) dv dw. \quad (2.15)$$

In the case of $d = 3$ and $s = 3/2$, $G_{\Lambda, 3/2}$ can be written as

$$G_{\Lambda, 3/2}(w) = -\frac{1}{2\pi^2} \log |w| + R_{\Lambda, 3/2}(w) \quad (2.16)$$

where $R_{\Lambda, 3/2}$ is smooth on $(\mathbb{R}^3 \setminus \Lambda) \cup \{(0, 0, 0)\}$; see Lemma 3.3. Note that

$$\int_{B_r} \int_{B_r} \log |w - \tilde{w}| dw d\tilde{w} = \frac{4\pi^2}{3} r^6 \log \frac{1}{r} - r^6 \int_{B_1} \int_{B_1} \log |v - \tilde{v}| dv d\tilde{v} \quad (2.17)$$

$$\begin{aligned} \int_{B_r} \int_{B_r} R_{\Lambda, 3/2}(w - \tilde{w}) dw d\tilde{w} &= \int_{B_r} \int_{B_r} R_{\Lambda, 3/2}(0) + O(r^2) dw d\tilde{w} \\ &= \frac{4\pi^2}{3} r^6 R_{\Lambda, 3/2}(0) + O(r^8). \end{aligned} \quad (2.18)$$

Here one used the fact $\nabla R(0) = 0$ since $G(w) = G(-w)$ for all $w \in \mathbb{R}^3 \setminus \Lambda$ to deduce the $O(r^2)$ term. Therefore

$$I_{\Lambda, 3/2}(B_r) = \frac{8r^6}{9} \log \frac{1}{r} - \frac{r^6}{2\pi^2} \int_{B_1} \int_{B_1} \log |v - \tilde{v}| dv d\tilde{v} + \frac{4\pi^2}{3} r^6 R_{\Lambda, 3/2}(0) + O(r^8). \quad (2.19)$$

Let

$$\begin{aligned} c_1(r) &= \frac{8r^6}{9} \log \frac{1}{r} - \frac{r^6}{2\pi^2} \int_{B_1} \int_{B_1} \log |v - \tilde{v}| dv d\tilde{v} \\ c_2(r) &= \frac{4\pi^2}{3} r^6 \end{aligned}$$

and the proposition follows from (2.19). $\square$

In the rest of the paper we show that $R_{\Lambda, 3/2}(0)$ is uniquely minimized by the BCC lattice. Let us briefly recall some basic facts in the lattice theory. A d -dimensional lattice Λ is a subset of $\mathbb{R}^d$ of the form

$$\Lambda = \{n_1 v_1 + n_2 v_2 + \dots + n_d v_d : n_j \in \mathbb{Z}\} \quad (2.20)$$

where $\{v_1, v_2, \dots, v_d\}$ is a set of linearly independent vectors in $\mathbb{R}^d$. Denote by $V \in GL(d, \mathbb{R})$ the $d \times d$ matrix whose j -th row is the row vector v_j ; V is called a generator matrix of Λ . The Gram matrix Q of V is a positive definite matrix given by

$$Q = V V' \quad (2.21)$$

where V' is the transpose of V .

The most important lattice in two dimensions is arguably the hexagonal lattice. For this lattice we can take $v_1 = (1, 0)$ and $v_2 = (1/2, \sqrt{3}/2)$. Then

$$V = \begin{pmatrix} 1 & 0 \\ \frac{1}{2} & \frac{\sqrt{3}}{2} \end{pmatrix}, \quad Q = \begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{pmatrix}. \quad (2.22)$$

When $d = 3$, Z^3 is a cubic lattice, generated by $(1, 0, 0)$, $(0, 1, 0)$, and $(0, 0, 1)$. Both the generator matrix and the Gram matrix are the identity matrix.

Adding *body centers* $(1/2, 1/2, 1/2) + \lambda$, $\lambda \in Z^3$, to Z^3 , we obtain a BCC lattice; see the left plot of Figure 1. This lattice has a generator matrix and a corresponding Gram matrix as follows:

$$V = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}, \quad Q = \begin{pmatrix} \frac{3}{4} & -\frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & \frac{3}{4} & -\frac{1}{4} \\ -\frac{1}{4} & -\frac{1}{4} & \frac{3}{4} \end{pmatrix}. \quad (2.23)$$

From the cubic lattice Z^3 , adding *face centers* $(0, 1/2, 1/2) + \lambda$, $(1/2, 0, 1/2) + \lambda$, and $(1/2, 1/2, 0) + \lambda$, $\lambda \in Z^3$, we have an FCC lattice; see the right plot of Figure 1. This lattice has

$$V = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}, \quad Q = \begin{pmatrix} \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{2} \end{pmatrix} \quad (2.24)$$

as a generator matrix and a corresponding Gram matrix.

The flat torus associated with Λ is the quotient space $\mathbb{R}^d/\Lambda$. The Lebesgue measure of $\mathbb{R}^d/\Lambda$ is

$$|\mathbb{R}^d/\Lambda| = |\Lambda| = |\det V| = (\det Q)^{1/2} \quad (2.25)$$

which we denote by $|\Lambda|$ for simplicity. It is also called the volume of the lattice Λ .

Two lattices are equivalent if one can be transformed to the other by a dilation and an orthogonal transform. Any lattice that is equivalent to the lattice described in (2.22), (2.23) or (2.24), respectively, is a hexagonal lattice, (BCC lattice or FCC lattice, respectively).

To understand this equivalence relation in terms of generator matrices, let $V \in GL(d, \mathbb{R})$ transform to $\tilde{V} \in GL(d, \mathbb{R})$ by the right action

$$V \rightarrow \tilde{V} = V\kappa U \quad (2.26)$$

where $\kappa \in \mathbb{R} \setminus \{0\}$ and U is a $d \times d$ orthogonal matrix and. The resulting space of left cosets is

$$H^d = GL(d, \mathbb{R})/O(d)\mathbb{R}^\times \quad (2.27)$$

where $O(d)$ is the group of $d \times d$ orthogonal matrices and $\mathbb{R}^\times$ in (2.27) denotes the space of nonzero scalar multiples of the $d \times d$ identity matrix. Note that this $\mathbb{R}^\times$ is the center of $GL(d, \mathbb{R})$.

When $d = 3$, by the Iwasawa decomposition [11], each point in H^3 can be uniquely represented by an upper triangular matrix of the form

$$\tau = \begin{pmatrix} & & \\ y_1 y_2 & y_1 x_2 & x_3 \\ & y_1 & x_1 \\ & & & 1 \end{pmatrix} \quad (2.28)$$

where $x_1, x_2, x_3, y_1, y_2 \in \mathbb{R}$ and $y_1, y_2 > 0$. More precisely, every generator matrix $V \in GL(3, \mathbb{R})$ can be written as

$$V = \tau \kappa U \quad (2.29)$$

where τ is of the form (2.28), $\kappa \in \mathbb{R}^{\times}$, and U is an orthogonal matrix. The Gram matrix Q corresponding to V is

$$Q = \kappa^2 \tau \tau'. \quad (2.30)$$

The generator matrix $V \in GL(3, \mathbb{R})$ of the BCC lattice in (2.23) is decomposed as in (2.29) with

$$\tau = \begin{bmatrix} \frac{\sqrt{2}}{3} & \frac{\sqrt{3}}{2} & \frac{\sqrt{2}}{3} & \sqrt{-\frac{1}{2}} & -\frac{1}{3} \\ \frac{\sqrt{2}}{3} & \frac{\sqrt{3}}{2} & \frac{\sqrt{2}}{3} & -\frac{1}{3} & -\frac{1}{3} \\ 1 & & & & \end{bmatrix}, \quad \kappa = \frac{\sqrt{3}}{2}, \quad U = \begin{bmatrix} 0 & \frac{\sqrt{1}}{2} & \frac{\sqrt{1}}{2} \\ \frac{\sqrt{2}}{6} & -\frac{\sqrt{1}}{6} & \frac{\sqrt{1}}{6} \\ \frac{\sqrt{1}}{3} & \frac{\sqrt{1}}{3} & -\frac{\sqrt{1}}{3} \end{bmatrix}. \quad (2.31)$$

For the FCC lattice in (2.24) the decomposition (2.29) is given by

$$\tau = \begin{bmatrix} \frac{\sqrt{3}}{2} & \frac{\sqrt{2}}{3} & \frac{\sqrt{3}}{2} & \frac{1}{3} & \frac{1}{2} \\ \frac{\sqrt{3}}{2} & \frac{\sqrt{2}}{3} & \frac{\sqrt{3}}{2} & \frac{1}{3} & \frac{1}{2} \\ 1 & & & & \end{bmatrix}, \quad \kappa = \frac{\sqrt{1}}{2}, \quad U = \begin{bmatrix} -\frac{\sqrt{1}}{3} & \frac{\sqrt{1}}{3} & \frac{\sqrt{1}}{3} \\ \frac{\sqrt{1}}{6} & -\frac{\sqrt{1}}{6} & \frac{\sqrt{2}}{6} \\ \frac{\sqrt{1}}{2} & \frac{\sqrt{1}}{2} & 0 \end{bmatrix}. \quad (2.32)$$

There is still more redundancy in H^d . If g is in the modular group $SL(d, \mathbb{Z})$ and V is a generator matrix, then gV is another generator matrix of the same lattice. This left action, $V \rightarrow gV$, gives rise to the double coset space

$$SL(d, \mathbb{Z}) \backslash H^d = SL(d, \mathbb{Z}) \backslash GL(d, \mathbb{R}) / O(d) \mathbb{R}^{\times} \quad (2.33)$$

which is the space of equivalent lattice classes.

If Λ is a lattice in $\mathbb{R}^d$, the dual lattice of Λ is

$$\Lambda^* = \{k \in \mathbb{R}^d : k \cdot \lambda \in \mathbb{Z} \text{ for all } \lambda \in \Lambda\}. \quad (2.34)$$

If V and Q are a generator matrix and a Gram matrix of Λ respectively, then we can take

$$V^* = (V^{-1})', \quad Q^* = V^* (V^*)' = Q^{-1} \quad (2.35)$$

to be a generator matrix and a Gram matrix of Λ^* respectively. The dual lattice of a hexagonal lattice is again a hexagonal lattice. By (2.23) and (2.24), the dual lattice of an FCC lattice is a BCC lattice, and vice versa.

As a function of $w \in \mathbb{R}^d$, $e^{2\pi i k \cdot w}$ is Λ -periodic if $k \in \Lambda^*$; it is an eigenfunction of the $-\Delta$ operator on $\mathbb{R}^d / \Lambda$, with the eigenvalue $(2\pi)^2 |k|^2$. For $s > 0$ let $G_{\Lambda, s}$ be Green's function of the operator $(-\Delta)^s$ on $\mathbb{R}^d / \Lambda$ so that

$$(-\Delta)^s G_{\Lambda, s} = \delta - \frac{1}{|\Lambda|}, \quad \int_{\mathbb{R}^d / \Lambda} G_{\Lambda, s}(w) dw = 0. \quad (2.36)$$

Now write $G_{\Lambda, s}$ as

$$G_{\Lambda, s}(w) = \sum_{k \in \Lambda^*} C_k e^{2\pi i k \cdot w}, \quad C_0 = 0$$

where the sum is assumed to converge in the sense of distributions on $\mathbb{R}^d / \Lambda$. Here $C_0 = 0$ because of the integral condition in (2.36). By the fact

$$\delta = \sum_{k \in \Lambda^*} \frac{1}{|\Lambda|} e^{2\pi i k \cdot w}, \quad (2.37)$$

the C_k 's satisfy

$$\sum_{k \in \Lambda^*} (2\pi)^{2s} |k|^{2s} C_k e^{2\pi i k \cdot w} = \sum_{k \in \Lambda^*} \frac{1}{|\Lambda|} e^{2\pi i k \cdot w} - \frac{1}{|\Lambda|}.$$

Hence $G_k = \frac{1}{(2\pi)^{2s} |k|^{2s} |\Lambda|}$ if $k \neq 0$ and $C_0 = 0$. Consequently

$$G_{\Lambda, s}(w) = \sum_{k \in \Lambda \setminus \{0\}} \frac{e^{2\pi i k \cdot w}}{(2\pi)^{2s} |k|^{2s} |\Lambda|}. \quad (2.38)$$

Let V^* be a generator matrix of Λ^* and $Q^* = V^* (V^*)'$ be the associated Gram matrix. If $k = mV^*$ for $m \in \mathbb{Z}^d$, then

$$|k|^2 = mV^* (mV^*)' = mQ^* m' := Q^*[m].$$

This allows us to write alternatively

$$G_{\Lambda, s}(w) = \sum_{m \in \mathbb{Z}^d \setminus \{0\}} \frac{e^{2\pi i m V^* \cdot w}}{(2\pi)^{2s} Q^*[m]^s |\Lambda|}. \quad (2.39)$$

3 $R_{\Lambda, 3/2}(0)$

The expression (2.39) for Green's function G_s is reminiscent of the twisted Epstein zeta function introduced by Siegel. Let Q be a positive definite $d \times d$ matrix, $u, v \in \mathbb{R}^d$, and define this zeta function by

$$\zeta(s, u, v, Q) = \sum_{m \in \mathbb{Z}^d, m+v \neq 0} \frac{e^{2\pi i m \cdot u}}{Q[m+v]^s}, \quad s \in \mathbb{C}, \operatorname{Re} s > \frac{d}{2}. \quad (3.1)$$

Lemma 3.1 ([8, Epstein], [21, Siegel]). *As a function of s , ζ admits an analytic continuation on $\mathbb{C}$. It is entire if $u \in \mathbb{Z}^d$, and has a simple pole at $s = d/2$ if $u \in \mathbb{Z}^d$. Furthermore, ζ satisfies the functional equation*

$$\pi^{-s} \Gamma(s) \zeta(s, u, v, Q) = e^{-2\pi i u \cdot v} (\det Q)^{-1/2} \pi^{(d/2-s)} \Gamma\left(\frac{d}{2} - s\right) \zeta\left(\frac{d}{2} - s, v, -u, Q^{-1}\right). \quad (3.2)$$

The case $u \in \mathbb{Z}^d$ was treated by Epstein and the case $u \in \mathbb{Z}^d$ by Siegel. In the latter case there is the question what $\zeta(d/2, u, v, Q)$ is? If $d = 2$, the answer is given by Kronecker's second limit formula. If $d = 3$ and $v = 0$, Efrat proved the result below.

By (2.29) and (2.30) we write

$$Q = (\det Q)^{1/3} (y_1^2 y_2)^{-2/3} \tau \tau' \quad (3.3)$$

where τ , together with the x_j 's and the y_j 's, is given in (2.28). Let

$$Z_1 = x_1 + iy_1, \quad Z_2 = x_2 + iy_2, \quad X_4 = x_3 - x_1 x_2. \quad (3.4)$$

Define a matrix Q_2 to be

$$Q_2 = \frac{1}{y_1} \begin{pmatrix} y_1 & x_1 & y_1 \\ 1 & x_1 & 1 \end{pmatrix} \quad (3.5)$$

and denote by ζ_2 this zeta function in two dimensions:

$$\begin{aligned} \zeta_2(s, \begin{pmatrix} u_2 \\ u_3 \end{pmatrix}, 0, Q) &= \sum_{(n_1, n_2) \in \mathbb{Z}^2 \setminus \{(0,0)\}} \frac{e^{2\pi i (n_1 u_2 + n_2 u_3)}}{Q_2[n]^s} \\ &= \sum_{(n_1, n_2) \in \mathbb{Z}^2 \setminus \{(0,0)\}} \frac{e^{2\pi i (n_1 u_2 + n_2 u_3)}}{|n_1 Z_1 + n_2|^s} \end{aligned} \quad (3.6)$$

which converges absolutely for $\operatorname{Re} s > 1$.

Lemma 3.2 ([6, Efrat]). Let $d = 3$, $v = 0$, and $u/\in \mathbb{Z}^3$. Then

$$(\det Q)^{1/2} \zeta \left(\frac{3}{2}, u, 0, Q \right) = y_1^{1/2} y_2 \zeta_2 \left(\frac{3}{2}, \begin{matrix} u_2 \\ u_3 \end{matrix}, 0, Q \right) \\ - 4\pi \log \prod_{(n_1, n_2) \in \mathbb{Z}^2} \left(1 - \exp \left(-2\pi y_2 |(n_2 - u_3)z_1 - (n_1 - u_2)| \right) \right) \\ \exp \left(2\pi i (u_1 + (n_1 - u_2)x_2 + (n_2 - u_3)x_4) \right).$$

A comparison of $G_{\Lambda, s}$ in (2.39) and ζ in (3.1) shows that

$$G_{\Lambda, s}(w) = (2\pi)^{-2s} |\Lambda|^{-1} \zeta(s, V^* w, 0, Q^*). \quad (3.7)$$

We proceed to find the fundamental solution of $G_{\Lambda, 3/2}$ and the regular part of $G_{\Lambda, 3/2}$ evaluated at 0. Let V^* be a generator matrix of the dual lattice Λ^* and $Q^* = V^* (V^*)'$ be its Gram matrix. By the Iwasawa decomposition one can write V^* and Q^* as

$$V^* = (\det V^*)^{1/3} (y_1^2 y_2)^{-1/3} \tau U \quad (3.8)$$

$$Q^* = (\det Q^*)^{1/3} (y_1^2 y_2)^{-2/3} \tau \tau'. \quad (3.9)$$

Here U is an orthogonal matrix and τ is a triangular matrix in the Iwasawa decomposition of V^* (not V); τ takes the form

$$\tau = \begin{pmatrix} 1 & & & \\ & y_1 y_2 & y_1 x_2 & x_3 \\ & & y_1 & x_1 \\ & & & 1 \end{pmatrix} \quad (3.10)$$

where $y_1, y_2 > 0$, and $x_1, x_2, x_3 \in \mathbb{R}$. Also set z_1, z_2 , and x_4 as in (3.4).

Lemma 3.3. When $d = 3$ and $s = 3/2$,

$$G_{\Lambda, 3/2}(w) = -\frac{1}{2\pi^2} \log |w| + R_{\Lambda, 3/2}(w)$$

where $R_{\Lambda, 3/2}$ is a smooth function near 0 and

$$R_{\Lambda, 3/2}(0) = \frac{y_1^{1/2} y_2}{(2\pi)^3} \left(\prod_{(n_1, n_2) \in \mathbb{Z}^2 \setminus \{(0,0)\}} \frac{x}{|n_1 z_1 + n_2|^3} \right) - \frac{1}{2\pi^2} \log \left(2\pi y_1^{1/3} y_2^{2/3} |\Lambda|^{-1/3} \right) \\ - \frac{1}{2\pi^2} \log \prod_{(n_1, n_2) \in \mathbb{Z}^2 \setminus \{(0,0)\}} \left(1 - \exp \left(-2\pi y_2 |n_2 z_1 - n_1| + 2\pi i (n_1 x_2 + n_2 x_4) \right) \right).$$

Here x_j, y_j , and z_j , given by (3.10) and (3.4), come from τ in the Iwasawa decomposition of V^* .

Proof. By (3.7) and Lemma 3.2

$$G_{\Lambda, 3/2}(w) = (2\pi)^{-3} (\det Q^*)^{1/2} \zeta \left(\frac{3}{2}, V^* w, 0, Q^* \right) \quad (3.11)$$

$$= \frac{y_1^{1/2} y_2}{(2\pi)^3} \zeta_2 \left(\frac{3}{2}, \begin{matrix} u_2 \\ u_3 \end{matrix}, 0, Q \right) \\ - \frac{1}{2\pi^2} \log \prod_{(n_1, n_2) \in \mathbb{Z}^2} \left(1 - \exp \left(-2\pi y_2 |(n_2 - u_3)z_1 - (n_1 - u_2)| \right) \right) \\ \exp \left(2\pi i (u_1 + (n_1 - u_2)x_2 + (n_2 - u_3)x_4) \right). \quad (3.12)$$

Here

$$u = V^* w \quad (3.13)$$

and

$$Q_2^* = \frac{1}{y_1} \begin{pmatrix} y_1 & x_1 \\ 1 & x_1 \end{pmatrix} \begin{pmatrix} y_1 \\ 1 \end{pmatrix}. \quad (3.14)$$

As $w \rightarrow 0$ in (3.12), $u \rightarrow 0$; since the function ζ_2 is regular at $u_2 = u_3 = 0$,

$$\zeta_2\left(\frac{3}{2}, 0, 0, Q\right) = \prod_{(n_1, n_2) \in \mathbb{Z}^2 \setminus \{(0,0)\}} \frac{y_1^{3/2}}{|n_1 z_1 + n_2|^3}. \quad (3.15)$$

The term on the right side of (3.15) is actually the real analytic Eisenstein series at $s = 3/2$ times twice the Riemann zeta function at 3.

In the infinite product of (3.12) the $n_1 = n_2 = 0$ term

$$1 - \exp\{-2\pi y_2| -u_3 z_1 + u_2| + 2\pi i(u_1 - u_2 x_2 - u_3 x_4)\} \quad (3.16)$$

causes a logarithmic singularity at $w = 0$. Let

$$\tilde{w} = Uw \quad (3.17)$$

where U is the orthogonal matrix in (3.8). Then by (3.8) and (3.13)

$$\begin{aligned} u &= (\det V^*)^{1/3} (y_1^2 y_2)^{-1/3} \tau U w \\ &= (\det V^*)^{1/3} (y_1^2 y_2)^{-1/3} \tau \tilde{w} \end{aligned} \quad (3.18)$$

namely

$$\begin{aligned} u_1 &= (\det V^*)^{1/3} (y_1^2 y_2)^{-1/3} (y_1 y_2 \tilde{w}_1 + y_1 x_2 \tilde{w}_2 + x_3 \tilde{w}_3) \\ u_2 &= (\det V^*)^{1/3} (y_1^2 y_2)^{-1/3} (y_1 \tilde{w}_2 + x_1 \tilde{w}_3) \\ u_3 &= (\det V^*)^{1/3} (y_1^2 y_2)^{-1/3} \tilde{w}_3. \end{aligned}$$

Calculations show that

$$q := -2\pi y_2| -u_3 z_1 + u_2| + 2\pi i(u_1 - u_2 x_2 - u_3 x_4) \quad (3.19)$$

$$= 2\pi y_1^{1/3} y_2^{2/3} (-|\tilde{w}_2 - i \tilde{w}_3| + i \tilde{w}_1) (\det V^*)^{1/3}. \quad (3.20)$$

Then (3.20) implies that

$$\begin{aligned} \log |1 - e^q| &= \log |q| + O(|q|) \\ &= \log |\tilde{w}| + \log 2\pi y_1^{1/3} y_2^{2/3} + \log |\det V^*|^{1/3} + O(y_1^{1/3} y_2^{2/3} |\tilde{w}| |\det V^*|^{1/3}) \\ &= \log |w| + \log 2\pi y_1^{1/3} y_2^{2/3} + \log |\det V^*|^{1/3} + O(y_1^{1/3} y_2^{2/3} |w| |\det V^*|^{1/3}). \end{aligned} \quad (3.21)$$

The remaining terms in the infinite product of (3.12) are regular; they give

$$\prod_{(n_1, n_2) \in \mathbb{Z}^2 \setminus \{(0,0)\}} 1 - \exp\{-2\pi y_2|n_2 z_1 - n_1| + 2\pi i(n_1 x_2 + n_2 x_4)\} \quad (3.22)$$

when $u = 0$, i.e. $w = 0$. Lemma 3.3 then follows from (3.12) with the help of (3.15), (3.21), and (3.22). $\square$

4 $k_3(Q^*)$ and $h(R^3/\Lambda^*)$

Now consider Epstein's zeta function

$$Z_Q(s) = \sum_{m \in \mathbb{Z}^d \setminus \{0\}} \frac{1}{Q[m]^s}, \quad s \in \mathbb{C}, \quad \operatorname{Re} s > \frac{d}{2} \quad (4.1)$$

where Q is a positive definite $d \times d$ matrix. Clearly Z_Q is a special case of the twisted Epstein zeta function considered earlier:

$$Z_Q(s) = \zeta(s, u, 0, Q), \quad \text{if } u \in \mathbb{Z}^d. \quad (4.2)$$

Lemma 4.1 ([8, Epstein]). *As a function of s , $Z_Q(s)$ has a meromorphic extension to $\mathbb{C}$ with only one simple pole at $d/2$ and its residue is $(\det Q)^{-1/2} \pi^{d/2} \Gamma(d/2)^{-1}$. Moreover, Z_Q satisfies the functional equation*

$$\pi^{-s} \Gamma(s) Z_Q(s) = (\det Q)^{-1/2} \pi^{-(d/2-s)} \Gamma\left(\frac{d}{2} - s\right) Z_{Q^{-1}}\left(\frac{d}{2} - s\right).$$

Let $k_d(Q)$ be

$$k_d(Q) = \lim_{s \rightarrow d/2} Z_Q(s) - \frac{(\det Q)^{-1/2} \pi^{d/2} \Gamma(d/2)^{-1}}{s - d/2} \quad (4.3)$$

the constant term in the Laurent series of Z_Q about $d/2$. When $d = 2$, $k_2(Q)$ is given by the first Kronecker limit formula. When $d = 3$, $k_3(Q)$ follows from a formula in [7, Efrat].

Lemma 4.2. *Let $d = 3$ and τ be the triangular matrix associate with Q as in (2.28), (2.29) and (2.30). Then*

$$k_3(Q) = 2\pi(\det Q)^{-1/2} \log(\det Q)^{-1/3} + 2\gamma - 2 - 2 \log y_1^{1/3} y_2^{2/3} - 4 \log g(\tau)$$

where $\gamma = 0.57721\dots$ is Euler's constant and

$$g(\tau) = \exp \left(-\frac{y_1^{1/2} y_2}{8\pi} \sum_{(n_1, n_2) \in \mathbb{Z}^2 \setminus \{(0,0)\}} \frac{y_1^{3/2}}{|n_1 z_1 + n_2|^3} \right) \prod_{(n_1, n_2) \in \mathbb{Z}^2 \setminus \{(0,0)\}} \frac{1 - \exp(-2\pi y_2 |n_2 z_1 - n_1| + 2\pi i(n_1 x_2 + n_2 x_4))}{1 - \exp(-2\pi y_2 |n_2 z_1 - n_1| + 2\pi i(n_1 x_2 + n_2 x_4))}. \quad (4.4)$$

Proof. As explained in [7], the Eisenstein series $E(\tau, t)$ associated with the maximal parabolic subgroup of $SL(3, \mathbb{Z})$ can be written as

$$E(\tau, t) = \sum_{(n_1, n_2, n_3) \neq 1} \frac{(y_1^2 y_2)^t}{(y_1^2 |n_3 z_2 + n_1|^2 + (n_3 x_3 + n_1 x_1 + n_2)^2)^{3t/2}} \quad (4.5)$$

where x_j , y_j , and z_j come from τ as in (2.28) and (3.4). Let

$$E^*(\tau, t) = \zeta^*(3t) E(\tau, t) \quad (4.6)$$

where $\zeta^*(s) = \pi^{-s/2} \Gamma(s/2) \zeta(s)$ and $\zeta(s)$ is the Riemann zeta function. $E^*(\tau, t)$ as a function of t admits a meromorphic continuation to $\mathbb{C}$ with poles at $t = 1, 0$ of residues $2/3, -2/3$ respectively. It is shown in [7] that

$$E^*(\tau, t) = \frac{2/3}{t-1} + \gamma - \log 4\pi - \frac{2}{3} \log y_1 y_2^2 - 4 \log g(\tau) + O(t-1) \quad (4.7)$$

where $g(\tau)$ is given in (4.4).

Let Q be a 3 by 3 positive definite matrix associated with τ as in (2.30) so that

$$Q = (\det Q)^{1/3} (y_1^2 y_2)^{-2/3} \tau \tau'.$$

One relates $Z_Q(s)$ to $E^*(\tau, t)$:

$$\begin{aligned} Z_Q(s) &= \sum_{m \in \mathbb{Z}^3 \setminus \{0\}} \frac{1}{Q[m]^s} \\ &= (\det Q)^{-s/3} \sum_{m \in \mathbb{Z}^3 \setminus \{0\}} \frac{(y_1^2 y_2)^{2s/3}}{|m\tau|^2s} \\ &= (\det Q)^{-s/3} \sum_{m \in \mathbb{Z}^3 \setminus \{0\}} \frac{(y_1^2 y_2)^{2s/3}}{((m_1 y_1 y_2)^2 + (m_1 y_1 x_2 + m_2 y_1)^2 + (m_1 x_3 + m_2 x_1 + m_3)^2)^s} \\ &= (\det Q)^{-s/3} \sum_{m \in \mathbb{Z}^3 \setminus \{0\}} \frac{(y_1^2 y_2)^{2s/3}}{(y_1^2 |m_1 z_2 + m_2|^2 + (m_1 x_3 + m_2 x_1 + m_3)^2)^s} \\ &= (\det Q)^{-s/3} \zeta(2s) \sum_{(m_1, m_2, m_3)=1} \frac{(y_1^2 y_2)^{2s/3}}{(y_1^2 |m_1 z_2 + m_2|^2 + (m_1 x_3 + m_2 x_1 + m_3)^2)^s} \\ &= (\det Q)^{-s/3} \zeta(2s) E^*\left(\tau, \frac{2s}{3}\right) \\ &= (\det Q)^{-s/3} \pi^s \Gamma(s)^{-1} E^*\left(\tau, \frac{2s}{3}\right). \end{aligned} \quad (4.8)$$

By (4.7) with $t = 2s/3$, (4.8) becomes

$$Z_Q(s) = (\det Q)^{-s/3} \pi^s \Gamma(s)^{-1} \frac{1}{s - 3/2} + \gamma - \log 4\pi - \frac{2}{3} \log y_1 y_2^2 - 4 \log g(\tau) + O\left(s - \frac{3}{2}\right). \quad (4.9)$$

Expand the other terms in (4.8) about $s = 3/2$ to find

$$(\det Q)^{-s/3} \pi^s = \pi^{3/2} (\det Q)^{-1/2} + \pi^{3/2} (\det Q)^{-1/2} \log \pi (\det Q)^{-1/3} \left(s - \frac{3}{2}\right) + O\left(s - \frac{3}{2}\right) \quad (4.10)$$

$$\Gamma(s) = \Gamma\left(\frac{3}{2}\right) + \Gamma'\left(\frac{3}{2}\right) \left(s - \frac{3}{2}\right) + O\left(s - \frac{3}{2}\right). \quad (4.11)$$

Note that

$$\Gamma\left(\frac{3}{2}\right) = \frac{\pi^{1/2}}{2}, \quad \frac{\Gamma'(3/2)}{\Gamma(3/2)} = \psi\left(\frac{3}{2}\right) = 2 - 2 \log 2 - \gamma$$

where $\psi = \Gamma'/\Gamma$ is the digamma function. Consequently by (4.10), and (4.11), (4.9) simplifies to

$$Z_Q(s) = \frac{2\pi(\det Q)^{-1/2}}{s - 3/2} + 2\pi(\det Q)^{-1/2} \log(\det Q)^{-1/3} + 2\gamma - 2 - 2 \log y_1^{1/3} y_2^{2/3} - 4 \log g(\tau) + O\left(s - \frac{3}{2}\right) \quad (4.12)$$

and the lemma follows. $\square$

Lemma 4.3. Let Λ be a three-dimensional lattice. Then

$$k_3(Q^*) = 2\pi(\det Q^*)^{-1/2} (2\gamma - 2 + 2 \log(2\pi) + (2\pi)^2 R_{\Lambda, 3/2}(0))$$

where Q^* is a Gram matrix associated with Λ^* .

Proof. Compare $R_{\Lambda, 3/2}(0)$ in Lemma 3.3 and $k_3(Q)$ in Lemma 4.2 with Q substituted by Q^* . $\square$

Recall the height $h(M)$ of a Riemannian manifold defined in (1.16). When M is a flat torus $\mathbb{R}^d/\Lambda$, the eigenfunctions of $-\Delta$ are $e^{2\pi i k \cdot w}$, $k \in \Lambda^*$, and the corresponding eigenvalues are $4\pi^2|k|^2$. Then the height of $\mathbb{R}^d/\Lambda$ is essentially given by Epstein's zeta function because

$$Z(\mathbb{R}^d/\Lambda, s) = \sum_{k \in \Lambda^* \setminus \{0\}} \frac{1}{(2\pi)^{2s} |k|^{2s}} = (2\pi)^{-2s} \sum_{m \in \mathbb{Z}^n \setminus \{0\}} \frac{1}{Q^*[m]^s} = (2\pi)^{-2s} Z_{Q^*}(s) \quad (4.13)$$

where Q^* is a Gram matrix associated with the dual lattice Λ^* .

We reprove a result in [3, Chiu], correcting a minor error.

Lemma 4.4. *Let Q be a Gram matrix associated with lattice Λ . Then*

$$h(\mathbb{R}^d/\Lambda) = (\det Q)^{-1/2} \pi^{-d/2} \Gamma\left(\frac{d}{2}\right) k_d(Q) + \psi\left(\frac{d}{2}\right) - \gamma + 2 \log 2$$

where $\psi = \Gamma'/\Gamma$ is the digamma function. In particular

$$h(\mathbb{R}^3/\Lambda^*) = (\det Q^*)^{1/2} (2\pi)^{-1} k_3(Q^*) - 2\gamma + 2.$$

Proof. By (4.13), the height of $\mathbb{R}^d/\Lambda$ is

$$\begin{aligned} h(\mathbb{R}^d/\Lambda) &= Z'(\mathbb{R}^d/\Lambda, 0) \\ &= -2 \log(2\pi) Z_{Q^*}(0) + Z'_{Q^*}(0). \end{aligned} \quad (4.14)$$

By Lemma 4.1,

$$Z_{Q^*}(s) = (\det Q^*)^{-1/2} \pi^{2s-d/2} \Gamma(s)^{-1} \Gamma\left(\frac{d}{2} - s\right) Z_Q\left(\frac{d}{2} - s\right). \quad (4.15)$$

For s near 0, expand

$$\pi^{2s-d/2} = \pi^{-d/2} + 2\pi^{-d/2} \log \pi s + O(s^2) \quad (4.16)$$

$$\Gamma(s)^{-1} = s + \gamma s^2 + O(s^3) \quad (4.17)$$

$$\Gamma\left(\frac{d}{2} - s\right) = \Gamma\left(\frac{d}{2}\right) - \Gamma'\left(\frac{d}{2}\right) s + O(s^2) \quad (4.18)$$

$$Z_Q\left(\frac{d}{2} - s\right) = -\frac{(\det Q)^{-1/2} \pi^{d/2} \Gamma\left(\frac{d}{2}\right)^{-1}}{s} + k_d(Q) + O(s) \quad (4.19)$$

where (4.19) follows from (4.3). Then

$$Z_{Q^*}(s) = -1 + (\det Q)^{1/2} \pi^{-d/2} \Gamma\left(\frac{d}{2}\right) k_d(Q) + \psi\left(\frac{d}{2}\right) - \gamma - 2 \log \pi s + O(s^2). \quad (4.20)$$

Hence

$$Z_{Q^*}(0) = -1 \quad (4.21)$$

$$Z'_{Q^*}(0) = (\det Q)^{1/2} \pi^{-d/2} \Gamma\left(\frac{d}{2}\right) k_d(Q) + \psi\left(\frac{d}{2}\right) - \gamma - 2 \log \pi \quad (4.22)$$

and consequently by (4.14)

$$h(\mathbb{R}^d/\Lambda) = (\det Q)^{-1/2} \pi^{-d/2} \Gamma\left(\frac{d}{2}\right) k_d(Q) + \psi\left(\frac{d}{2}\right) - \gamma + 2 \log 2 \quad (4.23)$$

from which the lemma follows. $\square$

We now state the key lemma in this paper.

Lemma 4.5. *If $d = 3$, then*

$$h(R^3/\Lambda^*) = (2\pi)^2 R_{\Lambda,3/2}(0) + 2 \log(2\pi).$$

Proof. Compare $R_{\Lambda,3/2}(0)$ in Lemma 4.3 and $h(R^3/\Lambda^*)$ in Lemma 4.4. □

To prove the main theorem, we need a deep result of Sarnak and Strömbergsson.

Theorem 4.6 ([20, Sarnak and Strömbergsson]). *Among three dimensional lattices Λ of unit volume, the height $h(R^3/\Lambda)$ is uniquely minimized by the FCC lattice.*

Proof of Theorem 1.2. By Lemma 4.5 and Theorem 4.6, $R_{\Lambda,3/2}(0)$ is uniquely minimized when Λ^* is the FCC lattice. Since the FCC lattice is the dual lattice of the BCC lattice by (2.23) and (2.24), Λ must be the BCC lattice. □

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