Discrete Minimal Energy on Flat Tori and Four-Point Maximal Polarization on S^2

By

Yujian Su

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Approved:

Professor Douglas Hardin

Professor Akram Aldroubi

Professor Kirill Bolotin

Professor Alexander Powell

Professor Edward Saff

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Introduction

Consider a finite collection of classical point charges constrained on the surface of a conductor and interacting through a Coulomb potential. In the absence of other forces, physics tells us these charges will arrange themselves in an optimal configuration so that the total potential energy attains its minimum. In this case the loss of potential energy is dissipated as heat. For a sphere conductor determining the stable configuration and the minimum potential energy is called the *Thomson Problem*.

This phenomenon leads us to the study of discrete minimum energy problems and we shall formulate this investigation in a more general setting, namely, we will study this question in various dimensions and the pairwise interaction will be from a larger class of potentials such as Riesz potentials. Specifically, we are interested in the positions of these charges and their minimal potential energy.

For a given potential $f : [0, \infty) \to \mathbb{R} \cup \{+\infty\}$ and any N-point configuration $\omega_N = (x_1, \ldots, x_N) \in (\mathbb{R}^d)^N$ we consider the *f-energy* of ω_N

$$E_f(\omega_N) := \sum_{j \neq k} f(|x_j - x_k|^2), \tag{1.1}$$

and for a subset $\Omega \subset \mathbb{R}^d$, we consider the *$N$-point minimal f-energy on Ω*

$$\mathscr{E}_f(\Omega, N) := \inf_{\omega_N \in \Omega^N} E_f(\omega_N). \tag{1.2}$$

A configuration that attains this infimum is called an *N-point optimal configuration on Ω*. If we further assume that f is lower-semicontinuous and Ω is compact then it is elementary to show an N-point optimal configuration on Ω always exists.

In this dissertation we are mostly concerned with the Riesz s-potentials $f_s(x) = |x|^{-\frac{s}{2}}$

for $s > 0$ and the logarithmic potential $f_{\log}(x) = \frac{1}{2}\log\frac{1}{|x|}$. It is easy to verify that Riesz potentials and logarithmic potential are indeed lower-semicontinuous. For simplicity, we shall write E_s, $E_{\log}$, $\mathscr{E}_s$, $\mathscr{E}_{\log}$ for E_{f_s}, $E_{f_{\log}}$, $\mathscr{E}_{f_s}$, $\mathscr{E}_{f_{\log}}$, respectively. However, it is worth considering a larger class of potential functions. A C^∞ function $f : I \to \mathbb{R} \cup \{+\infty\}$ is *completely monotonic* if $(-1)^k f^{(k)}(x) \geq 0$ for all $x \in I$ and all $k \geq 0$ and *strictly completely monotonic* if strict inequality always holds in the interior of I. An N-point configuration is *universally optimal* if it is optimal for each completely monotonic potential function. By Bernstein's theorem (cf. [1, Theorem 12b, page161]) a function is completely monotonic on $(0, \infty)$ if and only if there exists a non-decreasing function $\alpha(t)$ such that

$$f(x) = \int_0^\infty e^{-xt} d\alpha(t). \tag{1.3}$$

It is elementary to verify that all Riesz s-potentials are completely monotonic on $(0, \infty)$. We recall the Gamma function

$$\Gamma(s) = \int_0^\infty x^{s-1} e^{-x} dx.$$

It is then straightforward to show that any Riesz s-potential can be written as

$$\frac{1}{(|x|^2)^{\frac{s}{2}}} = \frac{1}{|x|^s} = \int_0^\infty e^{-|x|^2 t} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt. \tag{1.4}$$

Comparing (1.3) and (1.4) it again shows Riesz s-potentials are in the class of completely monotonic functions.

It turns out that many optimal configurations are also the most important configurations in geometry. For example, the vertices of a regular tetrahedron and the vertices of a regular icosahedron are universally optimal configurations on S^2. Many special configurations were studied and proved to be optimal in the past but it was not until 2007 that Cohn and Kumar([2]) proved that any sharp configuration is universally optimal on the unit sphere

S^{d-1}. Here a finite subset of S^{d-1} is a *sharp configuration* if there are m inner products between distinct points in it and it is a spherical $(2m-1)$-design. Recall that a finite subset ω_N of N points on S^{d-1} is a *spherical M-design* if every polynomial of degree up to M has the same average over the subset as over S^{d-1};

$$\int_{S^{d-1}} p(x) \, d\sigma(x) = \frac{1}{M} \sum_{x \in \omega_N} p(x),$$

where σ denotes normalized surface area measure on S^{d-1}. Sharp configurations have been well-studied in coding theory (cf. [3]) and Cohn and Kumar's result shows that a large class of important configurations are universally optimal on S^{d-1}.

What if these points are not confined in a compact set but in $\mathbb{R}^d$? If the interaction potential is strictly decreasing to 0, then all the points will simply go to infinity and the potential energy is 0. To make sense of this problem we need to add some constraints about the density of the points. They are required to be distributed in a uniform way. In nature there is a structure called the crystal structure. One can think of it as an array of boxes infinitely repeating in all directions, and the structure of the box is repeated as well. Therefore a crystal structure is determined by the shape of the box and the structure inside the box. In mathematics such a configuration is called a *periodic configuration*. For a $d \times d$ nonsingular matrix A, let $\Lambda := A\mathbb{Z}^d$ denote the *lattice generated by A*. The parallelotope $\Omega_\Lambda := A[0,1)^d$ is a fundamental domain for $\mathbb{R}^d/\Lambda$. The volume of Ω_Λ equals $|\det A|$ and is called the *co-volume of* Λ. Let $\omega_N = \{x_j\}_{j=1}^N$ be an N-point configuration in $\mathbb{R}^d$ such that $x_j - x_k \notin \Lambda$ for any $j \neq k$. Then $\omega_N + \Lambda$ is called an *N-point Λ-periodic configuration* generated by ω_N.

For a periodic configuration $\omega_N + \Lambda$ and a potential function f, we consider the f-energy of $\omega_N + \Lambda$

$$E_{f,\Lambda}^{cp}(\omega_N) = \sum_{j \neq k} \sum_{v \in \Lambda} f(|x_j - x_k + v|^2), \tag{1.5}$$

and the *N*-point minimal energy

$$\mathscr{E}^{cp}_{f,\Lambda}(N) = \inf_{\omega_N \in (\mathbb{R}^d)^N} E^{cp}_{f,\Lambda}(\omega_N).$$

For a Riesz *s*-potential where $s > d$, (1.5) can be written as

$$E^{cp}_{s,\Lambda}(\omega_N) = \sum_{j \neq k} \zeta_\Lambda(s; x_j - x_k),$$

where

$$\zeta_\Lambda(s; x) := \sum_{v \in \Lambda} \frac{1}{|x + v|^s}, \qquad s > d, x \in \mathbb{R}^d.$$

$\zeta_\Lambda(s; x)$ is called the *Epstein Hurwitz zeta function for the lattice* Λ and can be analytically continued to $\mathbb{C} \setminus d$. Notice that $\zeta_\Lambda(s; x)$ is Λ-periodic, that is, $\zeta_\Lambda(s; x + v) = \zeta_\Lambda(s; x)$ for all $v \in \Lambda$. More generally, for a Λ-periodic potential $F : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$, we consider the *F*-energy of an *N*-tuple $\omega_N = (x_1, \ldots, x_N) \in (\mathbb{R}^d)^N$

$$E_F(\omega_N) := \sum_{j \neq k} F(x_j - x_k), \tag{1.6}$$

and the *N-point minimal F-energy*

$$\mathscr{E}_F(N) := \inf_{\omega_N \in (\mathbb{R}^d)^N} E_F(\omega_N). \tag{1.7}$$

Unlike the sphere case, not much is known about optimal configurations in $\mathbb{R}^d$. In 1986, Montgomery proved (cf. [4]) that the hexagonal lattice A_2 is universally optimal among all lattice configurations; i.e.,

$$\zeta_{A_2}(s) < \zeta_\Lambda(s),$$

for each $s > 0$ and each lattice $\Lambda \subset \mathbb{R}^2$ of co-volume 1 not equal to A_2. In 2007, Cohn

and Kumar studied the one dimensional case of this problem and proved that any equally spaced configuration is universally optimal among periodic configurations in $\mathbb{R}^1$(cf. [2]). They also conjectured that the A_2 hexagonal lattice in $\mathbb{R}^2$, the E_8 root lattice in $\mathbb{R}^8$, and the Leech lattice in $\mathbb{R}^{24}$ are universally optimal. Coulangeon and Schurmann then proved (cf. [5]) that A_2, D_4, E_8 and the Leech lattice are locally universally optimal among periodic configurations. In chapter 4 we provide a new proof for the 1-dimensional case where we derive some nice properties about the classical theta function. We also study the cases for $N = 2, 3$ where the associated lattice Λ is the hexagonal lattice and prove the desired configurations are universally optimal. Specifically, we will prove the following theorem

Theorem 4.2.2. *Let the potential function $f : [0, \infty) \to \mathbb{R} \cup \{\infty\}$ be completely monotonic on $(0, \infty)$ with $f(0) = \lim\limits_{x \to 0^+} f(x)$ and satisfies $f(x) = O(|x|^{-\frac{1}{2} - \varepsilon})$ for some $\varepsilon > 0$ as $|x| \to \infty$. Let $u_1 = [1, 0]^T$, $u_2 = [\frac{1}{2}, \frac{\sqrt{3}}{2}]^T$, and $P = \frac{1}{3}(u_1 + u_2) = [\frac{1}{2}, \frac{\sqrt{3}}{6}]^T$, $Q = \frac{2}{3}(u_1 + u_2) = [1, \frac{\sqrt{3}}{3}]^T$. Consider the f-energy of ω_N associated to the lattice $\widetilde{A_2} := [u_1, u_2]\mathbb{Z}^2 = (\frac{\sqrt{3}}{2})^{\frac{1}{2}} A_2$.*

(1) For $N = 2$, let $\omega_2^* = \{0, P\}$ or $\{0, Q\}$ up to translations. Then for any 2-point config-uration $\omega_2 \in (\mathbb{R}^2)^2$,

$$E_{f, \widetilde{A_2}}^{cp}(\omega_2) \geq E_{f, \widetilde{A_2}}^{cp}(\omega_2^*).$$

(2) For $N = 3$, let $\omega_3^* = \{0, P, Q\}$ up to translations. Then for any 3-point configuration $\omega_3 \in (\mathbb{R}^2)^3$,

$$E_{f, \widetilde{A_2}}^{cp}(\omega_3) \geq E_{f, \widetilde{A_2}}^{cp}(\omega_3^*).$$

Another open problem concerns the asymptotic behaviour of minimal energy for Riesz s-potentials and logarithmic potential in $\mathbb{R}^d$. We would like to obtain a series expansion of minimal energy in terms of N as N approaches infinity. For the compact case, where we have N points confined in some nice d-Hausdorff dimensional compact space Ω, it is

known that the minimal energy $\mathcal{E}_s(\Omega, N)$ has the following asymptotic expansion:

$$\mathcal{E}_s(\Omega, N) = \frac{C_{s,d}}{\mathcal{H}_d(\Omega)^{\frac{s}{d}}} \cdot N^{1+\frac{s}{d}} + o\left(N^{1+\frac{s}{d}}\right), \qquad s > d,$$

$$\mathcal{E}_s(\Omega, N) = W_s(\Omega)N^2 + o\left(N^2\right), \qquad 0 < s < d \text{ or } s = \log.$$

where $W_s(\Omega)$ is the Wiener constant of Ω with respect to the Riesz s-potential and the logarithmic potential. We know that $W_s(\Omega)$ is determined by any weak* limit of the normalized counting measure generated by the optimal N-point configurations as $N \to \infty$. And it seems that it is the next order term in the asymptotic expansion that really reflects the local structure of the N-point optimal configurations as $N \to \infty$. In the paper [6] the next order term for the d-dimensional sphere case was surveyed and was conjectured to be of order $N^{1+\frac{s}{d}}$ for $s < d$.

We would like to investigate this problem for any periodic configuration in $\mathbb{R}^d$ with $s < d$ or $s = \log$. Notice that the sum in (1.5) does not converge in this case. It is suggested that (cf. [7]) the new periodic potential $F_{s,\Lambda}(x)$ and $F_{\log,\Lambda}(x)$ should be considered where

$$F_{s,\Lambda}(x) := \sum_{v \in \Lambda} \int_1^\infty e^{-|x+v|^2 t} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt + \frac{1}{|\Lambda|} \sum_{w \in \Lambda^* \setminus \{0\}} e^{2\pi i w \cdot x} \int_0^1 \frac{\pi^{\frac{d}{2}}}{t^{\frac{d}{2}}} e^{-\frac{\pi^2 |w|^2}{t}} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt, \qquad s > 0,$$

and

$$F_{\log,\Lambda}(x) := \sum_{v \in \Lambda} \int_1^\infty e^{-|x+v|^2 t} \frac{dt}{t} + \frac{1}{|\Lambda|} \sum_{w \in \Lambda^* \setminus \{0\}} e^{2\pi i w \cdot x} \int_0^1 \frac{\pi^{\frac{d}{2}}}{t^{\frac{d}{2}}} e^{-\frac{\pi^2 |w|^2}{t}} \frac{dt}{t}.$$

As discussed in Section 2.1, it turns out that $F_{s,\Lambda}(x)$ is an entire function of s satisfying

$$F_{s,\Lambda}(x) = \zeta_\Lambda(s; x) + \frac{2\pi^{\frac{d}{2}} |\Lambda|^{-1}}{\Gamma(\frac{s}{2})(d-s)},$$

for $s > d$ and, hence, provides an analytic continuation of $\zeta_\Lambda(s; x)$ for $s \in \mathbb{C} \setminus \{d\}$. Denote the respective periodic energy of ω_N and the minimal N-point periodic energy by $E_{s,\Lambda}(\omega_N)$, $E_{\log,\Lambda}(\omega_N)$, $\mathcal{E}_{s,\Lambda}(N)$ and $\mathcal{E}_{\log,\Lambda}(N)$. Our main result is that

Theorem 2.2.1. *Let Λ be a lattice in $\mathbb{R}^d$ with co-volume $|\Lambda| > 0$. Then, as $N \to \infty$,*

$$\mathscr{E}_{s,\Lambda}(N) = \frac{2\pi^{\frac{d}{2}}|\Lambda|^{-1}}{\Gamma(\frac{s}{2})(d-s)} N^2 + C_{s,d}|\Lambda|^{-s/d} N^{1+\frac{s}{d}} + o(N^{1+\frac{s}{d}}), \qquad 0 < s < d, \qquad (2.20)$$

$$\mathscr{E}_{\log,\Lambda}(N) = \frac{2\pi^{\frac{d}{2}}|\Lambda|^{-1}}{d} N(N-1) - \frac{2}{d}N\log N + \left(C_{\log,d} - 2\zeta_\Lambda'(0)\right)N + o(N). \qquad (2.21)$$

where $C_{\log,d}$ and $C_{s,d}$ are constants independent of Λ.

The second topic of this thesis focuses on the maximal polarization problem. Given a compact set Ω and a potential function f, any n-point configuration ω_N will generate some f-potential at each point x in Ω.

$$U^f(\omega_N; x) := \sum_{k=1}^{N} f(|x - x_k|^2). \qquad (1.8)$$

The minimal potential in Ω

$$M^f(\omega_N; \Omega) := \min_{x \in \Omega} U^f(\omega_N; x), \qquad (1.9)$$

is called the *f-polarization of ω_N*. The maximal polarization problem requires maximizing this quantity among all N-point configurations in Ω. An N-point configuration is called optimal for the N-point maximal polarization problem if it attains this maximum. The reason this problem is important is that it is considered to be a generalization of the minimal covering problem, that is, minimizing the radius of N balls centered in Ω that cover the set Ω.

Not much is known about optimal configurations for the maximal polarization problem. For example, finding a $(d+1)$-point optimal configuration in S^{d-1} for the polarization problem remains open for $d \geq 4$. The case when $\Omega = S^1$ is investigated in [8] and as a particular consequence any equally spaced configuration on S^1 is optimal for Riesz potentials. In this dissertation we are concerned with the case where $\Omega = S^2$ and $n = 4$ and we will

prove

Theorem 3.2.1. *Let $f : [0,4] \to [0,\infty]$ be non-increasing and strictly convex with $f(0) = \lim_{x \to 0^+} f(x)$. Then ω_4 is optimal for the 4-point maximal polarization problem on S^2, i.e., $M^f(\omega_4; S^2) = M_4^f(S^2)$, if and only if $\omega_4 = \omega_T$ up to rotations, where ω_T is a configuration that consists of vertices of a regular tetrahedron.*

We also conjecture that the vertices of any regular d-simplex is optimal for the maximal polarization problem on S^{d-1} for a large class of potentials.

Chapter 2

Second order asymptotics for long-range Riesz potentials on flat tori

2.1   Preliminaries

Let $A = [v_1, \ldots, v_d]$ be a $d \times d$ nonsingular matrix with j-th column v_j and let $\Lambda = \Lambda_A := A\mathbb{Z}^d$ denote the lattice generated by A. The set

$$\Omega = \Omega_\Lambda := \left\{ w : w = \sum_{j=1}^{d} \alpha_j v_j, \ \alpha_j \in [0,1), \ j = 1, 2, \ldots, d \right\}.$$

is a fundamental domain of the quotient space $\mathbb{R}^d / \Lambda$; i.e., the collection of sets $\{\Omega + v : v \in \Lambda\}$ tiles $\mathbb{R}^d$. The volume of Ω_Λ, denoted by $|\Lambda|$, equals $|\det A|$ and is called the *co-volume* of Λ (in fact, any measurable fundamental domain of Λ has the same volume). We will let Λ^* denote the the *dual lattice* of Λ which is the lattice generated by $(A^T)^{-1}$.

For an interaction potential $F : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$, we consider the *F-energy* of an N-tuple $\omega_N = (x_1, \ldots, x_N) \in (\mathbb{R}^d)^N$

$$E_F(\omega_N) := \sum_{k=1}^{N} \sum_{\substack{j=1 \\ j \neq k}}^{N} F(x_k - x_j), \tag{2.1}$$

and for a subset $A \subset \mathbb{R}^d$, we consider the *N-point minimal F-energy*

$$\mathscr{E}_F(A, N) := \inf_{\omega_N \in A^N} E_F(\omega_N). \tag{2.2}$$

In this chapter we are mostly concerned with Λ-periodic potentials F, that is, $F(x+v) = F(x)$ for all $v \in \Lambda$. For such an F, the energy $E_F(\omega_N) = E_F(x_1, \ldots, x_N)$ is Λ-periodic in each component x_k and so, without loss of generality, we may assume that $\omega_N \in (\Omega_\Lambda)^N$; i.e., $\mathscr{E}_F(\mathbb{R}^d, N) = \mathscr{E}_F(\Omega_\Lambda, N)$. Specifically, we consider periodized Riesz potentials and

periodized logarithmic potentials and $A = \mathbb{R}^d$ (or, equivalently $A = \Omega_\Lambda$) as we next describe.

For $s > d$, we consider the periodic potential generated by the Riesz s-potential as follows

$$\zeta_\Lambda(s;x) := \sum_{v \in \Lambda} \frac{1}{|x+v|^s}, \qquad s > d, x \in \mathbb{R}^d \setminus \Lambda, \tag{2.3}$$

which, as shown in Lemma 2.1.1, is finite for $x \notin \Lambda$ and equals $+\infty$ when $x \in \Lambda$, see Section 2.3 for further properties of $\zeta_\Lambda(s;x)$. Then $\zeta_\Lambda(s;x-y)$ can be considered to be the energy required to place a unit charge at location $x \in \mathbb{R}^d$ in the presence of unit charges placed at $y + \Lambda = \{y+v: v \in \Lambda\}$ with charges interacting through the Riesz s-potential. For $s \leq d$, the sum on the right side of (2.3) is infinite for all $x \in \mathbb{R}^d$. In [7], Λ-periodic energy problems for a class of long range potentials are considered and it is shown that for the case of the Riesz potential with $s \leq d$, the appropriate energy problem can be obtained through analytic continuation. Specifically, we define

$$F_{s,\Lambda}(x) := \sum_{v \in \Lambda} \int_1^\infty e^{-|x+v|^2 t} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt + \frac{1}{|\Lambda|} \sum_{w \in \Lambda^* \setminus \{0\}} e^{2\pi i w \cdot x} \int_0^1 \frac{\pi^{\frac{d}{2}}}{t^{\frac{d}{2}}} e^{-\frac{\pi^2|w|^2}{t}} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt, \tag{2.4}$$

and, in the following lemma, verify basic analytic properties of $F_{s,\Lambda}$.

Lemma 2.1.1. *$F_{s,\Lambda}(x)$ is finite for $x \in \mathbb{R}^d \setminus \Lambda$. Furthermore, for fixed $x \in \mathbb{R}^d \setminus \Lambda$, $F_{s,\Lambda}(x)$ is an entire function of s satisfying*

$$F_{s,\Lambda}(x) = \zeta_\Lambda(s;x) + \frac{2\pi^{\frac{d}{2}}|\Lambda|^{-1}}{\Gamma(\frac{s}{2})(d-s)}. \qquad s > d, \tag{2.5}$$

Proof. Let $x \in \mathbb{R}^d \setminus \Lambda$ and choose δ such that $0 < \delta < |x+v|^2$ for all $v \in \Lambda$. Consider the integrand

$$\int_1^\infty \sum_{v \in \Lambda} e^{-|x+v|^2 t} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt = \int_1^\infty \sum_{v \in \Lambda} e^{-(|x+v|^2-\delta)t} \frac{e^{-\delta t} t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt.$$

The sum $\sum_{v \in \Lambda} e^{-(|x+v|^2-\delta)t}$ is bounded on $[1,\infty)$ since it is finite at $t = 1$ and decreasing

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on $[1, \infty)$. Therefore the above integrand is finite and it follows from Tonelli's theorem that the first sum in (2.4) is finite. For the second sum in (2.4) let w_0 be an element in $\Lambda^* \setminus \{0\}$ with minimal length. Consider the integrand

$$\int_0^1 \sum_{w \in \Lambda^* \setminus \{0\}} e^{-\frac{\pi^2 |w|^2}{t}} \frac{t^{\frac{s-d}{2}-1}}{\Gamma(\frac{s}{2})} dt = \int_0^1 \sum_{w \in \Lambda^* \setminus \{0\}} e^{-\frac{\pi^2(|w|^2-|w_0|^2)}{t}} \frac{e^{-\frac{\pi^2 |w_0|^2}{t}} t^{\frac{s-d}{2}-1}}{\Gamma(\frac{s}{2})} dt.$$

The sum $\sum_{w \in \Lambda^* \setminus \{0\}} e^{-\frac{\pi^2(|w|^2-|w_0|^2)}{t}}$ is bounded on $(0, 1]$ since it is finite at $t = 1$ and increasing on $(0, 1]$. Therefore the above integrand is finite and it follows from Tonelli's theorem that the second sum in (2.4) converges absolutely. Notice that $\frac{1}{\Gamma(\frac{s}{2})}$ is an entire function and thus each term in both sums in (2.4) is an entire function of s. The uniform convergence of the sums for s in any compact subset of $\mathbb{C}$ then implies that $F_{s,\Lambda}(x)$ is an entire function of s. For $s > d$, using (1.4) and the Poisson summation formula (see appendix B) we get

$$\zeta_\Lambda(s;x) = \sum_{v \in \Lambda} \int_0^\infty e^{-|x+v|^2 t} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt = \sum_{v \in \Lambda} \int_1^\infty e^{-|x+v|^2 t} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt + \sum_{v \in \Lambda} \int_0^1 e^{-|x+v|^2 t} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt$$

$$= \sum_{v \in \Lambda} \int_1^\infty e^{-|x+v|^2 t} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt + \frac{1}{|\Lambda|} \sum_{w \in \Lambda^*} e^{2\pi i w \cdot x} \int_0^1 \frac{\pi^{\frac{d}{2}}}{t^{\frac{d}{2}}} e^{-\frac{\pi^2 |w|^2}{t}} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt$$

$$= \sum_{v \in \Lambda} \int_1^\infty e^{-|x+v|^2 t} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt + \frac{1}{|\Lambda|} \sum_{w \in \Lambda^* \setminus \{0\}} e^{2\pi i w \cdot x} \int_0^1 \frac{\pi^{\frac{d}{2}}}{t^{\frac{d}{2}}} e^{-\frac{\pi^2 |w|^2}{t}} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt$$

$$+ \frac{1}{|\Lambda|} \int_0^1 \frac{\pi^{\frac{d}{2}} t^{\frac{s-d}{2}-1}}{\Gamma(\frac{s}{2})} dt$$

$$= F_{s,\Lambda}(x) - \frac{2\pi^{\frac{d}{2}} |\Lambda|^{-1}}{\Gamma(\frac{s}{2})(d-s)}$$

$\square$

Lemma 2.1.1 shows that (2.4) provides an analytic continuation of $\zeta_\Lambda(\cdot;x)$ to $\mathbb{C} \setminus \{d\}$ (note that $\zeta_\Lambda(s;x)$ has a simple pole at $s = d$ for $x \notin \Lambda$). We refer to (the analytically extended) $\zeta_\Lambda(s;x)$ as the *Epstein Hurwitz zeta function for the lattice* Λ. We shall also need

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the *Epstein zeta function* defined for $s > d$ by

$$\zeta_\Lambda(s) := \sum_{v \in \Lambda \setminus \{0\}} \frac{1}{|v|^s}. \tag{2.6}$$

Using a similar argument and calculation as in the proof of Lemma 2.1.1, we can prove the following lemma:

Lemma 2.1.2 (cf. [9]). *The Epstein zeta function $\zeta_\Lambda(s)$ can be analytically continued to $\mathbb{C} \setminus \{d\}$ through the following formula :*

$$\zeta_\Lambda(s) = \frac{2}{\Gamma(\frac{s}{2})} \left(\frac{2\pi^{\frac{d}{2}} |\Lambda|^{-1}}{s-d} - \frac{1}{s} \right) + \sum_{v \in \Lambda \setminus \{0\}} \int_1^\infty e^{-|v|^2 t} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt$$

$$+ \frac{1}{|\Lambda|} \sum_{w \in \Lambda^* \setminus \{0\}} \int_0^1 \frac{\pi^{\frac{d}{2}}}{t^{\frac{d}{2}}} e^{-\frac{\pi^2 |w|^2}{t}} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt.$$

Remark 2.1.3. *From $\lim_{s \to 0+} \Gamma(\frac{s}{2}) = \infty$ and $\lim_{s \to 0+} \frac{s}{2}\Gamma(\frac{s}{2}) = \lim_{s \to 0+} \Gamma(\frac{s}{2}+1) = \Gamma(1) = 1$, it follows that $\zeta_\Lambda(0) = -1$ and $\zeta_\Lambda(0;x) \equiv 0$ for any lattice Λ.*

In [7], analytic continuation and periodized Riesz potentials are connected through the use of *convergence factors*; i.e., a parametrized family of functions $g_a : \mathbb{R}^d \to [0, \infty)$ such that

(a) for $a > 0$, $f_s(x)g_a(x)$ decays sufficiently rapidly as $|x| \to \infty$ so that

$$F_{s,a,\Lambda}(x) := \sum_{v \in \Lambda} f_s(x+v)g_a(x+v)$$

converges to a finite value for all $x \notin \Lambda$, and

(b) $\lim_{a \to 0^+} g_a(x) = 1$ for all $x \in \mathbb{R}^d \setminus \{0\}$.

For example, the family of Gaussians $g_a(x) = e^{-a|x|^2}$ is a convergence factor for Riesz potentials. In [7], it is shown that for a large class of convergence factors $\{g_a\}_{a>0}$ (including

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the Gaussian convergence family) one may choose C_a (depending on the convergence factor $\{g_a\}_{a>0}$) such that

$$F_{s,\Lambda}(x) = \lim_{a\to 0^+} \left(F_{s,a,\Lambda}(x) - C_a \right). \tag{2.7}$$

Then, for $a > 0$, $F_{s,a,\Lambda}(x-y)$ represents the energy required to place a unit charge at location x in the presence of unit charges placed at $y + \Lambda = \{y + v : v \in \Lambda\}$ with charges interacting through the potential $f_s(x)g_a(x)$. This leads us to consider, for $s > 0$, the *periodic Riesz s-energy of ω_N associated with the lattice Λ* defined by

$$E_{s,\Lambda}(\omega_N) := \sum_{\substack{1\leq k,j\leq N \\ k\neq j}} F_{s,\Lambda}(x_k - x_j), \tag{2.8}$$

as well as the *minimal N-point periodic Riesz s-energy*

$$\mathscr{E}_{s,\Lambda}(N) := \mathscr{E}_{F_{s,\Lambda}}(\mathbb{R}^d; N) = \inf_{\omega_N\in(\mathbb{R}^d)^N} E_{s,\Lambda}(\omega_N). \tag{2.9}$$

We shall also consider the *periodic logarithmic potential associated with Λ* generated from the logarithmic potential using convergence factors as above and resulting in the definition

$$F_{\log,\Lambda}(x) := \sum_{v\in\Lambda} \int_1^\infty e^{-|x+v|^2 t} \frac{\mathrm{d}t}{t} + \frac{1}{|\Lambda|} \sum_{w\in\Lambda^*\backslash\{0\}} e^{2\pi i w\cdot x} \int_0^1 \frac{\pi^{\frac{d}{2}}}{t^{\frac{d}{2}}} e^{-\frac{\pi^2|w|^2}{t}} \frac{\mathrm{d}t}{t}. \tag{2.10}$$

Comparing (2.10) and (2.4), it is not difficult to obtain (cf. [7]) the relations

$$F_{\log,\Lambda}(x) = \lim_{s\to 0} \Gamma\left(\frac{s}{2}\right) F_{s,\Lambda}(x) = 2\left(\frac{d}{ds}F_{s,\Lambda}(x)\right)\bigg|_{s=0} = 2\zeta'_\Lambda(0;x) + \frac{2\pi^{d/2}|\Lambda|^{-1}}{d}, \tag{2.11}$$

where the prime denotes differentiation with respect to the variable s. We then define the

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periodic logarithmic energy of $\omega_N = (x_1, \ldots, x_N)$,

$$E_{\log,\Lambda}(\omega_N) := \sum_{\substack{1 \le k,j \le N \\ k \ne j}} F_{\log,\Lambda}(x_j - x_k), \tag{2.12}$$

and also the *N-point minimal periodic logarithmic energy for* Λ,

$$\mathscr{E}_{\log,\Lambda}(N) := \inf_{\omega_N \in (\mathbb{R}^d)^N} E_{\log,\Lambda}(\omega_N). \tag{2.13}$$

For $0 < s < d$, the kernel $K_{s,\Lambda}(x,y) := F_{s,\Lambda}(x-y)$ is positive definite and integrable on $\Omega_\Lambda \times \Omega_\Lambda$ and so there is a unique probability measure μ_s (called the *Riesz s-equilibrium measure*) that minimizes the continuous Riesz *s*-energy

$$I_{s,\Lambda}(\mu) := \iint_{\Omega_\Lambda \times \Omega_\Lambda} K_{s,\Lambda}(x,y) \mathrm{d}\mu(x) \mathrm{d}\mu(y)$$

over all Borel probability measures μ on Ω_Λ. From the periodicity of $F_{s,\Lambda}$ and the uniqueness of the equilibrium measure, it follows that $\mu_s = \lambda_d$ where λ_d denotes Lebesgue measure restricted to Ω_Λ and normalized so that $\lambda_d(\Omega_\Lambda) = 1$; i.e., λ_d is the normalized Haar measure for $\Omega_\Lambda = \mathbb{R}^d/\Lambda$. The periodic logarithmic kernel $K_{\log,\Lambda}(x,y) := F_{\log,\Lambda}(x-y)$ is conditionally positive definite and integrable and it similarly follows that λ_d is the unique equilibrium measure minimizing the periodic logarithmic energy

$$I_{\log,\Lambda}(\mu) := \iint_{\Omega_\Lambda \times \Omega_\Lambda} K_{\log,\Lambda}(x,y) \mathrm{d}\mu(x) \mathrm{d}\mu(y)$$

over all Borel probability measures μ on Ω_Λ.

It is not difficult to verify (cf. [7]) that

$$\int_{\Omega_\Lambda} \zeta_\Lambda(s;x) \, \mathrm{d}\lambda_d(x) = 0, \qquad 0 < s < d, \tag{2.14}$$

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and

$$\int_{\Omega_\Lambda} \zeta_\Lambda'(0;x) \, d\lambda_d(x) = 0, \tag{2.15}$$

from which we obtain

$$I_{s,\Lambda}(\lambda_d) = \frac{2\pi^{\frac{d}{2}}|\Lambda|^{-1}}{\Gamma(\frac{s}{2})(d-s)}, \qquad 0 < s < d, \tag{2.16}$$

and

$$I_{\log,\Lambda}(\lambda_d) = \frac{2\pi^{d/2}|\Lambda|^{-1}}{d}. \tag{2.17}$$

It then follows (cf. [10]) that

$$\lim_{N\to\infty} \frac{\mathscr{E}_{s,\Lambda}(N)}{N^2} = \frac{2\pi^{\frac{d}{2}}|\Lambda|^{-1}}{\Gamma(\frac{s}{2})(d-s)}, \qquad 0 < s < d, \tag{2.18}$$

and

$$\lim_{N\to\infty} \frac{\mathscr{E}_{\log,\Lambda}(N)}{N^2} = \frac{2\pi^{d/2}|\Lambda|^{-1}}{d}. \tag{2.19}$$

2.2   Main Results

Our main result is the following asymptotic expansion of the periodic Riesz and logarithmic minimal energy as $N \to \infty$.

Theorem 2.2.1. *Let Λ be a lattice in $\mathbb{R}^d$ with co-volume $|\Lambda| > 0$. Then, as $N \to \infty$,*

$$\mathscr{E}_{s,\Lambda}(N) = \frac{2\pi^{\frac{d}{2}}|\Lambda|^{-1}}{\Gamma(\frac{s}{2})(d-s)}N^2 + C_{s,d}|\Lambda|^{-s/d}N^{1+\frac{s}{d}} + o(N^{1+\frac{s}{d}}), \qquad 0 < s < d, \tag{2.20}$$

$$\mathscr{E}_{\log,\Lambda}(N) = \frac{2\pi^{\frac{d}{2}}|\Lambda|^{-1}}{d}N(N-1) - \frac{2}{d}N\log N + \left(C_{\log,d} - 2\zeta_\Lambda'(0)\right)N + o(N). \tag{2.21}$$

where $C_{\log,d}$ and $C_{s,d}$ are constants independent of Λ.

Petrache and Serfaty establish in [11] a result closely related to (2.20) for point configurations interacting through a Riesz *s* potential and confined by an external field for values

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of the Riesz parameter $d - 2 \leq s \leq d$ and Sandier and Serfaty prove in [12] a result closely related to (2.21) for the case that $s = \log$ and $d = 2$.

For comparison, when $s \geq d$ it is known that the leading order term of $\mathscr{E}_{s,\Lambda}(N)$ is the same as that of $\mathscr{E}_s(\Omega_\Lambda, N) := \mathscr{E}_{f_s}(\Omega_\Lambda, N)$.

Theorem 2.2.2 ([13], [7]). *Let Λ be a lattice in $\mathbb{R}^d$ with co-volume $|\Lambda| > 0$. For $s > d$, there is a positive and finite constant $C_{s,d}$ such that*

$$\lim_{N \to \infty} \frac{\mathscr{E}_{s,\Lambda}(N)}{N^{1+s/d}} = \lim_{N \to \infty} \frac{\mathscr{E}_s(\Omega_\Lambda; N)}{N^{1+s/d}} = C_{s,d}|\Lambda|^{-s/d}, \qquad s > d, \tag{2.22}$$

$$\lim_{N \to \infty} \frac{\mathscr{E}_{d,\Lambda}(N)}{N^2 \log N} = \lim_{N \to \infty} \frac{\mathscr{E}_d(\Omega_\Lambda, N)}{N^2 \log N} = \frac{2\pi^{d/2}}{d\Gamma(\frac{d}{2})|\Lambda|}, . \tag{2.23}$$

By considering scaled lattice configurations (see Lemma 2.3.2) of the form $\omega_{m^d}^\Lambda := (1/m)\Lambda \cap \Omega_\Lambda$ for a lattice Λ of co-volume 1, we obtain the following upper bound for $C_{s,d}$ that holds both for $0 < s < d$ and $s = \log$ where $C_{s,d}$ is as in Theorem 2.2.1 as well as for $s > d$ where $C_{s,d}$ is as in Theorem 2.2.1.

Corollary 2.2.3. *Let Λ be a d-dimensional lattice with co-volume 1. Then,*

$$C_{s,d} \leq \begin{cases} \zeta_\Lambda(s), & s > 0, s \neq d, \\ 2\zeta_\Lambda'(0), & s = \log. \end{cases} \tag{2.24}$$

The constant $C_{s,d}$ for $s > d$ appearing in (2.22) is known only in the case $d = 1$ where $C_{s,1} = \zeta_\mathbb{Z}(s) = 2\zeta(s)$ and $\zeta(s)$ denotes the classical Riemann zeta function. For dimensions $d = 2, 4, 8$, and 24, it has been conjectured (cf. [2, 6] and references therein) that $C_{s,d}$ for $s > d$ is also given by an Epstein zeta function, specifically, that $C_{s,d} = \zeta_{\Lambda_d}(s)$ for Λ_d denoting the equilateral triangular (or hexagonal) lattice, the D_4 lattice, the E_8 lattice, and the Leech lattice (all scaled to have co-volume 1) in the dimensions $d = 2, 4, 8$, and 24, respectively. In [5], it is shown that periodized lattice configurations for these special lattices are *local* minima of the energy for a large class of energy potentials that includes

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periodic Riesz s-energy potentials for $s > d$.

2.3 The Epstein Hurwitz Zeta Function

In this section, we will review some relevant terminology and notation involving some special functions that will be crucial for our analysis in Section 2.4. We begin with the following observation.

Lemma 2.3.1. *Let Λ be a sublattice of Λ'. Then for any $s \in \mathbb{C} \setminus \{d\}$, it holds that*

$$\sum_{x \in \Lambda' \cap \Omega_\Lambda \setminus \{0\}} \zeta_\Lambda(s;x) = \zeta_\Lambda(s) - \zeta_{\Lambda'}(s). \tag{2.25}$$

Proof. It is sufficient to prove that (2.25) holds for $s > d$, since the general result follows from the fact that both sides of this relation are analytic on $\mathbb{C} \setminus \{d\}$. For $s > d$, we have by definition

$$\zeta_{\Lambda'}(s) = \sum_{x \in \Lambda' \setminus \{0\}} \frac{1}{|x|^s} = \sum_{x \in \Lambda' \cap \Omega_\Lambda \setminus \{0\}} \sum_{v \in \Lambda} \frac{1}{|x+v|^s} + \sum_{v \in \Lambda \setminus \{0\}} \frac{1}{|v|^s}$$

$$= \sum_{x \in \Lambda' \cap \Omega_\Lambda \setminus \{0\}} \zeta_\Lambda(s;x) + \zeta_\Lambda(s),$$

thus proving the lemma. $\square$

Using the above lemma and scaling properties of Epstein zeta functions we obtain the following:

Lemma 2.3.2. *For every $m \in \mathbb{N}$ and $s \in \mathbb{C} \setminus \{d\}$, it holds that*

$$\sum_{x \in \frac{1}{m}\Lambda \cap \Omega_\Lambda \setminus \{0\}} \zeta_\Lambda(s;x) = (m^s - 1)\zeta_\Lambda(s). \tag{2.26}$$

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Therefore,

$$\sum_{\substack{x,y\in\frac{1}{m}\Lambda\cap\Omega_\Lambda \\ x\neq y}} \zeta_\Lambda(s;x-y) = m^d(m^s-1)\zeta_\Lambda(s). \tag{2.27}$$

Proof. As in the proof of Lemma 2.3.2, we will prove the desired identities when $s > d$ and then rely on the uniqueness of the analytic continuation to obtain the desired conclusion for all $s \neq d$. The first equality of the lemma is an immediate consequence of the infinite series definition of $\zeta_\Lambda(s;q)$. To prove the second equality, notice that every $v \in \Lambda$ can be expressed uniquely as $r - t + u$ for some $t \in \Lambda \cap \Omega_{\Lambda'}$ and $u \in \Lambda'$. The desired equality now follows from the infinite sum (2.3) when $s > d$. $\qquad\square$

We will also require the following lemmas, which establish continuity properties of the Epstein Hurwitz Zeta function with respect to the lattice.

Lemma 2.3.3. *Let $\{P_m\}_{m\in\mathbb{N}}$ be a sequence of $d \times d$ matrices such that $P_m \to P$ in norm as $m \to \infty$. Fix any distinct x and y in Ω_Λ and suppose $\{x_m\}_{m\in\mathbb{N}}$ and $\{y_m\}_{m\in\mathbb{N}}$ are sequences in Ω_Λ converging to x and y, respectively. Then for any compact set $K \subset \mathbb{C} \setminus \{d\}$, $\zeta_{P_m\Lambda}(s;P_m(x_m-y_m))$ converges to $\zeta_{P\Lambda}(s;P(x-y))$ uniformly for s in K as $m \to \infty$.*

Proof. Let $R = \sup_{s\in K} \operatorname{Re}(s)$ and $r = \inf_{s\in K} \operatorname{Re}(s)$. Notice that $\sup_{s\in K} |1/\Gamma(\frac{s}{2})|$ is finite

since $1/\Gamma(\frac{s}{2})$ is entire. Let m be large enough so that $x_m - y_m \notin \Lambda$. Using (2.4), we have

$$|\zeta_{P_m\Lambda}(s;P_m(x_m-y_m)) - \zeta_{P\Lambda}(s;P(x-y))|$$

$$= |F_{s,P_m\Lambda}(P_mx_m - P_my_m) - F_{s,P\Lambda}(Px-Py)|$$

$$\leq \int_1^\infty \sum_{v\in\Lambda} \left| e^{-|P_m(x_m-y_m+v)|^2 t} - e^{-|P(x-y+v)|^2 t} \right| \frac{|t^{\frac{s}{2}-1}|}{|\Gamma(\frac{s}{2})|} dt$$

$$+ \int_0^1 \sum_{w\in\Lambda^*\backslash\{0\}} \left| e^{2\pi i w\cdot(x_m-y_m)} e^{-\frac{\pi^2|(P_m^{-1})^T w|^2}{t}} - e^{2\pi i w\cdot(x-y)} e^{-\frac{\pi^2|(P^{-1})^T w|^2}{t}} \right| \frac{\pi^{\frac{d}{2}}|t^{\frac{s-d}{2}-1}|}{|\Gamma(\frac{s}{2})|} dt$$

$$\leq \int_1^\infty \sum_{v\in\Lambda} \left| e^{-|P_m(x_m-y_m+v)|^2 t} - e^{-|P(x-y+v)|^2 t} \right| \frac{t^{\frac{R}{2}-1}}{\inf_{s\in K}|\Gamma(\frac{s}{2})|} dt$$

$$+ \int_0^1 \sum_{w\in\Lambda^*\backslash\{0\}} \left| e^{2\pi i w\cdot(x_m-y_m)} e^{-\frac{\pi^2|(P_m^{-1})^T w|^2}{t}} - e^{2\pi i w\cdot(x-y)} e^{-\frac{\pi^2|(P^{-1})^T w|^2}{t}} \right| \frac{\pi^{\frac{d}{2}} t^{\frac{r-d}{2}-1}}{\inf_{s\in K}|\Gamma(\frac{s}{2})|} dt.$$

$$(2.28)$$

As in [7], it is elementary to establish that integrals of the form

$$\int_1^\infty \sum_{v\in\Lambda} e^{-|P(x-y+v)|^2 t} t^{\frac{R}{2}-1} dt \quad \text{and} \quad \int_0^1 \sum_{w\in\Lambda^*\backslash\{0\}} e^{-\frac{\pi^2|(P^{-1})^T w|^2}{t}} \pi^{\frac{d}{2}} t^{\frac{r-d}{2}-1} dt$$

are finite and thus, by dominated convergence, it follows that the expressions in (2.28) tend to zero as $m \to \infty$. $\qquad\square$

We remark that the proof of Lemma 2.3.3 shows that $F_{s,P_m\Lambda}(P_mx_m - P_my_m)$ converges to $F_{s,P\Lambda}(Px - Py)$ as $m \to \infty$ uniformly for s in any compact set of $\mathbb{C}$.

Corollary 2.3.4. *Let $\{P_m\}_{m\in\mathbb{N}}$ be a sequence of $d \times d$ matrices such that $P_m \to P$ in norm as $m \to \infty$ and suppose $s > 0$. Then, for all $N \geq 2$, we have $\mathscr{E}_{s,P_m\Lambda}(N) \to \mathscr{E}_{s,P\Lambda}(N)$ as $m \to \infty$.*

Proof. Let $\omega_N^* \subset \Omega_\Lambda$ be such that $P\omega_N^*$ is an $E_{s,P\Lambda}$ optimal N-point configuration. Then,

$$\limsup_{m\to\infty} \mathscr{E}_{s,P_m\Lambda}(N) \leq \limsup_{m\to\infty} E_{s,P_m\Lambda}(P_m\omega_N^*) = E_{s,P\Lambda}(P\omega_N^*) = \mathscr{E}_{s,P\Lambda}(N),$$

where the next to last equality follows from Lemma 2.3.3.

Next let $\omega_N^m = \{x_1^m, \ldots, x_N^m\} \subset \Omega_\Lambda$ be such that $P_m \omega_N^m$ is an optimal N-point configuration for $F_{s,P_m\Lambda}$. Let $\{\omega_N^{m_k}\}_{k\in\mathbb{N}}$ be a subsequence such that

$$\lim_{k\to\infty} E_{s,P_{m_k}\Lambda}(P_{m_k}\omega_N^{m_k}) = \liminf_{m\to\infty} \mathscr{E}_{s,P_m\Lambda}(N).$$

Using the compactness of Ω_Λ in the 'flat torus' topology, we may assume without loss of generality that $\{\omega_N^{m_k}\}_{k\in\mathbb{N}}$ converges to some N-point configuration $\tilde{\omega}_N = \{\tilde{x}_1, \ldots, \tilde{x}_N\}$; i.e., $x_j^{m_k} \to \tilde{x}_j$ as $k \to \infty$ for each $j = 1, \ldots, N$. Then we have

$$\liminf_{m\to\infty} \mathscr{E}_{s,P_m\Lambda}(N) = \lim_{k\to\infty} E_{s,P_{m_k}\Lambda}(P_{m_k}\omega_N^{m_k}) = E_{s,P\Lambda}(P\tilde{\omega}_N) \geq \mathscr{E}_{s,P\Lambda}(N),$$

where the next to last equality follows from Lemma 2.3.3. $\qquad\square$

Finally, the following result expresses continuity properties of the Epstein zeta function with respect to the lattice similar to the results in Lemma 2.3.3 for the Epstein Hurwitz zeta function.

Lemma 2.3.5. *Let $\{P_m\}_{m\in\mathbb{N}}$ be a sequence of $d \times d$ matrices such that $P_m \to P$ in norm as $m \to \infty$. Then for any compact set $K \subset \mathbb{C} \setminus \{d\}$, $\zeta_{P_m\Lambda}(s)$ converges to $\zeta_{P\Lambda}(s)$ uniformly in K and hence $\zeta'_{P_m\Lambda}(s) \to \zeta'_{P\Lambda}(s)$ for all $s \in \mathbb{C} \setminus \{d\}$ as $m \to \infty$.*

Proof. Using Lemma 2.1.2, a similar argument as in the proof of Lemma 2.3.3 implies that $\zeta_{P_m\Lambda}(s)$ converges uniformly to $\zeta_{P\Lambda}(s)$ on compact sets $K \subset \mathbb{C} \setminus \{d\}$. The convergence of the derivatives then follows from Cauchy's integral formula for derivatives. $\qquad\square$

2.4   Proof of Theorem 2.2.1

Throughout this section and the next we shall assume that $\Lambda = A\mathbb{Z}^d$ denotes a d-dimensional lattice in $\mathbb{R}^d$ with fundamental domain $\Omega = \Omega_\Lambda$, co-volume 1, and generating matrix A. Then Theorem 2.2.1 follows from a simple rescaling. We shall find it

convenient to use what we call the *classical periodic Riesz s-potential* $F_{s,\Lambda}^{\text{cp}}(x) := \zeta_\Lambda(s;x)$ which, for $s \neq d$, differs from $F_{s,\Lambda}$ only by the constant $\frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{s}{2})(d-s)}$. Similarly, we call $F_{\log,\Lambda}^{\text{cp}}(x) := 2\zeta_\Lambda'(0;x)$ the *classical periodic logarithmic potential*. The energies associated with these potentials are given by

$$E_{s,\Lambda}^{\text{cp}}(\omega_N) := \sum_{j \neq k} \zeta_\Lambda(s;x_j - x_k), \qquad (s > 0), \tag{2.29}$$

and, similarly,

$$E_{\log,\Lambda}^{\text{cp}}(\omega_N) := 2 \sum_{j \neq k} \zeta_\Lambda'(0;x_j - x_k), \tag{2.30}$$

and we denote the respective minimal N-point energies by $\mathcal{E}_{s,\Lambda}^{\text{cp}}(N)$ and $\mathcal{E}_{\log,\Lambda}^{\text{cp}}(N)$.

From (2.5), we obtain

$$\mathcal{E}_{s,\Lambda}(N) = \mathcal{E}_{s,\Lambda}^{\text{cp}}(N) + \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{s}{2})(d-s)} N(N-1), \tag{2.31}$$

and

$$\mathcal{E}_{\log,\Lambda}(N) = \mathcal{E}_{\log,\Lambda}^{\text{cp}}(N) + \frac{2\pi^{\frac{d}{2}}}{d} N(N-1), \tag{2.32}$$

Define

$$\underline{g}_{s,d}(\Lambda) := \liminf_{N \to \infty} \frac{\mathcal{E}_{s,\Lambda}^{\text{cp}}(N)}{N^{1+s/d}},$$

$$\overline{g}_{s,d}(\Lambda) := \limsup_{N \to \infty} \frac{\mathcal{E}_{s,\Lambda}^{\text{cp}}(N)}{N^{1+s/d}},$$

$$\underline{g}_{\log,d}(\Lambda) := \liminf_{N \to \infty} \frac{\mathcal{E}_{\log,\Lambda}^{\text{cp}}(N) + \frac{2}{d}N \log N}{N},$$

$$\overline{g}_{\log,d}(\Lambda) := \limsup_{N \to \infty} \frac{\mathcal{E}_{\log,\Lambda}^{\text{cp}}(N) + \frac{2}{d}N \log N}{N}.$$

Our use of these quantities is motivated by the proof of the main results in [13], and indeed the general strategy of our proofs is similar to that of [13]. More precisely, we shall prove $\underline{g}_{s,d}(\Lambda) = \overline{g}_{s,d}(\Lambda)$ and $\underline{g}_{\log,d}(\Lambda) = \overline{g}_{\log,d}(\Lambda)$ and that these limits are finite. We first need

estimates on quantities appearing in (2.4) and (2.10).

Lemma 2.4.1. *Let $s > 0$ and Λ be a d-dimensional lattice with co-volume 1 and $l_0 :=$ $\min_{0 \neq v \in \Lambda} \{|v|\}$. The following relations hold.*

$$\sum_{w \in \Lambda^*} e^{-\frac{\pi^2 |w|^2}{t}} t^{-\frac{d}{2}} = \pi^{-\frac{d}{2}} + O(e^{-l_0^2 t}), \qquad as \ t \to \infty, \tag{2.33}$$

$$\sum_{w \in \Lambda^*} \int_1^{\frac{1}{\delta}} e^{-\frac{\pi^2 |w|^2}{t}} t^{\frac{s-d}{2}-1} dt = \frac{2\pi^{-\frac{d}{2}}}{s} \delta^{-\frac{s}{2}} + O(1), \qquad as \ \delta \to 0^+, \tag{2.34}$$

$$\sum_{w \in \Lambda^*} \int_1^{\frac{1}{\delta}} e^{-\frac{\pi^2 |w|^2}{t}} t^{-\frac{d}{2}-1} dt = \pi^{-\frac{d}{2}} \log \delta^{-1} + O(1), \qquad as \ \delta \to 0^+ \tag{2.35}$$

Proof. Applying Poisson Summation, we obtain

$$\sum_{w \in \Lambda^*} e^{-\frac{\pi^2 |w|^2}{t}} t^{-\frac{d}{2}} = \pi^{-d/2} \sum_{v \in \Lambda} e^{-|v|^2 t} = \pi^{-d/2} + \pi^{-d/2} e^{-l_0^2 t} \sum_{v \in \Lambda \setminus \{0\}} e^{-(|v|^2 - l_0^2)t}$$

$$= \pi^{-d/2} + O(e^{-l_0^2 t}),$$

proving (2.33). Hence, there exists a constant C_1 such that

$$\left| \sum_{w \in \Lambda^*} e^{-\frac{\pi^2 |w|^2}{t}} t^{-\frac{d}{2}} - \pi^{-\frac{d}{2}} \right| \le C_1 e^{-l_0^2 t},$$

and so, multiplying both sides of the above by $t^{\frac{s}{2}-1}$, we have

$$\left| \sum_{w \in \Lambda^*} e^{-\frac{\pi^2 |w|^2}{t}} t^{\frac{s-d}{2}-1} - \pi^{-\frac{d}{2}} t^{\frac{s}{2}-1} \right| \le C_1 t^{\frac{s}{2}-1} e^{-l_0^2 t}$$

and so

$$\left| \int_1^{\frac{1}{\delta}} \left(\sum_{w \in \Lambda^*} e^{-\frac{\pi^2 |w|^2}{t}} t^{\frac{s-d}{2}-1} - \pi^{-\frac{d}{2}} t^{\frac{s}{2}-1} \right) dt \right| \le \int_1^{\frac{1}{\delta}} C_1 t^{\frac{s}{2}-1} e^{-l_0^2 t} dt$$

$$\le \int_1^{\infty} C_1 t^{\frac{s}{2}-1} e^{-l_0^2 t} dt =: C_2(s). \tag{2.36}$$

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Therefore,

$$\left| \sum_{w \in \Lambda^*} \int_1^{\frac{1}{\delta}} e^{-\frac{\pi^2 |w|^2}{t}} t^{\frac{s-d}{2}-1} dt - \frac{2\pi^{-\frac{d}{2}}}{s} (\delta^{-\frac{s}{2}} - 1) \right| \leq C_2(s), \qquad s > 0$$

proving (2.34), while substituting $s = 0$ into (2.36) yields

$$\left| \sum_{w \in \Lambda^*} \int_1^{\frac{1}{\delta}} e^{-\frac{\pi^2 |w|^2}{t}} t^{-\frac{d}{2}-1} dt - \pi^{-\frac{d}{2}} \log \delta^{-1} \right| \leq C_2(0), \qquad s = 0.$$

proving (2.35). □

The following lemma is the key calculation that allows us to apply the method of [13]. Once we have established this lemma, the only remaining technical difficulty will be to establish the fact that the constants $C_{s,d}$ and $C_{\log,d}$ are independent of the lattice Λ.

Lemma 2.4.2. *With Λ as in Lemma 2.4.1 and $s > 0$, the following inequalities hold:*

$$-\infty < \underline{g}_{s,d}(\Lambda) \leq \overline{g}_{s,d}(\Lambda) \leq \zeta_\Lambda(s) < \infty,$$

$$-\infty < \underline{g}_{\log,d}(\Lambda) \leq \overline{g}_{\log,d}(\Lambda) \leq 0.$$

Proof. Let us first consider the case $s > 0$. For any configuration $\omega_N = (x_j)_{j=1}^N$ in Ω_Λ and any $\delta \in (0, 1]$,

$$E_{s,\Lambda}(\omega_N) = \sum_{j \neq k} K_{s,\Lambda}(x_j, x_k) =: I_1 + I_2.$$

where

$$I_1 = \sum_{j \neq k} \sum_{v \in \Lambda} \int_1^\infty e^{-|x_j - x_k + v|^2 t} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt,$$

$$I_2 = \sum_{j \neq k} \sum_{w \in \Lambda^* \setminus \{0\}} e^{2\pi i w \cdot (x_j - x_k)} \int_0^1 \frac{\pi^{\frac{d}{2}}}{t^{\frac{d}{2}}} e^{-\frac{\pi^2 |w|^2}{t}} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt.$$

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Let

$$h_\delta(x) := \int_1^{\frac{1}{\delta}} e^{-|x|^2 t} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt.$$

then

$$\hat{h}_\delta(\xi) = \int_1^{\frac{1}{\delta}} \left(\frac{\pi}{t}\right)^{\frac{d}{2}} e^{-\frac{\pi^2|\xi|^2}{t}} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt \geq 0, \quad \hat{h}_\delta(0) = \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{s}{2})(d-s)} \left(1 - \delta^{\frac{d-s}{2}}\right).$$

Notice that since the upper limit of the integral defining h_δ is finite, it is easy to verify that h_δ satisfies the hypotheses of Poisson Summation. Applying it gives us the following inequalities:

$$
\begin{aligned}
I_1 &\geq \sum_{j \neq k} \sum_{v \in \Lambda} h_\delta(x_j - x_k + v) \\
&= \sum_{j \neq k} \sum_{w \in \Lambda^*} \hat{h}_\delta(w) e^{2\pi i w \cdot (x_j - x_k)} \\
&= \sum_{w \in \Lambda^*} \hat{h}_\delta(w) \left(\sum_{j,k} e^{2\pi i w \cdot (x_j - x_k)} - N \right) \\
&= \sum_{w \in \Lambda^*} \hat{h}_\delta(w) \left(\left| \sum_j e^{2\pi i w \cdot x_j} \right|^2 - N \right) \\
&\geq N^2 \hat{h}_\delta(0) - N \sum_{w \in \Lambda^*} \hat{h}_\delta(w) \\
&= N^2 \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{s}{2})(d-s)} \left(1 - \delta^{\frac{d-s}{2}}\right) - N \frac{\pi^{\frac{d}{2}}}{\Gamma(\frac{s}{2})} \sum_{w \in \Lambda^*} \int_1^{\frac{1}{\delta}} e^{-\frac{\pi^2|w|^2}{t}} t^{\frac{s-d}{2}-1} dt.
\end{aligned}
$$

(2.37)

By Lemma 2.4.1, we conclude

$$
\begin{aligned}
I_1 &\geq N^2 \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{s}{2})(d-s)} \left(1 - \delta^{\frac{d-s}{2}}\right) - N \frac{2\pi^{\frac{d}{2}}}{s\Gamma(\frac{s}{2})} \left(\pi^{-\frac{d}{2}} \delta^{-\frac{s}{2}} + O(1)\right) \\
&= \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{s}{2})(d-s)} N^2 - \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{s}{2})(d-s)} N^2 \delta^{\frac{d-s}{2}} - \frac{2}{s\Gamma(\frac{s}{2})} N \delta^{-\frac{s}{2}} - O(N),
\end{aligned}
$$

(2.38)

To obtain lower bounds on I_2, we calculate

$$
\begin{aligned}
I_2 &= \sum_{w \in \Lambda^* \setminus \{0\}} \left(\sum_{j,k} e^{2\pi i w \cdot (x_j - x_k)} - N \right) \int_0^1 \frac{\pi^{\frac{d}{2}}}{t^{\frac{d}{2}}} e^{-\frac{\pi^2 |w|^2}{t}} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt \\
&= \sum_{w \in \Lambda^* \setminus \{0\}} \left(\left| \sum_j e^{2\pi i w \cdot x_j} \right|^2 - N \right) \int_0^1 \frac{\pi^{\frac{d}{2}}}{t^{\frac{d}{2}}} e^{-\frac{\pi^2 |w|^2}{t}} \frac{t^{\frac{s}{2}-1}}{\Gamma(\frac{s}{2})} dt \\
&\geq -N \cdot \frac{\pi^{\frac{d}{2}}}{\Gamma(\frac{s}{2})} \sum_{w \in \Lambda^* \setminus \{0\}} \int_0^1 e^{-\frac{\pi^2 |w|^2}{t}} t^{\frac{s-d}{2}-1} dt \\
&= O(N).
\end{aligned}
\tag{2.39}
$$

Therefore

$$
E_{s,\Lambda}(\omega_N) = I_1 + I_2 \geq \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{s}{2})(d-s)} N^2 - \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{s}{2})(d-s)} N^2 \delta^{\frac{d-s}{2}} - \frac{2}{s\Gamma(\frac{s}{2})} N \delta^{-\frac{s}{2}} - O(N).
$$

If we let $\delta = \pi^{-1} N^{-\frac{2}{d}}$, then this lower bound becomes

$$
E_{s,\Lambda}(\omega_N) \geq \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{s}{2})(d-s)} N^2 + C^* N^{1+\frac{s}{d}} + O(N).
\tag{2.40}
$$

where

$$
C^* = -\frac{2\pi^{\frac{s}{2}} d}{\Gamma(\frac{s}{2}) s (d-s)}.
$$

The right hand side of (2.40) is independent of ω_N and thus

$$
\mathscr{E}_{s,\Lambda}(N) \geq \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{s}{2})(d-s)} N^2 + C^* N^{1+\frac{s}{d}} + O(N),
$$

$$
\mathscr{E}_{s,\Lambda}^{\mathrm{cp}}(N) \geq C^* N^{1+\frac{s}{d}} + O(N).
$$

We conclude that $\underline{g}_{s,d}(\Lambda) \geq C^*$.

To establish the finiteness of $\overline{g}_{s,d}$, we will use the same method as was used in [13]. For

any natural number N, let $m = m_N$ be a positive integer such that $(m-1)^d < N \leq m^d$. Let $\omega^m = \frac{1}{m}\Lambda \cap \Omega_\Lambda$. Then

$$\mathscr{E}_{s,\Lambda}^{\mathrm{cp}}(m^d) \leq E_{s,\Lambda}^{\mathrm{cp}}(\omega^m) = \sum_{\substack{x_j,x_k \in \frac{1}{m}\Lambda \cap \Omega_\Lambda \\ x_j \neq x_k}} \zeta_\Lambda(s; x_j - x_k) = m^d(m^s - 1)\zeta_\Lambda(s), \qquad (2.41)$$

where we used Lemma 2.3.2

As $\left\{ \dfrac{\mathscr{E}_{s,\Lambda}^{\mathrm{cp}}(N)}{N(N-1)} \right\}_{N=2}^{\infty}$ is an increasing sequence (see, e.g., [10, Chapter II §3.12, page 160]) we arrive at the following:

$$\begin{aligned}
\overline{g}_{s,d}(\Lambda) &= \limsup_{N\to\infty} \frac{\mathscr{E}_{s,\Lambda}^{\mathrm{cp}}(N)}{N^{1+s/d}} = \limsup_{N\to\infty} \frac{\mathscr{E}_{s,\Lambda}^{\mathrm{cp}}(N)}{N(N-1)} \cdot \frac{N-1}{N^{\frac{s}{d}}} \\
&\leq \limsup_{N\to\infty} \frac{\mathscr{E}_{s,\Lambda}^{\mathrm{cp}}(\Omega_\Lambda, m^d)}{m^d(m^d-1)} \cdot \frac{N-1}{N^{\frac{s}{d}}} \\
&\leq \limsup_{N\to\infty} \frac{m^d(m^s-1)\zeta_\Lambda(s)}{m^d(m^d-1)} \cdot \frac{N-1}{N^{\frac{s}{d}}} = \zeta_\Lambda(s) < \infty.
\end{aligned}$$

Now we turn our attention to the classical periodic logarithmic energy. Using (2.11), (2.38), and (2.39), we obtain

$$\begin{aligned}
E_{\log,\Lambda}(\omega_N) &= \lim_{s\to 0^+} \Gamma\left(\frac{s}{2}\right) E_{s,\Lambda}(\omega_N) = \lim_{s\to 0^+} \Gamma\left(\frac{s}{2}\right)(I_1 + I_2) \\
&\geq N^2 \frac{2\pi^{\frac{d}{2}}}{d}\left(1 - \delta^{\frac{d}{2}}\right) - N\pi^{\frac{d}{2}} \sum_{w\in\Lambda^*} \int_1^{\frac{1}{\delta}} e^{-\frac{\pi^2|w|^2}{t}} t^{-\frac{d}{2}-1}\,\mathrm{d}t + O(N) \\
&= N^2 \frac{2\pi^{\frac{d}{2}}}{d}\left(1 - \delta^{\frac{d}{2}}\right) - N\pi^{\frac{d}{2}}\left(\pi^{-\frac{d}{2}}\log\delta^{-1} + O(1)\right) + O(N) \\
&= \frac{2\pi^{\frac{d}{2}}}{d}N^2 - \frac{2\pi^{\frac{d}{2}}}{d}N^2\delta^{\frac{d}{2}} - N\log\delta^{-1} + O(N).
\end{aligned}$$

If we let $\delta = N^{-\frac{2}{d}}$, then we get

$$E_{\log,\Lambda}(\omega_N) = \frac{2\pi^{\frac{d}{2}}}{d}N^2 - \frac{2}{d}N\log N + O(N).$$

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Thus

$$\mathscr{E}_{\log,\Lambda}(N) \geq \frac{2\pi^{\frac{d}{2}}}{d}N^2 - \frac{2}{d}N\log N + O(N),$$

$$\mathscr{E}^{\mathrm{cp}}_{\log,\Lambda}(N) + \frac{2}{d}N\log N \geq O(N),$$

and we conclude that $\underline{g}_{\log,d}(\Lambda) > -\infty$.

To establish the finiteness of $\overline{g}_{s,d}$, let $m = m_N$ be a positive integer such that $(m-1)^d < N \leq m^d$. Let $\omega^m = \frac{1}{m}\Lambda \cap \Omega_\Lambda$. Then by (2.41)

$$E^{\mathrm{cp}}_{s,\Lambda}(\omega^m) = m^d(m^s - 1)\zeta_\Lambda(s).$$

By definition,

$$\begin{aligned}
\mathscr{E}^{\mathrm{cp}}_{\log,\Lambda}(m^d) &\leq E^{\mathrm{cp}}_{\log,\Lambda}(\omega^m) = 2\left.\frac{\mathrm{d}}{\mathrm{d}s}E^{\mathrm{cp}}_{s,\Lambda}(\omega_N)\right|_{s=0} \\
&= 2\left.m^d\left(m^s\log m \cdot \zeta_\Lambda(s) + (m^s - 1)\zeta'(s)\right)\right|_{s=0} \\
&= 2m^d\log m \cdot \zeta_\Lambda(0) = -2m^d\log m = -\frac{2}{d}m^d\log m^d
\end{aligned}$$

Here we use the fact that $\zeta_\Lambda(0) = -1$ for every lattice Λ (cf. [9, Theorem 1, Section 1.4, page 59]). We conclude that

$$\frac{\mathscr{E}^{\mathrm{cp}}_{s,\Lambda}(N)}{N} = \frac{\mathscr{E}^{\mathrm{cp}}_{s,\Lambda}(N)}{N(N-1)} \cdot (N-1) \leq \frac{\mathscr{E}^{\mathrm{cp}}_{s,\Lambda}(m^d)}{m^d(m^d-1)} \cdot (N-1) \leq -\frac{2}{d}\log m^d \cdot \frac{N-1}{m^d-1}$$

This implies

$$\frac{\mathscr{E}^{\mathrm{cp}}_{s,\Lambda}(N) + \frac{2}{d}N\log N}{N} \leq -\frac{2}{d}\log m^d \cdot \frac{N-1}{m^d-1} + \frac{2}{d}\log N,$$

which tends to 0 as $N \to \infty$, and hence $\overline{g}_{\log,d}(\Lambda) \leq 0$. $\qquad\square$

The following lemma establishes scaling properties of the classical periodic energy and

will be helpful in establishing independence of the constants $C_{s,d}$ and $C_{\log,d}$ of the lattice Λ.

Lemma 2.4.3. *Let Λ be a lattice and $\Lambda' = B\Lambda$ be a sublattice of Λ (i.e. $B \in GL(d,\mathbb{Z})$), then for any $N > 0$,*

$$\mathscr{E}^{\mathrm{cp}}_{s,\Lambda'}(N|\det B|) \leq |\det B|\mathscr{E}^{\mathrm{cp}}_{s,\Lambda}(N) + N|\det B|(\zeta_\Lambda(s) - \zeta_{\Lambda'}(s)),$$

$$\mathscr{E}^{\mathrm{cp}}_{\log,\Lambda'}(N|\det B|) \leq |\det B|\mathscr{E}^{\mathrm{cp}}_{\log,\Lambda}(N) + 2N|\det B|(\zeta'_\Lambda(0) - \zeta'_{\Lambda'}(0)).$$

Proof. For any $\omega_N = (x_j)_{j=1}^N \in (\Omega_\Lambda)^N$, let $S(\omega_N) = (\omega_N + \Lambda) \cap \Omega_{\Lambda'}$. Then $S(\omega_N)$ is a $(N|\det B|)$-point configuration in $\Omega_{\Lambda'}$ and

$$E^{\mathrm{cp}}_{s,\Lambda'}(S(\omega_N)) = \sum_{\substack{x,y \in S(\omega_N) \\ x \neq y}} \zeta_{\Lambda'}(s, x-y) = \sum_{j,k} \sum_{\substack{r \in \Lambda, x_j + r \in \Omega_{\Lambda'} \\ t \in \Lambda, x_k + t \in \Omega_{\Lambda'} \\ x_j + r \neq x_k + t}} \zeta_{\Lambda'}(s; x_j + r - x_k - t)$$

$$= \sum_{j \neq k} \sum_{\substack{r \in \Lambda \cap \Omega_{\Lambda'} \\ t \in \Lambda \cap \Omega_{\Lambda'}}} \zeta_{\Lambda'}(s; x_j - x_k + r - t) + \sum_{j=1}^N \sum_{\substack{r \in \Lambda \cap \Omega_{\Lambda'} \\ t \in \Lambda \cap \Omega_{\Lambda'} \\ r \neq t}} \zeta_{\Lambda'}(s; r - t)$$

$$= \sum_{j \neq k} \sum_{r \in \Lambda \cap \Omega_{\Lambda'}} \zeta_\Lambda(s; x_j - x_k) + N \sum_{r \in \Lambda \cap \Omega_{\Lambda'}} (\zeta_\Lambda(s) - \zeta_{\Lambda'}(s))$$

$$= |\det B| \cdot E^{\mathrm{cp}}_{s,\Lambda}(\omega_N) + N|\det B|(\zeta_\Lambda(s) - \zeta_{\Lambda'}(s)), \tag{2.42}$$

where we used Lemma 2.3.1. Taking the infimum over all configurations $(x_j)_{j=1}^N \in (\Omega_\Lambda)^N$, we conclude that

$$\mathscr{E}^{\mathrm{cp}}_{s,\Lambda'}(N|\det B|) \leq \inf_{\omega_N \in (\Omega_\Lambda)^N} E^{\mathrm{cp}}_{s,\Lambda'}(S(\omega_N)) = |\det B| \cdot \mathscr{E}^{\mathrm{cp}}_{s,\Lambda}(N) + N|\det B|(\zeta_\Lambda(s) - \zeta_{\Lambda'}(s)).$$

The logarithmic case follows from this by differentiating (2.42) and evaluating at $s = 0$. $\quad\square$

Corollary 2.4.4. *For any positive integers m and N, we have*

$$\frac{\mathscr{E}^{\mathrm{cp}}_{s,\Lambda}(m^d N)}{(m^d N)^{1+\frac{s}{d}}} \leq \frac{\mathscr{E}^{\mathrm{cp}}_{s,\Lambda}(N)}{N^{1+\frac{s}{d}}} + \frac{(1-m^{-s})\zeta_\Lambda(s)}{N^{\frac{s}{d}}},$$

$$\frac{\mathscr{E}^{\mathrm{cp}}_{\log,\Lambda}(m^d N) + \frac{2}{d}m^d N \log(m^d N)}{m^d N} \leq \frac{\mathscr{E}^{\mathrm{cp}}_{\log,\Lambda}(N) + \frac{2}{d}N \log N}{N}.$$

Proof. Both of the inequalities follow from Lemma 2.4.3

$$\mathscr{E}^{\mathrm{cp}}_{s,m\Lambda}(m^d N) \leq m^d \cdot \mathscr{E}^{\mathrm{cp}}_{s,\Lambda}(N) + m^d N \left(\zeta_\Lambda(s) - \zeta_{m\Lambda}(s)\right),$$

$$\mathscr{E}^{\mathrm{cp}}_{\log,m\Lambda}(m^d N) \leq m^d \cdot \mathscr{E}^{\mathrm{cp}}_{\log,\Lambda}(N) + 2m^d N \left(\zeta'_\Lambda(0) - \zeta'_{m\Lambda}(0)\right)$$

and the facts that

$$\mathscr{E}^{\mathrm{cp}}_{s,m\Lambda}(m^d N) = m^{-s}\mathscr{E}^{\mathrm{cp}}_{s,\Lambda}(m^d N), \qquad \zeta_{m\Lambda}(s) = m^{-s}\zeta_\Lambda(s), \tag{2.43}$$

$$\mathscr{E}^{\mathrm{cp}}_{\log,m\Lambda}(m^d N) = \mathscr{E}^{\mathrm{cp}}_{\log,\Lambda}(m^d N), \qquad \zeta'_{m\Lambda}(0) = \log m + \zeta'_\Lambda(0). \tag{2.44}$$

Note that the first identity in (2.44) is obtained from the first identity in (2.43) using (2.11) while the second identity in (2.44) follows by differentiating the second identity in (2.43) and evaluating at $s = 0$. $\qquad\square$

We are now ready to prove our main result.

Proof of Theorem 2.2.1. By (2.31) and (2.32) it suffices to show

$$\overline{g}_{s,d}(\Lambda) = \underline{g}_{s,d}(\Lambda) = C_{s,d},$$

$$\overline{g}_{\log,d}(\Lambda) = \underline{g}_{\log,d}(\Lambda) = C_{\log,d} - 2\zeta'_\Lambda(0).$$

Fix some positive integer N_0. For any $N > N_0$ there exists $m \in \mathbb{N}$ such that $(m-1)^d N_0 \leq N < m^d N_0$, using Corollary 2.4.4 and the fact that $\{\frac{\mathscr{E}^{\mathrm{cp}}_{s,\Lambda}(N)}{N(N-1)}\}_{N=2}^{\infty}$ is an increasing sequence

we obtain

$$\frac{\mathscr{E}_{s,\Lambda}^{\mathrm{cp}}(N)}{N^{1+\frac{s}{d}}} = \frac{\mathscr{E}_{s,\Lambda}^{\mathrm{cp}}(N)}{N(N-1)} \cdot \frac{N-1}{N^{\frac{s}{d}}} \leq \frac{\mathscr{E}_{s,\Lambda}^{\mathrm{cp}}(m^d N_0)}{m^d N_0(m^d N_0-1)} \cdot \frac{N-1}{N^{\frac{s}{d}}}$$

$$= \frac{\mathscr{E}_{s,\Lambda}^{\mathrm{cp}}(m^d N_0)}{(m^d N_0)^{1+\frac{s}{d}}} \cdot \frac{(m^d N_0)^{\frac{s}{d}}}{(m^d N_0-1)} \cdot \frac{N-1}{N^{\frac{s}{d}}}$$

$$\leq \left(\frac{\mathscr{E}_{s,\Lambda}^{\mathrm{cp}}(N_0)}{N_0^{1+\frac{s}{d}}} + \frac{(1-m^{-s})\zeta_\Lambda(s)}{N_0^{\frac{s}{d}}} \right) \cdot \frac{(m^d N_0)^{\frac{s}{d}}}{N^{\frac{s}{d}}} \cdot \frac{N-1}{(m^d N_0-1)}.$$

Similarly

$$\frac{\mathscr{E}_{\log,\Lambda}^{\mathrm{cp}}(N) + \frac{2}{d} N \log N}{N}$$

$$= \frac{\mathscr{E}_{\log,\Lambda}^{\mathrm{cp}}(N)}{N(N-1)} \cdot (N-1) + \frac{2}{d} \log N$$

$$\leq \frac{\mathscr{E}_{\log,\Lambda}^{\mathrm{cp}}(m^d N_0)}{m^d N_0(m^d N_0-1)} \cdot (N-1) + \frac{2}{d} \log(m^d N_0)$$

$$= \left(\frac{\mathscr{E}_{\log,\Lambda}^{\mathrm{cp}}(m^d N_0) + \frac{2}{d} m^d N_0 \log(m^d N_0)}{m^d N_0} - \frac{2}{d} \log(m^d N_0) \right) \cdot \frac{N-1}{m^d N_0-1} + \frac{2}{d} \log(m^d N_0)$$

$$\leq \left(\frac{\mathscr{E}_{\log,\Lambda}^{\mathrm{cp}}(N_0) + \frac{2}{d} N_0 \log N_0}{N_0} - \frac{2}{d} \log(m^d N_0) \right) \cdot \frac{N-1}{m^d N_0-1} + \frac{2}{d} \log(m^d N_0).$$

Letting $N \to \infty$ yields

$$\overline{g}_{s,d}(\Lambda) = \limsup_{N\to\infty} \frac{\mathscr{E}_{s,\Lambda}^{\mathrm{cp}}(N)}{N^{1+s/d}} \leq \left(\frac{\mathscr{E}_{s,\Lambda}^{\mathrm{cp}}(N_0)}{N_0^{1+\frac{s}{d}}} + \frac{\zeta_\Lambda(s)}{N_0^{\frac{s}{d}}} \right),$$

$$\overline{g}_{\log,d}(\Lambda) = \limsup_{N\to\infty} \frac{\mathscr{E}_{\log,\Lambda}^{\mathrm{cp}}(N) + \frac{2}{d} N \log N}{N} \leq \frac{\mathscr{E}_{\log,\Lambda}^{\mathrm{cp}}(N_0) + \frac{2}{d} N_0 \log N_0}{N_0}.$$

Letting $N_0 \to \infty$ through an appropriate subsequence yields

$$\overline{g}_{s,d}(\Lambda) \leq \liminf_{N_0\to\infty} \frac{\mathscr{E}_{s,\Lambda}^{\mathrm{cp}}(N_0)}{N_0^{1+\frac{s}{d}}} = \underline{g}_{s,d}(\Lambda),$$

$$\overline{g}_{\log,d}(\Lambda) \leq \liminf_{N_0\to\infty} \frac{\mathscr{E}_{\log,\Lambda}^{\mathrm{cp}}(N_0) + \frac{2}{d} N_0 \log N_0}{N_0} = \underline{g}_{\log,d}(\Lambda).$$

Therefore $\overline{g}_{s,d}(\Lambda) = \underline{g}_{s,d}(\Lambda) =: C_{s,d}(\Lambda)$ and $\overline{g}_{\log,d}(\Lambda) = \underline{g}_{\log,d}(\Lambda) =: C_{\log,d}(\Lambda)$.

To show $C_{s,d}(\Lambda)$ is independent of Λ, let $\Lambda_1 = A_1 \mathbb{Z}^d$ and $\Lambda_2 = A_2 \mathbb{Z}^d$ be any two lattices with co-volume 1. Then $\Lambda_2 = Q\Lambda_1$ where $Q = A_2 A_1^{-1}$. We can use rational matrices to approximate Q, namely, there exists a sequence $Q_m \in \frac{1}{m} GL(d;\mathbb{Z})$ such that $Q_m \to Q$.

For any lattice Λ, $mQ_m\Lambda = (mQ_m)\Lambda$ is a sublattice of Λ since $mQ_m \in GL(d;\mathbb{Z})$. Applying Lemma 2.4.3 to $mQ_m\Lambda$ and Λ we get

$$\mathscr{E}_{s,mQ_m\Lambda}^{\mathrm{cp}}(Nm^d |\det Q_m|) \leq m^d |\det Q_m| \mathscr{E}_{s,\Lambda}^{\mathrm{cp}}(N) + Nm^d |\det Q_m| \left(\zeta_\Lambda(s) - \zeta_{mQ_m\Lambda}(s) \right).$$

Now if we let $\Lambda = Q_m^{-1}\Lambda_2$ we get

$$\mathscr{E}_{s,m\Lambda_2}^{\mathrm{cp}}(Nm^d |\det Q_m|) \leq m^d |\det Q_m| \mathscr{E}_{s,Q_m^{-1}\Lambda_2}^{\mathrm{cp}}(N) + Nm^d |\det Q_m| \left(\zeta_{Q_m^{-1}\Lambda_2}(s) - \zeta_{m\Lambda_2}(s) \right).$$

Using relation (2.43) again implies

$$m^{-s} \mathscr{E}_{s,\Lambda_2}^{\mathrm{cp}}(Nm^d |\det Q_m|)$$
$$\leq m^d |\det Q_m| \mathscr{E}_{s,Q_m^{-1}\Lambda_2}^{\mathrm{cp}}(N) + Nm^d |\det Q_m| \left(\zeta_{Q_m^{-1}\Lambda_2}(s) - m^{-s} \zeta_{\Lambda_2}(s) \right),$$

which can be rewritten as

$$\frac{\mathscr{E}_{s,\Lambda_2}^{\mathrm{cp}}(Nm^d |\det Q_m|)}{(Nm^d |\det Q_m|)^{1+\frac{s}{d}}} \leq \frac{\mathscr{E}_{s,Q_m^{-1}\Lambda_2}^{\mathrm{cp}}(N)}{N^{1+\frac{s}{d}} |\det Q_m|^{\frac{s}{d}}} + \frac{\zeta_{Q_m^{-1}\Lambda_2}(s) - m^{-s} \zeta_{\Lambda_2}(s)}{N^{\frac{s}{d}} |\det Q_m|^{\frac{s}{d}}}.$$

Lettin $m \to \infty$ and using Corollary 2.3.4 and Lemma 2.3.5, we obtain

$$C_{s,d}(\Lambda_2) \leq \frac{\mathscr{E}_{s,Q^{-1}\Lambda_2}^{\mathrm{cp}}(N)}{N^{1+\frac{s}{d}}} + \frac{\zeta_{Q^{-1}\Lambda_2}(s)}{N^{\frac{s}{d}}} = \frac{\mathscr{E}_{s,\Lambda_1}^{\mathrm{cp}}(N)}{N^{1+\frac{s}{d}}} + \frac{\zeta_{\Lambda_1}(s)}{N^{\frac{s}{d}}}.$$

Taking $N \to \infty$ implies

$$C_{s,d}(\Lambda_2) \leq C_{s,d}(\Lambda_1).$$

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By the arbitrariness of Λ_1 and Λ_2 we must have $C_{s,d}(\Lambda) \equiv C_{s,d}$ which is independent of Λ.

For the logarithmic case, we apply Lemma 2.4.3 to $mQ_m\Lambda$ and Λ to deduce

$$\mathscr{E}_{\log,mQ_m\Lambda}^{cp}(Nm^d|\det Q_m|) \leq m^d|\det Q_m|\mathscr{E}_{\log,\Lambda}^{cp}(N) + 2Nm^d|\det Q_m|\left(\zeta'_\Lambda(0) - \zeta'_{mQ_m\Lambda}(0)\right).$$

Now if we let $\Lambda = Q_m^{-1}\Lambda_2$ we have

$$\mathscr{E}_{\log,m\Lambda_2}^{cp}(Nm^d|\det Q_m|)$$
$$\leq m^d|\det Q_m|\mathscr{E}_{\log,Q_m^{-1}\Lambda_2}^{cp}(N) + 2Nm^d|\det Q_m|\left(\zeta'_{Q_m^{-1}\Lambda_2}(0) - \zeta'_{m\Lambda_2}(0)\right).$$

Using relation (2.43) again implies

$$\mathscr{E}_{\log,\Lambda_2}^{cp}(Nm^d|\det Q_m|)$$
$$\leq m^d|\det Q_m|\mathscr{E}_{\log,Q_m^{-1}\Lambda_2}^{cp}(N) + 2Nm^d|\det Q_m|\left(\zeta'_{Q_m^{-1}\Lambda_2}(0) - \log m - \zeta'_{\Lambda_2}(0)\right),$$

which can be rewritten as

$$\frac{\mathscr{E}_{\log,\Lambda_2}^{cp}(Nm^d|\det Q_m|)}{Nm^d|\det Q_m|} \leq \frac{\mathscr{E}_{\log,Q_m^{-1}\Lambda_2}^{cp}(N)}{N} + 2\left(\zeta'_{Q_m^{-1}\Lambda_2}(0) - \log m - \zeta'_{\Lambda_2}(0)\right).$$

Therefore,

$$\frac{\mathscr{E}_{\log,\Lambda_2}^{cp}(Nm^d|\det Q_m|) + \frac{2}{d}Nm^d|\det Q_m|\log(Nm^d|\det Q_m|)}{Nm^d|\det Q_m|}$$
$$\leq \frac{\mathscr{E}_{\log,Q_m^{-1}\Lambda_2}^{cp}(N) + \frac{2}{d}N\log N}{N} + 2\left(\zeta'_{Q_m^{-1}\Lambda_2}(0) - \zeta'_{\Lambda_2}(0)\right) + \frac{2}{d}\log|\det Q_m|.$$

Now let $m \to \infty$ and recall that Lemma 2.3.5 implies that $\zeta'_{Q_m^{-1}\Lambda_2}(0) \to \zeta'_{Q^{-1}\Lambda_2}(0)$ as $m \to \infty$
to conclude

$$C_{\log,d}(\Lambda_2) \leq \frac{\mathscr{E}_{\log,Q^{-1}\Lambda_2}^{cp}(N) + \frac{2}{d}N\log N}{N} + 2\left(\zeta'_{Q^{-1}\Lambda_2}(0) - \zeta'_{\Lambda_2}(0)\right).$$

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Taking $N \to \infty$ implies

$$C_{\log,d}(\Lambda_2) \leq C_{\log,d}(\Lambda_1) + 2\left(\zeta'_{\Lambda_1}(0) - \zeta'_{\Lambda_2}(0)\right).$$

By symmetry

$$C_{\log,d}(\Lambda_1) \leq C_{\log,d}(\Lambda_2) + 2\left(\zeta'_{\Lambda_2}(0) - \zeta'_{\Lambda_1}(0)\right).$$

It follows that

$$C_{\log,d}(\Lambda_1) + 2\zeta'_{\Lambda_1}(0) = C_{\log,d}(\Lambda_2) + 2\zeta'_{\Lambda_2}(0).$$

Hence, if we define $C_{\log,d} := C_{\log,d}(\Lambda) + 2\zeta'_{\Lambda}(0)$ for any lattice Λ of co-volume 1, then this quantity is in fact independent of the choice of lattice Λ, which is what we wanted to show. $\qquad\square$

Chapter 3

4-point maximal polarization problem on S^2

3.1   Introduction

Let Ω be a set in $\mathbb{R}^d$. For any nonnegative function f and any N-point configuration $\omega_N = (A_1, \ldots, A_N) \in \Omega^N$ and $A \in \Omega$ we recall the *f-potential* of ω_N at A defined in (1.8)

$$U^f(\omega_N; A) := \sum_{k=1}^{N} f(|A - A_k|^2),$$

and the *f-polarization* of ω_N defined in (1.9)

$$M^f(\omega_N; \Omega) := \inf_{A \in \Omega} U^f(\omega_N; A). \tag{3.1}$$

The maximal f-polarization problem on Ω requires finding ω_N that maximizes $M^f(\omega_N; \Omega)$ and we shall call

$$M_n^f(\Omega) := \sup_{\omega_N \in \Omega^N} M^f(\omega_N; \Omega) = \sup_{\omega_N \in \Omega^N} \inf_{A \in \Omega} U^f(\omega_N; A). \tag{3.2}$$

the *maximal n-point f-polarization* of Ω. In the case of a Riesz-*s* potential we shall use the superscript *s* instead of *f*.

If we further assume that Ω is compact and f is lower semi-continuous then the infimum in (3.1) and the supremum in (3.2) are always attained. One reason we are interested in the maximal polarization problem is that, just as the minimal energy problem is a generalization of the best packing problem, the maximal polarization problem is a generalization of the minimal covering problem.

Let Ω be a set in $\mathbb{R}^d$. The covering radius of a *n*-point configuration $\omega_N = (A_1, \ldots, A_N)$

in Ω is defined as

$$\eta(\omega_N;\Omega) := \sup_{A \in \Omega} \min_{1 \le k \le N} |A - A_k|.$$

And the minimal n-point covering radius of Ω is defined as

$$\eta_N(\Omega) := \inf_{\omega_N} \eta(\omega_N;\Omega).$$

This quantity is the minimal radius of n balls centered in Ω that cover the set Ω. The following proposition establishes the connection between the maximal polarization problem and the minimal covering problem:

Proposition 3.1.1. *[14, Theorem III.2.1] Let Ω be a compact set in $\mathbb{R}^d$. Then for any $N > 0$ and $s > 0$,*

$$\lim_{s \to \infty} (M_N^s(\Omega))^{\frac{1}{s}} = \frac{1}{\eta_N(\Omega)}.$$

Proof. For any N-point configuration $\omega_N = (A_1,\ldots,A_N) \in \Omega^N$ we have

$$\frac{1}{\min_{1 \le i \le N} |A - A_i|} \le \left(\sum_{k=1}^{N} \frac{1}{|A - A_k|^s} \right)^{\frac{1}{s}} \le \frac{N^{\frac{1}{s}}}{\min_{1 \le i \le N} |A - A_i|}. \tag{3.3}$$

It then follows

$$\frac{1}{\inf_{\omega_N \in \Omega^N} \sup_{A \in \Omega} \min_{1 \le i \le N} |A - A_i|} \le \sup_{\omega_N \in \Omega^N} \inf_{A \in \Omega} \left(\sum_{k=1}^{N} \frac{1}{|A - A_k|^s} \right)^{\frac{1}{s}} \le \frac{N^{\frac{1}{s}}}{\inf_{\omega_N \in \Omega^N} \sup_{A \in \Omega} \min_{1 \le i \le N} |A - A_i|},$$

i.e.,

$$\frac{1}{\eta_N(\Omega)} \le (M_N^s(\Omega))^{\frac{1}{s}} \le \frac{N^{\frac{1}{s}}}{\eta_N(\Omega)}$$

Thus

$$\lim_{s \to \infty} \left(M_N^s(\Omega) \right)^{\frac{1}{s}} = \frac{1}{\eta_N(\Omega)}.$$

$\square$

It is also helpful to have the following beautiful result about minimal covering problem in mind:

Theorem 3.1.2. *[15, Theorem 6.5.1] A $(d+1)$-point configuration is optimal for the minimal covering problem on S^{d-1} if and only if it consists of the vertices of a regular d-simplex.*

To prove this theorem we need the following lemma

Lemma 3.1.3. *Spherical caps of angular radius $\varphi < \frac{\pi}{2}$ cover S^{d-1} if and only if the convex hull of their centers in $\mathbb{R}^d$ contains the ball $B(O; \cos\varphi)$ that is centered at the origin and is of radius $\cos\varphi$.*

Proof. First we assume that some spherical caps of angular radius $\varphi < \frac{\pi}{2}$ cover S^{d-1} and denote the convex hull of their centers by P. Since $\varphi < \frac{\pi}{2}$ the dimension of P is d. For any facet F of P, the $(d-1)$-dimensional affine space that contains F cuts S^{d-1} into two spherical caps. Let $S(y, \psi)$ be the one that does not contain any interior point of P where y is the center and ψ is the angular radius of the spherical cap. Since y is covered by some spherical caps centered at a vertex of P of radius φ it follows that $\psi \leq \varphi$. Hence the Euclidean distance from O to F is at least $\cos\varphi$. In other words, P contains $B(O; \cos\varphi)$.

Assume now there are some spherical caps of angular radius $\varphi < \frac{\pi}{2}$ and the convex hull of their centers P contains $B(O; \cos\varphi)$. We are going to show these spherical caps cover S^{d-1}. For any $y \in S^{d-1}$, the distance from O to the convex hull of the spherical cap $S(y, \varphi)$ is $\cos\varphi$. Therefore the intersection of P and the convex hull of $S(y, \varphi)$ is nonempty and must contain a vertex v of P. The spherical cap $S(z, \varphi)$ then covers y. $\square$

Let H be a hyperplane in $\mathbb{R}^d$ and let $\mathrm{ref}_H : \mathbb{R}^d \to \mathbb{R}^d$ denote the reflection about H. For any set X in $\mathbb{R}^d$, recall the *Steiner symmetrization* of X with respect to H is defined as

$$X' := \bigcup_{l \in \mathscr{A}} \bigcup_{x,y \in X \cap l} \frac{1}{2}(x + \mathrm{ref}_H y),$$

where $\mathscr{A}$ is the set of lines in $\mathbb{R}^d$ that are perpendicular to H. For any point $x \in \mathbb{R}^d$, denote its projection onto H by $\mathrm{proj}_H x$.

Lemma 3.1.4. *Let Δ be a d-simplex in $\mathbb{R}^d$ with vertices $v_1, v_2, \ldots, v_{d+1}$ and let H be a hyperplane in $\mathbb{R}^d$ that is perpendicular to $v_1 v_2$, i.e., $\mathrm{proj}_H v_1 = \mathrm{proj}_H v_2$. Then Δ', the Steiner symmetrization of Δ, is a d-simplex with vertices $v'_1 := \mathrm{proj}_H v_1 + \frac{1}{2}(v_1 - v_2)$, $v'_2 := \mathrm{proj}_H v_1 - \frac{1}{2}(v_1 - v_2)$, $v'_3 := \mathrm{proj}_H v_3, \ldots v'_{d+1} := \mathrm{proj}_H v_{d+1}$.*

Proof. Denote the simplex generated from $v'_1, v'_2, \ldots, v'_{d+1}$ by Δ''. We will show $\Delta' = \Delta''$. First of all Δ'' is a d-simplex. Since $v_2 - v_1, \ldots, v_{d+1} - v_1$ are linearly independent it follows that the projection of $v_3 - v_1, \ldots, v_{d+1} - v_1$ onto the orthogonal complement of $v_2 - v_1$ is still linearly independent. It then implies $\mathrm{proj}_H v_1, v'_3 \ldots v'_{d+1}$ forms a $(d-1)$-simplex in H and hence Δ'' is a d-simplex.

Secondly, it holds that $\Delta' \subset \Delta''$. For each $l \in \mathscr{A}$ and any $x, y \in \Delta \cap l$, there exist real $\{\alpha_i\}_{i=1}^{d+1}$ and β such that

$$x = \sum_{i=1}^{d+1} \alpha_i v_i, \qquad \sum_{i=1}^{d+1} \alpha_i = 1, \qquad \alpha_i \geq 0,$$

and

$$y = x + \beta(v_1 - v_2).$$

It follows that

$$y = \sum_{i=1}^{d+1} \alpha_i v_i + \beta(v_1 - v_2) = (\alpha_1 + \beta)v_1 + (\alpha_2 - \beta)v_2 + \sum_{i=3}^{d+1} \alpha_i v_i.$$

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Since $y \in \Delta$ it then implies

$$\alpha_1 + \beta \geq 0, \qquad \alpha_2 - \beta \geq 0.$$

Then

$$\frac{1}{2}(x + \mathrm{ref}_H y) = \frac{1}{2}(x + \mathrm{ref}_H x - \beta(v_1 - v_2)) = \sum_{i=1}^{d+2} \alpha_i \mathrm{proj}_H v_i - \frac{1}{2}\beta(v_1 - v_2)$$

$$= \sum_{i=3}^{d+2} \alpha_i \mathrm{proj}_H v_i + (\alpha_1 + \alpha_2)\mathrm{proj}_H v_1 - \frac{1}{2}\beta(v_1 - v_2)$$

$$= \sum_{i=3}^{d+2} \alpha_i v_i' + \frac{1}{2}(\alpha_1 + \alpha_2)(v_1' + v_2') - \frac{1}{2}\beta(v_1' - v_2')$$

$$= \sum_{i=3}^{d+2} \alpha_i v_i' + \frac{1}{2}(\alpha_1 + \alpha_2 - \beta)v_1' + \frac{1}{2}(\alpha_1 + \alpha_2 + \beta)v_2'.$$

Since both $\alpha_1 + \alpha_2 - \beta$ and $\alpha_1 + \alpha_2 + \beta$ are positive we conclude that $\frac{1}{2}(x + \mathrm{ref}_H y) \in \Delta''$.

Clearly, $v_i' \in \Delta'$ for each $1 \leq i \leq d+1$. It remains to show Δ' is a convex set and hence $\Delta' = \Delta''$. Let $\frac{1}{2}(x_1 + \mathrm{ref}_H y_1)$, $\frac{1}{2}(x_2 + \mathrm{ref}_H y_2)$ be two points in Δ' where $x_1, y_1 \in \Delta \cap l_1$, $x_1, y_1 \in \Delta \cap l_1$ and $l_1, l_2 \in \mathscr{A}$. Then for any $\lambda \in [0,1]$,

$$\lambda \cdot \frac{1}{2}(x_1 + \mathrm{ref}_H y_1) + (1 - \lambda) \cdot \frac{1}{2} * x_2 + \mathrm{ref}_H y_2)$$

$$= \frac{1}{2}((\lambda x_1 + (1 - \lambda)x_2) + \mathrm{ref}_H(\lambda y_1 + (1 - \lambda)y_2))$$

lies in Δ' since $\lambda x_1 + (1 - \lambda)x_2$, $\lambda y_1 + (1 - \lambda)y_2 \in \Delta \cap l$ where $l = \lambda l_1 + (1 - \lambda)l_2$ is a straight line perpendicular to H. Therefore Δ' is convex completing the proof of our lemma. $\qquad \square$

Proof of Theorem 3.1.2. For any d-simplex Δ in $B(O; 1)$ that contains O, let $r(\Delta)$ be the maximum radius of balls that are centered at O and are contained in Δ. If Δ is inscribed in S^{d-1} then Lemma 3.1.3 implies that the minimal angular radius of spherical caps centered at vertices of Δ that cover S^{d-1} is $\arccos r(\Delta)$. Therefore, it is sufficient to show that

the maximum of $r(\Delta)$ among all d-simplices in $B(O;1)$ is attained if and only if Δ is a regular d-simplex. Note that if Δ is not inscribed in S^{d-1} we can always perturb the vertices of Δ and strictly increase $r(\Delta)$. Hence we may assume Δ maximizes $r(\Delta)$ and Δ is inscribed in S^{d-1}. Assume to the contrary that Δ is not regular, then there exist vertices u, v, w of Δ such that $|u-v| \neq |u-w|$. Let H be the hyperplane that bisects the edge vw perpendicularly and let $\text{ref}_H : \mathbb{R}^d \to \mathbb{R}^d$ denote the reflection about H. For any set X in $\mathbb{R}^d$, denote its Steiner symmetrization by X'. Since $B(O;r(\Delta)) \subset \Delta \subset B(O;1)$ it follows that $B(O;r(\Delta)) = B'(O;r(\Delta)) \subset \Delta' \subset B'(O;1) = B(O;1)$. Therefore $r(\Delta')$ equals $r(\Delta)$ and Δ' is also an optimal simplex. By Lemma 3.1.4 $\text{proj}_H u$ is a vertex of Δ'. It contradicts the maximality of $r(\Delta)$ since $\text{proj}_H u$ lies in the interior of $B(O;1)$. $\qquad \square$

3.2   Main results

In this chapter we are concerned with the case when $\Omega = S^2$ and $n = 4$ and we shall prove the following theorem which is our main result.

Theorem 3.2.1. *Let $f : [0,4] \to [0,\infty]$ be non-increasing and strictly convex with $f(0) = \lim\limits_{x \to 0^+} f(x)$. Then ω_4 is optimal for the 4-point maximal polarization problem on S^2, i.e., $M^f(\omega_4;S^2) = M_4^f(S^2)$, if and only if $\omega_4 = \omega_T$ up to rotations, where ω_T is a configuration that consists of vertices of a regular tetrahedron.*

We remark that the convexity of f and left continuity of f at 0 implies f is a continuous extended real-valued function on $[0,4]$. According to [16] $M^f(\omega_T;S^2)$ is attained by the antipodes of the vertices of ω_T, i.e., $M^f(\omega_T;S^2) = U^f(\omega_T;S(\omega_T))$ where $S(\omega_T)$ is any antipode of vertices of ω_T.

We also conjecture that

Conjecture 3.2.2. *Let $f : [0,4] \to [0,\infty]$ be non-increasing and strictly convex. Then ω_{d+1} is optimal for the $(d+1)$-point maximal polarization problem on S^{d-1} if and only if it consists of vertices of a regular d-simplex.*

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Lemma 3.2.3. *Let* $f : [0,4] \to [0,\infty]$ *be non-increasing and strictly convex with* $f(0) = \lim_{x \to 0^+} f(x)$. *Then for any* $\omega_4 \in (S^2)^4$, *there exists a point* $A(\omega_4) \in S^2$ *such that*

$$U^f(\omega_4, A(\omega_4)) \leq U^f(\omega_T, S(\omega_T)). \tag{3.4}$$

Equality holds if and only if $\omega_4 = \omega_T$ *up to rotations.*

The proof of Theorem 3.2.1 is straightforward once Lemma 3.2.3 is established.

Proof of Theorem 3.2.1. For any $\omega_4 \in (S^2)^4$, by Lemma 3.2.3,

$$\min_{A \in S^2} U^f(\omega_4; A) \leq U^f(\omega_4; A(\omega_4)) \leq U^f(\omega_T; S(\omega_T)).$$

Therefore

$$\max_{\omega_4 \in (S^2)^4} \min_{A \in S^2} U^f(\omega_4; A) \leq U^f(\omega_T; S(\omega_T)).$$

Equality holds if and only if $\omega_4 = \omega_T$ up to rotations. $\square$

Before proving Lemma 3.2.3 we will first introduce some notations and establish some lemmas we are going to use.

Let $\omega_4 = (A_1, A_2, A_3, A_4) \in (S^2)^4$. If all 4 points are on a hemisphere, say the one that is given by $\{(x,y,z)|x^2 + y^2 + z^2 = 1, z \leq 0\}$, then, as shown below (see proof of Lemma 3.2.3), inequality (3.4) holds with $A(\omega_4)$ simply chosen to be the pole $(0,0,1)$. Thus we may assume A_1, A_2, A_3, A_4 are all different (otherwise there would be four points on a hemisphere). For any three different points A_i, A_j, A_k in ω_4, let $d(O, A_i A_j A_k)$ be the distance from the origin O to the plane $A_i A_j A_k$. Without loss of generality we may assume $d(O, A_1 A_2 A_3)$ is the smallest, i.e. A_1, A_2, A_3 form the largest spherical cap. Here the spherical cap determined by A_i, A_j, A_k is chosen to be the one whose boundary contains A_i, A_j, A_k and the cap does not contain the fourth point. Let (x_i, y_i, z_i) be the Cartesian coordinates

of A_i. As the potential energy of ω_4 is invariant under rotations we may further assume that A_1, A_2, A_3 are arranged horizontally so that $z_1 = z_2 = z_3 < z_4$. As we said it is sufficient to consider the case when none of these 4 points are on the same hemisphere. Thus for each $\theta \in [0, \frac{\pi}{2})$, we consider

$$\Omega(\theta) := \{(A_1, A_2, A_3, A_4) \in (S^2)^4 | \triangle A_1 A_2 A_3 \text{ is an acute triangle}, d(O, A_1 A_2 A_3)$$
$$= \min_{1 \leq i < j < k \leq 4} d(O, A_i A_i A_k), z_1 = z_2 = z_3 = -\cos\theta \leq 0, z_4 > -\cos\theta\}.$$

Here θ is the angular radius of the spherical cap determined by A_1, A_2, A_3, see Figure 3.1.

Lemma 3.2.4. $\Omega(\theta)$ *is nonempty if and only if* $\theta \in [\arccos\frac{1}{3}, \frac{\pi}{2})$. *Furthermore,*

$$\Omega\left(\arccos\frac{1}{3}\right) = \{\rho\omega_T | \rho \text{ is any rotation about the z-axis}\}.$$

Proof. Let $\theta \in [\arccos\frac{1}{3}, \frac{\pi}{2})$ and let $A_1 A_2 A_3$ be an equilateral triangle with z-coordinate equal to $-\cos\theta$ and A_4 be the north pole. Then the spherical cap $A_1 A_2 A_3$ is the largest spherical cap determined by $A_i A_j A_k$ and it follows that $\omega_4 = \{A_1, A_2, A_3, A_4\} \in \Omega(\theta)$. If $\theta < \arccos\frac{1}{3}$, assume to the contrary that there exists $\omega_4 \in \Omega(\theta)$. Then the covering radius of ω_4 is determined by the largest spherical cap $A_1 A_2 A_3$ which is less than that of ω_T. This contradicts the fact that ω_T is the unique configuration that has the minimal covering radius among all 4-point configurations up to rotations (cf. [15, theorem 6.5.1]). $\square$

Let A_1, A_2, A_3 be points on S^2 with $z_1 = z_2 = z_3 = -\cos\theta$ and such that $\triangle A_1 A_2 A_3$ is acute. If $\theta < \frac{\pi}{2}$ then $d(O, A_1 A_2 A_3) > 0$. Let $\Pi_{ij}(i, j \in \{1, 2, 3\}, i \neq j)$ be the reflection of plane $A_1 A_2 A_3$ about plane $OA_i A_j$, i.e., Π_{ij} satisfies

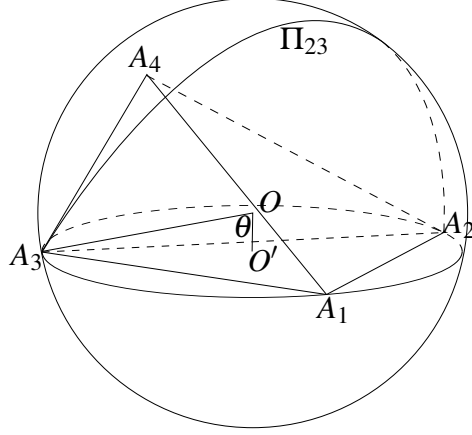$$d(O, \Pi_{ij}) = d(O, A_1 A_2 A_3) \leq d(O, A_i A_j A_4).$$

Figure 3.1: Π_{23} satisfies $d(O,\Pi_{23}) = d(O,A_1A_2A_3) \leq d(O,A_1A_2A_4)$
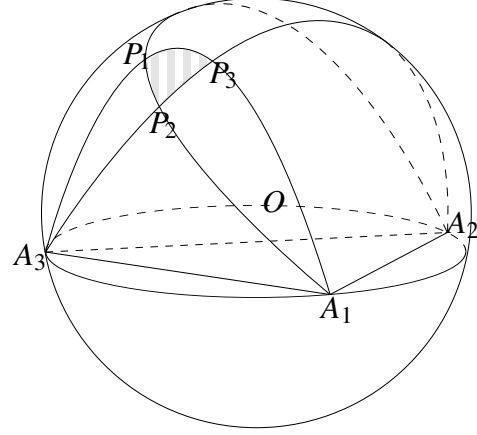
Figure 3.2: $\widetilde{\triangle}P_1P_2P_3$ is the domain of A_4. It is a spherical triangle if nonempty.

Π_{12}, Π_{23}, Π_{31} determine a region on S^2 (See Figure 3.2):

$$\bigcap_{i \neq j, i,j \in \{1,2,3\}} \{A_4 \in S^2 | d(O,A_1A_2A_3) \leq d(O,A_iA_jA_4), z_4 > -\cos\theta\}$$

$$= \{A_4 \in S^2 | (A_1,A_2,A_3,A_4) \in \Omega(\theta)\}.$$

If this set is nonempty it is in fact a spherical triangle $\widetilde{\triangle}P_1P_2P_3$ where P_1 is the intersection of Π_{12} and Π_{13} on the unit sphere, and so on for P_2 and P_3. It is easy to see that $\widetilde{\triangle}P_1P_2P_3$ is either a spherical triangle or degenerates to a single point if nonempty. Namely, $\widetilde{\triangle}P_1P_2P_3$ is the set of A_4 such that A_1, A_2, A_3 form the largest spherical cap. $\Omega(\theta)$ can be rewritten as

$$\Omega(\theta) = \Big\{ (A_1,A_2,A_3,A_4) \in (S^2)^4 | \triangle A_1A_2A_3 \text{ is an acute triangle,}$$

$$z_1 = z_2 = z_3 = -\cos\theta, A_4 \in \widetilde{\triangle}P_1P_2P_3 \Big\}.$$

The following calculation is crucial for our analysis.

Lemma 3.2.5. *Let A_1, A_2, A_3 be different points on the sphere with z-coordinate equal $-\cos\theta(0 < \theta < \frac{\pi}{2})$. Denote by O' the projection of O to the plane $A_1A_2A_3$ (i.e., $O' =$*

$(0, 0, -\cos\theta))$, *and let ϕ_1, ϕ_2, ϕ_3 denote the angles $\angle A_2 O' A_3$, $\angle A_3 O' A_1$, $\angle A_1 O' A_2$, respectively. Then the z-coordinate of P_3 is given by*

$$z_{P_3} = \cos\theta \left[-1 + \frac{4\tan^2\theta}{\sec^2\theta - \tan\frac{\phi_1}{2}\tan\frac{\phi_2}{2} + \frac{(\tan\frac{\phi_1}{2} + \tan\frac{\phi_2}{2})^2}{\sec^2\theta - \tan\frac{\phi_1}{2}\tan\frac{\phi_2}{2}}} \right]. \tag{3.5}$$

Proof. See section 3.3. $\qquad\square$

Corollary 3.2.6. *Let $(A_1, A_2, A_3, A_4) \in \Omega(\theta)$ and ϕ_1, ϕ_2, ϕ_2 be as described in Lemma 3.2.5, then for any $1 \le i < j \le 3$ it holds*

$$\sec^2\theta > \tan\frac{\phi_i}{2}\tan\frac{\phi_j}{2}. \tag{3.6}$$

In addition, there exist $C_1(\theta), C_2(\theta) \in \left(0, \frac{\pi}{2}\right)$ such that for any $i \in \{1, 2, 3\}$ it holds that

$$C_1(\theta) < \frac{\phi_i}{2} < C_2(\theta),$$

where $C_1(\theta), C_2(\theta)$ only depend on θ.

Proof. The existence of (A_1, A_2, A_3, A_4) suggests $\widetilde{\triangle} P_1 P_2 P_3$ is well-defined and nonempty. Since $P_3 \in \widetilde{\triangle} P_1 P_2 P_3$, the definition of $\widetilde{\triangle} P_1 P_2 P_3$ implies $z_{P_3} > -\cos\theta$. The first desired inequality then follows immediately from identity (3.5).

To prove the second inequality, without loss of generality we may assume $i = 3$. Using trigonometric identities we have

$$\tan\frac{\phi_3}{2} = \tan\left(\pi - \frac{\phi_1}{2} - \frac{\phi_2}{2}\right) = -\tan\left(\frac{\phi_1}{2} + \frac{\phi_2}{2}\right) = \frac{\tan\frac{\phi_1}{2} + \tan\frac{\phi_2}{2}}{\tan\frac{\phi_1}{2}\tan\frac{\phi_2}{2} - 1}$$

$$\ge \frac{2\sqrt{\tan\frac{\phi_1}{2}\tan\frac{\phi_2}{2}}}{\tan\frac{\phi_1}{2}\tan\frac{\phi_2}{2} - 1} = \frac{2}{\sqrt{\tan\frac{\phi_1}{2}\tan\frac{\phi_2}{2}} - \frac{1}{\sqrt{\tan\frac{\phi_1}{2}\tan\frac{\phi_2}{2}}}} > \frac{2}{\sec\theta - \frac{1}{\sec\theta}}.$$

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Using inequality (3.6) and the above inequality for ϕ_1 we get

$$\tan \frac{\phi_3}{2} < \frac{\sec^2 \theta}{\tan \frac{\phi_1}{2}} < \sec^2 \theta \left(\frac{\sec \theta - \frac{1}{\sec \theta}}{2} \right) = \frac{\sec^3 \theta - \sec \theta}{2}.$$

Therefore $C_1(\theta) := \arctan \left(\frac{2}{\sec \theta - \frac{1}{\sec \theta}} \right)$ and $C_2(\theta) := \arctan \left(\frac{\sec^3 \theta - \sec \theta}{2} \right)$ satisfy the desired inequalities. $\quad\square$

Lemma 3.2.7. $\Omega(\theta)$ *is closed for each* $\theta \in [\arccos \frac{1}{3}, \frac{\pi}{2})$.

Proof. Let $\left(A_1^{(n)}, A_2^{(n)}, A_3^{(n)}, A_4^{(n)} \right)$ be a sequence in $\Omega(\theta)$ such that $\left(A_1^{(n)}, A_2^{(n)}, A_3^{(n)}, A_4^{(n)} \right) \to (A_1, A_2, A_3, A_4)$. It follows immediately from Corollary 3.2.6 that $\triangle A_1 A_2 A_3$ is still an acute triangle. Using the definition of $\Omega(\theta)$ and limit properties we get $d(O, A_1 A_2 A_3) = \min_{1 \le i \le j \le k} d(O, A_i A_i A_k)$ and $z_4 = \lim_{n \to \infty} z_4^{(n)} \ge -\cos \theta$. It remains to show $z_4 > -\cos \theta$. Assume to the contrary that $z_4 = -\cos \theta$. Then A_1, A_2, A_3, A_4 are on the plane $\{ (x, y, z) \in S^2 | z = -\cos \theta \}$. Since A_1, A_2, A_3 are distinct points without loss of generality we may assume A_4 is on the arc $A_1 A_2$ and $A_4 \ne A_1$. Therefore $A_1^{(n)}, A_3^{(n)}, A_4^{(n)}$ will still be distinct when n is sufficiently large. Notice that $z_4^{(n)} > -\cos \theta$ and $\lim_{n \to \infty} z_4^{(n)} = -\cos \theta < 0$ it follows that $d \left(O, A_1^{(n)} A_3^{(n)} A_4^{(n)} \right)$ increases to but does not equal $d(O, A_1 A_3 A_4) = \cos \theta = d \left(O, A_1^{(n)} A_2^{(n)} A_3^{(n)} \right)$ as $n \to \infty$, which contradicts the fact that

$$d \left(O, A_1^{(n)} A_2^{(n)} A_3^{(n)} \right) = \min_{1 \le i < j < k \le 4} d \left(O, A_i^{(n)} A_j^{(n)} A_k^{(n)} \right).$$

$\quad\square$

Lemma 3.2.8. *For* $\theta \in [\arccos \frac{1}{3}, \frac{\pi}{2})$, $\min_{\Omega(\theta)} z_4$ *is attained by some* $(A_1, A_2, A_3, A_4) \in \Omega(\theta)$ *only if the spherical triangle* $\widetilde{\triangle} P_1 P_2 P_3$ *determined by* A_1, A_2, A_3 *degenerates to a single point.*

The idea of this proof is that if $\widetilde{\triangle} P_1 P_2 P_3$ is not a single point we can always perturb A_1, A_2, A_3 so that $\widetilde{\triangle} P_1 P_2 P_3$ is still nonempty and z_4 decreases.

Proof. $\Omega(\theta)$ is closed and nonempty by Lemma 3.2.7 and Lemma 3.2.4. Thus $\min\limits_{\Omega(\theta)} z_4$ exists. Assume by contradiction that $\min\limits_{\Omega(\theta)} z_4$ is attained by A_1, A_2, A_3 but $\widetilde{\triangle P_1 P_2 P_3}$ is not a single point. In other words, P_1, P_2, P_3 are distinct. It is clear that $\min z_4$ is either z_{P_1}, z_{P_2} or z_{P_3}. By (3.5) we can consider z_{P_3} as a function of $x = \tan\frac{\phi_1}{2}$ and $y = \tan\frac{\phi_2}{2}$:

$$z_{P_3}(x,y) = \cos\theta \left[-1 + \frac{4\tan^2\theta}{\sec^2\theta - xy + \frac{(x+y)^2}{\sec^2\theta - xy}} \right]. \tag{3.7}$$

Without loss of generality we may assume

$$\min_{\Omega(\theta)} z_4 = \min_{\substack{z_1 = z_2 = z_3 = -\cos\theta \\ A_4 \in \widetilde{\triangle P_1 P_2 P_3}}} z_4 = \min_{\substack{x = \tan\frac{\phi_1}{2} \\ y = \tan\frac{\phi_2}{2} \\ \widetilde{\triangle P_1 P_2 P_3} \neq \emptyset}} \min_i z_{P_i}(x,y) = z_{P_3}(x_0, y_0).$$

We claim that

$$\left. \frac{\partial z_{P_3}}{\partial x} \right|_{(x_0, y_0)} = \left. \frac{\partial z_{P_3}}{\partial y} \right|_{(x_0, y_0)} = 0. \tag{3.8}$$

Otherwise we can perturb ϕ_1 and ϕ_2 so that: (1) z_{P_3} strictly decreases since the derivative is nonzero; (2) $\widetilde{\triangle P_1 P_2 P_3}$ is still nonempty since P_1, P_2, P_3 is continuous with respect to ϕ_1 and ϕ_2. This contradicts to the minimality of $z_{P_3}(x_0, y_0)$.

Let $A = \sec\theta$, then $A > 3$ (if $A = 3$, then by Lemma 3.2.4 ω_T is the only configuration in $\Omega(\theta)$ and hence P_1, P_2, P_3 coincide). It follows from (3.7) and (3.8) that

$$(x+y)(2A^2 - xy + y^2) = y(A^2 - xy)^2, \tag{3.9}$$

$$(x+y)(2A^2 - xy + x^2) = x(A^2 - xy)^2. \tag{3.10}$$

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Subtracting these two equations we get

$$(x+y)^2(y-x) = (A^2-xy)^2(y-x).$$

Notice that it follows from Corollary 3.2.6 that $A^2-xy > 0$, and so we conclude

$$y = x, \qquad \text{or} \qquad x+y = A^2-xy.$$

If $x+y = A^2-xy$ then (3.9) yields

$$2A^2-xy+y^2 = y(x+y).$$

Thus $A^2 = xy$ which contradicts Corollary 3.2.6.

If $x = y$ then (3.9) yields

$$2x \cdot 2A^2 = x(A^2-x^2)^2$$

$$\implies x^2 = y^2 = A^2-2A > 3^2-2\cdot3 = 3$$

$$\implies \tan\frac{\phi_1}{2} = \tan\frac{\phi_2}{2} > \sqrt{3} \implies \phi_1 = \phi_2 > \frac{2\pi}{3} > \phi_3 = 2\pi-\phi_1-\phi_2.$$

We will show $z_{P_1} = z_{P_2} < z_{P_3}$ and hence it contradicts our assumption. In fact,

$$\tan\frac{\phi_3}{2} = \tan\left(\pi-\frac{\phi_1}{2}-\frac{\phi_2}{2}\right) = -\tan\left(\frac{\phi_1}{2}+\frac{\phi_2}{2}\right) = \frac{\tan\frac{\phi_1}{2}+\tan\frac{\phi_2}{2}}{\tan\frac{\phi_1}{2}\tan\frac{\phi_2}{2}-1} = \frac{2x}{x^2-1}.$$

Thus

$$\left(A^2 - \tan\frac{\phi_2}{2}\tan\frac{\phi_3}{2} + \frac{(\tan\frac{\phi_2}{2}+\tan\frac{\phi_3}{2})^2}{A^2 - \tan\frac{\phi_2}{2}\tan\frac{\phi_3}{2}} \right) -$$

$$\left(A^2 - \tan\frac{\phi_2}{2}\tan\frac{\phi_1}{2} + \frac{(\tan\frac{\phi_2}{2}+\tan\frac{\phi_1}{2})^2}{A^2 - \tan\frac{\phi_2}{2}\tan\frac{\phi_1}{2}} \right)$$

$$= \left(A^2 - x\cdot\frac{2x}{x^2-1} + \frac{(x+\frac{2x}{x^2-1})^2}{A^2 - x\cdot\frac{2x}{x^2-1}} \right) - \left(A^2 - x^2 + \frac{4x^2}{A^2-x^2} \right)$$

$$= \frac{x^2(x^2-3)(A^2-1)[(A^2-1)x^2-A^2-x^4]}{(x^2-1)(A^2-x^2)[(A^2-2)x^2-A^2]}$$

$$= \frac{x^2(x^2-3)(A^2-1)2A(A-1)(A-2))}{(x^2-1)(A^2-x^2)A[A(A+1)(A-3)+4]} > 0. \qquad \text{(substitute } x^2 = A^2 - 2A.\text{)}$$

By (3.5) we have $z_{P_1} < z_{P_3}$, a contradiction to the minimality of z_{P_3}.

The above argument shows that our assumption at the beginning of the proof is false. Therefore $\min\limits_{\Omega(\theta)} z_4$ is attained by A_1, A_2, A_3 only if $\widetilde{\triangle}P_1P_2P_3$ is a single point. □

Lemma 3.2.9. *The following are equivalent*

(a) $\widetilde{\triangle}P_1P_2P_3$ *is a single point.*

(b) The incenter and the circumcenter of $A_1A_2A_3A_4$ coincide.

(c) $A_1A_2A_3A_4$ is equiareal, i.e., all its facets have the same area.

Proof. $(a) \Leftrightarrow (b)$ is trivial. For a proof of the equivalence of (b) and (c), see [17] for example. □

Remark 3.2.10. *It is known that (cf. [17]) for any d-simplex Δ, the circumcenter and the incenter of Δ coincide if and only if Δ is equiradial, i.e., all the facets of Δ have the same circumradius. The incenter and the centroid of Δ coincide if and only if Δ is equiareal. It is also known that a tetrahedron is equiradial if and only if it is equiareal. It then follows that the circumcenter and the incenter of a tetrahedron coincide if and only if it is isosceles. But for $d \geq 4$, there are equiradial d-simplices which are not equiareal. And this is one obstacle we come across when we try to extend our proof to higher dimensions.*

Corollary 3.2.11. *For $\theta \in [\arccos \frac{1}{3}, \frac{\pi}{2}]$, $\min\limits_{\Omega(\theta)} z_4 = 3\cos\theta$.*

Proof. If $\theta = \frac{\pi}{2}$ this is trivial. Assume that $\theta < \frac{\pi}{2}$. Suppose $\min\limits_{\Omega(\theta)} z_4$ is attained by some configuration (A_1, A_2, A_3, A_4). By Lemma 3.2.8 and Lemma 3.2.9 the tetrahedron $A_1 A_2 A_3 A_4$ is equiareal and hence all its four faces have the same area. Let S_0 be this face area. On the one hand the volume of $A_1 A_2 A_3 A_4$ equals

$$V_{A_1 A_2 A_3 A_4} = \frac{1}{3} S_0 \cdot (z_4 - (-\cos\theta)).$$

On the other hand, the center O of $A_1 A_2 A_3 A_4$ divides the whole tetrahedron into four small tetrahedron $OA_i A_j A_k$. Thus

$$V_{A_1 A_2 A_3 A_4} = 4 V_{OA_1 A_2 A_3} = 4 \cdot \frac{1}{3} S_0 \cdot \cos\theta.$$

Therefore,

$$z_4 + \cos\theta = 4\cos\theta \implies z_4 = 3\cos\theta.$$

$\square$

Lemma 3.2.12. *Let $f : [0,4] \to [0,\infty]$ be non-increasing and strictly convex and let $g(t) := 3f(2-2t) + f(2+6t)$, $t \in [0, \frac{1}{3}]$. Then $g(t)$ is a strictly decreasing function.*

Proof. For any $0 \leq t_1 < t_2 \leq \frac{1}{3}$, it follows that $2 - 2t_2 \leq 2 - 2t_1 \leq 2 + 6t_1 \leq 2 + 6t_2$. Using properties of strictly convex functions we obtain

$$\frac{f(2-2t_1) - f(2-2t_2)}{(2-2t_1) - (2-2t_2)} < \frac{f(2+6t_2) - f(2+6t_1)}{(2+6t_2) - (2+6t_1)}.$$

Therefore,

$$g(t_1) \leq g(t_2)$$

□

Proof of Lemma 3.2.3. It is elementary to compute that

$$U^f(\omega_T, S(\omega_T)) = 3f(4/3) + f(4) = g(1/3).$$

Let $\omega_4 = (A_1, A_2, A_3, A_4)$ be in $(S^2)^4$. If they are on a hemisphere, without loss of generality we may assume $z_1, z_2, z_3, z_3 \leq 0$. Let $A(\omega_4) = (0, 0, 1)$. Using Lemma 3.2.12 we get

$$\begin{aligned}
U^f(\omega_4, A(\omega_4)) &= \sum_{j=1}^4 f(|A(\omega_4)A_i|^2) = \sum_{j=1}^4 f(2(1 - z_i)) \\
&\leq \sum_{j=1}^4 f(2) = g(0) < g(1/3) = U^f(\omega_T, S(\omega_T)).
\end{aligned}$$

Therefore we may assume A_1, A_2, A_3, A_4 are not on any hemisphere. In particular, A_1, A_2, A_3, A_4 are distinct. Without loss of generality we may assume $A_1 A_2 A_3$ is the largest spherical cap and $z_1 = z_2 = z_3 = -\cos\theta < z_4, \theta \in [0, \frac{\pi}{2})$.

If $\triangle A_1 A_2 A_3$ is not acute assume that $\frac{\phi_1}{2} \geq \frac{\pi}{2}$. The plane Π_{23} cuts $B(0; 1)$ into two sets, the one that contains O and the one that doesn't. $\triangle A_1 A_2 A_3$ being not acute implies that A_1, A_2, A_3, A_4 are in the set that does not contain O. Therefore A_1, A_2, A_3, A_4 are on a hemisphere and hence (A_1, A_2, A_3, A_4) is not optimal. It remains to consider the case when $\triangle A_1 A_2 A_3$ is acute. In other words, $\omega_4 \in \Omega(\theta)$. By Lemma 3.2.4 we have $\theta \in [\arccos \frac{1}{3}, \frac{\pi}{2}]$. Let $A(\omega_4) = S = (0, 0, -1)$. Using Corollary 3.2.11

$$\begin{aligned}
U^f(\omega_4, S) &= \sum_{j=1}^4 f(|SA_i|^2) = \sum_{j=1}^4 f(2(1 + z_i)) \\
&\leq 3f(2(1 - \cos\theta)) + f(2(1 + \min_{\Omega(\theta)} z_4)) \\
&= 3f(2(1 - \cos\theta)) + f(2(1 + 3\cos\theta)) = g(\cos\theta).
\end{aligned}$$

Therefore for any $\theta \in \left[\arccos \frac{1}{3}, \frac{\pi}{2} \right)$,

$$U^f(\omega_4, S) = g(\cos \theta) \leq g(1/3) = U^f(\omega_T, S(\omega_T)).$$

Equality holds if and only if $\theta = \arccos \frac{1}{3}$, i.e., ω_4 equal ω_T up to rotations.

$\square$

3.3 Proof of Lemma 3.2.5

Assume that (see figure 3.1)

$$A_1 = (\sin \theta \cos \phi_2, -\sin \theta \sin \phi_2, -\cos \theta),$$

$$A_2 = (\sin \theta \cos \phi_1, \sin \theta \sin \phi_1, -\cos \theta),$$

$$A_3 = (\sin \theta, 0, -\cos \theta),$$

$$P_3 = (x_0, y_0, z_0).$$

We will solve (x_0, y_0, z_0) from the equations

$$\begin{cases} d(O, P_3 A_1 A_3) = d(O, P_3 A_2 A_3) = d(O, A_1 A_2 A_3) = \cos \theta \\ x_0^2 + y_0^2 + z_0^2 = 1 \end{cases} \tag{3.11}$$

Clearly,

$$\overrightarrow{A_2 A_3} = (\sin \theta (1 - \cos \phi_1), -\sin \theta \sin \phi_1, 0),$$

$$\overrightarrow{A_3 P_3} = (x_0 - \sin \theta, y_0, z_0 + \cos \theta),$$

We then obtain a normal vector of the plane $P_3A_2A_3$

$$
\vec{n} = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ x_0 - \sin\theta & y_0 & z_0 + \cos\theta \\ \sin\theta(1 - \cos\phi_1) & -\sin\theta\sin\phi_1 & 0 \end{vmatrix}
$$

$$
= ((z_0 + \cos\theta)\sin\theta\sin\phi_1, (z_0 + \cos\theta)\sin\theta(1 - \cos\phi_1),
$$

$$
- (x_0 - \sin\theta)\sin\theta\sin\phi_1 - y_0\sin\theta(1 - \cos\phi_1)
$$

$$
=: (a_1, b_1, c_1).
$$

Thus the equation of the plane $P_3A_2A_3$ has the form

$$
a_1(x - \sin\theta) + b_1 y + c_1(z + \cos\theta) = d_1
$$

and

$$
d(O, P_3A_2A_3) = \frac{|a_1\sin\theta - c_1\cos\theta|}{\sqrt{a_1^2 + b_1^2 + c_1^2}}.
$$

Similarly if we let (replacing ϕ_1 by $-\phi_2$)

$$
(a_2, b_2, c_2) := (-(z_0 + \cos\theta)\sin\theta\sin\phi_2, (z_0 + \cos\theta)\sin\theta(1 - \cos\phi_2),
$$

$$
(x_0 - \sin\theta)\sin\theta\sin\phi_2 - y_0\sin\theta(1 - \cos\phi_2))
$$

then

$$
d(O, P_3A_1A_3) = \frac{|a_2\sin\theta - c_2\cos\theta|}{\sqrt{a_2^2 + b_2^2 + c_2^2}}.
$$

Thus

$$(3.11) \iff \begin{cases} \dfrac{|a_1\sin\theta - c_1\cos\theta|}{\sqrt{a_1^2+b_1^2+c_1^2}} = \dfrac{|a_2\sin\theta - c_2\cos\theta|}{\sqrt{a_2^2+b_2^2+c_2^2}} = \cos\theta \\ x_0^2 + y_0^2 + z_0^2 = 1 \end{cases}. \qquad (3.12)$$

$$\frac{|a_1\sin\theta - c_1\cos\theta|}{\sqrt{a_1^2+b_1^2+c_1^2}} = \cos\theta$$

$$\iff (a_1\sin\theta - c_1\cos\theta)^2 = (a_1^2+b_1^2+c_1^2)\cos^2(\theta)$$

$$\iff a_1^2(\tan^2\theta - 1) = 2a_1c_1\tan\theta + b_1^2$$

$$\iff (z_0+\cos\theta)\sin^2(\phi_1)(\tan^2\theta - 1) = 2\sin\phi_1\tan\theta \cdot$$

$$[-(x_0-\sin\theta)\sin\phi_1 - y_0(1-\cos\phi_1] + (z_0+\cos\theta)(1-\cos\phi_1)^2$$

$$\iff (z_0+\cos\theta)\left(\tan^2\theta - \tan^2\frac{\phi_1}{2} - 1\right) = 2\tan\theta\left[-(x_0-\sin\theta) - y_0\tan\frac{\phi_1}{2}\right]. \qquad (3.13)$$

Similarly we have

$$(z_0+\cos\theta)\left(\tan^2\theta - \tan^2\frac{\phi_2}{2} - 1\right) = 2\tan\theta\left[-(x_0-\sin\theta) + y_0\tan\frac{\phi_2}{2}\right]. \qquad (3.14)$$

Now we can solve for z_0:

$$(3.13)-(3.14) \implies y_0 = \frac{(z_0+\cos\theta)(\tan\frac{\phi_2}{2} - \tan\frac{\phi_1}{2})}{2\tan\theta}$$

$$(3.13) \implies x_0 = \sin\theta + \frac{(z_0+\cos\theta)(\tan\frac{\phi_1}{2}\tan\frac{\phi_2}{2} + 2 - \sec^2\theta)}{2\tan\theta}.$$

$$x_0^2 + y_0^2 + z_0^2 = 1 \implies (x_0-\sin\theta)^2 + 2(x_0-\sin\theta)\sin\theta + y_0^2 + (z_0-\cos\theta)(z_0+\cos\theta) = 0$$

Therefore,

$$\frac{z_0 + \cos\theta}{4\tan^2\theta} \left[(z_0 + \cos\theta)\left(\tan\frac{\phi_1}{2}\tan\frac{\phi_2}{2} + 2 - \sec^2\theta\right)^2 + \right.$$

$$4\cos\theta\tan^2\theta\left(\tan\frac{\phi_1}{2}\tan\frac{\phi_2}{2} + 2 - \sec^2\theta\right) +$$

$$\left. (z_0 + \cos\theta)\left(\tan\frac{\phi_2}{2} - \tan\frac{\phi_1}{2}\right)^2 + 4\tan^2\theta(z_0 + \cos\theta) - 8\cos\theta\tan^2\theta \right] = 0$$

$$\Longrightarrow z_0 = -\cos\theta \text{ or}$$

$$z_0 = \cos\theta\left[-1 + \frac{4\tan^2\theta(\sec^2\theta - \tan\frac{\phi_1}{2}\tan\frac{\phi_2}{2})}{(\sec^2\theta - \tan\frac{\phi_1}{2}\tan\frac{\phi_2}{2})^2 + (\tan\frac{\phi_1}{2} + \tan\frac{\phi_2}{2})^2} \right].$$

Chapter 4

Universally Optimal Periodic Configurations in $\mathbb{R}^d$

4.1 The 1 dimensional case

Recall that a spherical $(2m-1)$-design of S^{d-1} is *sharp* if there are at most m different inner products between distinct points in the design. In [2] Cohn and Kumar show that any sharp design is universally optimal among configurations with the same number of points in S^{d-1}. This result can be applied to a large class of configurations in S^{d-1}. In particular when $d = 2$ we have the following:

Theorem 4.1.1. *Let the potential function* $f : [0,4] \to \mathbb{R} \cup \{\infty\}$ *be strictly completely monotonic on* $(0,4]$ *with* $f(0) = \lim\limits_{x \to 0^+} f(x)$. *Then an N-point configuration* ω_N *on* S^1 *minimizes* $E_f(\omega_N)$ *if and only if* ω_N *consists of N equally spaced points on* S^1.

Proof. See Theorem 1.2 in [2]. □

We remark that there is a classical result for the case where $f(x^2) = g(x)$ for some function g that is convex and decreasing.

Theorem 4.1.2. *[18] Let* $g : [0,2] \to \mathbb{R} \cup \{\infty\}$ *be convex and decreasing on* $(0,2]$ *with* $g(0) = \lim\limits_{x \to 0^+} g(x)$. *Let* $f : [0,4] \to \mathbb{R} \cup \{\infty\}$ *be the function that satisfies* $f(x^2) = g(x)$ *for any* $x \in [0,2]$. *Then any configuration of equally spaced points on* S^1 *minimizes the energy* $E_f(\omega_N)$.

Proof. For any configuration $\omega_N = (x_1, \ldots, x_N)$ on S^1, without loss of generality we may assume $x_j = e^{i\theta_j}$ where $0 \le \theta_1 \le \theta_2 \cdots \le \theta_N \le 2\pi$. Let $x_{N+j} := x_j$ and $\theta_{N+j} := \theta_j$, $j =$

$1, \dots, N-1$. Using the convexity of g we obtain

$$E_f(\omega_N) = \sum_{j \neq k} f(|x_j - x_k|^2) = \sum_{j \neq k} g(|x_j - x_k|) = \sum_{k=1}^{N-1} \sum_{j=1}^{N} g(|x_{j+k} - x_j|)$$

$$\geq \sum_{k=1}^{N-1} g\left(\frac{1}{N} \sum_{j=1}^{N} |x_{j+k} - x_j|\right) \geq \sum_{k=1}^{N-1} g\left(\frac{1}{N} \sum_{j=1}^{N} 2\sin \frac{|\theta_j - \theta_{j+k}|}{2}\right).$$

Since $\sin t$ is concave on $[0, \pi]$ and g is decreasing it then follows

$$E_f(\omega_N) \geq \sum_{k=1}^{N-1} g\left(2\sin \frac{1}{N} \sum_{j=1}^{N} \frac{|\theta_j - \theta_{j+k}|}{2}\right) = \sum_{k=1}^{N-1} g\left(2\sin \frac{k\pi}{N}\right).$$

where the last quantity is the f-energy of any N equally points on S^1. $\qquad \square$

Remark 4.1.3. *The above two theorems hold for Riesz s-potentials with $s > 0$. In addition, Theorem 4.1.1 holds for all Gaussian potentials $f(x) = e^{-ax}$ with $a > 0$.*

Let $\omega_N + \Lambda$ be an N-point Λ-periodic configuration. We shall call $N/|\Lambda|$ the *density* of $\omega_N + \Lambda$. In the last chapter of [2] they study the Euclidean case and prove the following 1-dimensional case.

Theorem 4.1.4. *Let $f : [0, \infty) \to \mathbb{R} \cup \{\infty\}$ be completely monotonic on $(0, \infty)$ with $f(0) = \lim_{x \to 0^+} f(x)$ and satisfies $f(x) = O(|x|^{-\frac{1}{2}-\varepsilon})$ for some $\varepsilon > 0$ as $|x| \to \infty$. Then any equally s-paced space configuration has the minimal f-potential energy of any periodic configuration in $\mathbb{R}$ with its density.*

In this section we will establish a connection between these two theorems and provide a simple proof for Theorem 4.1.4.

We start with some notations. For any $c > 0$ and $x \in \mathbb{R}$, the *classical one dimensional theta function* $\theta(c;x)$ is defined by

$$\begin{aligned}
\theta(c;x) &= \sum_{k=-\infty}^{\infty} e^{-\pi k^2 c} e^{i2\pi kx} \\
&= c^{-\frac{1}{2}} \sum_{n=-\infty}^{\infty} e^{-\frac{\pi(n+x)^2}{c}},
\end{aligned} \qquad (4.1)$$

where the second equality follows from the Poisson summation formula (See section B).

Notice that $\theta(c;\cdot)$ is $\mathbb{Z}$-periodic. We shall find it useful to also consider

$$\tilde{\theta}(c;t) := \theta\left(c; \frac{\arccos t}{2\pi}\right), \qquad t \in [-1,1].$$

In other words for any $x \in \mathbb{R}$ it holds that

$$\tilde{\theta}(c; \cos 2\pi x) = \theta(c;x).$$

A C^∞ function $f : I \to \mathbb{R} \cup \{+\infty\}$ is *absolutely monotonic* if $f^{(k)}(x) \geq 0$ for all $x \in I$ and all $k \geq 0$ and *strictly absolutely monotonic* if strict inequality always holds in the interior of I. We shall need the Jacobi triple product formula.

Lemma 4.1.5 (Jacobi triple product formula). *For any complex q and z with $|q| < 1$ and $z \neq 0$ we have*

$$\prod_{r=1}^{\infty}\left(1 - q^{2r}\right)\left(1 + q^{2r-1}z^2\right)\left(1 + q^{2r-1}z^{-2}\right) = \sum_{k=-\infty}^{\infty} q^{k^2} z^{2k}.$$

Proof. See Section C. □

Lemma 4.1.6. *For any $c > 0$, $\tilde{\theta}(c;\cdot) : [-1,1] \longrightarrow (0,\infty)$ is a strictly absolutely monotonic function.*

Proof. Apply Lemma 4.1.5 for $q = e^{-\pi c}$ and $z = e^{i\pi x}$ it follows

$$\begin{aligned}
\theta(c;x) &= \sum_{k=-\infty}^{\infty} e^{-\pi k^2 c} e^{i2\pi kx} \\
&= \prod_{r=1}^{\infty}\left(1 - e^{-2\pi rc}\right)\left(1 + e^{-(2r-1)\pi c} e^{i2\pi x}\right)\left(1 + e^{-(2r-1)\pi c} e^{-i2\pi x}\right) \\
&= \prod_{r=1}^{\infty}\left(1 - e^{-2\pi rc}\right)\left(1 + 2e^{-(2r-1)\pi c}\cos 2\pi x + e^{-2(2r-1)\pi c}\right).
\end{aligned}$$

Thus

$$\tilde{\theta}(c;t) = \prod_{r=1}^{\infty}(1 - e^{-2\pi rc})\left(1 + 2e^{-(2r-1)\pi c}t + e^{-2(2r-1)\pi c}\right). \tag{4.2}$$

It is elementary to show that

$$\sum_{r=1}^{\infty}\left|1 - (1 - e^{-2\pi rc})(1 + 2e^{-(2r-1)\pi c}t + e^{-2(2r-1)\pi c})\right|$$

converges uniformly on compact subsets of $\mathbb{C}$. It then follows from a theorem in complex analysis (cf. [19, Theorem 15.6]) that $\tilde{\theta}(c;t)$ converges uniformly on compact subsets of $\mathbb{C}$ and hence $\tilde{\theta}(c;\cdot)$ is holomorphic. In particular, $\tilde{\theta}(c;t)$ is smooth as a real function. Differentiating (4.2) yields for any $n \geq 0$, $c > 0$, $t \in [-1,1]$

$$\frac{\partial^n \tilde{\theta}}{\partial t^n}(c;t) > 0.$$

$\square$

Proof of Theorem 4.1.4. By Bernstein's theorem(cf. [1, Theorem 12b, page161]) there exists a non-decreasing function $\alpha : [0,\infty) \to \mathbb{R}$ such that for all $x > 0$,

$$f(x) = \int_0^{\infty} e^{-cx}\mathrm{d}\alpha(c).$$

There is no contribution from $c = 0$ since f approaches to 0 as $x \to \infty$. Therefore it is sufficient to prove the optimality of equally spaced configurations for $f(x) = e^{-cx}$ for some $c > 0$.

Let $\mathbb{Z} + \omega_N$ be an N-point Z-periodic configuration in $\mathbb{R}$ generated by $\omega_N = \{x_j\}_{j=1}^N$.

Then

$$E_{f,\mathbb{Z}}^{cp}(\omega_N) = \sum_{j\neq k}\sum_{n\in\mathbb{Z}} e^{-c(x_j-x_k+n)^2}$$

$$= \left(\frac{\pi}{c}\right)^{\frac{1}{2}} \sum_{j\neq k} \theta\left(\frac{\pi}{c};x_j-x_k\right)$$

$$= \left(\frac{\pi}{c}\right)^{\frac{1}{2}} \sum_{j\neq k} \tilde{\theta}\left(\frac{\pi}{c};\cos(2\pi(x_j-x_k))\right).$$

For any $t \in [-1,1]$, let $g(2-2t) = \tilde{\theta}(\frac{\pi}{c};t)$. By Lemma 4.1.6, $\tilde{\theta}\left(\frac{\pi}{c};\cdot\right)$ is strictly absolutely monotonic on [-1,1] and so it follows that $g : [0,4] \longrightarrow (0,\infty)$ is strictly completely monotonic on [0,4].

Consider the map $\varphi : \mathbb{R} \longrightarrow S^1$, $\varphi(x) = e^{2\pi i x}$. Notice that $|\varphi(x_j) - \varphi(x_k)|^2 = |e^{2\pi i x_j} - e^{2\pi i x_k}|^2 = 2 - 2\cos(2\pi(x_j-x_k))$. It then follows

$$E_{f,\mathbb{Z}}^{cp}(\omega_N) = \left(\frac{\pi}{c}\right)^{\frac{1}{2}} \sum_{j\neq k} g\left(2 - 2\cos(2\pi(x_j-x_k))\right)$$

$$= \left(\frac{\pi}{c}\right)^{\frac{1}{2}} \sum_{j\neq k} g(|\varphi(x_j) - \varphi(x_k)|^2)$$

$$= \left(\frac{\pi}{c}\right)^{\frac{1}{2}} E_g(\varphi(\omega_N)).$$

By Lemma 4.1.1, the energy $E_g(\varphi(\omega_N))$ attains its minimum at any N-point equally spaced configuration on S^1. Therefore $E_{f,\mathbb{Z}}^{cp}(\omega_N)$ attains its minimum at any N-point equally spaced configuration in $\mathbb{R}$. $\qquad\square$

4.2   The case for $n = 2,3$ and Λ is a Hexagonal lattice

Although we are not able to verify the universal optimality of hexagonal lattice A_2, we will investigate some simple cases in this section. Namely, we only consider A_2-periodic configurations with $N = 2,3$.

Conjecture 4.2.1. *Let the potential function $f : [0,\infty) \to \mathbb{R}\cup\{\infty\}$ be completely monotonic*

on $(0, \infty)$ *with* $f(0) = \lim\limits_{x \to 0^+} f(x)$ *and satisfies* $f(x) = O(|x|^{-1-\varepsilon})$ *for some* $\varepsilon > 0$ *as* $|x| \to \infty$.
If there exists a constant $\lambda \in (0, 1)$ *and an orthogonal* 2×2 *matrix such that* λQA_2 *is a finer lattice of* A_2 *and* $|(\lambda QA_2) \cap \Omega_{A_2}| = N$, *then* λQA_2 *is optimal among all* N-*point* A_2-*periodic configurations.*

This is a less general conjecture than Cohn and Kumar's [2]. First of all we only consider A_2-periodic configurations rather than all Λ-periodic configurations where Λ is any lattice with co-volume 1. Secondly this conjecture only makes sense when N is some special integer. In fact, it is not difficult to show that such N must have the form $N = m^2 + mn + n^2$ where m and n are both integers. As we mentioned before it is known that for any nice d-dimensional space $\Omega \subset \mathbb{R}^d$ with Lebesgue measure 1, it holds that

$$\lim_{N \to \infty} \frac{\mathcal{E}_s(\Omega; N)}{N^{1 + \frac{s}{d}}} = C_{s,d}, \qquad s > d$$

In particular, for the fundamental domain of A_2 (assuming $|\det A_2| = 1$), if the above conjecture is true, then by Theorem 2.2.2, we will obtain the constant

$$
\begin{aligned}
C_{s,2} &= \lim_{N \to \infty} \frac{\mathcal{E}_s(\Omega_{A_2}; N)}{N^{1 + \frac{s}{2}}} = \lim_{N \to \infty} \frac{\mathcal{E}_{s,A_2}(N)}{N^{1 + \frac{s}{2}}} \\
&= \lim_{m \to \infty} \frac{\mathcal{E}_{s,A_2}(m^2)}{(m^2)^{1 + \frac{s}{2}}} \\
&= \lim_{m \to \infty} \frac{E_{s,A_2}(\frac{1}{m}A_2 \cap \Omega_{A_2})}{m^{2+s}} \qquad \text{(conjecture 4.2.1)} \\
&= \lim_{m \to \infty} \frac{m^2 \cdot m^s \zeta_{A_2}(s)}{m^{2+s}} = \zeta_{A_2}(s).
\end{aligned}
$$

Recall our main result is that

Theorem 4.2.2. *Let the potential function* $f : [0, \infty) \to \mathbb{R} \cup \{\infty\}$ *be completely monotonic on* $(0, \infty)$ *with* $f(0) = \lim\limits_{x \to 0^+} f(x)$ *and satisfies* $f(x) = O(|x|^{-\frac{1}{2} - \varepsilon})$ *for some* $\varepsilon > 0$ *as* $|x| \to \infty$. *Let* $u_1 = [1, 0]^T$, $u_2 = [\frac{1}{2}, \frac{\sqrt{3}}{2}]^T$, *and* $P = \frac{1}{3}(u_1 + u_2) = [\frac{1}{2}, \frac{\sqrt{3}}{6}]^T$, $Q = \frac{2}{3}(u_1 + u_2) = [1, \frac{\sqrt{3}}{3}]^T$. *Consider the* f-*energy of* ω_N *associated to the lattice* $\widetilde{A_2} := [u_1, u_2]\mathbb{Z}^2 = (\frac{\sqrt{3}}{2})^{\frac{1}{2}} A_2$.
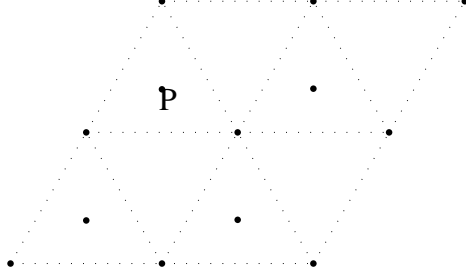
Figure 4.1: A universally optimal configuration for $N = 2$, $\Lambda = \widetilde{A_2}$. It is not a lattice but a "honeycomb" configuration.
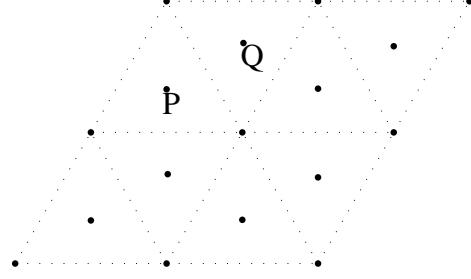
Figure 4.2: The universally optimal configuration for $N = 3$. $\Lambda = \widetilde{A_2}$ is a finer lattice of $\widetilde{A_2}$.

(1) For $N = 2$, let $\omega_2^* = \{0, P\}$ or $\{0, Q\}$ up to translations. Then for any 2-point configuration $\omega_2 \in (\mathbb{R}^2)^2$,

$$E^{cp}_{f,\widetilde{A_2}}(\omega_2) \geq E^{cp}_{f,\widetilde{A_2}}(\omega_2^*).$$

(2) For $N = 3$, let $\omega_3^* = \{0, P, Q\}$ up to translations. Then for any 3-point configuration $\omega_3 \in (\mathbb{R}^2)^3$,

$$E^{cp}_{f,\widetilde{A_2}}(\omega_3) \geq E^{cp}_{f,\widetilde{A_2}}(\omega_3^*).$$

By Bernstein's theorem we may assume $f(x) = e^{-ax}$ for some $a > 0$. Consider the $\widetilde{A_2}$-periodic function

$$F(x,y) := \sum_{v \in \widetilde{A_2}} e^{-a\left|[x,y]^T + v\right|^2}.$$

Then for any $\omega_N = \left((x_j, y_j)\right)_{j=1}^N \in (\mathbb{R}^2)^N$,

$$E^{cp}_{f,\widetilde{A_2}}(\omega_N) = \sum_{j \neq k} F(x_j - x_k, y_j - y_k). \tag{4.3}$$

Lemma 4.2.3. *F is uniquely determined by its values on the region $\Omega_0 := \{(x,y)|0 \leq x \leq$*

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$\frac{1}{2}, 0 \le y \le \frac{\sqrt{3}}{6}, y \le \frac{\sqrt{3}}{3}x\}$. *Furthermore,*

$$\nabla F|_P = \nabla F|_Q = \vec{0}.$$

Proof. Let G be the group of affine transformations that fix $\widetilde{A_2}$ and preserve distance in $\mathbb{R}^2$. Then for any $g \in G$,

$$\begin{aligned}
F(gx, gy) &= \sum_{v \in \widetilde{A_2}} e^{-a\left|g[x,y]^T + v\right|^2} \\
&= \sum_{v \in \widetilde{A_2}} e^{-a\left|g\left([x,y]^T + g^{-1}v\right)\right|^2} \\
&= \sum_{v \in \widetilde{A_2}} e^{-a\left|[x,y]^T + g^{-1}v\right|^2} = F(x,y).
\end{aligned}$$

It is not difficult to verify that $G\Omega_0$ is the whole plane. Thus F is determined by its values on Ω_0.

To prove $\nabla F|_P = 0$, consider the transformation g that rotates points about P by $\frac{2\pi}{3}$, namely, for any $[x,y]^T \in \mathbb{R}^2$,

$$g\left([x,y]^T\right) = \rho\left([x,y]^T - P\right) + P,$$

where ρ is the rotation of vectors by $\frac{2\pi}{3}$. Then $g \in G$ and hence

$$F(x,y) = F(g(x,y)).$$

Taking the gradient on both sides yields

$$\nabla F(x,y) = \rho \nabla F(g(x,y)).$$

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Evaluating the above identity at P implies

$$\nabla F|_P = \rho \nabla F|_{gP} = \rho \nabla F|_P.$$

Therefore

$$\nabla F|_P = 0.$$

The same argument shows that $\nabla F|_Q = 0$ as well. $\qquad\square$

Lemma 4.2.4. *For any* $[x,y]^T \in \mathbb{R}^2$,

$$F(x,y) = \frac{\pi}{\sqrt{3}a}\left[\theta\left(\frac{\pi}{3a};\frac{y}{\sqrt{3}}\right) \theta\left(\frac{\pi}{a};x\right) + \theta\left(\frac{\pi}{3a};\frac{y}{\sqrt{3}}+\frac{1}{2}\right) \theta\left(\frac{\pi}{a};x+\frac{1}{2}\right)\right].$$

Proof.

$$F(x,y) = \sum_{v\in[u_1,u_2]\mathbb{Z}^2} e^{-a\left|[x,y]^T+v\right|^2}$$

$$= \sum_{m,n\in\mathbb{Z}} e^{-a\left|[x,y]^T+(mu_1+nu_2)\right|^2}$$

$$= \sum_{m,n\in\mathbb{Z}} e^{-a\left[\left(x+m+\frac{n}{2}\right)^2+\left(y+\frac{\sqrt{3}}{2}n\right)^2\right]}$$

$$= \sum_{n\in\mathbb{Z}} e^{-a\left(y+\frac{\sqrt{3}}{2}n\right)^2} \sum_{m\in\mathbb{Z}} e^{-a\left(x+m+\frac{n}{2}\right)^2}$$

$$= \sum_{2|n} e^{-a\left(y+\frac{\sqrt{3}}{2}n\right)^2} \sqrt{\frac{\pi}{a}}\theta\left(\frac{\pi}{a};x\right) + \sum_{2\nmid n} e^{-a\left(y+\frac{\sqrt{3}}{2}n\right)^2} \sqrt{\frac{\pi}{a}}\theta\left(\frac{\pi}{a};x+\frac{1}{2}\right)$$

$$= \sum_{n\in\mathbb{Z}} e^{-a(y+\sqrt{3}n)^2} \sqrt{\frac{\pi}{a}}\theta\left(\frac{\pi}{a};x\right) + \sum_{n\in\mathbb{Z}} e^{-a\left[y+\frac{\sqrt{3}}{2}(2n+1)^2\right]} \sqrt{\frac{\pi}{a}}\theta\left(\frac{\pi}{a};x+\frac{1}{2}\right)$$

$$= \sqrt{\frac{\pi}{3a}}\theta\left(\frac{\pi}{3a};\frac{y}{\sqrt{3}}\right) \sqrt{\frac{\pi}{a}}\theta\left(\frac{\pi}{a};x\right) + \sqrt{\frac{\pi}{3a}}\theta\left(\frac{\pi}{3a};\frac{y}{\sqrt{3}}+\frac{1}{2}\right) \sqrt{\frac{\pi}{a}}\theta\left(\frac{\pi}{a};x+\frac{1}{2}\right)$$

$$= \frac{\pi}{\sqrt{3}a}\left[\theta\left(\frac{\pi}{3a};\frac{y}{\sqrt{3}}\right) \theta\left(\frac{\pi}{a};x\right) + \theta\left(\frac{\pi}{3a};\frac{y}{\sqrt{3}}+\frac{1}{2}\right) \theta\left(\frac{\pi}{a};x+\frac{1}{2}\right)\right].$$

$\qquad\square$

Let

$$\widetilde{F}(t_1, t_2) := F\left(\frac{\arccos t_1}{2\pi}, \frac{\sqrt{3}\arccos t_2}{2\pi}\right) \tag{4.4}$$

$$= \frac{\pi}{\sqrt{3}a}\left[\tilde{\theta}\left(\frac{\pi}{3a}; t_2\right)\tilde{\theta}\left(\frac{\pi}{a}; t_1\right) + \tilde{\theta}\left(\frac{\pi}{3a}; -t_2\right)\tilde{\theta}\left(\frac{\pi}{a}; -t_1\right)\right]. \tag{4.5}$$

In this section we always assume the relations

$$t_1 = \cos(2\pi x), \qquad t_1 = \cos(2\pi y/\sqrt{3}).$$

Lemma 4.2.5. *For any integers l_1 and l_2 satisfying $2|l_1 + l_2$,*

$$\frac{\partial^{l_1+l_2}\widetilde{F}}{\partial t_1^{l_1}\partial t_2^{l_2}}(t_1, t_2) > 0, \qquad \forall t_1, t_2 \in [-1, 1].$$

In particular,

$$\frac{\partial^2\widetilde{F}}{\partial t_1^2}(t_1, t_2) > 0, \qquad \frac{\partial^2\widetilde{F}}{\partial t_2^2}(t_1, t_2) > 0,$$

$$\frac{\partial^2\widetilde{F}}{\partial t_1\partial t_2}(t_1, t_2) = \frac{\partial^2\widetilde{F}}{\partial t_2\partial t_1}(t_1, t_2) > 0, \qquad \forall t_1, t_2 \in [-1, 1].$$

Proof. This follows immediately from (4.5) and Lemma 4.1.6. $\qquad\square$

Lemma 4.2.6.

$$\frac{\partial\widetilde{F}}{\partial t_2}(t_1, t_2) \geq 0, \qquad \forall t_1 \in [-1, 1], \quad \forall t_2 \in \left[\frac{1}{2}, 1\right].$$

$$\frac{\partial F}{\partial y}(x, y) \leq 0, \qquad \forall x \in \mathbb{R}, \forall y \in \left[0, \frac{\sqrt{3}}{6}\right].$$

The first "=" holds if and only if $(t_1, t_2) = \left(-1, \frac{1}{2}\right)$. The second "=" holds if and only if $y = 0$ or $(x, y) = \left(\frac{1}{2}, \frac{\sqrt{3}}{6}\right) = P$.

Proof. By Lemma 4.2.5 and Lemma 4.2.3,

$$\frac{\partial \widetilde{F}}{\partial t_2}(t_1, t_2) \geq \frac{\partial \widetilde{F}}{\partial t_2}\left(-1, \frac{1}{2}\right)$$

$$= \frac{\partial F}{\partial y}\left(\frac{\arccos t_1}{2\pi}, \frac{\sqrt{3}\arccos t_2}{2\pi}\right) \cdot \frac{\sqrt{3}}{2\pi} \cdot \left(-\frac{1}{\sqrt{1-t_2^2}}\right)\Bigg|_{t_1=-1, t_2=\frac{1}{2}}$$

$$= \frac{\partial F}{\partial y}\Bigg|_P \cdot \left(-\frac{\sqrt{3}}{2\pi} \cdot \frac{1}{\sqrt{1-t_2^2}}\right)\Bigg|_{t_1=-1, t_2=\frac{1}{2}} = 0.$$

Thus for any $x \in \mathbb{R}$ and $y \in [0, \frac{\sqrt{3}}{6}]$,

$$\frac{\partial F}{\partial y}(x, y) = \frac{\partial \widetilde{F}}{\partial t_2}(\cos(2\pi x), \cos(2\pi y/\sqrt{3})) \cdot \left(-\frac{2\pi}{\sqrt{3}}\sin(2\pi y/\sqrt{3})\right) \leq 0.$$

$\square$

Lemma 4.2.7.

$$\frac{\partial \widetilde{F}}{\partial t_1}(t_1, t_2) > 0, \qquad \forall t_1 \in [-1, 1], \quad \forall t_2 \in \left[\frac{1}{2}, 1\right]. \tag{4.6}$$

$$\frac{\partial F}{\partial x}(x, y) \leq 0, \qquad \forall x \in \left[0, \frac{1}{2}\right], \quad \forall y \in \left[0, \frac{\sqrt{3}}{6}\right]. \tag{4.7}$$

"=" holds if and only if $x = 0$ or $x = \frac{1}{2}$.

Proof. (4.7) follows immediately from (4.6) since

$$\frac{\partial F}{\partial x}(x, y) = \frac{\partial \widetilde{F}}{\partial t_1}(\cos(2\pi x), \cos(2\pi y/\sqrt{3})) \cdot (-2\pi \sin(2\pi x)).$$

By Lemma 4.2.5 and (4.5) it suffices to show

$$\frac{\partial \widetilde{F}}{\partial t_1}\left(-1, \frac{1}{2}\right) = \frac{\pi}{\sqrt{3}a}\left[\tilde{\theta}\left(\frac{\pi}{3a}; \frac{1}{2}\right)\frac{\partial \tilde{\theta}}{\partial t}\left(\frac{\pi}{a}; -1\right) - \tilde{\theta}\left(\frac{\pi}{3a}; -\frac{1}{2}\right)\frac{\partial \tilde{\theta}}{\partial t}\left(\frac{\pi}{a}; 1\right)\right] > 0.$$

(1) If $a \le \frac{\pi^2}{3 \ln \frac{\sqrt{5}+1}{2}}$, then $e^{-\frac{\pi^2}{3a}} \le \frac{\sqrt{5}-1}{2}$. Applying formula (4.2), we get

$$
\frac{\partial \widetilde{F}}{\partial t_1}\left(-1, \frac{1}{2}\right)
$$

$$
= \frac{\pi}{\sqrt{3}a}\left[\tilde{\theta}\left(\frac{\pi}{3a}; \frac{1}{2}\right) \frac{\partial \tilde{\theta}}{\partial t}\left(\frac{\pi}{a}; -1\right) - \tilde{\theta}\left(\frac{\pi}{3a}; -\frac{1}{2}\right) \frac{\partial \tilde{\theta}}{\partial t}\left(\frac{\pi}{a}; 1\right)\right]
$$

$$
= \frac{\pi}{\sqrt{3}a}\left[\prod_{r=1}^{\infty}\left(1 - e^{-2r\frac{\pi^2}{3a}}\right)\left(1 + e^{-(2r-1)\frac{\pi^2}{3a}} + e^{-2(2r-1)\frac{\pi^2}{3a}}\right) \cdot \right.
$$

$$
\sum_{j=1}^{\infty}\left(1 - e^{-2j\frac{\pi^2}{a}}\right) 2e^{-(2j-1)\frac{\pi^2}{a}} \prod_{r \ne j}\left(1 - e^{-2r\frac{\pi^2}{a}}\right)\left(1 - 2e^{-(2r-1)\frac{\pi^2}{a}} + e^{-2(2r-1)\frac{\pi^2}{a}}\right)
$$

$$
- \prod_{r=1}^{\infty}\left(1 - e^{-2r\frac{\pi^2}{3a}}\right)\left(1 - e^{-(2r-1)\frac{\pi^2}{3a}} + e^{-2(2r-1)\frac{\pi^2}{3a}}\right) \cdot
$$

$$
\left. \sum_{j=1}^{\infty}\left(1 - e^{-2j\frac{\pi^2}{a}}\right) 2e^{-(2r-1)\frac{\pi^2}{a}} \prod_{r \ne j}\left(1 - e^{-2r\frac{\pi^2}{a}}\right)\left(1 + 2e^{-(2r-1)\frac{\pi^2}{a}} + e^{-2(2r-1)\frac{\pi^2}{a}}\right)\right]
$$

$$
= \frac{\pi}{\sqrt{3}a}\prod_{r=1}^{\infty}(1 - q^{2r})\sum_{j=1}^{\infty} 2q^{-3(2j-1)}\left((1 - q^{6j})\left[\left((1 + q^{-(2j-1)} + q^{-2(2j-1)}\right) \cdot \right.\right.
$$

$$
\prod_{r \ne j}\left(1 + q^{-(2r-1)} + q^{-2(2r-1)}\right)\left(1 - 2q^{-3(2r-1)} + q^{-6(2r-1)}\right)
$$

$$
- \left(1 - q^{-(2j-1)} + q^{-2(2j-1)}\right)\prod_{r \ne j}\left(1 - q^{-(2r-1)} + q^{-2(2r-1)}\right) \cdot
$$

$$
\left. \left(1 + 2q^{-3(2r-1)} + q^{-6(2r-1)}\right)\right],
$$

where $q = e^{-\frac{\pi^2}{3a}} \le \frac{\sqrt{5}-1}{2}$. Therefore to prove $\frac{\partial \widetilde{F}}{\partial t_1}(t_1, t_2) > 0$ it suffices to show for any $r \ge 1$,

$$
\left(1 + q^{-(2r-1)} + q^{-2(2r-1)}\right)\left(1 - 2q^{-3(2r-1)} + q^{-6(2r-1)}\right)
$$

$$
\ge \left(1 - q^{-(2r-1)} + q^{-2(2r-1)}\right)\left(1 + 2q^{-3(2r-1)} + q^{-6(2r-1)}\right)
$$

$$
\iff 2q^{-(2r-1)}\left(q^{-2(2r-1)} + 1\right)\left(q^{-2(2r-1)} - \frac{3+\sqrt{5}}{2}\right)\left(q^{-2(2r-1)} - \frac{3-\sqrt{5}}{2}\right) \ge 0.
$$

The above inequality holds since

$$q^{-2(2r-1)} \geq q^{-2} \geq \left(\frac{\sqrt{5}-1}{2}\right)^{-2} = \frac{3+\sqrt{5}}{2}, \qquad \forall r \geq 1.$$

(2) If $a > \frac{\pi^2}{3\ln\frac{\sqrt{5}+1}{2}} > 4$, for any $t' \in [-1,1]$ let

$$x' = \frac{\arccos t'}{2\pi}.$$

Then

$$\frac{\partial \tilde{\theta}}{\partial t}\left(\frac{\pi}{a};t'\right) = \frac{\partial \theta}{\partial x}\left(\frac{\pi}{a};x'\right)\frac{\partial x}{\partial t}(t')$$
$$= -\frac{\frac{\partial \theta}{\partial x}\left(\frac{\pi}{a};x'\right)}{2\pi \sin(2\pi x')}.$$

Using L'hospital's rule we get

$$\frac{\partial \tilde{\theta}}{\partial t}\left(\frac{\pi}{a};-1\right) = -\frac{\frac{\partial^2 \theta}{\partial x^2}\left(\frac{\pi}{a};x'\right)}{4\pi^2 \cos(2\pi x')}\Bigg|_{x'=\frac{1}{2}} = \frac{\frac{\partial^2 \theta}{\partial x^2}\left(\frac{\pi}{a};\frac{1}{2}\right)}{4\pi^2}$$
$$= \frac{1}{2\pi}\left(\frac{\pi}{a}\right)^{-\frac{3}{2}}\sum_{n=-\infty}^{\infty}\left[2a(n-\frac{1}{2})^2 - 1\right]e^{-a(n-\frac{1}{2})^2}$$
$$> \frac{1}{2\pi}\left(\frac{\pi}{a}\right)^{-\frac{3}{2}}\sum_{n=-\infty}^{\infty}\left(\frac{a}{2} - 1\right)e^{-a(n-\frac{1}{2})^2}$$
$$> \frac{1}{2\pi}\left(\frac{\pi}{a}\right)^{-\frac{3}{2}}\sum_{n=-\infty}^{\infty}e^{-a\left(n-\frac{1}{2}\right)^2},$$

and

$$\frac{\partial \tilde{\theta}}{\partial t}\left(\frac{\pi}{a};1\right) = -\frac{\frac{\partial^2 \theta}{\partial x^2}\left(\frac{\pi}{a};x'\right)}{4\pi^2 \cos(2\pi x')}\bigg|_{x'=0} = \frac{\frac{\partial^2 \theta}{\partial x^2}\left(\frac{\pi}{a};0\right)}{4\pi^2}$$

$$= \frac{1}{2\pi}\left(\frac{\pi}{a}\right)^{-\frac{3}{2}} \sum_{n=-\infty}^{\infty}\left(1-2an^2\right)e^{-an^2} < \frac{1}{2\pi}\left(\frac{\pi}{a}\right)^{-\frac{3}{2}}.$$

Thus

$$\frac{\partial \widetilde{F}}{\partial t_1}\left(-1,\frac{1}{2}\right)$$

$$= \frac{\pi}{\sqrt{3}a}\left[\tilde{\theta}\left(\frac{\pi}{3a};\frac{1}{2}\right)\frac{\partial \tilde{\theta}}{\partial t}\left(\frac{\pi}{a};-1\right) - \tilde{\theta}\left(\frac{\pi}{3a};-\frac{1}{2}\right)\frac{\partial \tilde{\theta}}{\partial t}\left(\frac{\pi}{a};1\right)\right]$$

$$= \frac{\pi}{\sqrt{3}a}\left[\theta\left(\frac{\pi}{3a};\frac{1}{6}\right)\frac{\partial \tilde{\theta}}{\partial t}\left(\frac{\pi}{a};-1\right) - \theta\left(\frac{\pi}{3a};-\frac{1}{3}\right)\frac{\partial \tilde{\theta}}{\partial t}\left(\frac{\pi}{a};1\right)\right]$$

$$> \frac{a}{2\sqrt{3}\pi^2}\left[e^{-3a\cdot\left(\frac{1}{6}\right)^2}\sum_{n=-\infty}^{\infty}e^{-a\left(n-\frac{1}{2}\right)^2} - \sum_{n=-\infty}^{\infty}e^{-3a\left(n-\frac{1}{3}\right)^2}\cdot 1\right]$$

$$= \frac{a}{2\sqrt{3}\pi^2}\left[\sum_{n=-\infty}^{\infty}e^{-a\left(n^2-n+\frac{1}{3}\right)} - \sum_{n=-\infty}^{\infty}e^{-a\left(3n^2-2n+\frac{1}{3}\right)}\right]$$

$$= \frac{a}{2\sqrt{3}\pi^2}\sum_{n=-\infty}^{\infty}e^{-a\left(3n^2-2n+\frac{1}{3}\right)}\left(e^{an(2n-1)}-1\right) > 0.$$

$\square$

Corollary 4.2.8. *For any* $x,y \in \Omega_{\widetilde{A_2}}$,

$$F(x,y) \geq F\left(\frac{1}{2},\frac{\sqrt{3}}{6}\right) = F|_P = F|_Q.$$

"=" holds if and only if $(x,y) = P$ *or* Q.

Proof. For any x and y, by Lemma 4.2.3 there exists some affine transformation g such that $(gx,gy) \in \Omega_0$ and $F(x,y) = F(gx,gy)$. Thus by Lemma 4.2.6 and Lemma 4.2.7

$$F(x,y) = F(gx,gy) \geq F\left(gx,\frac{\sqrt{3}}{6}\right) \geq F\left(\frac{1}{2},\frac{\sqrt{3}}{6}\right).$$

□

Proof of Theorem 4.2.2. For any $\omega_2 \in (\mathbb{R}^2)^2$, using the minimality of $F|_P$ and (4.3) we obtain

$$E^{cp}_{f,\widetilde{A_2}}(\omega_2) \geq 2F|_P = E^{cp}_{f,\widetilde{A_2}}(\omega_2^*).$$

Similarly, for any $\omega_3 \in (\mathbb{R}^2)^3$,

$$E^{cp}_{f,\widetilde{A_2}}(\omega_3) \geq 6F|_P = E^{cp}_{f,\widetilde{A_2}}(\omega_3^*).$$

Note that "=" holds in the above relation if and only if $\omega_2 = \{0, P\}$ or $\{0, Q\}$ and $\omega_3 = \{0, P, Q\}$ up to translations respectively. □

We will end this section with a discussion of the polarization problem for N-point periodic configurations in $\mathbb{R}^d$. Recall in Chapter 3 we have discussed the polarization problem for N-point configurations in a compact set. For any nonnegative function f and any N-point Λ-periodic configuration $\omega_N + \Lambda$ in $\mathbb{R}^d$ and any $x \in \mathbb{R}^d$, we define the *f-polarization of $\omega_N + \Lambda$ at x*

$$U^f(\Lambda + \omega_N; x) := \sum_{k=1}^{N} \sum_{v \in \Lambda} f(|x - x_k + v|^2),$$

and the *f-polarization of ω_N*

$$M^f(\Lambda + \omega_N) = \inf_{x \in \mathbb{R}^d} U^f(\Lambda + \omega_N; x).$$

Our main result shows that if Λ is a hexagonal lattice and f satisfies the conditions in Theorem 4.2.2, then the *f*-polarization of Λ is attained at P and Q, and the *f*-polarization of $\Lambda + \{0, P\}$ is attained at Q.

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Corollary 4.2.9. *Suppose f, $\tilde{A}_2$, and P are as in Theorem 4.2.2. Then*

$$M^f(\widetilde{A_2}) = U^f(\widetilde{A_2}, P) \text{ and } M^f(\widetilde{A_2} + \{0, P\}) = U^f(\widetilde{A_2} + \{0, P\}, Q) = 2U^f(\widetilde{A_2}, P).$$

In the case $f = f_s$ is a Riesz potential, we have

$$U^s(\widetilde{A_2}, P) = \zeta_{\widetilde{A_2}}(s; P) = \left(\frac{3^{\frac{s}{2}} - 1}{2}\right) \zeta_{\widetilde{A_2}}(s).$$

Proof. It suffices to prove the last identity. Notice that $\Lambda_1 := \widetilde{A_2} + \{0, P, Q\}$ is also a hexagonal lattice. Using the same techniques as in the proof of Lemma 2.3.2 we obtain

$$\sum_{x \in \Lambda_1 \cap \Omega_{\widetilde{A_2}} \setminus \{0\}} \zeta_{\widetilde{A_2}}(s; x) = ((\sqrt{3})^s - 1) \zeta_{\widetilde{A_2}}(s).$$

Since

$$\sum_{x \in \Lambda_1 \cap \Omega_{\widetilde{A_2}} \setminus \{0\}} \zeta_{\widetilde{A_2}}(s; x) = \zeta_{\widetilde{A_2}}(s; P) + \zeta_{\widetilde{A_2}}(s; Q) = 2\zeta_{\widetilde{A_2}}(s; P).$$

The desired identity then follows immediately. $\qquad \square$

Appendix A

Bernstein's Theorem on completely monotonic functions

In this section we will present the proof of Bernstein's Theorem which characterizes the class of completely monotonic functions on the nonnegative real axis.

Theorem A.0.10. *A function* $f : [0, \infty) \to \mathbb{R}$ *is completely monotonic on* $[0, \infty)$ *if and only if*

$$f(x) = \int_0^\infty e^{-xt} \mathrm{d}\alpha(t),$$

where $\alpha(t)$ *is bounded and non-decreasing and the integral converges for* $0 \leq x < \infty$.

A weaker version of this theorem states that

Theorem A.0.11. *A function* $f : (0, \infty) \to \mathbb{R}$ *is completely monotonic on* $[0, \infty)$ *if and only if*

$$f(x) = \int_0^\infty e^{-xt} \mathrm{d}\alpha(t),$$

where $\alpha(t)$ *is bounded and non-decreasing and the integral converges for* $0 < x < \infty$.

Before proving the above theorems we will first introduce some lemmas and Hausdorff Theorem which we are going to use. Given a sequence $\{\mu_n\}_{n=0}^\infty$, let

$$\Delta\mu_n := \mu_{n+1} - \mu_n, \qquad \Delta^k\mu_n := \Delta(\Delta^{k-1}\mu_n).$$

It is not difficult to prove by induction that

$$\Delta^k\mu_n = \sum_{m=0}^k (-1)^{m-k} \binom{k}{m} \mu_{n+m}. \tag{A.1}$$

A sequence $\{\mu_n\}_{n=0}^{\infty}$ is called *completely monotonic* if $(-1)^k \Delta^k \mu_n \geq 0$ for any $n, k \geq 0$.

Lemma A.0.12. *If f is completely monotonic on $[a, \infty)$, then for any $h > 0$, the sequence $\{f(a + nh)\}_{n=0}^{\infty}$ is completely monotonic.*

Proof. For each $k \geq 0$ and $n \geq 0$, let $P(t)$ be the Lagrange interpolation polynomial of f at points $a + nh, \ldots, a + (n+k)h$. Since $f(t) - p(t)$ vanishes at $k + 1$ distinct points it follows from the Rolle's theorem that there exists $\xi \in (a + nh, a + (n+k)h)$ such that $f^{(k)}(\xi) = p^{(k)}(\xi) = k!b_k$ where b_k is the leading coefficient of $p(t)$. Therefore $(-1)^k b_k \geq 0$. It is well-known that

$$p(t) = \sum_{m=0}^{k} f(a + (n+m)h) \prod_{\substack{i=0 \\ i \neq m}}^{k} \frac{t - a(n+i)h}{(m-i)h}.$$

Thus,

$$b_k = \sum_{m=0}^{k} f(a + (n+m)h) \prod_{\substack{i=0 \\ i \neq m}}^{k} \frac{1}{(m-i)h} = \sum_{m=0}^{k} \frac{(-1)^{m-k} f(a + (n+m)h)}{m!(k-m)!h^k}$$

$$= \frac{1}{k!h^k} \sum_{m=0}^{k} (-1)^{m-k} \binom{k}{m} f(a + (n+m)h) = \frac{1}{k!h^k} \Delta^k f(a + nh),$$

where we use (A.1) in the last equality. Therefore $(-1)^k \Delta^k f(a + nh) \geq 0$. $\square$

Theorem A.0.13 (Hausdorff Theorem). *A sequence $\{\mu_n\}_{n=0}^{\infty}$ is completely monotonic if and only if*

$$\mu_n = \int_0^1 t^n d\alpha(t), \qquad n = 0, 1, 2, \ldots \tag{A.2}$$

where $\alpha(t)$ is bounded and non-decreasing on $[0, 1]$.

Proof. Assuming (A.2), then for each $k \geq 0$ we have

$$(-1)^k \Delta^k \mu_n = \int_0^1 (-1)^k \Delta^k t^n d\alpha(t) = \int_0^1 (-1)^k \sum_{m=0}^k (-1)^{m-k} \binom{k}{m} t^{n+m} d\alpha(t)$$

$$= \int_0^1 (-1)^k t^n (t-1)^k d\alpha(t) = \int_0^1 t^n (1-t)^k d\alpha(t) \geq 0.$$

Suppose now $\{\mu_n\}_{n=0}^\infty$ is completely monotonic. For each $k \geq 0$ and $m \leq k$ consider

$$\lambda_{k,m} := \binom{k}{m} (-1)^{k-m} \Delta^{k-m} \mu_m \geq 0.$$

Let $\alpha_k(t)$ be the normalized step function that has jumps $\lambda_{k,m}$ at points $\frac{k}{m}$. Then

$$\sum_{m=0}^k \lambda_{k,m} = \sum_{m=0}^k \binom{k}{m} (-1)^{k-m} \Delta^{k-m} \mu_m$$

$$= \sum_{m=0}^k \binom{k}{m} (-1)^{k-m} \sum_{i=0}^{k-m} (-1)^{i-(k-m)} \binom{k-m}{i} \mu_{m+i}$$

$$= \sum_{m=0}^k \sum_{i=0}^{k-m} (-1)^i \binom{k}{m} \binom{k-m}{i} \mu_{m+i}$$

$$= \sum_{m=0}^k \sum_{j=m}^k (-1)^{j-m} \binom{k}{m} \binom{k-m}{j-m} \mu_j$$

$$= \sum_{j=0}^k \sum_{m=0}^j (-1)^{j-m} \binom{k}{m} \binom{k-m}{j-m} \mu_j$$

$$= \sum_{j=0}^k \binom{k}{j} \mu_j \sum_{m=0}^j (-1)^{j-m} \binom{j}{m} = \sum_{j=0}^k \binom{k}{j} \mu_j (1-1)^j = \mu_0.$$

Therefore $\alpha_k(t)$ are bounded and non-decreasing. We claim that

$$\mu_n = \lim_{k \to \infty} \int_0^1 t^n d\alpha_k(t).$$

Let $g_n(t) = \prod_{i=0}^{n-1} \frac{kt-i}{k-i}$ for $n \geq 1$ and $g_0(x) = 1$. Then

$$\sum_{m=n}^k g_k \left(\frac{m}{k} \right) \lambda_{k,m}$$

$$= \sum_{m=n}^k \frac{m!(k-n)!}{(m-n)!k!} \begin{pmatrix} k \\ m \end{pmatrix} (-1)^{k-m} \Delta^{k-m} \mu_m$$

$$= \sum_{m=n}^k \frac{m!(k-n)!}{(m-n)!k!} \begin{pmatrix} k \\ m \end{pmatrix} (-1)^{k-m} \sum_{i=0}^{k-m} (-1)^{i-(k-m)} \begin{pmatrix} k-m \\ i \end{pmatrix} \mu_{m+i}$$

$$= \sum_{m=n}^k \sum_{i=0}^{k-m} (-1)^i \begin{pmatrix} k-n \\ m+in \end{pmatrix} \begin{pmatrix} m+i-n \\ i \end{pmatrix} \mu_{m+i}$$

$$= \sum_{m=n}^k \sum_{j=m}^k (-1)^{j-m} \begin{pmatrix} k-n \\ j-n \end{pmatrix} \begin{pmatrix} j-n \\ j-m \end{pmatrix} \mu_j$$

$$= \sum_{j=n}^k \begin{pmatrix} k-n \\ j-n \end{pmatrix} \mu_j \sum_{m=0}^j (-1)^{j-m} \begin{pmatrix} j-n \\ j-m \end{pmatrix} = \sum_{j=n}^k \begin{pmatrix} k-n \\ j-n \end{pmatrix} \mu_j (1-1)^{j-n} = \mu_n.$$

(A.3)

Since each factor in $g(t)$ converges uniformly to t in $[0,1]$ as $k \to \infty$, it is clear that

$$\lim_{k \to \infty} \prod_{i=0}^{n-1} \frac{kt-i}{k-i} = t^n$$

uniformly for $0 \leq t \leq 1$. Therefore for any $\varepsilon > 0$, there exists a positive integer k_0 such that

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for any $k \geq k_0$ it holds that

$$|g_k(t) - t^n| < \varepsilon, \qquad t \in [0, 1],$$

and

$$\left(\frac{n}{k}\right)^n < \varepsilon.$$

Using (A.3) we get

$$\left| \mu_n - \int_0^1 t^n \mathrm{d}\alpha_k(t) \right| = \left| \sum_{m=n}^{k} g_k\left(\frac{m}{k}\right) \lambda_{k,m} - \sum_{m=0}^{k} \left(\frac{m}{k}\right)^n \lambda_{k,m} \right|$$

$$\leq \sum_{m=n}^{k} \left| g_k\left(\frac{m}{k}\right) - \left(\frac{m}{k}\right)^n \right| \lambda_{k,m} + \sum_{m=0}^{n-1} \left(\frac{m}{k}\right)^n \lambda_{k,m}$$

$$\leq \sum_{m=n}^{k} \left| g_k\left(\frac{m}{k}\right) - \left(\frac{m}{k}\right)^n \right| \lambda_{k,m} + \sum_{m=0}^{n-1} \left(\frac{n}{k}\right)^n \lambda_{k,m}$$

$$\leq \sum_{m=n}^{k} \varepsilon \lambda_{k,m} + \sum_{m=0}^{n-1} \varepsilon \lambda_{k,m} = \varepsilon \sum_{m=0}^{k} \lambda_{k,m} = \varepsilon \mu_0.$$

Therefore,

$$\mu_n = \lim_{k \to \infty} \int_0^1 t^n \mathrm{d}\alpha_k(t).$$

By Helly's selectoin theorem there exists a subsequence of $\{\alpha_k(t)\}$ that approaches a limit $\alpha(t)$ with bounded variation. The function $\alpha(t)$ is then non-decreasing and satisfies

$$\mu_n = \int_0^1 t^n \mathrm{d}\alpha(t).$$

$\square$

We are now ready to prove Theorem A.0.10

Proof of Theorem A.0.10. Suppose that

$$f(x) = \int_0^\infty e^{-xt} d\alpha(t).$$

Then f is clearly completely monotonic by successive differentiation. Now assume that f is completely monotonic on $[0, \infty)$. By Lemma 2.1.1 for any positive integer m, the sequence $\{f\left(\frac{n}{m}\right)\}_{n=0}^\infty$ is completely monotonic. By Hasdorff Theorem there exists a non-decreasing bounded function $\beta_m(t)$ such that

$$f\left(\frac{n}{m}\right) = \int_0^1 t^n d\beta_m(t), \qquad n = 0, 1, 2, \dots \tag{A.4}$$

Then

$$f(n) = \int_0^1 t^{mn} d\beta_m(t) = \int_0^1 t^n d\beta_m\left(t^{\frac{1}{m}}\right).$$

On the other hand,

$$f(n) = \int_0^1 t^n d\beta_1(t).$$

Therefore,

$$\int_0^1 t^n d\beta_m\left(t^{\frac{1}{m}}\right) = \int_0^1 t^n d\beta_1(t), \qquad n = 0, 1, 2 \dots$$

Using Weierstrass approximation theorem on $[0, 1]$ we conclude that

$$\int_0^1 t^{\frac{n}{m}} d\beta_m\left(t^{\frac{1}{m}}\right) = \int_0^1 t^{\frac{n}{m}} d\beta_1(t), \qquad n = 0, 1, 2 \dots$$

Thus after changing of variable (A.4) becomes

$$f\left(\frac{n}{m}\right) = \int_0^1 t^n \mathrm{d}\beta_m(t) = \int_0^1 t^{\frac{n}{m}} \mathrm{d}\beta_m(t^{\frac{1}{m}}) = \int_0^1 t^{\frac{n}{m}} \mathrm{d}\beta_1(t)$$

$$= \int_{0+}^1 t^{\frac{n}{m}} \mathrm{d}\beta_1(t) = \int_0^\infty e^{-nt/m} \mathrm{d}\alpha(t), \qquad n = 0, 1, 2 \ldots$$

where $\alpha(t) = -\beta_1(e^{-t})$. Since both $f(x)$ and $\int_0^\infty e^{-tx}\mathrm{d}\alpha(t)$ are continuous on $[0,\infty)$ it follows that

$$f(x) = \int_0^\infty e^{-xt} \mathrm{d}\alpha(t)$$

for any x in $[0,\infty)$. $\qquad\qquad\square$

Proof of Theorem A.0.11. Suppose that

$$f(x) = \int_0^\infty e^{-xt} \mathrm{d}\alpha(t).$$

Then f is clearly completely monotonic by successive differentiation. Now assume that f is completely monotonic on $(0,\infty)$. For any $0 < \delta < 1$, the function $f(x+\delta)$ is completely monotonic on $[0,\infty)$ as a function of x. Therefore the proof of Theorem A.0.10 shows that there exists a non-decreasing bounded function $\beta_\delta(t)$ such that

$$f(x+\delta) = \int_0^1 t^x \mathrm{d}\beta_\delta(t).$$

Then for any $x > \delta$,

$$f(x) = \int_0^1 t^{x-\delta} \mathrm{d}\beta_\delta(t) = \int_0^1 t^x t^{-\delta} \mathrm{d}\beta_\delta(t).$$

In particular, for any $n \geq 1$,

$$f(n) = \int_0^1 t^n t^{-\delta} \mathrm{d}\beta_\delta(t).$$

In other words, the integral $\int_0^1 t^x t^{-\delta} \mathrm{d}\beta_\delta(t)$ is independent of δ. Using Weierstrass Theorem on $[0,1]$ we conclude that for any continuous function $h(x)$ on $[0,1)$ with $h(0) = 0$, the integral $\int_0^1 h(t)t^{-\delta} \mathrm{d}\beta_\delta(t)$ is independent of δ. In particular the integral, for any fixed $x > 0$, the integral

$$f(x) = \int_0^1 t^x t^{-\delta} \mathrm{d}\beta_\delta(t)$$

is independent of δ. Therefore if we choose a $\delta_0 \in (0,1)$, then for any $x > 0$ it holds that

$$f(x) = \int_0^1 t^x t^{-\delta} \mathrm{d}\beta_{\delta_0}(t) = -\int_0^\infty e^{-tx} e^{t\delta} \mathrm{d}\beta_{\delta_0}(e^{-t}) = \int_0^\infty e^{-tx} \mathrm{d}\alpha(t)$$

where $\alpha(t) := -\int_0^u e^{u\delta} \mathrm{d}\beta_{\delta_0}(e^{-t})$ so that $\mathrm{d}\alpha(t) = -e^{-t\delta} \mathrm{d}\beta_{\delta_0}(e^{-t})$ and $\alpha(t)$ is the desired funcion. $\qquad \square$

Appendix B

Poisson summation formula

For any complex function $f \in L^1(\mathbb{R}^d)$, its *Fourier Transform* is defined by

$$\hat{f}(\xi) = \int_{\mathbb{R}^d} f(x)e^{-2\pi i \xi \cdot x} dx.$$

Theorem B.0.14. *Suppose f satisfies $|f(x)| \leq C(1+|x|)^{-d-\varepsilon}$ and $|\hat{f}(\xi)| \leq C(1+|\xi|)^{-d-\varepsilon}$ for some $C > 0$ and $\varepsilon > 0$. Then*

$$\sum_{n \in \mathbb{Z}^d} f(x+n) = \sum_{k \in \mathbb{Z}^d} \hat{f}(k)e^{2\pi i k \cdot x}.$$

In particular, taking $x = 0$ we have

$$\sum_{n \in \mathbb{Z}^d} f(n) = \sum_{k \in \mathbb{Z}^d} \hat{f}(k).$$

Proof. Let

$$F(x) = \sum_{n \in \mathbb{Z}^d} f(x+n).$$

Clearly F is $\mathbb{Z}^d$-periodic. Since $\sum_{n \in \mathbb{Z}^d}(1+|n|)^{-d-\varepsilon} < \infty$ it follows that the series

$$\sum_{n \in \mathbb{Z}^d} f(x+n)$$

and

$$\sum_{k \in \mathbb{Z}^d} \hat{f}(k)e^{2\pi i k \cdot x}$$

converge uniformly and absolutely in $\mathbb{R}^d$. Therefore $F(x)$ is continuous and can be considered as a function in $L^2([0,1]^d)$. Let $\{F_k; k \in \mathbb{Z}\}$ be its Fourier coefficients in the orthogonal

basis $\{e^{2\pi ik\cdot x}; k \in \mathbb{Z}\}$. Then

$$F_k = \int_{[0,1]^d} F(x)e^{-2\pi ik\cdot x}\mathrm{d}x = \int_{[0,1]^d} \sum_{n\in\mathbb{Z}^d} f(x+n)e^{-2\pi ik\cdot x}\mathrm{d}x$$

$$= \int_{[0,1]^d} \sum_{n\in\mathbb{Z}^d} f(x+n)e^{-2\pi ik\cdot(x+n)}\mathrm{d}x = \hat{f}(k).$$

Therefore $\sum_{k\in\mathbb{Z}^d} \hat{f}(k)e^{2\pi ik\cdot x}$ is the Fourier series of $F(x)$ and converge to F in $L^2([0,1]^d)$. Since the convergence is uniform it follows that $\sum_{k\in\mathbb{Z}^d} \hat{f}(k)e^{2\pi ik\cdot x} = F(x)$ pointwise. □

Corollary B.0.15. *Let Λ be a lattice and $c > 0$. Then for any $x \in \mathbb{R}^d$,*

$$\sum_{v\in\Lambda} e^{-c|x+v|^2} = \frac{\pi^{\frac{d}{2}}}{c^{\frac{d}{2}}|\Lambda|} \sum_{\omega\in\Lambda^*} e^{2\pi i\omega\cdot x}e^{-\frac{\pi^2|\omega|^2}{c}}$$

Proof. Assume that $\Lambda = A\mathbb{Z}^d$ for some $d\times d$ nonsingular matrix. Let $f(x) = e^{-c|Ax|^2}$, then its Fourier transform is

$$\hat{f}(\xi) = \int_{\mathbb{R}^d} e^{-c|Ax|^2}e^{-2\pi i\xi\cdot x}\mathrm{d}x = \frac{1}{\det A}\int_{\mathbb{R}^d} e^{-c|Ax|^2}e^{-2\pi i(A^{-T}\xi)\cdot Ax}\mathrm{d}(Ax) \qquad \text{(B.1)}$$

$$= \frac{1}{\det A}\int_{\mathbb{R}^d} e^{-c|y|^2}e^{-2\pi i(A^{-T}\xi)\cdot y}\mathrm{d}y = \frac{\pi^{\frac{d}{2}}}{c^{\frac{d}{2}}|\Lambda|}e^{-\frac{\pi^2|A^{-T}\xi|^2}{c}}. \qquad \text{(B.2)}$$

Then by Poisson summation formula

$$\sum_{v\in\Lambda} e^{-c|x+v|^2} = \sum_{n\in\mathbb{Z}^d} e^{-c|A(A^{-1}x+n)|^2} = \sum_{n\in\mathbb{Z}^d} f(A^{-1}x+n) = \sum_{k\in\mathbb{Z}^d} \hat{f}(k)e^{2\pi ik\cdot(A^{-1}x)}$$

$$= \sum_{k\in\mathbb{Z}^d} \frac{\pi^{\frac{d}{2}}}{c^{\frac{d}{2}}|\Lambda|}e^{-\frac{\pi^2|A^{-T}k|^2}{c}}e^{2\pi i(A^{-T}k)\cdot x} = \frac{\pi^{\frac{d}{2}}}{c^{\frac{d}{2}}|\Lambda|} \sum_{\omega\in\Lambda^*} e^{-\frac{\pi^2|\omega|^2}{c}}e^{2\pi i\omega\cdot x}.$$

□

Appendix C

Jacobi triple product formula

Lemma C.0.16 (Jacobi triple product formula)**.** *For any complex q and z with $|q| < 1$ and $z \neq 0$ we have*

$$\prod_{r=1}^{\infty} \left(1 - q^{2r}\right) \left(1 + q^{2r-1} z^2\right) \left(1 + q^{2r-1} z^{-2}\right) = \sum_{k=-\infty}^{\infty} q^{k^2} z^{2k}. \tag{C.1}$$

Proof. It is elementary to verify that for any q and z with $|q| < 1$ and $z \neq 0$ the infinite products

$$\prod_{r=1}^{\infty} \left(1 - q^{2r}\right), \qquad \prod_{r=1}^{\infty} \left(1 + q^{2r-1} z^2\right), \qquad \prod_{r=1}^{\infty} \left(1 + q^{2r-1} z^{-2}\right)$$

converge. For fixed q with $|q| < 1$ and any $z \neq 0$, let

$$F_q(z) = \prod_{r=1}^{\infty} \left(1 + q^{2r-1} z^2\right) \left(1 + q^{2r-1} z^{-2}\right).$$

Then

$$\begin{aligned}
qz^2 F_q(qz) &= qz^2 \prod_{r=1}^{\infty} \left(1 + q^{2r+1} z^2\right) \left(1 + q^{2r-3} z^{-2}\right) \\
&= qz^2 \prod_{r=2}^{\infty} \left(1 + q^{2r-1} z^2\right) \prod_{r=0}^{\infty} \left(1 + q^{2r-1} z^{-2}\right) \\
&= qz^2 \left(1 + q^{-1} z^{-2}\right) \prod_{r=2}^{\infty} \left(1 + q^{2r-1} z^2\right) \prod_{r=1}^{\infty} \left(1 + q^{2r-1} z^{-2}\right) \\
&= \left(1 + qz^2\right) \prod_{r=2}^{\infty} \left(1 + q^{2r-1} z^2\right) \prod_{r=1}^{\infty} \left(1 + q^{2r-1} z^{-2}\right) \\
&= \prod_{r=1}^{\infty} \left(1 + q^{2r-1} z^2\right) \prod_{r=1}^{\infty} \left(1 + q^{2r-1} z^{-2}\right).
\end{aligned}$$

Therefore, $F_q(z)$ satisfies the functional equation

$$qz^2 F_q(qz) = F_q(z). \tag{C.2}$$

Let $G_q(z)$ be the left hand side of (C.1), then

$$G_q(z) = F_q(z) \prod_{r=1}^{\infty} \left(1 - q^{2r}\right) \tag{C.3}$$

It follows from (C.2) that $G_q(z)$ also satisfies

$$qz^2 G_q(qz) = G_q(z). \tag{C.4}$$

For fixed q with $|q| < 1$ the infinite product in (C.1) converges uniformly on compact subsets of $\{z \in \mathbb{C}; z \neq 0\}$. Thus $G(z)$ is analytic for $z \neq 0$. Notice that $G_q(z)$ is an even function, its Laurent expansion can be written as

$$G_q(z) = \sum_{k=-\infty}^{\infty} a_k z^{2k}. \tag{C.5}$$

Equation (C.4) then implies

$$\sum_{k=-\infty}^{\infty} a_k z^{2k} = qz^2 \sum_{k=-\infty}^{\infty} a_k q^{2k} z^{2k} = \sum_{k=-\infty}^{\infty} a_k q^{2k+1} z^{2k+2} = \sum_{k=-\infty}^{\infty} a_{k-1} q^{2k-1} z^{2k}.$$

Thus we obtain the recursion formula

$$a_k = a_{k-1} q^{2k-1}.$$

and hence for any $k \in \mathbb{Z}$,

$$a_k = a_0 q^{k^2}.$$

Now we have

$$G(z) = a_0(q) \sum_{k=-\infty}^{\infty} q^{k^2} z^{2k}. \qquad\qquad (C.6)$$

To show $a_0(q) \equiv 1$, we shall prove

$$G_q\left(e^{\frac{\pi i}{4}}\right) = G_{q^4}(i). \qquad\qquad (C.7)$$

In fact,

$$G_q\left(e^{\frac{\pi i}{4}}\right) = \prod_{r=1}^{\infty} \left(1 - q^{2r}\right)\left(1 + q^{2r-1}i\right)\left(1 - q^{2r-1}i\right) = \prod_{r=1}^{\infty} \left(1 - q^{2r}\right)\left(1 + q^{4r-2}\right)$$

$$= \prod_{r=1}^{\infty} \left(1 - q^{4r}\right)\left(1 - q^{4r-2}\right)\left(1 + q^{4r-2}\right) = \prod_{r=1}^{\infty} \left(1 - q^{4r}\right)\left(1 - q^{8r-4}\right)$$

$$= \prod_{r=1}^{\infty} \left(1 - q^{8r}\right)\left(1 - q^{8r-4}\right)\left(1 - q^{8r-4}\right) = G_{q^4}(i).$$

Using (C.6) and (C.7) we obtain

$$a_0(q) = a_0(q^4).$$

Note that for fixed $z \neq 0$, the left hand side of (C.1) converges uniformly in $\{q \in \mathbb{C}, q \leq r\}$ for each $r < 1$ and hence is analytic as a function of q. In particular, $a_0(q)$ is analytic. Therefore, for any q with $|q| < 1$,

$$a_0(q) = \lim_{k \to \infty} a_0\left(q^{4k}\right) = a_0(0) = 1.$$

$\square$

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