UNIVERSITÀ DEGLI STUDI DI PADOVA

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MASTER'S THESIS

ON UNIVERSALLY OPTIMAL CONFIGURATIONS OF POINTS

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To my grandparents
I dedicate this work.

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Isagoge

Rem tene, verba sequentur

The present work deals mainly with two important results in the theory of universally optimal configurations of points with respect to potential energy minimisation. Namely, a theorem of Cohn and Kumar published in [CK07] about universally optimal spherical configurations and a very recent theorem of Coulangeon and Schürmann contained in [CS10], about periodical point configurations in $\mathbb{R}^d$, which seems to prelude to new results in this theory. Let us spend some words here to explain the meaning of the above expressions: what a potential energy minimisation problem is, what a (universally) optimal configuration of points is, and why the quest for such mathematical objects is truly worthwile. We will discover a fascinating subject, which shows connections with many other mathematical topics, such as sphere packing theory, lattice and coding theory, interpolation, orthogonal polynomials and harmonic analysis.

Genetics of symmetrical figures

We could say that at the origin of our subject there is the observation that symmetry is all around us, in the physical world as well as in mathematics, not to mention the artistic human outputs. We can observe it in an enormous number of different situations, from the beauty of a small snowflake to the solemn elegance of polychromatic plane ornaments, which can be admired in the famous Arab or Renaissance buildings, remarkable examples of science in the service of art. In other times, art is in the service of science, as in the case of the regular solids drawn by Leonardo da Vinci for Luca Pacioli's treatise *De divina proportione*; and we could go on.

However, while the last examples raise more admiration than wonder, as they are the product of educated minds, there is no apparent reason why nature should provide us with such a regular figure as a snowflake. Besides, it is true that only a few of the many possible symmetric groups are actually realised in nature, notwithstanding, we see more of them than we apparently have any right to expect: since symmetry is by its very nature delicate and easily disturbed by perturbations, any occurrence of it in the natural world demands a mathematical explanation. This is what L. Fejes Tóth in his classical book *Regular figures* [FT64] refers to as the *genetics of regular figures*: it is not sufficient to recognise and describe symmetrical structures, we also have to understand the causes and circumstances that generate them and make them stable.

Let us consider a couple of further examples: certain mathematical objects, such as the icosahedron, viewed as a finite set of points on $\mathbb{S}^2$, have always attracted the interest of mathematicians, for their symmetry and elegance, and they have been a source of deep mathematics since the Grecian times. Coming forth to more "modern" structures, which are going to appear in the following chapters, we can mention here the E_8 root lattice in $\mathbb{R}^8$ and the Leech lattice Λ_{24} in $\mathbb{R}^{24}$, as examples of extraordinarily rich mathematical objects. They bring together numerous topics, including sphere packing, finite simple groups, combinatorial and spherical designs, error-correcting codes, lattices and quadratic forms, and so on, thanks to their symmetries and other remarkable properties. As these objects solve, or seem to solve, a broad range of problems, we would like to characterise them via the genetics of the regular figures.

Energy minimisation

Unfortunately, in this matter, even if much is known, far more remains to be discovered, and many natural questions appear to be totally intractable. Nevertheless, a good framework to this subject is to try to present regular figures as solutions of optimisation problems. Please notice that this approach does not always work, as conjecturing a symmetrical solution sometimes leads to the true optimum, but sometimes it is misleading.

Here we will focus on a particular *energy minimisation* problem, which is a generalisation of the *Thomson problem.* Thomson, in his 1904 paper "On the structure of the atom" asked for the minimal-energy configuration of N classical electrons confined to the unit sphere $\mathbb{S}^2$; in other words, the particles interact via the Coulomb potential $1/r$ at Euclidean distance r. This model was originally intended to describe atoms, before quantum mechanics or even the discovery of the nucleus. Now, although subsequent discoveries have shown that this atomic model is far from being adequate, it remains all the same of great interest, both to describe real-world phenomena* and, from a mathematical point of view, to try to characterise our special symmetrical structures as optimal solutions. Indeed, if we constrain a finite number of identically charged particles to move on the surface of a (d-dimensional) sphere, how will they arrange themselves? They will eventually spread out so as to minimise their electrical potential energy, assuming that their kinetic energy dissipates according to a force such as viscosity.

We can hence formulate the problem in these terms: given a finite set $\mathcal{C}$ of points on the sphere, $\mathcal{C} \subset \mathbb{S}^{d-1}$, and a *potential function* $f : (0,4] \to \mathbb{R}$, we define the *potential energy* of $\mathcal{C}$ as

$$E_f(\mathcal{C}) = \sum_{\substack{x,y\in\mathcal{C} \\ x\neq y}} f(|x-y|^2)$$

and we look for the configuration $\mathcal{C}$ which is a global minimum for this quantity. That we call an *optimal solution.*

*For example, think of two different liquids separated by colloidal particles which adsorb on the contact surface: in many cases the particles spread out into a regular arrangement due to their mutual repulsion.

Universal optimality

However, we are more interested here in the effect caused by varying the potential function: how will the optimal configuration change as we let f run into a selected family of functions? Notice that from the physical perspective, the question appears silly, as the potential is usually given as a datum of the problem. But in mathematics, the question is critical, as our nice symmetrical configurations arise as "fixed points", i.e. arrangements that minimise energy for a broad family of functions. For the sake of precision, we deal with *completely monotonic* potentials, i.e., smooth functions satisfying $(-1)^k f^{(k)} \geq 0$ for all integers $k \geq 0$, and we call a configuration *universally optimal* if it minimises energy for any completely monotonic potential function.

The first two chapters of this thesis are devoted to the study of universally optimal *spherical* configurations of points: much work has been done in the last 50 years to try to characterise these arrangements, which by the way seem to be quite rare objects. For example, on $\mathbb{S}^1$ there is an N-point universal optimum for each N, namely the vertices of a regular N-gon. Instead, in $\mathbb{S}^2$, aside from degenerate cases with three or fewer points, there are only three universal optima, namely the tetrahedron, the octahedron and the icosahedron. Thus from the Platonic solids, we have to drop out the cube and the dodecahedron: indeed they are not even optimal, let alone universally optimal, as one can lower energy by rotating a facet. In higher dimensions, there are the root systems of E_8 and the minimal vectors of Λ_{24}, suitably rescaled to the respective unitary sphere.

How to prove that these configurations are indeed universally optimal? How to discover such new arrangements, if they exist, besides those listed in Table 1.1? And what properties do they share in order to be universally optimal? A crucial, though partial, result is given by Cohn and Kumar's cited theorem, which relies on the concept of spherical design. A *spherical k-design* in $\mathbb{S}^{d-1}$ is a finite subset $\mathcal{C}$ of the sphere such that for every polynomial $p : \mathbb{R}^d \to \mathbb{R}$ of total degree at most k, the average of p over $\mathcal{C}$ is equal to its average on the entire sphere. Then the theorem states: *suppose that in $\mathcal{C}$ there are m possible distances between distinct points, and that $\mathcal{C}$ is a spherical $(2m-1)$-design (that is, $\mathcal{C}$ is a so-called* sharp configuration*); then $\mathcal{C}$ is universally optimal* (Theorem 2.4).

The theorem, as we said, is not a characterisation of universally optimal configurations: the only known case not covered by it is the regular 600-cell in $\mathbb{R}^4$, which needs a different argument to be shewn universally optimal. On the other hand, extensive computer searches done by Cohn and others in [Exp09] suggest that Table 1.1 is probably not complete, but anyhow not far from being complete, with only two more configurations that are conjectured to be universally optimal. Thus the theorem is a powerful tool, which has the advantage of relating the search of universal optima to the theory of spherical designs.

Proof techniques: an outline

Theorem 2.4 is a generalisation of a result of Levenshtein [L92], which states that our configurations are all optimal spherical codes. Indeed, a universal optimum is automatically an optimal spherical code, since for the potential function $f(r) = 1/r^s$ with s large, the energy is asymptotically determined by the minimal distance; unfortunately, the converse is far from being true!

The proof of 2.4 rests on lower bounds for the potential energy of a finite set of points on $\mathbb{S}^{d-1}$, which come from linear programming. They were originally developed by Delsarte for discrete problems in coding theory [D72], then extended to continuous packing problems in [DGS77, KL78] and adapted for potential energy minimisation by Yudin and his collaborators Kolushov and Andreev in [Y92, KY94, KY97, A96, A97]. In those papers, they showed that certain configurations minimise specific sorts of energy, raising the question of how generally the techniques could be applied.

To apply the bounds to sharp configurations, we need an auxiliary function h, chosen from the potential function f through *Hermite interpolation*. Then the energy of $\mathcal{C}$ is bounded from below by

$$|\mathcal{C}|^2\alpha_0 - |\mathcal{C}|h(1). \qquad (*)$$

The hypotheses h must satisfy, as well as the condition for $(*)$ to prove a sharp bound, are expressed in terms of a family of orthogonal polynomials, the *ultraspherical*, or *Gegenbauer polynomials*, which are going to play an important role throughout chapters 1 and 2. We will deal with several other families of orthogonal polynomials, which arise as *the* orthogonal polynomials for certain Borel measures on $\mathbb{R}$.

Finally, the third ingredient in the proof of 2.4 are some properties and characterisations of spherical designs, a subject which deserves our interest on its own and which has been greatly developed by Delsarte, Goethals and Seidel in their classical article [DGS77]: we will make an extensive use of the results contained there.

The Euclidean case

Slightly adapting the definition of potential energy to infinite sets of points, we wish to investigate the problem of universal optimality for configurations in the Euclidean space. Here we choose to deal only with discrete periodic point sets, i.e. unions of finitely many translates of a given lattice, to avoid some worries of defining energy in pathological cases. Letting Fourier analysis take the place of ultraspherical polynomials, we can develop the theory analogously to the case of the sphere, but unfortunately, the Euclidean case seems much more difficult than the former, and the degree of advancement is far smaller. Many of the results we wish to obtain remain conjectures for the moment: we do not even know whether universally optimal Euclidean configurations do exist, although Cohn and Kumar have conjectured that the hexagonal lattice in $\mathbb{R}^2$, E_8 and the Leech lattice actually are so.

In this perspective, what appears a crucial step is the result of Coulangeon and Schürmann, which states that *lattices for which all shells are spherical 4-designs are locally universally optimal (among all periodic configurations) if and only if they are locally universally optimal among lattices*; in particular this holds for D_4, E_8 and the Leech lattice. This theorem uses earlier results of Coulangeon [Cou06], Schürmann [S10] and Sarnak and Strömbergsson [SS07]; we devote chapter 3 to prove it. The key technique consists in expanding the functional $E_f(\mathcal{C})$ into its Taylor series and studying gradient and Hessian in order to detect critical points. By the way, this implies dealing with two important maps associated to lattices, namely the Epstein zeta function $\zeta(\Lambda, s)$ and the theta series $\theta_\Lambda(s)$, which are the main sources of information about a lattice.

Future prospects

As said above, a great deal of work is still to be done both for spherical and for Euclidean configurations of points: in our wishlist, we must include the complete classification of universally optimal spherical configurations, and the proof of existence or non-existence of universally optimal Euclidean configurations. However, the state of the art is in continual evolution, as a good number of skilful mathematicians is working on it, so it is reasonable to expect new results on this subject quite soon.

Acknowledgements

[Warning: the content of the following lines is not mathematical, but reading it is recommended all the same.]

While completing this thesis, I have realised how far I have arrived since the beginnings of my student life (when I could not even imagine I would study mathematics), and how much is still to be done. I owe a huge debt of gratitude to many people who have helped and supported me throughout these last two years. So, first of all, let me thank Christine Bachoc, for letting me doing my thesis with her, and for introducing me a new and fascinating subject; thanks also to Renaud Coulangeon, for allowing me to use a non-negligible part of his article in my thesis. Then I am grateful to Marco Garuti, the person who is in charge of the ALGANT programme in Padua: thank you, Marco, for trusting and encouraging me! I owe him, as well as to my former supervisor Maurizio Candilera who advised me to apply, the chance of taking part in this project and of spending a year and a half in Bordeaux. May ALGANT grow both in the number of universities involved and in participants. I also would like to thank Yuri Bilu, who is in charge of the ALGANT master programme here in Bordeaux and Jean-Paul Cerri, whose classes I attended with great pleasure.

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Bordeaux, January 2011
Giovanni Lazzarini

Chapter 1

Spherical designs and sharp configurations

In this first chapter, we study the properties of particular finite sets of points on the unit sphere in $\mathbb{R}^d$, called *spherical t-designs*, which have essentially the property that every polynomial on $\mathbb{R}^d$ of total degree at most t has the same average over the design as over the entire sphere. The concept is due to Delsarte, Goethals and Seidel, in their classical paper of 1977 [DGS77], from which much of the material of this chapter is taken: sharp configurations, which we are going to prove being universally optimal, are in fact introduced at the end of the chapter as an élite type of spherical designs.

We begin introducing the primary tool to handle spherical designs, namely orthogonal and harmonic polynomials, then we start with generic spherical codes and end listing the currently known sharp configurations.

1.1 Orthogonal polynomials

Let $\mu(x)$ denote a non-decreasing function with an infinite number of points of increase in the interval $[a, b]$. The latter interval may be infinite. We assume that moments of all orders exist, that is, $\int_a^b x^n d\mu(x)$ exist for $n = 0, 1, 2, \ldots$.

Definition 1.1. We say that a sequence of polynomials $\{p_n(x)\}_0^\infty$, where $p_n(x)$ has exact degree n, is *orthogonal* with respect to the measure $d\mu(x)$ if

$$\int_a^b p_n(x)p_m(x)d\mu(x) = h_n\delta_{m,n}. \tag{1.1}$$

One fundamental property of any sequence of orthogonal polynomials is that they satisfy a three-term recurrence relation.

Theorem 1.2. *A sequence of orthogonal polynomials $\{p_n(x)\}$ satisfies*

$$p_{n+1}(x) = (A_n x + B_n)p_n(x) - C_n p_{n-1}(x) \quad \text{for } n \geq 0, \tag{1.2}$$

where we set $p_{-1}(x) = 0$. A_n, B_n and C_n are real constants, $n = 0, 1, 2, \ldots$, and $A_{n-1}A_nC_n > 0$, $n = 1, 2, \ldots$. If the highest coefficient of $p_n(x)$ is k_n, then

$$A_n = \frac{k_{n+1}}{k_n}, \quad C_{n+1} = \frac{A_{n+1}}{A_n}\frac{h_{n+1}}{h_n},$$

where h_n is the constant appearing in (1.1).

Proof. Determine A_n such that $p_{n+1} - A_n x p_n(x)$ is a polynomial of degree n. Then

$$p_{n+1}(x) - A_n x p_n(x) = \sum_{k=0}^{n} b_k p_k(x) \tag{1.3}$$

for some coefficients b_k. Notice that, if $Q(x)$ is a polynomial of degree $m < n$, then by (1.1)

$$\int_a^b p_n(x) Q(x) d\mu(x) = 0.$$

This implies that $b_k = 0$ for $k < n-1$, as can be seen by multiplying both sides of (1.3) by $p_k(x)$ and integrating. This shows (1.2).

It is clear that $A_n = k_{n+1}/k_n$, and to derive the final result, multiply (1.2) by $p_{n-1}(x)$ and integrate to get

$$0 = A_n \int_a^b p_n(x) x p_{n-1}(x) d\mu(x) - C_n \int_a^b p_{n-1}^2(x) d\mu(x).$$

As

$$x p_{n-1}(x) = \frac{k_{n-1}}{k_n} p_n(x) + \sum_{k=0}^{n-1} d_k p_k(x),$$

we obtain

$$\frac{A_n}{A_{n-1}} h_n - C_n h_{n-1} = 0.$$

This proves the theorem. □

We give here another important result concerning orthogonal polynomials, the *Christoffel-Darboux formula.*

Theorem 1.3. *Suppose that the $p_n(x)$ are normalised so that*

$$h_n = \int_a^b p_n^2(x) d\mu(x) = 1.$$

Then

$$\sum_{m=0}^{n} p_m(y) p_m(x) = \frac{k_n}{k_{n+1}} \frac{p_{n+1}(x) p_n(y) - p_{n+1}(y) p_n(x)}{x - y}, \tag{1.4}$$

where k_n is the highest coefficient of $p_n(x)$.

Proof. The recurrence relation (1.2) implies that

$$p_n(y) p_{n+1}(x) = (A_n x + B_n) p_n(x) p_n(y) - C_n p_{n-1}(x) p_n(y)$$
$$p_n(x) p_{n+1}(y) = (A_n y + B_n) p_n(y) p_n(x) - C_n p_{n-1}(y) p_n(x).$$

Subtract the two equations and divide by $A_n(x - y)$ to get

$$\frac{1}{A_n} \frac{p_n(y) p_{n+1}(x) - p_n(x) p_{n+1}(y)}{x - y} =$$
$$= p_n(x) p_n(y) + \frac{1}{A_{n-1}} \frac{p_{n-1}(y) p_n(x) - p_{n-1}(x) p_n(y)}{x - y}. \tag{1.5}$$

We have used the fact that $C_n = A_n/A_{n-1}$, for $h_n = 1$. Iterating (1.5) and observing that $A_n = k_{n+1}/k_n$, we get the required result. □

Proposition 1.4. *When $h_n = 1$, then*

$$\sum_{k=0}^{n} p_k^2(x) = \frac{k_n}{k_{n+1}} (p'_{n+1}(x)p_n(x) - p_{n+1}(x)p'_n(x)). \tag{1.6}$$

Proof. Rewrite the right side of (1.4) as

$$\frac{k_n}{k_{n+1}} \frac{(p_{n+1}(x) - p_{n+1}(y))p_n(y) - (p_n(x) - p_n(y))p_{n+1}(y)}{x - y}$$

and let $y \to x$. □

Corollary 1.5. $p'_{n+1}(x)p_n(x) - p_{n+1}(x)p'_n(x) > 0$ *for all* x.

Now we state and prove a couple of results concerning the zeroes of orthogonal polynomials, namely their simplicity and their property of being interlaced (in the sense specified below).

Proposition 1.6. *With* $\{p_n(x)\}$, $d\mu(x)$ *and* $[a, b]$ *as above,* $p_n(x)$ *has* n *simple zeroes in* $[a, b]$ *for every* n.

Proof. Suppose $p_n(x)$ has m distinct zeroes $x_1, x_2, \ldots, x_m$ in $[a, b]$ that are of odd order. Then

$$Q(x) = p_n(x) \prod_{k_1}^{m} (x - x_k) \geq 0 \tag{1.7}$$

for all x in $[a, b]$. If $m < n$, then by orthogonality

$$\int_a^b Q(x)d\mu(x) = 0. \tag{1.8}$$

However, the inequality in (1.7) implies that the integral in (1.8) should be strictly positive. The contradiction implies that $m = n$ and that the zeroes must be simple. □

Denote the zeroes of $p_n(x)$ by $x_{1,n} < x_{2,n} < \cdots < x_{n,n}$.

Proposition 1.7. *The zeroes of* $p_n(x)$ *and* $p_{n+1}(x)$ *separate each other, i.e.*

$$x_{n+1,1} < x_{n,1} < x_{n+1,2} < x_{n,2} < \cdots < x_{n,n} < x_{n+1,n+1}.$$

Proof. From Corollary 1.5,

$$p_{n+1}(x)p'_n(x) - p_n(x)p'_{n+1}(x) < 0.$$

Since $x_{k,n+1}$ is a zero of $p_{n+1}(x)$, we get

$$p_n(x_{k,n+1})p'_{n+1}(x_{k,n+1}) > 0.$$

The simplicity of the zeroes implies that $p'_{n+1}(x_{k,n+1})$ and $p'_{n+1}(x_{k+1,n+1})$ have different signs. Hence $p_n(x_{k,n+1})$ and $p_n(x_{k+1,n+1})$ have different signs. By the continuity, p_n has a zero between $x_{k,n+1}$ and $x_{k+1,n+1}$ for $k = 1, 2, \ldots,$ and the result follows. □

We limit ourselves to state the following result, which can be proved by means of the Gauss quadrature formula (cfr. [AAR99])

Proposition 1.8. *Let* $m < n$. *Between any two zeroes of* $p_m(x)$ *there is a zero of* $p_n(x)$.

1.1.1 Gegenbauer (ultraspherical) polynomials

The most important family of orthogonal polynomials we shall need to deal with spherical configurations of points are the ultraspherical polynomials $\{Q_k(x), k \in \mathbb{N}\}$, defined for a fixed $d \geq 2$.

Definition 1.9. The *Gegenbauer (or ultraspherical polynomial)* $Q_k(x)$, of degree k is defined by the recurrence

$$\begin{aligned} Q_0(1) &= 1; \\ Q_1(x) &= dx; \\ \lambda_{k+1}Q_{k+1}(x) &= xQ_k(x) - (1-\lambda_{k-1})Q_{k-1}(x), \quad \text{with } \lambda_k = \frac{k}{d+2k-2} \end{aligned}$$

We give here the first few Gegenbauer polynomials:

$$\begin{aligned} 2Q_2(x) &= (d+2)(dx^2-1) \\ 6Q_3(x) &= d(d+4)((d+2)x^3-3x) \\ 24Q_4(x) &= d(d+6)((d+2)(d+4)x^4-6(d+2)x^2+3) \\ 120Q_5(x) &= d(d+2)(d+8)((d+4)(d+6)x^5-10(d+4)x^3+15x). \end{aligned}$$

In what follows the $Q_k(x)$'s will be used together with the *classical Gegenbauer polynomials* $C_k^m(x)$, which are related to the former by

$$Q_k(x) = \frac{d+2k-2}{d-2}\, C_k^{d/2-1}(x) : \tag{1.9}$$

in particular

$$C_0^{d/2-1}(1) = Q_0(1) = 1;$$

the latter formulation is more suitable to deal with sharp configurations (see Section 1.6). For $d = 2$, $k \geq 1$, ultraspherical polynomials are related to the Chebyshev polynomials of the first kind $T_k(x)$ by the relation

$$Q_k(x) = kC_k^0(x) = 2T_k(x).$$

Notice also that if we set

$$C_k(x) := \sum_{i=0}^{\lfloor k/2 \rfloor} Q_{k-2i}(x),$$

then $C_k(x)$ is the classical Gegenbauer polynomial $C_k^{d/2}(x)$. From the definitions it is easy to prove that

$$\begin{aligned} Q_k(1) &= \binom{d+k-1}{d-1} - \binom{d+k-3}{d-1}, \\ C_k(1) &= \binom{d+k-1}{d-1}, \quad \text{for } k \geq 1. \end{aligned}$$

The Gegenbauer polynomials are indeed orthogonal polynomials, namely

$$\int_{-1}^{1} Q_k(x)Q_l(x)(1-x^2)^{(d-3)/2}dx = a_d Q_k(1)\delta_{k,l},$$

where a_d is some positive constant: we will show it in Section 2.2.2.

To any polynomials $F(x) \in \mathbb{R}[x]$ we associate its Gegenbauer expansion

$$F(x) = \sum_{k=0}^{\infty} f_k Q_k(x),$$

for uniquely determined coefficients f_k, which of course are non-zero only for finitely many k's. We list here three useful lemmas with standard properties of Gegenbauer polynomials:

Lemma 1.10. *Let*

$$Q_i(x)Q_j(x) = \sum_{k=0}^{i+j} q_k(i,j)Q_k(x).$$

Then

$$q_0(i,j) = Q_i(1)\delta_{i,j} \quad \textit{and} \quad q_k(i,j) \geq 0$$

for all i, j, k, *with* $q_k(i,j) > 0$ *if and only if*

$$|i-j| \leq k \leq i+j \textit{ and } k \equiv i+j \mod 2.$$

Lemma 1.11. *Let* $G(x) = Q_l(x)F(x)/Q_l(1)$ *for some* $l \in \mathbb{N}$. *Then* $g_0 = f_1$, *and if* $f_k \geq 0$ *for all* $k \in \mathbb{N}$, *then also* $g_k \geq 0$ *for all* $k \in \mathbb{N}$.

Lemma 1.12. *Let* $G(x) = x^l F(x)$ *for some* $l \in \mathbb{N}$. *Then, for each* $k \in \mathbb{N}$, *the number* g_k *is a convex linear combination, with strictly positive coefficients, of the numbers* f_{k+l-2i}, *for* $i = 0, 1, \ldots, \min(l \lfloor \frac{1}{2}(k+l) \rfloor)$.

1.2 Harmonic polynomials

Let $\mathbb{S}^{d-1}$, with surface measure σ_d, denote the unit sphere in the Euclidean space $\mathbb{R}^d$, endowed with the usual inner product $\langle\, , \rangle$. For every $k \geq 0$, let

$$\mathrm{Hom}(k) = \mathrm{Hom}_d(k)$$

be the linear space of all functions $V : \mathbb{S}^{d-1} \to \mathbb{R}$ which are represented by polynomials

$$V(\xi) = V(\xi_1, \ldots, \xi_d),$$

homogeneous of total degree k in the k variables ξ_i.

Let also $\mathrm{Harm}(k)$ denote the subspace of $\mathrm{Hom}(k)$ consisting of all functions represented by *harmonic polynomials* of degree k. Then $\mathrm{Harm}(k)$ is invariant under the orthogonal group $\mathrm{O}(d)$ of $\mathbb{R}^d$. Any function $V \in \mathrm{Hom}(k)$ can be uniquely written as

$$V(\xi) = \sum_{i=0}^{\lfloor k/2 \rfloor} \langle \xi, \xi \rangle^i W_{k-2i}(\xi), \quad W_l \in \mathrm{Harm}(l).$$

Therefore we have the following decomposition:

Theorem 1.13.

$$\mathrm{Hom}(k) = \sum_{i=0}^{\lfloor k/2 \rfloor} \mathrm{Harm}(k-2i)$$

$$\mathrm{Hom}(k) \oplus \mathrm{Hom}(k-1) = \sum_{i=0}^{k} \mathrm{Harm}(i).$$

Notice that the linear space in the second line consists of all functions on $\mathbb{S}^{d-1}$ represented by (not necessarily homogeneous) polynomials of total degree at most k in d variables.

For the dimensions, we have the following result, cfr. [DGS77], Theorem 3.2:

Theorem 1.14.

$$\begin{aligned} \dim \mathrm{Hom}(k) &= C_k(1), \\ \dim \mathrm{Harm}(k) &= Q_k(1), \\ \dim \mathrm{Hom}(k) \oplus \mathrm{Hom}(k-1) &= \binom{d+k-1}{d-1} + \binom{d+k-2}{d-1} =: R_k. \end{aligned}$$

The *addition formula* relates the Gegenbauer polynomial $Q_k(x)$ and any orthogonal basis $\{W_{k,i}, i = 1, 2, \dots, Q_k(1)\}$ of $\mathrm{Harm}(k)$, with norm $W_{k,i} = \sigma_d^{1/2}$, as follows:

Theorem 1.15.

$$\sum_{i=1}^{Q_k(1)} W_{k,i}(x) W_{k,i}(y) = Q_k(\langle x, y \rangle), \quad \textit{for } x, y \in \mathbb{S}^{d-1} \tag{1.10}$$

Proof. See for example [AAR99]. □

An important invariant associated to a finite (non-empty) set $\mathcal{C}$ of $\mathbb{S}^{d-1}$ is its characteristic matrix:

Definition 1.16. For any finite non-empty set $\mathcal{C} \subset \mathbb{S}^{d-1}$ of cardinality N, for any orthogonal basis $\{W_{k,i}\}$ of *Harm*(k), with norm $W_{k,i} = \sigma_d^{1/2}$, and for any fixed numbering of these, the $N \times Q_k(1)$ matrix

$$H_k := (W_{k,i}(x))_{k,i}, \quad x \in \mathcal{C},\ i = 1, 2, \dots, Q_k(1)\},$$

is called the k-th *characteristic matrix*. Thus, H_0 is the all-one vector of size N.

Definition 1.17. For any $\mathcal{C} \subset \mathbb{S}^{d-1}$ of cardinality N, and for any $\alpha \in \mathbb{R}$, $-1 \leq \alpha \leq 1$, the $N \times N$ *distance matrix* D_α is defined by its elements $D_\alpha(x, y) = 1$ for $\langle x, y \rangle = \alpha$, and $D_\alpha(x, y) = 0$ otherwise, for $x, y \in \mathcal{C}$. The sum of the elements of D_α is denoted by d_α.

By how it has been defined, it is clear that D_α is a symmetric matrix.

Theorem 1.18. *Let $\mathcal{C} \subset \mathbb{S}^{d-1}$, and let A' be a finite set containing all inner products of the vectors of $\mathcal{C}$. Then*

$$H_k H_k^t = \sum_{\alpha \in A'} Q_k(\alpha) D_\alpha,$$

where the $Q_k(x)$ are the Gegenbauer polynomials, H_k the characteristic matrices, and D_α the distance matrices.

Proof. Just a straightforward verification: the addition formula (1.10) and Definition 1.16 yield

$$H_k H_k^t = (Q_k(\langle x, y\rangle))_{x,y\in\mathcal{C}}.$$

Now apply Definition 1.17. □

Corollary 1.19.

$$|H_k^t H_0|^2 = \sum_{\alpha\in A'} Q_k(\alpha) d_\alpha.$$

Proof. As $|H_k^t H_0|^2 = H_0^t(H_k H_k^t)H_0$, and H_0 is the all-one vector of size N, take the sum of the elements of the matrices in the formula of Theorem 1.18. □

Corollary 1.20. *For any polynomial* $p(x)$ *with Gegenbauer coefficients* $p_0, p_1, \dots,$ *the following holds:*

$$p_0 N^2 + \sum_{k=1}^{\infty} p_k |H_k^t H_0|^2 = \sum_{\alpha\in A'} p(\alpha) d_\alpha.$$

Proof. Use the expansion

$$p(x) = \sum_k p_k Q_k(x)$$

with Theorem 1.18 to get

$$\sum_{k=0}^{\infty} p_k H_k H_k^t = \sum_{\alpha\in A'} p(\alpha) D_\alpha,$$

then take the sum of the elements of the matrices. □

Lemma 1.21.

$$|H_i^t H_j - N\Delta_{i,j}|^2 = \sum_{k=1}^{i+j} q_k(i,j) |H_k^t H_0|^2,$$

where $q_k(i,j)$ *is as in Lemma 1.10 and* $\Delta_{i,j}$ *denotes the suitable zero matrix for* $i \neq j$ *and unit matrix for* $i = j$.

Proof. See [DGS75], Lemma 4.5. □

1.3 Spherical codes

Definition 1.22. Let A be a subset of the interval $[-1, 1)$. A *spherical* A*-code*, for short an A*-code*, is a non-empty subset $\mathcal{C}$ of the unit sphere in $\mathbb{R}^d$, satisfying $\langle x, y\rangle \in A$ for all $x \neq y \in \mathcal{C}$.

Thus, an A-code is a set of unit vectors with angles from the prescribed set $\arccos A$, or a set of points on $\mathbb{S}^{d-1}$ with distances from the prescribed set $(2 - 2A)^{1/2}$. We shall use the notation $A' := A \cup \{1\}$.

Definition 1.23. A polynomial $p(x) \in \mathbb{R}[x]$ is *compatible* with the set A if

$$p(\alpha) \leq 0 \text{ for all } \alpha \in A.$$

Theorem 1.24. *Let $p(x)$, with Gegenbauer coefficients $f_0 > 0$ and $f_k \leq 0$. for all k, be compatible with the set A. Then the cardinality N of any A-code $\mathcal{C}$ satisfies*

$$N \leq p(1)/p_0.$$

Equality holds if and only if, for all $x \neq y \in \mathcal{C}$ and for all $k \geq 1$,

$$p(\langle x, y \rangle) = 0, \quad f_k H_k^t H_0 = 0.$$

Proof. This is a consequence of Corollary 1.20, since $d_1 = N$: explicitely, we have

$$p_0 N^2 + \sum_{k=1}^{\infty} f_k |H_k^t H_0|^2 = p(1)N + \sum_{\alpha \in A} p(\alpha) d_\alpha$$

which implies

$$f_0 N^2 - p(1)N = -\sum_{k=1}^{\infty} f_k |H_k^t H_0|^2 + \sum_{\alpha \in A} p(\alpha) d_\alpha \leq 0,$$

whence $p(0)N^2 \leq p(1)N$. The statement on equality is straightforward. □

Example 1.25. For a given β, $-1 \leq \beta < 0$, let A be any subset of the interval $[-1, \beta]$. The polynomial $P(x) = x - \beta$ is compatible with A, and $P_0 = -\beta$, $P_1 = 1/d > 0$. Hence Theorem 1.24 applies, yielding $N \leq 1 - 1/\beta$. An A-code $\mathcal{C}$ of given dimension $r \leq d$ achieves ths bound if and only $\mathcal{C}$ is an r- dimensional regular simplex, with $\beta = -1/r$.

Before introducing the fundamental notion of spherical design, we prove another bound for the cardinality of an A-code $\mathcal{C}$. This so-called absolute bound only depends on the cardinality of A, not on its specific elements.

Theorem 1.26. *For given $s = |A| < \infty$, the cardinality N of any A-code $\mathcal{C}$ satisfies*

$$N \leq R_s.$$

.

Proof. Define the annihilator polynomial for A

$$P(x) := \prod_{\alpha \in A} \frac{x - \alpha}{1 - \alpha},$$

and for any $y \in \mathcal{C}$ define the function $P_y : \mathbb{S}^{d-1} \to \mathbb{R}$ by

$$P_y(x) := P(\langle x, y \rangle), \quad x \in \mathbb{S}^{d-1}.$$

Thus P_y belongs to the linear space $\mathrm{Hom}(s) \oplus \mathrm{Hom}(s-1)$, whose dimension is exactly the number appearing in our bound. By definition we have

$$P_y(y) = P(\langle y, y \rangle) = P(1) = \prod_{\alpha \in A} \frac{1 - \alpha}{1 - \alpha} = 1,$$
$$P_y(x) = 0 \quad \text{for } x \in \mathcal{C}, \ x \neq y,$$

so that the functions P_y are linearly independent. Hence their number $N = |\mathcal{C}|$ cannot exceed the dimension of the linear space, which proves the theorem. □

Example 1.27. For $s = 1$, we have $N \leq d + 1$, with equality if and only if $\mathcal{C}$ is a regular d-simplex, as in Example 1.25.

1.4 Spherical t-designs

The concept on which the recent results about universally optimal configurations rest is that of spherical design, which is a property of some finite subsets of $\mathbb{S}^{d-1}$ that can be characterised in several equivalent ways. What follows is one of the possible definitions:

Definition 1.28. A finite non-empty set $\mathcal{C} \subset \mathbb{S}^{d-1}$ is a *spherical t-design*, for short a *t-design*, for some $t \in \mathbb{N}$, if the following holds for $k = 0, 1, \ldots, t$:

$$\forall V \in \mathrm{Hom}(k),\ \forall T \in \mathrm{O}(d), \quad \sum_{x \in \mathcal{C}} V(Tx) = \sum_{x \in \mathcal{C}} V(x).$$

Since $\mathrm{Hom}(k)$ is spanned by the monomials

$$x_1^{k_1} x_2^{k_2} \cdots x_d^{k_d}, \quad k_i \in \mathbb{N}, \quad \sum_{i=1}^{d} k_i = k,$$

Definition 1.28 amounts to requiring that the kth moments of $\mathcal{C}$ are invariants with respect to orthogonal transformations, for $k = 0, 1, \ldots, t$.

Actually, Definition 1.28 is not the most commonly used, although it is that we find in the original paper of Delsarte, Goethals and Seidel [DGS77], to whom the concept of a spherical design is due, and indeed it can seem a little abstract at a first sight: to give the most usual definition, we observe that another way to express the t-design property is that, for $k = 0, 1, \ldots, t$,

$$\forall V \in \mathrm{Hom}(k),\ \forall T \in \mathrm{O}(d), \quad \frac{1}{N} \sum_{x \in \mathcal{C}} V(Tx) = \frac{1}{\sigma_d} \int_{\mathbb{S}^{d-1}} V(x)\, d\sigma(x), \qquad (1.11)$$

that is, the kth moments of $T\mathcal{C}$ are equal to the corresponding kth moments of $\mathbb{S}^{d-1}$, for all $T \in \mathrm{O}(d)$. Hence we get the simpler equivalent formulation, which we shall repeatedly use:

Definition. A finite non-empty set $\mathcal{C} \subset \mathbb{S}^{d-1}$ is a t-design if for every polynomial p of degree less or equal than t,

$$\boxed{\frac{1}{N} \sum_{x \in \mathcal{C}} p(x) = \frac{1}{\sigma_d} \int_{\mathbb{S}^{d-1}} p(x) d\sigma(x),} \qquad (1.12)$$

i.e. the average of p on the entire sphere is the same as its average on $\mathcal{C}$.

Since for any $V \in \mathrm{Harm}(k)$, with $k \geq 1$, the integral in (1.11) vanishes, Theorem 1.13 yields the following important criterion for spherical t-designs:

Theorem 1.29. *A finite subset $\mathcal{C}$ of $\mathbb{S}^{d-1}$ is a spherical t-design if and only if*

$$\sum_{x \in \mathcal{C}} W(x) = 0 \quad \textit{for all } W \in \sum_{k=1}^{t} \mathrm{Harm}(k).$$

As we have said, there are several equivalent characterisations of t-designs: for example in terms of their characteristic matrices we have the following theorem:

Theorem 1.30. *A finite set $\mathcal{C} \subset \mathbb{S}^{d-1}$ is a t-design if and only if its characteristic matrices satisfy any one of the following conditions:*

(i) $H_k^t H_0 = 0$ *for* $k = 1, 2, \ldots, t$, *or*

(ii) $H_k^t H_l = n\Delta_{k,l}$ *for* $0 \leq k + l \leq t$.

Proof. The equivalence of Definition 1.28 and *(i)* follows from Theorem 1.29 and Definition 1.16.

The equivalence of *(i)* and *(ii)* follows from Lemma 1.21. □

Remark 1.31. For $t \leq 2$, let $e := \lfloor t/2 \rfloor$ and $r := e - (-1)^t$. Then

$$H_e^t H_e = nI \text{ and } H_e^t H_r = 0$$

are necessary and sufficient conditions for a t-design. This is a consequence of Theorem 1.30 and Lemmas 1.10 and 1.21.

Theorem 1.32. *For any A-code $\mathcal{C}$, let $A' = A \cup \{1\}$ and denote by d_α the sum of the elements of the distance matrix D_α. Then*

$$\sum_{\alpha \in A'} d_\alpha Q_k(\alpha) \geq 0,$$

and equality holds for $k = 1, 2, \ldots, t$ if and only if $\mathcal{C}$ is a t-design.

Proof. Apply Corollary 1.19 and Theorem 1.30. □

Remark 1.33. In other words, theorem 1.32 gives a simple test for spherical design strength: a configuration $\mathcal{C} \subset \mathbb{S}^{d-1}$ is a spherical t-design if and only if

$$\sum_{x,y \in \mathcal{C}} C_i^{d/2-1}(\langle x, y \rangle) = 0$$

for $1 \leq i \leq t$. This shall be essential in Chapter 2.

Example 1.34. Remark 1.31 says that 2-designs $\mathcal{C}$ are characterised by

$$H_0^t H_1 = 0 \text{ and } H_1^t H_1 = nI.$$

Example 1.35. A set $\mathcal{C}$ is *antipodal* whenever $-x \in \mathcal{C}$ for all $x \in \mathcal{C}$, equivalently $-\mathcal{C} = \mathcal{C}$. Antipodal A-codes provide 1-designs, since

$$A'(\mathcal{C}) = -A'(\mathcal{C}), \quad d_\alpha = d_{-\alpha}, \quad \sum_{\alpha \in A'} d_\alpha Q_k(\alpha) = 0 \text{ for odd } k.$$

Example 1.36. For $d = 3$, the six vertices of the octahedron, and also the eight vertices of the cube, provide a 3-design. Further examples shall be given when dealing with spherical sharp configurations.

There is no upper bound to the number of points of a t-design, since the union of disjoint t-designs again is a t-design (this is evident if we think at the average property). The following theorem, which to some extent is dual to Theorem 1.24, provides a lower bound for $|\mathcal{C}|$.

Theorem 1.37. *Let $p(x)$, with Gegenbauer coefficients f_0 and $f_k \leq 0$ for all $k > t$, satisfy $p(1) > 0$ and $p(\alpha) \leq 0$ for all $\alpha \in [-1,1]$. Then the cardinality of any t-design $\mathcal{C}$ satisfies*

$$n \geq \frac{p(1)}{f_0}.$$

Equality holds if and only if, for all $x \neq y \in \mathcal{C}$, and for all $k > t$,

$$p(\langle x, y\rangle) = 0, \quad f_k H_k^t H_0.$$

Proof. This is a consequence of Theorem 1.30 and Corollary 1.20. □

Theorem 1.38. *Let $\mathcal{C}$ be a $(2e)$-design (e as above). Then*

$$n = |\mathcal{C}| \geq R_e.$$

Equality holds if and only if $A(\mathcal{C})$ consists of the zeroes of

$$R_e(x) := \sum_{i=0}^{e} Q_i(x).$$

Proof. See [DGS77], Theorem 5.11. □

Theorem 1.39. *Let $\mathcal{C}$ be a $(2e+1)$-design. Then*

$$n = |\mathcal{C}| \geq 2C_e(1).$$

Equality holds if and only if $A(\mathcal{C})$ consists of -1 and the zeroes of $C_e(\mathcal{C})$. Moreover, in the case of equality, X is antipodal.

Proof. See [DGS77], Theorem 5.12. □

Definition 1.40. A t-design is called *tight* if any of the bounds mentioned in Theorems 1.38 and 1.39 is attained.

Clearly, a tight t-design cannot be a $(t+1)$-design (check cardinalities). We conclude this section giving some simple examples of tight t-designs.

Example 1.41. For $d = 2$ and any t, a tight t-design is nothing but a regular $(t+1)$-gon.

Example 1.42. For any d, the $d+1$ vertices of a regular simplex in $\mathbb{R}^d$ provide a tight 2-design.

The $2d$ vertices of the cross polytope provide a tight 3-design. Notice that the 2^d vertices of the cube also provide a 3-design (not a 4-design), but not a tight 3-design for $d \geq 3$.

Example 1.43. For $d = 3$, the icosahedron is the only tight 5-design.

1.5 Spherical (d, N, s, t)-configurations

Definition 1.44. A *(spherical) (d, N, s, t)-configuration* is a finite subset $\mathcal{C} \subset \mathbb{S}^{d-1}$ of cardinality N, which is a t-design and an A-code with $|A| = s$.

Given $\mathcal{C} \subset \mathbb{S}^{d-1}$, $|\mathcal{C}| = N$, we denote by $s(\mathcal{C})$ and $t(\mathcal{C})$ the minimum s and the maximum t for which $\mathcal{C}$ is a (d, N, s, t)-configuration. Theorem 1.48 will provide a criterion for an A-code to be a t-design, in terms of the Gegenbauer coefficients $f_0, f_1, \dots, f_s$ of an annihilator polynomial $p(x)$ of degree s for the set A.

Definition 1.45. A polynomial $p(x) \in \mathbb{R}[x]$ is an *annihilator* for a finite set $A \neq \emptyset$ with $1 \notin A$ if

$$p(1) = 1, \quad \forall \alpha \in A\ p(\alpha) = 0.$$

Lemma 1.46. *Let $\mathcal{C}$ be an A-code, and let $p(x)$ be an annihilator for A with Gegenbauer coefficients $p_0, p_1, \dots$. Then*

$$N(1 - np_0) = \sum_{k=1}^{\infty} p_k |H_k^t H_0|^2.$$

Proof. Apply Corollary 1.20, it is a direct computation. □

Theorem 1.47. *Let $\mathcal{C}$ be an A-code, $|\mathcal{C}| = N$, $|A| = s$. The Gegenbauer coefficients of an annihilator $p(x)$ of degree s for A have the following property:*

$$\text{if } \forall 0 \leq i \leq s\ p_i \geq 0, \text{ then } \forall 0 \leq j \leq s\ f_j \leq 1/N.$$

If, in addition, $f_j = 1/N$ for some $j \leq s$, then $\mathcal{C}$ is an A-code of maximum cardinality.

Proof. For any fixed $j \in \{0, 1, \dots, s\}$, define

$$G(x) := \frac{p(x)Q_j(x)}{Q_j(1)}.$$

Then $G(x)$ is clearly an annihilator for A. Lemma 1.11 implies that $g_0 = p_j$ and $g_k \geq 0$ for all k. Hence Lemma 1.46 gives

$$1 - np_j = 1 - ng_0 \geq 0.$$

Furthermore, if equality holds, then the bound of Theorem 1.24 is attained, and $\mathcal{C}$ is an A-code of maximum cardinality. □

Theorem 1.48. *Let $\mathcal{C}$ be an A-code, with $|\mathcal{C}| = N$, $|A| = s$, and let $p(x)$ be an annihilator of degree s for A, with Gegenbauer coefficients $p_0, p_1, \dots, p_s$. If $\mathcal{C}$ is a t-design with $t \geq s$, then $p_0 = p_1 = \dots = p_{t-s} = 1/N$.*

Conversely, if $p_0 = p_1 = \dots = p_r = 1/N$, and $p_{r+1} > 0, \dots, p_s > 0$ for some $r \leq s$, then $\mathcal{C}$ is an $(r+s)$-design.

Proof. First, suppose $\mathcal{C}$ a $t-$*design* with $t \geq s$. For any fixed $j \in \{0, 1, \dots, t-s\}$, the polynomial

$$G(x) := \frac{p(x)Q_j(x)}{Q_j(1)}$$

is an annihilator for A of degree $j + s \geq t$. Hence Theorem 1.30 and Lemma 1.46 yield

$$0 = 1 - Ng_0 = 1 - Np_j$$

by use of Lemma 1.11.

Conversely, take the annihilator

$$G(x) := x^r p(x)$$

for A of degree $r+s$. Assuming $p_0 = \cdots = p_r = 1/N$ and all $p_i > 0$, we conclude from Lemma 1.12 that $g_0 = 1/N$, $g_k > 0$ for $0 \leq k \leq r+s$. Lemma 1.46 then implies that $H_k^t H_0 = 0$ for $1 \leq k \leq r+s$, whence $\mathcal{C}$ is an $(r+s)$-design. □

Theorem 1.49. *Any (d, N, s, t)-configuration $\mathcal{C}$ satisfies*

$$t \leq 2s \quad \textit{and} \quad N \leq R_s.$$

If equality holds in any of the above bounds, then $\mathcal{C}$ is a tight $(2s)$-design.

Proof. Let $p(x)$ be the annihilator of degree s for A. First apply Theorem 1.48: if $t \geq s$, then $p_{t-s} \neq 0$, hence $t - s \leq s$, i.e. $t \leq 2s$.

In the case of equality, Theorem 1.38 implies $N \geq R_s$, whence equality holds by 1.26, and $\mathcal{C}$ is thus a tight $(2s)$-design.

For the second part of the theorem, we observe that Theorem 1.18 implies

$$\sum_{k=0}^{s} p_k H_k H_k^t = \sum_{k=0}^{s} f_k \left(\sum_{\alpha \in A'} Q_k(\alpha) D_\alpha \right) =$$

$$= \sum_{\alpha \in A'} \left(\sum_{k_0}^{s} f_k Q_k(\alpha) \right) D_\alpha = \sum_{\alpha \in A'} p(\alpha) D_\alpha = D_1 = I.$$

Hence the $N \times R_s$-matrix

$$H := \begin{bmatrix} H_0 & H_1 & \cdots & H_s \end{bmatrix}$$

has rank N, proving once again $N \leq R_s$ of Theorem 1.26.

Now suppose $N = R_s$, then H is non-singular, and all p_k are positive. Therefore Theorem 1.47 implies that all $p_k \leq 1/N$. This yields

$$N \sum_{k=0}^{s} p_k Q_k(1) = N = R_s = \sum_{k=0}^{s} Q_k(1)$$

whence $p_0 = p_1 = \cdots = p_s = 1/N$, $Np(x) = R_s(x)$, and it follows from Theorem 1.48 that $\mathcal{C}$ is a $(2s)$-design. This concludes the proof; it is interesting to observe that in case of equality we have

$$HH^t = H^t H = NI.$$

□

Theorem 1.50. *Every (d, N, s, t)-configuration $\mathcal{C}$, which is an A-code with $A' = -A'$, $|A| = s$, satisfies*

$$t \leq 2s - 1 \quad \textit{and} \quad N \leq 2C_{s-1}.$$

If equality holds in any of the above bounds, then $\mathcal{C}$ is an antipodal tight $(2s-1)$-design.

Proof. See [DGS77], Theorem 6.8. □

For any A-code $\mathcal{C}$, the *valencies* $v_\alpha(x)$ and the *intersection numbers* $p_{\alpha,\beta}(x,y)$ are defined as follows:

Definition 1.51.

$$v_\alpha(x) := |\{z \in \mathcal{C} : \langle x,z\rangle = \alpha\}|, \ \alpha \in A', \ x \in \mathcal{C},$$
$$p_{\alpha,\beta}(x,y) := |\{z \in \mathcal{C} : \langle x,z\rangle = \alpha, \ \langle y,z\rangle = \beta\}|, \ \alpha,\beta \in A', \ x,y \in \mathcal{C}.$$

Definition 1.52. $\mathcal{C}$ is *distance invariant* if for all $x \in A'$ the valency $v_\alpha(x)$ is independent of $x \in \mathcal{C}$.

$\mathcal{C}$ carries an *s-class association scheme* if for all $\alpha, \beta \in A'$ the intersection number $p_{\alpha,\beta}(x,y)$ depends only on $\langle x,y\rangle$.

We observe that the triangle inequality on the sphere imposes restrictions on the intersection numbers, namely we have

$$p_{\alpha,\beta}(x,y) \neq 0 \Rightarrow (2(1-\alpha)(1-\beta)(1+\langle x,y\rangle)) \geq (1-\alpha-\beta+\langle x,y\rangle)^2).$$

For any integer $i \geq 0$, let x^i have the Gegenbauer expansion

$$x^i = \sum_{k=0}^{i} f_{i,k} Q_k(x.)$$

The *convolution* of x^i and x^j is defined to be the polynomial

$$F_{i,j}(x) := \sum_{k=0}^{\min(i,j)} f_{i,k} f_{j,k} Q_k(x).$$

Lemma 1.53. *For $0 \leq i+j \leq t$ and for fixed $\gamma = \langle x,y\rangle$, the intersection numbers $p_{\alpha,\beta(x,y)}$ of a (d,N,s,t)-configuration satisfy the linear equation*

$$\sum_{\alpha,\beta \in A} \alpha^i \beta^j p_{\alpha,\beta}(x,y) = NF_{i,j}(\gamma) - \gamma^j - \gamma^i + \delta_{1,\gamma}.$$

Proof. By Theorem 1.30*(ii)*, the t-design property implies

$$\left(\sum_{k=0}^{i} f_{i,k} H_k H_k^t\right)\left(\sum_{k=0}^{j} f_{j,k} H_k H_k^t\right) = n \sum_{k=0}^{\min(i,j)} f_{i,k} f_{j,k} H_k H_k^t.$$

Rewrite this using Theorem 1.18 which reads

$$H_k H_k^t = (Q_k(\langle x,y\rangle))_{x,y\in\mathcal{C}}.$$

Equate the (x,y)-entries on both sides of the formula above, and use the definition of $f_{i,k}$: we get

$$\sum_{\alpha,\beta \in A'} \alpha^i \beta^j p_{\alpha,\beta}(x,y) = nF_{i,j}(\langle x,y\rangle).$$

This yields the desired formula, since for $\langle x,y\rangle = \gamma$

$$p_{\alpha,1}(x,y) = p_{1,\alpha}(x,y) = \delta_{\alpha,\gamma}.$$

□

Theorem 1.54. *Let $\mathcal{C}$ be a (d, N, s, t)-configuration.*

(i) If $t \geq s-1$, then $\mathcal{C}$ is distance invariant;

(ii) if $t \geq 2s-2$, then $\mathcal{C}$ carries an $s(\mathcal{C})$-class association scheme;

(iii) if $t \geq 2s-3$, then, for any fixed $\langle x, y\rangle = \gamma$, the intersection numbers $p_{\alpha,\beta}(x, y)$ are uniquely determined by $p_{\gamma,\gamma}(x, y)$.

Proof. *(i)* Suppose $t \geq s-1$, and apply Lemma 1.53 with $j = 0$, $x = y$, $\gamma = 1$:

$$\sum_{\alpha \in A} \alpha^i v_\alpha(x) = nF_{i,0}(1) - 1; \quad 0 \leq i \leq s-1.$$

This linear system of s equations with s unknows $v_\alpha(x)$ has a Vandermonde, hence non-singular, matrix. Therefore, the valencies are uniquely determined, and are independent of x.

(ii) Next suppose $t \geq 2s-2$. Now Lemma 1.53 yields a linear system of s^2 equations for $0 \leq i,\ j \leq s-1$, with s^2 unknows $p_{\alpha,\beta}(x, y)$. The matrix of this system is the direct product of two Vandermonde matrices, hence is non-singular. Therefore, for fixed $\gamma = \langle x, y\rangle$, the intersection numbers are uniquely determined.

The third part of the theorem is proved analogously. □

Theorem 1.55. *Any tight t-design carries an s-class association scheme, with $s = \lceil t/2 \rceil$.*

Proof. Apply Theorems 1.38, 1.39 and 1.54. □

We conclude this section quoting the following non-existence theorem:

Theorem 1.56. *The only tight 6-design is the regular heptagon in $\mathbb{R}^2$.*

Proof. See [DGS77], Theorem 7.7. □

1.6 Sharp configurations

Definition 1.57. A finite subset of the unit sphere $\mathbb{S}^{d-1}$ is a *sharp configuration* if there are m inner products between distinct points in it and it is a spherical $(2m-1)$-design.

Remark 1.58. Observe that replacing $2m-1$ with $2m+1$ in Definition 1.57 would be impossible, for the following reason: if $t_1, \ldots, t_m$ are the inner products that occur between distinct points in a configuration and y is a point in the configuration, then the polynomial

$$x \to (1 - \langle x, y\rangle) \prod_{i=1}^{m} (\langle x, y\rangle - t_i)^2$$

of degree $2m+1$ vanishes on the entire configuration. However, its integral over the sphere does not vanish, because the polynomial is non-negative on the sphere and not identically zero. Thus, sharp configurations are spherical designs of nearly the greatest possible strength given the number of distances occurring in them. (Some, but not all sharp configurations are actually $2m$-designs.)

Table 1.1 lists all sharp configurations we know, together with the 600-cell, which is not sharp but to which our techniques nevertheless apply almost the same way as for sharp configurations. In the table, the columns list the dimension d of the ambient Euclidean space, then the number N of points, the largest m such that the code is a spherical m-design, the inner products other than 1 which occur between points in the code, and the name of the code, if any exists. If t denotes the largest inner product, then each of these codes is the unique (d, N, t) spherical code, except for some of those listed on the last line of the table (the isotropic subspace codes); see Appendix A for details about uniqueness. Let us describe briefly these configurations, as some of them

Table 1.1: The known sharp configurations, together with the 600-cell

d	N	t	Inner products	Name
2	N	$N-1$	$\cos(2\pi j/N)$ $(1 \leq j \leq N/2)$	N-gon
d	$N \leq d$	1	$-1/(N-1)$	simplex
d	$d+1$	2	$-1/d$	simplex
d	$2d$	3	-1, 0	cross polytope
3	12	5	-1, $\pm 1/\sqrt{5}$	icosahedron
4	120	11	$-1, \pm 1/2, 0, (\pm 1 \pm \sqrt{5})/4$	600-cell
8	240	7	$-1, \pm 1/2, 0$	E_8 roots
7	56	5	$-1, \pm 1/3$	kissing
6	27	4	$-1/2, 1/4$	kissing/Schläfli
5	16	3	$-3/5, 1/5$	kissing
24	196560	11	$-1, \pm 1/2, \pm 1/4, 0$	Leech lattice Λ_{24}
23	4600	7	$-1, \pm 1/3, 0$	kissing
22	891	5	$-1/2, -1/8, 1/4$	kissing
23	552	5	$-1, \pm 1/5$	equiangular lines
22	275	4	$-1/4, 1/6$	kissing
21	162	3	$-2/7, 1/7$	kissing
22	100	3	$-4/11, 1/11$	Higman-Sims
$q\frac{q^3+1}{q+1}$	$(q+1)(q^3+1)$	3 (4 if $q=2$)	$-1/q, 1/q^2$	isotropic subspaces (q a prime power)

are well-known mathematical objects while some other are more mysterious. The first six configurations listed in the table are the vertices of certain full-dimensional regular polytopes (specifically, those regular polytopes whose faces are simplices), together with lower-dimensional simplices. The next seven cases are derived from the E_8 root lattice in $\mathbb{R}^8$ and the Leech lattice in $\mathbb{R}^{24}$. Indeed, the 240-point and 196560-point configurations are just the systems of minimal non-zero vectors, suitably rescaled to $\mathbb{S}^{d-1}$; the others are what in sphere packing terms are called the *kissing configurations*, i.e. the points of tangency in the corresponding sphere packings. Each arrangement with the label "kissing" is the kissing configuration of the arrangement above it: each configuration yields a sphere packing in spherical geometry by centring congruent spherical caps at the points, with radius as large as possible without making their interiors overlap. The points of tangency of a given cap form a spherical code in a space of one fewer dimension. In general different spheres in a packing can have different kissing configurations, but this does not occur here because the automorphism group of each configuration acts transitively on it (See [CS99], in particular Chapter 14, for more details).

Some of the kissing configurations are interesting on their own. For example, the sharp configuration of 552 points in $\mathbb{R}^{23}$ comes from an equiangular arrangement of 276 lines in $\mathbb{R}^{23}$ described by the unique regular two-graph on 276 vertices (see Chapter 11 of [GR01]). It can also be derived from the Leech lattice Λ_{24} in the following way: choose any $w \in \Lambda_{24}$ with $|w|^2 = 6$. Then the 552 points are the vectors $v \in \Lambda_{24}$ satisfying $|v|^2 = |w - v|^2 = 4$. These points all lie on a hyperplane, but it does not pass through the origin, so subtract $w/2$ from each vector to obtain points on a sphere centred at the origin.

The *Higman-Sims* configuration of 100 points in $\mathbb{R}^{22}$ can be constructed similarly: choose w_1 and w_2 in Λ_{24} satisfying $|w_1|^2 = |w_2|^2 = 6$ and $|w_1 - w_2|^2 = 4$. Then there are 100 points $v \in \Lambda_{24}$ satisfying

$$|v|^2 = |w_1 - v|^2 = |w_2 - v|^2 = 4,$$

and they form the Higman-Sims configuration (on an affine subspace as above).

By the way, one might imitate the last two constructions by using the E_8 lattice instead of the Leech lattice and replacing the norms 6 and 4 with the smallest two norms in E_8, namely 4 and 2. This works, but it merely yields the cross polytope in $\mathbb{R}^7$ and the simplex in $\mathbb{R}^6$.

Finally, the last line describes a remarkable family of sharp configurations from [CGS78]. They are the only known sharp configurations not derived from regular polytopes, the E_8 lattice, or the Leech lattice. The parameter q must be a prime power; when $q = 2$, this arrangement is exactly the Schläfly configuration (and it is a spherical 4-design), but for $q > 2$ it is different from all the other elements in the table. Points in the configuration correspond to totally isotropic 2-dimensional subspaces of a 4-dimensional Hermitian space over $\mathbb{F}_{q^2}$, with the distances between points determined by the dimensions of the intersections of the corresponding subspaces (inner product $-1/q$ corresponds to intersection dimension 1).

By Theorem 1.50, antipodal sharp configurations are the same as antipodal tight spherical designs. Much progress has been made for the purpose of classifying such designs, see [BMV04] for more information. Here, it suffices to say that Table 1 contains all of the antipodal sharp configurations in at most 103 dimensions.

Chapter 2

Universally optimal spherical configurations

2.1 Energy minimisation

As we have said in the introduction, we are interested in sharp configurations because they turn out to be universally optimal solutions to an energy minimisation problem. More precisely, let

$$f : (0, 4] \to [0, \infty)$$

be any decreasing, continuous function. Given a finite subset $\mathcal{C}$ of the unit sphere $\mathbb{S}^{d-1}$, we define the *f-potential energy* of $\mathcal{C}$ to be

$$E_f(\mathcal{C}) = \sum_{\substack{x,y \in \mathcal{C} \\ x \neq y}} f(|x-y|^2) \tag{2.1}$$

Remark 2.1. It is important to notice that:

- since each pair x, y is counted twice in both orders, our potential energy is twice that from physics: this normalisation is absolutely equivalent and makes the formulae prettier;
- we view potentials as functions of squared distance between points, rather than of distance: this fits better to the class of functions we are going to deal with.

What are the properties we should reasonably require of f? Well, without loss of generality we can assume that f is non-negative (only distances between 0 and 2 occur on the sphere, and one can clearly add a constant to ensure non-negativity). Besides, since the force between points is repulsive, the potential must be decreasing, and it is natural to require convexity as well. The results shown here require a strongest condition, namely complete monotonicity.

Definition 2.2. A C^∞ function $f : I \to \mathbb{R}$ on an interval I is *completely monotonic* if

$$(-1)^k f^{(k)}(x) \geq 0$$

for all $k \geq 0$, and *strictly completely monotonic* if strictly inequality always holds in the interior of I.

For example, all *inverse power laws* $f(r) = r^{-s}$ with $s > 0$ are strictly completely monotonic on $(0, \infty)$; another instance is provided by *exponential laws* $f(r) = e^{-cr}$ with $c > 0$. These are by far the most important cases for our purposes.

It might seem more reasonable to use complete monotonic functions of distance, rather than squared distance, but squared distance simplifies formulas appearing later on, and it is more general than using distance: indeed, if $r \to f(r^2)$ is completely monotonic on a subinterval (a, b) of $(0, \infty)$, then f is completely monotonic on (a^2, b^2), but not vice versa.

Definition 2.3. A finite subset $\mathcal{C} \subset \mathbb{S}^{d-1}$ is *universally optimal* if it (weakly) minimises f-potential energy among all configurations of $|\mathcal{C}|$ points on $\mathbb{S}^{d-1}$ for every completely monotonic potential function f.

Now we can fully state the main theorem for universally optimal spherical configurations, namely that sharp configurations and also the 600-cell are globally universally optimal:

Theorem 2.4 (Cohn and Kumar)**.** *Let $f : (0, 4] \to \mathbb{R}$ be a completely monotonic function, and let $\mathcal{C} \subset \mathbb{S}^{d-1}$ be a sharp configuration or the vertices of a regular* 600*-cell. If $\mathcal{C}' \subset \mathbb{S}^{d-1}$ is any set satisfying $|\mathcal{C}'| = |\mathcal{C}|$, then*

$$E_f(\mathcal{C}') \geq E_f(\mathcal{C}). \tag{2.2}$$

Moreover, if f is strictly completely monotonic, then equality in (2.2) *implies that $\mathcal{C}'$ is also a sharp configuration (resp. the vertices of the* 600*-cell) and the distances between points of $\mathcal{C}'$ are the same occurring in $\mathcal{C}$. In that case, if $\mathcal{C}$ appears on Table* (1.1)*, but not on the last line, then*

$$\mathcal{C}' = A\,\mathcal{C} \text{ for some } A \in O(d),$$

i.e. $\mathcal{C}'$ and $\mathcal{C}$ are isometric.

Uniqueness does not necessarily hold if the hypothesis that f must be strictly completely monotonic is removed (consider for example a constant potential function); furthermore, the configurations from the last line in Table 1.1 are not always unique.

It is interesting, as a demonstration of the techniques used in the proof of Theorem 2.4, to prove it in the simplest possible case, namely when $|\mathcal{C}| \leq d + 1$ (in which case $\mathcal{C}$ is a simplex), while the general proof is in Section 2.6

Proof of special case. Suppose $N = |\mathcal{C}| \leq d + 1$. Then $\mathcal{C}$ is a regular simplex with inner product $-1/(N-1)$ between distinct points, so the squared Euclidean distance between distinct points is $2 + 2/(N-1) =: \delta^2$. For this special case we only require f to be decreasing and convex.

Let

$$h(x) = f(\delta^2) + f'(\delta^2)(x - \delta^2),$$

so that h is the tangent line to f at δ^2. Because f is convex, $f(x) \geq h(x)$ for all $x \in (0, 4]$, and if f is strictly convex, the equality holds if and only if $x = \delta^2$.

Now suppose that $\mathcal{C}'$ is any subset of $\mathbb{S}^{d-1}$ with $|\mathcal{C}'| = N$; then

$$E_f(\mathcal{C}') = \sum_{\substack{x,y\in\mathcal{C}'\\ x\neq y}} f(|x-y|^2) \geq \sum_{\substack{x,y\in\mathcal{C}'\\ x\neq y}} h(|x-y|^2),$$

and the right side equals

$$\sum_{\substack{x,y\in\mathcal{C}'\\ x\neq y}} f(\delta^2) + f'(\delta^2)(|x-y|^2 - \delta^2) =$$

$$= N(N-1)f(\delta^2) + f'(\delta^2) \sum_{x,y\in\mathcal{C}'} |x-y|^2 - N(N-1)f'(\delta^2)\delta^2.$$

We have

$$\begin{aligned}\sum_{x,y\in\mathcal{C}'} |x-y|^2 &= \sum_{x,y\in\mathcal{C}'} (2 - 2\langle x,y\rangle)\\ &= 2N^2 - 2\sum_{x,y\in\mathcal{C}'} \langle x,y\rangle\\ &= 2N^2 - 2\left|\sum_{x\in\mathcal{C}'} x\right|^2 \leq 2N^2,\end{aligned}$$

and since $f'(\delta^2) \leq 0$, we get

$$\begin{aligned}E_f(\mathcal{C}') &\geq N(N-1)f(\delta^2) + 2N^2 f'(\delta^2) - \delta^2 N(N-1)f'(\delta^2)\\ &= N(N-1)f(\delta^2)\\ &= \sum_{\substack{x,y\in\mathcal{C}\\ x\neq y}} f(|x-y|^2)\\ &= E_f(\mathcal{C})\end{aligned}$$

as we wanted to show. When f is strictly convex, then equality holds only if $|x-y|^2 = \delta^2$ for all $x, y \in \mathcal{C}'$ with $x \neq y$, in which case $\mathcal{C}'$ is a regular simplex. □

Remark 2.5. A useful remark, while testing whether a configuration is universally optimal, is that we can restrict ourselves to a smaller class of potential functions. Theorem 9b in [W41] implies that on each compact subinterval of $(0, 4]$, every completely monotonic function on $(0, 4]$ can be approximated uniformly by non-negative linear combinations of the functions $r \to (4-r)^k$ with $k \in \{0, 1, 2, \dots\}$. For example,

$$\frac{1}{r^s} = \sum_{k\geq 0} \binom{s+k-1}{k} \frac{(4-r)^k}{4^{k+s}}.$$

Thus, a configuration is universally optimal if and only if it is optimal for each of the potential functions $f(r) = (4-r)^k$.

Before proving the main result, we show here a negative result, namely that there are no universal optimal configurations in between the simplex and cross polytope:

Proposition 2.6. *If $d+1 < N < 2d$, then there is no N-point universally optimal configuration on $\mathbb{S}^{d-1}$.*

Proof. An optimal code of this size has the following structure, according to [B04] (see Theorem 6.2.1 and the remark following it). There are $N-d$ parwise orthogonal subspaces of $\mathbb{R}^d$ whose span is $\mathbb{R}^d$, each containing $h+1$ points of the code if its dimension is h. If the code is universally optimal, then each of these subspaces must contain a regular simplex: because of orthogonality, distances between points in different subspaces are constant, so within each subspace we must have a universally optimal code. For the same reason, every union of some of the component simplices must be universally optimal as well. Thus, without loss of generality, we can assume that $N = d+2$. We can also assume that $d \geq 4$ because the case of $d = 3$ and $N = 5$ was dealt with above in this section.

Suppose that the two regular simplices have $i+1$ and $d-i+1$ points. For the potential function

$$f(r) = (4-r)^k,$$

the energy of the configuration equals

$$i(i+1)\left(2 - \frac{2}{i}\right)^k + (d-i)(d-i+1)\left(2 - \frac{2}{d-i}\right)^k + (i+1)(d-i+1)2^{k+1}.$$

For $k = 2$ that equals

$$4d(d+1) - \frac{4d}{i(d-i)},$$

from which it follows that the potential energy is minimised exactly when $i = \lfloor d/2 \rfloor$ or $i = \lceil d/2 \rceil$. As $k \to \infty$, the energy is asymptotic to $(i+1)(d-i+1)2^{k+1}$, which is minimised exactly when $i = 1$ or $i = d-1$ (and hence not at $i = \lfloor d/2 \rfloor$ or $i = \lceil d/2 \rceil$, because $d \geq 4$). Thus, universal optimality is impossible, as we wanted to prove. □

2.2 More tools: technical interlude

Before addressing the proof of Theorem 2.4, we have to introduce some further tools.

2.2.1 Hermite interpolation

Hermite interpolation is a generalisation of well-known Lagrange interpolation in which one computes a polynomial that agrees with a given function not only at the values, but also up to a certain derivative, at some specified set of points. More precisely, suppose we are given $f \in C^\infty([a,b])$, distinct points $t_1, \ldots, t_m \in [a,b]$ and positive integers $k_1, \ldots, k_m$. Our aim is to find a polynomial p of degree strictly less than $D = k_1 + k_2 + \cdots + k_m$ such that for $1 \leq i \leq m$ and $0 \leq k < k_i$,

$$p^{(k)}(t_i) = f^{(k)}(t_i),$$

that is, p and f agree to order k_i at t_i. We immediately observe that such a polynomial always exists and is unique, for the linear map

$$\begin{aligned} \Phi : \mathbb{R}_{\leq D-1}[X] &\to \mathbb{R}^{k_1+\cdots+k_m} = \mathbb{R}^D \\ p &\mapsto (p(t_1), p'(t_1), \ldots, p^{k_1-1}(t_1), \ldots, p(t_m), \ldots, p^{k_m-1}(t_m)) \end{aligned}$$

is injective (and hence also surjective).

The following remainder formula will be a fundamental tool when dealing with spherical configurations (cfr. [D63], Theorem 3.5.1):

Lemma 2.7. *With the above notation, for each $t \in [a,b]$ there exists $\xi \in (a,b)$ such that*

$$\min(t, t_1, \dots, t_m) < \xi < \max(t, t_1, \dots, t_m) \quad \textit{and}$$
$$f(t) - f(p) = \frac{f^{(D)}(\xi)}{D!} \prod_{i=1}^{m} (t - t_i)^{k_i}.$$

Proof. For $t \in \{t_1, \dots, t_m\}$ the lemma is trivial; otherwise let

$$g(t) = \frac{f(t) - p(t)}{\prod_{i=1}^{m} (t - t_i)^{k_i}},$$

and we want to show that $g(t) = f^{(D)}(\xi)/D!$. Consider the function

$$\begin{aligned} s \mapsto f(s) - p(s) - g(t) \prod_{i=1}^{m} (s - t_i)^{k_i} \\ = f(s) - p(s) - \frac{f(t) - p(t)}{\prod_{i=1}^{m} (t - t_i)^{k_i}} \prod_{i=1}^{m} (s - t_i)^{k_i}. \end{aligned}$$

By construction, for each i it vanishes at t_i to order k_i, and it also vanishes at t, so it has $D+1$ roots in the interval

$$[\min(t, t_1, \dots, t_m), \max(t, t_1, \dots, t_m)].$$

By iterated use of Rolle's theorem, there exists ξ in the interior of this interval at which the D-th derivative vanishes, i.e.

$$f^{(D)}(\xi) - g(t) D! = 0,$$

as desired. ☐

This formula will play a crucial role later, but we also need a stronger result.

Definition 2.8. A function $f : [a,b] \to [0,\infty)$ is *absolutely monotonic* on $[a,b]$ if it is C^∞ and

$$f^{(k)}(t) \geq 0 \quad \text{for every } t \in [a,b] \text{ and } k \geq 0.$$

f is called *strictly absolutely monotonic* on an interval if it is absolutely monotonic and it and its derivatives are strictly positive on the interior of the interval.

Be careful no to confuse the two definitions of completely monotonicity and absolutely monotonicity, although they sound similar.

Proposition 2.9. *Under the hypotheses above, suppose further that f is absolutely monotonic (resp. strictly absolutely monotonic) on (a,b). Then*

$$\frac{f(t) - p(t)}{\prod_{i=1}^{m} (t - t_i)^{k_i}}$$

is also absolutely monotonic (resp. strictly absolutely monotonic) on (a,b).

Cleary, quotients such as the above are defined by continuity when $t = t_i$ for some i so that they become C^∞ functions. We underline that the fact that $t_1, \dots, t_m$ lie in $\in [a, b]$ is a crucial hypotheses.

Before proving Proposition 2.9, it is worthwile to introduce systematic notation for Hermite interpolations. Given a polynomial g with $\deg(g) \geq 1$, let $H(f, g)$ denote the polynomial of degree less than $\deg(g)$ that agrees with f at each root of g to the order of that root. Notice that if f is a polynomial, then $H(f, g)$ is just its remainder modulo g in polynomial division; in other words, if $g(t)$ vanishes to order k at $t = s$, then

$$f(t) - H(f, g)(t) = O((t - s)^k) \quad \text{for } t \to s.$$

Therefore the function $Q(f, g)$ defined by

$$Q(f, g)(t) = \frac{f(t) - H(f, g)(t)}{g(t)}$$

extends to a C^∞ function at the roots of g. Then Proposition 2.9 states that if $g(t) = \prod_{i=1}^{m} (t - t_i)^{k_i}$, then $Q(f, g)$ is absolutely monotonic.

Proof of Proposition 2.9. The proof is based on two properties of $Q(f, g)$. The first is that

$$Q(f, g_1 g_2) = Q(Q(f, g_1), g_2),$$

which follows from the uniqueness of the Hermite interpolation:

$$\begin{aligned} Q(Q(f, g_1), g_2) &= \frac{Q(f, g_1) - H(Q(f, g_1), g_2)}{g_2} \\ &= \frac{(f - H(f, g_1))/g_1 - H(Q(f, g_1), g_2)}{g_2} \\ &= \frac{f - H(f, g_1) - g_1 H(Q(f, g_1), g_2)}{g_1 g_2}, \end{aligned}$$

but $H(f, g_1 g_2)$ is the unique polynomial of degree less than $\deg(g_1) + \deg(g_2)$ such that

$$\frac{f - H(f, g_1 g_2)}{g_1 g_2}$$

extends to a C^∞ function everywhere, whence we deduce that

$$H(f, g_1 g_2) = H(f, g_1) + g_1 H(Q(f, g_1), g_2)$$

and consequently

$$Q(f, g_1 g_2) = Q(Q(f, g_1), g_2).$$

The second property is that if $g_0(t) = (t - s_0)^n$, then

$$Q(f, g_0)(s_0) = \frac{f^{(n)}(s_0)}{n!} :$$

indeed expanding into Taylor series we have

$$f(t) = \underbrace{f(s_0) + f'(s_0)(t - s_0) + \cdots + \frac{f^{(n-1)}(s_0)}{(n-1)!}(t - s_0)^{n-1}}_{H(f, g_0)} + \frac{f^{(n)}(s_0)}{n!}(t - s_0)^n + O(t - s_0)^{n+1}.$$

To prove the proposition we must show that for $n \geq 0$ and $t \in (a, b)$,

$$Q(f, g)^{(n)}(t) \geq 0.$$

When $n = 0$, that follows from Lemma 2.7, which states the existence of $\xi \in (a, b)$ (depending on t) such that

$$Q(f, g)(t) = \frac{f^{(\deg(g))}(\xi)}{\deg(g)!} \geq 0.$$

When $n > 0$, given $s_0 \in (a, b)$, define $g_0(t) = (t - s_0)^n$. Then

$$\frac{Q(f, g)^{(n)}(s_0)}{n!} = Q(Q(f, g), g_0)(s_0) = Q(f, gg_0)(s_0) \geq 0.$$

This completes the proof when f is absolutely monotonic. The case of strictly absolutely monotonicity works exactly the same way. □

Remark 2.10. It follows from continuity that Proposition 2.9 still holds when the open interval (a, b) is replaced with a half-open or closed interval.

2.2.2 Positive-definite kernels

In this section we develop further the relation between orthogonal polynomials and spherical designs, partly reviewing what has been said in the first sections of Chapter 1, and partly adding new details; in particular, we prove that Gegenbauer polynomials are orthogonal with respect to the measure $(1 - t^2)^{(d-3)/2}$.

Definition 2.11. A continuous function

$$K : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to \mathbb{R}$$

is a *positive-definite kernel* if for all k and all $x_1, \dots, x_k \in \mathbb{S}^{d-1}$, the $k \times k$ matrix whose (i, j) entry is $K(x_i, x_j)$ is positive semidefinite.

In other words, for all $t_1, \dots, t_k \in \mathbb{R}$,

$$\sum_{i,j=1}^{k} t_i t_j K(x_i, x_j) \geq 0.$$

The most important particular case is when $t_1 = \cdots = t_k = 1$: for every finite subset $\mathcal{C} \subset \mathbb{S}^{d-1}$,

$$\sum_{x,y \in \mathcal{C}} K(x, y) \geq 0.$$

Positive-definite kernels K such that $K(x, y)$ depends only on the distance $|x - y|$ between x and y are particularly important for us. There is a simple representation-theoretic construction of such kernels, which Schoenberg in [S42] proved gives all of them.

We have seen in Section 1.2 that as a unitary representation of $O(d)$, the Hilbert space $L^2(\mathbb{S}^{d-1})$ splits as a completed orthogonal direct sum of infinitely many finite-dimensional representations:

$$L^2(\mathbb{S}^{d-1}) = \widehat{\bigoplus_{l \geq 0}} \operatorname{Harm}(l),$$

where Harm(l) is the space of spherical harmonics of degree l, i.e. the restrictions to $\mathbb{S}^{d-1}$) of homogeneous polynomials on $\mathbb{R}^d$ of degree l that are in the kernel of the Euclidean Laplacian. Recall also that spherical harmonics of different degrees are orthogonal, and that every polynomial on $\mathbb{R}^d$ has the same restriction to $\mathbb{S}^{d-1}$ as some unique linear combination of spherical harmonics.

For each $l \geq 0$ and each $x \in \mathbb{S}^{d-1}$, there is a unique *reproducing kernel* $\mathrm{ev}_{l,x} \in V_l$, defined by requiring that for all $f \in V_l$,

$$\langle f, \mathrm{ev}_{l,x} \rangle = f(x).$$

(Warning: we use Hermitian forms that are conjugate linear in the second variable.) To construct $\mathrm{ev}_{l,x}$ explicitely, choose an orthonormal basis $e_{l,1}, \dots, e_{l,\dim V_l}$ of V_l and define

$$\mathrm{ev}_{l,x}(y) = \overline{e_{l,1}(x)}\, e_{l,1}(y) + \cdots + \overline{e_{l,\dim V_l}(x)}\, e_{l,\dim V_l}(y).$$

Define the function $K_l : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to \mathbb{C}$ by

$$K_l(x, y) = \langle \mathrm{ev}_{l,x}, \mathrm{ev}_{l,y} \rangle = \mathrm{ev}_{l,x}(y).$$

We have that

$$\mathrm{ev}_{l,Ax} = \mathrm{ev}_{l,x} \circ A^{-1} \quad \text{for } A \in O(d).$$

Since $O(d)$ acts distance-transitively on $\mathbb{S}^{d-1}$ (i.e., if $|x'-y'| = |x-y|$, then there is $A \in O(d)$ such that $Ax' = x$ and $Ay' = y$), we have that $K_l(x, y)$ depends only on the distance between x and y. This implies that it is real-valued, for

$$K_l(x, y) = \overline{K_l(y, x)}$$

follows directly from the definition while $K_l(x, y) = K_l(y, x)$ since $|x - y| = |y - x|$. The crucial property of K_l is that it is a positive-definite kernel:

$$\sum_{i,j=1}^{k} t_i t_j K_l(x_i, x_j) = \left| \sum_{i=1}^{k} t_i \, \mathrm{ev}_{l,x_i} \right|^2 \geq 0.$$

All convergent non-negative infinite linear combinations of these functions are still positive-definite kernels, and Schoenberg showed that those are the only continuous positive-definite kernels that depend only on the distance between points.

One can compute K_l explicitely: since $K_l(x, y)$ depends only on the distance between x and y, we can write $K_l(x, y) = C_l(\langle x, y \rangle)$ for some function C_l. To compute C_l, we use the orthogonality between spherical harmonics of different degrees: if we fix a point on the sphere and project orthogonally onto the line through the origin at that point, then the surface measure $d\sigma_d$ on the sphere projects to a constant times the measure

$$(1 - t^2)^{(d-3)/2} dt$$

on the interval $[-1, 1]$, and the orthogonality property amounts to saying that $C_0, C_1, \dots$ are orthogonal polynomials with respect to that measure, with C_i having degree i. The following calculation shows that the measure is proportional to $(1 - t^2)^{(d-3)/2} dt$: consider the spherical shell defined by

$$1 \leq x_1^2 + \cdots + x_d^2 \leq 1 + \varepsilon.$$

If we set $x_1 = t$, then the remaining coordinates satisfy

$$1 - t^2 \le x_2^2 + \cdots + x_d^2 \le 1 - t^2 + \varepsilon,$$

and the volume is proportional to

$$(1 - t^2 + \varepsilon)^{(d-1)/2} - (1 - t^2)^{(d-1)/2}.$$

Now divide by ε to normalise, then as $\varepsilon \to 0$ we find that the density of the surface measure with $x_1 = t$ is proportional to $(1 - t^2)^{(d-3)/2}$, as desired.

As we have seen in Section 1.1.1, the orthogonal polynomials obtained this way are determined up to multiplication by a positive scalar (which we can normalise with no troubles), and they are exactly the ultraspherical polynomials:

$$C_k^\lambda(t), \quad \deg C_k^\lambda = k$$

(here $\lambda = d/2-1$ because usually one prefers to write that the C_k^λ are orthogonal with respect to $(1 - t^2)$). The normalisation is chosen such that $C_0^\lambda(t) = 1$ and $C_1^\lambda(t) = 2\lambda t$.

Whenever we refer to the *ultraspherical coefficients* of a function, we mean its coefficients in terms of ultraspherical polynomials (where the parameter λ is implicit in the context). A *positive-definite function* will be a function whose ultraspherical coefficients are non-negative.

One fundamental fact about positive-definite functions is that they are close under taking products. Equivalently, the product of two ultraspherical polynomials is a non-negative linear combination of ultraspherical polynomials (for $\lambda \ge 0$). By orthogonality, proving this amounts to showing that

$$\int_{-1}^{1} C_i(t)C_j(t)C_k(t)(1 - t^2)^{(d-3)/2} dt \ge 0 \tag{2.3}$$

for all $i, j, k \ge 0$. Let μ denote the surface measure on $\mathbb{S}^{d-1}$. Then using the expansion

$$K_l(x, y) = \sum_{m=1}^{\dim V_l} \overline{e_{l,m}(x)}\, e_{l,m}(y)$$

in terms of a choice of orthonormal basis $e_{l,1}, \ldots, e_{l,\dim V_l}$ for each V_l shows that (2.3) holds if and only if

$$\sum_{a=1}^{\dim V_i} \sum_{b=1}^{\dim V_j} \sum_{c=1}^{\dim V_k} \int e_{i,a}(x)e_{j,b}(x)e_{k,c}(x)d\mu(x)\overline{e_{i,a}(y)}\,\overline{e_{j,b}(y)}\,\overline{e_{k,c}(y)} \ge 0$$

for some (equivalently, all) $y \in \mathbb{S}^{d-1}$. Integrating over y yields

$$\sum_{a=1}^{\dim V_i} \sum_{b=1}^{\dim V_j} \sum_{c=1}^{\dim V_k} \left| \int e_{i,a}(x)e_{j,b}(x)e_{k,c}(x)d\mu(x) \right|^2,$$

which is clearly non-negative.

Finally, we call a polynomial *strictly positive definite* if all its ultraspherical coefficients are strictly positive (up to its degree). The product of strictly positive-definite polynomials is strictly positive-definite; the proof rests on the fact that that in the expansion of $C_i^\lambda C_j^\lambda$, the coefficient of C_{i+j}^λ is positive (because all these polynomials have positive leading coefficients).

2.3 Use of orthogonal polynomials

The proof of Theorem 2.4 involves expansions of polynomials as non-negative linear combinations of orthogonal polynomials. In this section we prove a theorem about such expansions which we will need to find a bound from below for the energy of a point configuration.

Let μ be any Borel measure on $\mathbb{R}$ such every polynomial p is integrable with respect to μ and if p is not identically zero

$$\int p(t)^2 d\mu(t) > 0.$$

Equivalently, for all polynomials p such that $p(t) \geq 0$ for all t but p is not identically zero,

$$\int p(t) d\mu(t) > 0.$$

Let $p_0, p_1, \dots$ be the monic orthogonal polynomials for μ, with $\deg(p_i) = i$, i.e.

$$\int p_i(t) p_j(t) d\mu(t) = 0 \quad \text{for } i \neq j;$$

in particular, taking $i = 0$, we have

$$\int p_j(t) d\mu(t) = 0 \quad \text{for } j > 0.$$

We know that for each $\alpha \in \mathbb{R}$, the polynomial $p_n + \alpha p_{n-1}$ has n distinct real roots, which are interlaced with the roots of p_{n-1}. The result we need is the following one:

Theorem 2.12. *Let α be any real number, and let*

$$r_1 < r_2 < \cdots < r_n$$

be the roots of $p_n + \alpha p_{n-1}$. Then for $k < n$,

$$\prod_{i=1}^{k} (t - r_i)$$

has positive coefficients in terms of $p_0(t), p_1(t), \dots, p_k(t)$.

The section is devoted to prove this theorem, which, albeit not conceptually difficult, involves some technical details. We begin with the easy case, namely when $k = n - 1$.

Proposition 2.13. *Let α be any real number, and let $r = r_n$ be the largest root of $p_n + \alpha p_{n-1}$. Then*

$$\frac{p_n(t) + \alpha p_{n-1(t)}}{t - r}$$

has positive coefficients in terms of $p_0(t), p_1(t), \dots, p_{n-1}(t)$.

Proposition 2.13 follows from the Christoffel-Darboux formula (Proposition 1.3), but we prove it directly to illustrate the technique we will apply to the general case.

Proof. Define $c_0, \dots, c_{n-1}$ so that

$$\frac{p_n(t) + \alpha p_{n-1}(t)}{t - r} = \sum_{l=0}^{n-1} c_l p_l(t). \tag{2.4}$$

For $l \leq n-1$ it follows from orthogonality that

$$\int (p_n(t) + \alpha p_{n-1}(t)) \frac{p_l(t) - p_l(r)}{t - r} d\mu(t) = 0, \tag{2.5}$$

because the polynomial

$$\frac{p_l(t) - p_l(r)}{t - r}$$

has degree $l - 1 < n - 1$, hence it is orthogonal to both $p_n(t)$ and $p_{n-1}(t)$. Rearranging (2.5), we get

$$\int \frac{p_n(t) + \alpha p_{n-1}(t)}{t - r} p_l(t) d\mu(t) = p_l(r) \int \frac{p_n(t) + \alpha p_{n-1}(t)}{t - r} d\mu(t),$$

which by (2.4) and by orthogonality yields

$$c_l \int p_l^2(t) d\mu(t) = c_0 p_l(r) \int d\mu(t).$$

Since the roots of $p_n + \alpha p_{n-1}$ and p_{n-1} are interlaced, r is greater than the largest root of p_{n-1} and hence greater than the largest root of p_l. It follows that $p_l(r) > 0$, and thus $c_0, \dots, c_{n-1}$ have all the same sign. Comparing leading coefficients shows that $c_{n-1} = 1$, hence every coefficient must be (strictly) positive. □

Now our aim is to generalise this proof to the case of arbitrary k in Theorem 2.12. The idea is to use orthogonality with respect to a *signed measure*, because for $k < n$,

$$\prod_{i=1}^{k} (t - r_i)$$

is the monic orthogonal polynomial of degree k for the signed measure

$$(t - r_{k+1}) \cdots (t - r_n) d\mu(t),$$

assuming there is a unique such polynomial, as we will prove below. To verify that, we simply need to show that it is orthogonal to all polynomials of degree less than k, which is equivalent to the orthogonality of $p_n + \alpha p_{n-1}(t)$ to all such polynomials with respect to $d\mu(t)$. (Notice that for $k = n$ the conclusion is false unless $\alpha = 0$). More generally, we prove the following lemma:

Lemma 2.14. *Suppose ν is a signed measure that has monotonic orthogonal polynomials $q_0, q_1, \dots, q_{M+1}$, where $\deg(q_i) = i$. For $i \leq M$, if $q_i(r) \neq 0$ and $(t - r)d\nu(t)$ has a unique degree i orthogonal polynomial, then it equals*

$$\frac{q_{i+1}(t) + \alpha_i q_i(t)}{t - r},$$

where α_i is chosen so that $q_{i+1}(r) + \alpha_i q_i(r) = 0$ (in particular the above function is indeed a polynomial).

Proof. The orthogonality of this polynomial with respect to $(t-r)$ amounts to the orthogonality with respect to $d\nu(t)$ of $q_{i+1}(t)+\alpha_i q_i(t)$ to all polynomials of degree at most $i-1$. □

In order to prove Theorem 2.12, we imitate the proof of Proposition 2.13, by removing successive roots of $p_n+\alpha p_{n-1}$, but theoretically is not obvious at all that this approach works: in fact, as soon as one introduces linear factors such as $t-s$ into the measure, it is no longer a positive measure, but rather a signed measure. This technical difficulty makes a priori many of the properties of orthogonal polynomials fail, that is, orthogonal polynomials may not exist or be unique, and the roots of p_i and p_{i+1} may not be interlaced. Besides, the proof of Proposition 2.13 depends on the positivity of

$$\int p_l^2(t)d\mu(t) \text{ and } \int d\mu(t),$$

neither of which is generally positive for a signed measure.

Fortunately, the measures that actually arise in the proof will be considerably better behaved than a typical signed measure; in particular they will all have the following property for some M:

Definition 2.15. Let ν be a signed Borel measure on $\mathbb{R}$ such that all polynomials are integrable with respect to it. ν is said to be *positive definite up to degree* M if for all polynomials f such that $\deg(f)\geq M$

$$\int f(t)^2 d\nu \geq 0,$$

with equality if and only if f is identically zero.

Such a ν is therefore a signed measure which behaves positively to a certain extent; the advantage of dealing with this kind of measures is that many of the usual properties still hold for orthogonal polynomials of degrees up to $M+1$. More precisely, we have the following

Lemma 2.16. *Let ν be positive up to degree M. Then there exist unique monic polynomials $q_0, q_1, \ldots, q_{M+1}$ such that $\deg(q_i)=i$ for each i and*

$$\int q_i(t)q_j(t)d\nu(t) = 0.$$

for $i\neq j$. For each i, q_i has i distinct real roots, and the roots of q_i and q_{i-1} are interlaced.

As we see, this is the analogue of Propositions 1.6 and 1.7, and indeed a similar proof can be implemented; here we use instead a proof of Simon [S05]:

Proof. The proof consists in finding the orthogonal polynomials for ν by applying Gram-Schmidt orthogonalisation technique to the basis $1, t, \ldots, t^{M+1}$:

$$q_i(t) = t^i - \sum_{j=0}^{i-1} q_j(t)\frac{\int s^j q_j(s)d\nu(s)}{\int q_j(s)^2 d\nu(s)}$$

which makes sense for $i\leq M+1$ because the norm of q_j is the denominator is always non-zero. These polynomials are unique, for the quotiens of integrals which appear as coefficients in such an expansion are forced by the condition of orthogonality.

The next step is to prove the three-term recurrence relation. The polynomial $q_i(t) - tq_{i-1}(t)$ is orthogonal to all polynomials of degree less than $i-2$, and hence we can write

$$q_i(t) = (t + a_i)q_{i-1}(t) + b_i q_{i-2}(t)$$

for some constants a_i and b_i. Multiplying by q_{i-2} and integrating yields

$$b_i \int q_{i-2}(t)^2 d\nu(t) = -\int q_{i-1}(t) t q_{i-2}(t) d\nu(t),$$

by orthogonality. The polynomials $tq_{i-2}(t)$ and $q_{i-1}(t)$ differ by a polynomial of degree at most $i-2$, hence

$$\int q_{i-1}(t) t q_{i-2}(t) d\nu(t) = \int q_{i-1}^2(t);$$

by the two last equations we deduce that $b_i < 0$, which we will use to conclude the proof.

We now prove by induction that the roots of q_i and q_{i-1} are interlaced. The base case of $i = 1$ is trivial. For the induction step, suppose the roots of q_{i-1} and q_{i-2} are interlaced; for each root r of q_{i-1}, we have

$$q_i(r) = b_i q_{i-2}(r),$$

by the three-term recurrence relation. By hypothesis, q_{i-2} alternates in sign at the roots of q_{i-1}. Since b_i is negative, q_i and q_{i-2} have opposite signs at the roots of q_{i-1}. That implies by continuity that $q_i(t)$ has a root between each pair of consecutive roots of q_{i-1}. Because $q_i(t)$ and $q_{i-2}(t)$ have the same sign when $|t|$ is sufficiently large, q_i must also have a root greater than every root of q_{i-1} and a root less than every root of q_{i-1}. All i roots of q_i are now accounted for, so all the roots of q_i are real and interlaced with those of q_{i-1}. Now the proof is complete. □

Now we need to prove this minor variant of Gauss-Jacobi quadrature to understand the signed measure that appear in our proof of 2.12:

Lemma 2.17. *Let α be any real number, and let*

$$r_1 < r_2 < \cdots < r_n$$

be the roots of $p_n + \alpha p_{n-1}$. Then there are positive numbers $\lambda_1, \ldots, \lambda_n$ such that for every polynomial f of degree at most $2n-2$

$$\int f(t) d\mu(t) = \sum_{i=1}^{n} \lambda_i f(r_i). \tag{2.6}$$

Proof. It is easy to see that for $\deg(f) < n$ there exist coefficients $\lambda_1, \ldots, \lambda_n$ such that (2.6) holds, because a polynomial of degree less than n is completely determined by its values at $r_1, \ldots, r_n$ and the map taking these values to the integral is linear and injective.

For $\deg(f) \leq 2n-2$, do Euclidean division and write

$$f = (p_n + \alpha p_{n-1})g + h$$

with $\deg(g) \leq n-2$ and $\deg(h) < n$. By orthogonality,

$$\begin{aligned}\int f(t)d\mu(t) &= \int p_n(t)g(t)d\mu(t) + \alpha \int p_{n-1}(t)g(t)d\mu(t) + \int h(t)d\mu(t) \\ &= \int h(t)d\mu(t),\end{aligned}$$

and $f(r_i) = h(r_i)$ for each i because $p_n(r_i) + \alpha p_{n-1}(r_i) = 0$ by definition. It follows that

$$\int f(t)d\mu(t) = \sum_{i=1}^{n} \lambda_i f(r_i)$$

holds whenever $\deg(f) \leq 2n-2$. What remains to prove is positivity of the coefficients. For fixed i, let

$$f(t) = \prod_{j \neq i} (t - r_j)^2.$$

Then

$$\int f(t)d\mu(t) = \sum_{i=1}^{n} \lambda_i f(r_i) = \lambda_i f(r_i)^2$$

whence it follows that $\lambda_i > 0$. □

Let $r_1 < \cdots < r_n$ be the roots of $p_n + \alpha p_{n-1}$, and for $0 \leq j \leq n$ define the measure μ_j by

$$d\mu_j(t) = \prod_{i=0}^{j-1} (r_{n-i} - t)d\mu(t)$$

(of course $\mu_0 = \mu$).

Lemma 2.18. *For $0 \leq j \leq n-1$, the measure μ_j is positive definite up to degree $n-j-1$.*

In other words, more factors we add, less positive definite the measure μ_j is.

Proof. If $\deg(f) \leq n - 1 - j/2$, then by Lemma 2.17,

$$\int f(t)^2 \prod_{i=0}^{j-1} (r_{n-i} - t)d\mu(t) = \sum_{i=1}^{n} \lambda_i f(r_i)^2 \prod_{l=0}^{j-1} (r_{n-l} - r_i) \geq 0;$$

equality holds if and only if f vanishes at $r_i, \ldots, r_{n-j}$, which is impossible for a polynomial of degree at most $n-j-1$ unless it vanishes identically. □

Let $q_{j,i}$ be the monic orthogonal polynomial of degree i for μ_j. (Note that $q_{0,i} = p_i$.) When $i = n-j$, the polynomial $q_{j,i}$ is simpler, for we have

$$q_{j,n-j}(t) = (t - r_1) \cdots (t - r_{n-j}),$$

as pointed out in Lemma 2.14. Hence for $i < n-j$ the largest root of $q_{j,i}$ is less than r_{n-j}, being the roots interlaced.

Equivalently, for $i \le n-j$, the largest root of $q_{j-1,i}$ is less than r_{n-j+1}, so $q_{j-1,i}(r_{n-j+1}) \ne 0$. Hence Lemma 2.14 implies that for $i \le n-j$, there are constants $\alpha_{j,i}$ such that

$$q_{j,i}(t) = \frac{q_{j-1,i-1}(t) + \alpha_{j,i} q_{j-1,i}(t)}{t - r_{n-j+1}}.$$

Lemma 2.19. *For $i \le j \le n$ and $i \le n-j$, the polynomial $q_{i,j}$ is a positive linear combination*

$$q_{i,j}(t) = \sum_{l=0}^{i} c_l q_{j-1,l}(t)$$

of the polynomials $q_{j-1,0}, \dots, q_{j-1,i}$.

Proof. Define $c_0, \dots, c_i$ so that

$$q_{j,i}(t) = \sum_{l=0}^{i} c_l q_{j-1,l}(t).$$

We argue in the same way as in the proof of Proposition 2.13. For $l \le i$, we have that

$$\int (q_{j-1,i+1}(t) + \alpha_{j,i} q_{j-1,i}(t)) \frac{q_{j-1,l}(t) - q_{j-1,l}(r_{n-j+1})}{t - r_{n-j+1}} d\mu_{j-1}(t) = 0 \qquad (2.7)$$

by orthogonality, because

$$\frac{q_{j-1,l}(t) - q_{j-1,l}(r_{n-j+1})}{t - r_{n-j+1}} d\mu_{j-1}(t)$$

is a polynomial of degree $l-1$, which is less than i. Now from

$$q_{j,i}(t) = \frac{q_{j-1,i+1}(t) + \alpha_{j,i} q_{j-1,i}(t)}{t - r_{n-j+1}} \qquad (2.8)$$

and (2.7) it follows that

$$\int q_{i,j}(t) q_{j-1,l}(t) d\mu_{j-1}(t) = q_{j-1,l}(r_{n-j+1}) \int q_{j,i}(t) d\mu_{j-1}(t).$$

Thus,

$$c_l \int q_{j-1,l}^2(t) d\mu_{j-1}(t) = c_0 q_{j-1,l}(r_{n-j+1}) \int d\mu_{j-1}(t).$$

Since $l \le i \le n-j$, both integrals are positive by Lemma 2.18. The largest root of $q_{j-1,l}$ is less than r_{n-j+1}, so

$$q_{j-1,l}(r_{n-j+1}) > 0.$$

Thus, $c_0, \dots, c_i$ all have the same sign, which is positive because $c_i = 1$. □

Now Theorem 2.12 follows from applying Lemma 2.19 repeatedly, starting with $q_{n-k,k}$.

2.4 Linear programming bounds

Theorem 2.4 is deduced from the following proposition, which provides a lower bound for the f-energy of a finite set of points on the sphere through choosing an auxiliary polynomial h:

Proposition 2.20. *Let $f : (0, 4] \to \mathbb{R}$ be any function. Suppose $h : [-1, 1] \to \mathbb{R}$ is a polynomial such that*

$$h(t) \leq f(2 - 2t)$$

for all $t \in [-1, 1)$, and suppose there are non-negative coefficients $\alpha_0, \ldots, \alpha_d$ such that h has the expansion

$$h(t) = \sum_{i=0}^{d} \alpha_i C_i^{d/2-1}(t)$$

in terms of ultraspherical polynomials. Then for every set $\mathcal{C}$ of N points on $\mathbb{S}^{d-1}$, the f-energy satisfies

$$E_f(\mathcal{C}) \geq N^2 \alpha_0 - N h(1). \tag{2.9}$$

Proof. We have by assumption

$$\sum_{\substack{x,y \in \mathcal{C} \\ x \neq y}} f(|x-y|^2) \geq \sum_{\substack{x,y \in \mathcal{C} \\ x \neq y}} h(\langle x, y \rangle),$$

for $|x-y|^2 = 2 - 2\langle x, y \rangle$. On the other hand,

$$\begin{aligned}\sum_{\substack{x,y \in \mathcal{C} \\ x \neq y}} h(\langle x, y \rangle) &= \sum_{x,y \in \mathcal{C}} h(\langle x, y \rangle) - N h(1) \\ &= \sum_{i=0}^{d} \alpha_i \sum_{x,y \in \mathcal{C}} C_i^{d/2-1}(\langle x, y \rangle) - N h(1).\end{aligned}$$

Since $C_i^{d/2-1}$ is a positive-definite kernel, as we saw in 2.2.2,

$$\sum_{x,y \in \mathcal{C}} C_i^{d/2-1}(\langle x, y \rangle) \geq 0,$$

whence we deduce, as $C_0^{d/2-1} = 1$, that

$$\sum_{\substack{x,y \in \mathcal{C} \\ x \neq y}} h(\langle x, y \rangle) \geq \alpha_0 \sum_{x,y \in \mathcal{C}} C_0^{d/2-1}(\langle x, y \rangle) - N h(1) = N^2 \alpha_0 - N h(1).$$

□

Remark 2.21. The above bound given by an auxiliary polynomial h is sharp for a configuration $\mathcal{C}$ and potential function f if and only if two conditions hold:

i) $h(t) = f(2 - 2t)$ at for every inner product t between distinct points of $\mathcal{C}$;

ii) whenever the ultraspherical coefficient α_i is positive with $i > 0$, we must have
$$\sum_{x,y\in\mathcal{C}} C_i^{d/2-1}(\langle x, y\rangle) = 0.$$

In particular, if h is strictly positive definite, $\mathcal{C}$ must be a spherical $\deg(h)$-design, by Theorem 1.32.

This proposition is a generalisation of the linear programming bounds for spherical codes, due independently to Kabatiansky and Levenshtein in [KL78] and Delsarte, Goethals and Seidel in [DGS77] (the topic is also developed in Chapter 9 of [CS99]). One can derive those bounds for spherical codes with minimal angle θ from proposition 2.20 by setting

$$f(2-2t) = \begin{cases} \infty \text{ if } t > \cos\theta, \text{ and} \\ 0 \text{ otherwise.} \end{cases}$$

(of course f takes values in $\mathbb{R} \cup \infty$, but this is not a problem.) The f-potential energy is thus 0 for a spherical code with minimal angle at least θ and ∞ otherwise; then Proposition 2.20 implies that no such code can exist if $N > h(1)/\alpha_0$.

Choosing the optimal function h amounts to solving an infinite-dimensional linear programming problem: we have that the potential energy is a linear functional of h, and the only restrictions we make on h are the linear constraints on its values and ultraspherical coefficients. However, it is not difficult to approximate the optimal h numerically, by solving a finite-dimensional linear programming problem in which one imposes the constraint $h(t) \leq f(2-2t)$ for only finitely many t's.

The bound is usually not sharp (even if it is often quite close), but in the case of sharp configurations, for every completely monotonic potential function there does exist an auxiliary function that proves a sharp bound, as we show in Section 2.6.

2.5 Choosing auxiliary functions

We describe here an explicit choice for the auxiliary function h in Proposition 2.20; although we will not require this function later, it provides an concrete way to apply Proposition 2.20 and the techniques employed here will be important in the proof of Theorem 2.4.

Let $f : (0, 4] \to \mathbb{R}$ be completely monotonic: from the proof of Proposition 2.20 we know that it is more convenient to work with $a(t) = f(2-2t)$, as $|x-y|^2 = 2-2\langle x, y\rangle$. The function a is absolutely monotonic on $[-1, 1)$ because f is completely monotonic on $(0, 4]$, and it is strictly absolutely monotonic if and only if f is strictly completely monotonic.

To construct h, we require three inputs:

1) the dimension $d-1$ of $\mathbb{S}^{d-1}$;

2) a natural number $m \geq 1$, and

3) a real number $\alpha \geq 0$.

Let

$$t_1 < \cdots < t_m$$

be the roots of the polynomial $C_m^{d/2-1} + \alpha C_{m-1}^{d/2-1}$. We require that $t_1 \geq -1$ and thus $\{t_1, \ldots, t_m\} \subset [-1, 1)$; by Theorem 3.3.4 in [Sz75], that amounts to

$$\alpha \leq -C_m^{d/2-1}/C_{m-1}^{d/2-1}$$

(which is positive because $C_i^{d/2}$ has sign $(-1)^i$).

Let $h(t)$ be the Hermite interpolating polynomial that coincides with $a(t)$ up to order 2 at each t_i, i.e. $h(t_i) = a(t_i)$ and $h'(t_i) = a'(t_i)$.

Lemma 2.22. *For all* $t \in [-1, 1)$,

$$h(t) \leq a(t).$$

Proof. By Lemma 2.7, there exists a point ξ such that

$$\min(t, t_1, \ldots, t_m) < \xi < \max(t, t_1, \ldots, t_m)$$

and

$$a(t) - h(t) = \frac{a^{(2m)}(\xi)}{(2m)!} \prod_{i=1}^{m} (t - t_i)^2.$$

The right side is non-negative, hence $a(t) \geq h(t)$. □

Before we can apply Proposition 2.20, we have to show that h is positive definite, and that it more subtle. Let

$$F(t) = C_m^{d/2-1}(t) + \alpha\, C_{m-1}^{d/2-1}(t) = \prod_{i=1}^{m} (t - t_i),$$

then in our notation $h = H(a, F^2)$. We will show that F^2 has a stronger property called conductivity:

Definition 2.23. A non-constant polynomial g with all its roots in $[-1, 1)$ is said to be *conductive* if for all absolutely monotonic functions a on $[-1, 1)$, $H(a, g)$ is positive definite. It is *strictly conductive* if it is conductive and for all strictly absolutely monotonic a, $H(a, g)$ is strictly positive definite of degree $\deg(g) - 1$.

Lemma 2.24. *(i) If g_1 and g_2 are conductive and g_1 is positive definite, then $g_1 g_2$ is conductive.*

(ii) If g_1 is conductive and strictly positive definite and g_2 is strictly conductive, then $g_1 g_2$ is strictly conductive.

Proof. We know from the proof of Proposition 2.9 that for every absolutely monotonic function a on $[-1, 1)$,

$$H(a, g_1 g_2) = H(a, g_1) + g_1 H(Q(a, g_1), g_2).$$

The lemma now follows from Proposition 2.9 and the fact that the positive-definite (or strictly positive-definite) functions are closed under taking (sums and) products. □

Now for $r \in [-1, 1)$, let ℓ_r denote the linear polynomial $\ell_r(t) = t - r$. Clearly ℓ_r is conductive, for $H(a, \ell_r) = a(r) \geq 0$, and even strictly conductive if $r \neq -1$. Lemma 2.24 implies that if g is conductive and positive definite, then $g\,\ell_r$ is conductive.

Consider the partial products

$$\prod_{i=1}^{j}(t - t_i), \quad j \leq m.$$

By Theorem 2.12 they are strictly positive definite for $j < m$, and positive definite for $j = m$ because $F(t) = C_m^{d/2-1}(t) + \alpha C_{m-1}^{d/2-1}(t)$ with $\alpha \geq 0$. Then by Lemma 2.24 and by what we have just said, each product is conductive, hence also F and still by Lemma 2.24, its square F^2 is conductive as well. As $h = H(a, F^2)$, we conclude that h is positive definite, as desired.

Remark 2.25. These auxiliary polynomials are seldom optimal, as pointed out in [CK07]; however, they provide a reasonably good bound, in view of the simplicity of their construction.

Remark 2.26. One can generalise the construction from this section in the following way: let $p_0, p_1, \ldots$ be *any* family of orthogonal polynomials such that each is positive definite. Given m and α, choose $t_1, \ldots, t_m$ to be the roots of $p_m + \alpha p_{m-1}$. The construction of the correspondent polymonial h and the proof are essentially the same as before. In fact, the proof of Theorem 2.4 will be based on this approach.

2.6 Proof of Theorem 2.4

Let $f : (0, 4] \to \mathbb{R}$ be our completely monotonic function, define $a(t) = f(2-2t)$ as in Section 2.4, and let $\mathcal{C} \subset \mathbb{S}^{d-1}$ be a sharp configuration with $|\mathcal{C}| = N$. To prove Theorem 2.4, we shall construct an auxiliary polynomial h that satisfies the hypotheses of Proposition 2.20 and proves a sharp bound. The case of the 600-cell needs a particular treatment, and shall be dealt with in section 2.7.

Call $t_1, \ldots, t_m$ the possible inner products between distinct points in $\mathcal{C}$, ordered so that

$$-1 \leq t_1 < \cdots < t_m < 1.$$

Finally, let $h(t)$ be the Hermite interpolating polynomial that agrees with $a(t)$ to order 2 at each t_i, i.e. $h = H(a, F^2)$, where $F(t) = (t - t_1) \cdots (t - t_m)$.

Remark 2.27. If $t_1 = -1$, it might seem more natural to interpolate only to first order there: indeed the purpose of second-order interpolation is to avoid sign changes in $h(t) - a(t)$ when $t = t_i$, and that is clearly not a concern when $t = -1$. In fact

Lemma 2.28. *For all* $t \in [-1, 1)$*,*

$$h(t) \leq a(t).$$

Proof. Identical to that of Lemma 2.22. □

Thus, the first hypothesis of Proposition 2.20 is satisfied, and what remains to show is that h is a positive-definite function and that the bound is sharp to have universal optimality. (The bound deived from this function h is not sharp for the 600-cell, which is why that case must be treated separately).

The sharpness of the bound follows from the fact that $\mathcal{C}$, being a sharp configuration, is a spherical $\deg(h)$-design. Thus,

$$\sum_{x,y\in\mathcal{C}} C_i^{d/2-1}(\langle x,y\rangle) = 0$$

whenever $0 < i \le \deg(h)$, and since h agrees with a at the inner products $t_1, \dots, t_m$ from $\mathcal{C}$, the conditions for a sharp bound we listed in Remark 2.21 are satisfied.

The proof that h is positive definite is analogous to the one in Section 2.5, but it involves more elaborate machinery. We will do it by showing that F^2 is strictly conductive, which will also allow us to deduce uniqueness.

Lemma 2.29. *The function F is strictly positive definite.*

Proof. The leading coefficient of F (in the usual t^i expansion) is 1, which implies that its leading ultraspherical coefficient is positive. For the others, apply orthogonality to see that the i-th ultraspherical coefficient of F equals a positive constant (depending on i) times

$$\int_{\mathbb{S}^{d-1}} F(\langle x,y\rangle) C_i^{d/2-1}(\langle x,y\rangle) d\sigma(x),$$

where y is an arbitrary point on $\mathbb{S}^{d-1}$ and $d\sigma(x)$ denotes the surface measure on $\mathbb{S}^{d-1}$.

Now choose $y \in \mathcal{C}$: as the leading ultraspherical coefficient of F is positive, we can take $i < \deg(F)$. Thus, $\deg(F) + i \le 2\deg(F) - 1$, and since $\mathcal{C}$ is a spherical $(2\deg(F) - 1)$-design, it follows that the integral above equals a positive constant times

$$\sum_{x\in\mathcal{C}} F(\langle x,y\rangle) C_i^{d/2-1}(\langle x,y\rangle) = F(1) C_i^{d/2-1}(1),$$

since by the construction of F each term of the sum vanishes except for $x = y$. Both factors are positive, as desired. □

In order to deal with the partial products

$$\prod_{i=1}^{j} (t - t_i),$$

we must express F in terms of orthogonal polynomials. Recall that the ultraspherical polynomials $C_i^{d/2-1}$ are orthogonal with respect to the measure

$$d\mu = (1 - t^2)^{(d-3)/2} dt$$

on $[-1, 1]$. Let $p_0, p_1, \dots$ denote the monic orthogonal polynomials with respect to $(1-t)d\mu(t)$. These polynomials are a special case of Jacobi polynomials, but we will require only on fact about them: they are non-negative linear combinations of the ultraspherical polynomials $C_i^{d/2-1}$. This follows from Lemma 2.14 and Proposition 2.13.

Lemma 2.30. *There exists a constant* α *such that* $F = p_m + \alpha p_{m-1}$.

Proof. We simply need to show that F is orthogonal to al polynomials of degree at most $m-2$ with respect to the measure $(1-t)d\mu(t)$, and this is equivalent to showing that $(1-t)F(t)$ is orthogonal to all such polynomials with respect to $d\mu(t)$. Let then p be any polynomial of degree at most $m-2$. Since $\mathcal{C}$ is a sharp configuration, it is a spherical $(2m-1)$-design. It follows as in the previous proof that

$$\int(1-t)F(t)p(t)d\mu(t)$$

equals a positive linear combination of

$$(1-t_1)F(t_1)p(t_1), \dots, (1-t_m)F(t_m)p(t_m), (1-1)F(1)p(1).$$

Each of these vanishes because F vanishes at $t_1, \dots, t_m$. Therefore,

$$\int F(t)p(t)(1-t)d\mu(t) = 0$$

as desired. □

Combining Lemma 2.30 with Theorem 2.12 shows that for $j < m$ the polynomial

$$\prod_{i_1}^{j}(t-t_i)$$

is strictly positive definite, and the case $j = m$ is given by Lemma 2.29; now to conclude that F and F^2 are conductive it suffices to follow the argument in Section 2.5, using Lemma 2.24 iteratedly.

With the above Lemmas, we have eventually shown that $h = H(a, F^2)$ is positive definite, which was what we wanted to use the (sharp) bound given by Proposition 2.20: *therefore we have proved the universal optimality of sharp configurations.*

To prove the additional uniqueness results when f is strictly completely monotonic, we use the following lemma:

Lemma 2.31. *If* a *satisfies* $a^{(k)}(t) > 0$ *for all* $k \geq 0$ *and* $t \in (-1, 1)$ *(i.e.* a *is strictly absolutely monotonic), then* $a(t) - h(t)$ *has at most* $\deg(h) + 1$ *roots in* $[-1, 1)$*, taking into account multiplicities.*

Proof. By Rolle's theorem, $a(t) - h(t)$ has at most one more root than $a'(t) - h'(t)$. Repeated differentiation reduces to the case in which $\deg(h) = 0$, which is trivial: if $h = C$ constant, then $a(t) - C$ has at most one root, for a is strictly completely monotonic. □

Conclusion. Thus, counting multiplicities, the only roots of $a(t)-h(t)$ in $(-1, 1]$ are at $t = t_i$ for some i; then from Remark 2.21 it follows that if $\mathcal{C}'$ is another potential energy minimum with $|\mathcal{C}'| = |\mathcal{C}|$, then the bound of Proposition 2.20 being again sharp, all inner products between distinct points of $\mathcal{C}'$ occur among $t_1, \dots, t_m$. Therefore we have that $\mathcal{C}'$ is a spherical code with the same parameters as $\mathcal{C}$, and each sharp configuration listed in Table 1.1 except on the last line is known to be the *unique* spherical code with its parameters, of course up to orthogonal transformations. See Appendix A for details.

Even when the spherical code is not unique, we can still conclude from the fact that a is strictly absolute monotonic that $\mathcal{C}'$ must be sharp. The key observation is that F^2 is strictly conductive (by 2.29, 2.30 and 2.24), except in the trivial case when $\mathcal{C}$ consists of two antipodal points. This implies that h is a strictly positive-definite polynomial of degree $2m-1$. Then the sharpness of the bound in Proposition 2.20 implies that $\mathcal{C}$ must be a spherical $\deg(h)$-design (by Theorem 1.32), hence by definition a sharp configuration. Furthermore, each of $t_1, \dots, t_m$ must occur as an inner product in $\mathcal{C}'$, from switching the role of $\mathcal{C}$ and $\mathcal{C}'$. □

2.7 The 600-cell

The final configuration of points is given by the vertices of the regular 600-cell. The construction given in the previous section does not work in this case, and overall the 600-cell appears to be intrinsically more complicated than the sharp configurations. The fundamental problem is that it is only a spherical 11-design, but the polynomial h constructed as above would have degree 15 (or 14 if we use the alternate construction for antipodal configurations). Recall that being a spherical $\deg(h)$-design was crucial to have a sharp bound: in fact, h does turn out to be a positive-definite function also in this case, but it proves a suboptimal bound.

Fortunately, what saves the proof is that although the 600-cell is not a spherical 12-design, all spherical harmonics of degrees from 13 to 19 do indeed sum to 0 over it. The degree 12 spherical harmonic is the only problem, and it can be solved by requiring that the 12th ultraspherical coefficient of h vanishes. The fact that spherical harmonics of degree 13 through 19 do sum to 0 over the 600-cell can be checked using the distance distribution from Table 2.1, which tells for each vertex how many others have a given inner product with it.

For the 600-cell, we have $m = 8$ and $\{t_1, \dots, t_m\} = \{-1, 0, \pm 1/2, (\pm 1 \pm \sqrt{5})/4\}$; we order the inner products so that $t_1 < \cdots < t_8$, that is,

$$
\begin{array}{llll}
t_1 = -1, & t_2 = (-1-\sqrt{5})/4, & t_3 = -1/2, & t_4 = (1-\sqrt{5})/4, \\
t_5 = 0, & t_6 = (-1+\sqrt{5})/4, & t_7 = 1/2, & t_8 = (1+\sqrt{5})/4.
\end{array}
$$

Let $h(t)$ be the unique polynomial of degree at most 17 such that $h(t_i) = a(t_i)$ for $1 \le i \le 8$, $h'(t_i) = a'(t_i)$ for $2 \le i \le 8$, and $\alpha_{11} = \alpha_{12} = \alpha_{13} = 0$, where α_i denotes the i-th ultraspherical coefficient of h. Notice that we do *not* require that $h'(-1) = a'(-1)$.

If $h(t) \le a(t)$ for all t and h is positive definite, then it proves a sharp bound (as said above, because $\alpha_{12} = 0$). We are going to prove that these two conditions hold, although no simple reason is known why it should happen; the computations that follow can be done performed on a computer algebra sysem, and they use exact arithmetic in $\mathbb{Q}(\sqrt{5})$.

2.7.1 Proof that h is positive definite

We want to show that $h(t)$ is a non-negative linear combination

$$h(t) = \sum_{i=0}^{17} \alpha_i C_i^1(t)$$

Inner product	Count
± 1	1
$(\pm 1 \pm \sqrt{5})/4$	12
$\pm 1/2$	20
0	30

Table 2.1: The distance distribution of the 600-cell

of the ultraspherical polynomials $C_i^1(t)$ (indeed, here $d/2 - 1 = 4/2 - 1 = 1$). Each ultraspherical coefficient of $h(t)$ is a linear function of $a(t_i)$ and $a'(t_i)$ for $1 \leq i \leq m$. In other words,

$$\begin{aligned}\alpha_i &= \alpha_i(a(t_1), \ldots, a(t_8), a'(t_1), \ldots, a'(t_8)) \\ &= \sum_{j=1}^{8} u_j\, a(t_j) + \sum_{j=1}^{8} v_j a'(t_j).\end{aligned}$$

As we have explained in Remark 2.5, it suffices to consider the potential functions

$$f(r) = (4 - r)^k, \quad k \in \{0, 1, 2, \ldots, \};$$

then we have

$$a(t) = f(2 - 2t) = (4 - (2 - 2t))^k = 2^k(1 + t)^k,$$

and up to rescaling, that amounts to taking $a(t) = (1 + t)^k$, with $a'(t) = k(1 + k)^{k-1}$. Our linear combination thus becomes

$$\sum_{j=1}^{8} (u_j(1 + t_j)^k + v_j k(1 + t_j)^{k-1}). \tag{2.10}$$

If $v_8 > 0$, then the last expression is positive for all sufficiently big k; to prove that it is non-negative for all k, we calculate a bound l such that (2.10) is guaranteed to be positive for all $k \geq l$ and then check non-negativity for $0 \leq h < l$.

Let then

$$\chi(x) = \begin{cases} x & \text{if } x \leq 0 \\ 0 & \text{if } x > 0. \end{cases}$$

If we choose l so that

$$\sum_{j=1}^{8} (\chi(u_j)(1 + t_j)^l + \chi(v_j) l (1 + t_j)^{l-1}) + v_8 l (1 + t_8)^{l-1} \geq 0, \tag{2.11}$$

then

$$\sum_{j=1}^{8} (u_j(1 + t_j)^k + v_j k(1 + t_j)^{k-1}) \geq 0$$

for all $k \geq l$, i.e., once the asymptotically dominant term becomes bigger than all the negative terms, it continues to do so forever, because whenever k increases, the dominant term increases by a larger factor than any other term does.

To prove that h is positive definite, one deals with eighteen cases, one for each ultraspherical coefficient of h. In each case, one computes the coefficients

$$u_1, \dots, u_8, v_1, \dots, v_8$$

explicitely (they are in $\mathbb{Q}(\sqrt{5})$). Then one checks that v_8 *is* positive, and that (2.11) holds with $l = 32$. Finally, one checks that the ultraspherical coefficient is non-negative for $k \in \{0, 1, \dots, 31\}$. These calculations have been done by Conway and Cumar using a computer algebra system.

2.7.2 Proof that $h(t) \leq a(t)$

The simple proof of the inequality $h(t) \leq a(t)$ we have given in the case of the sharp configurations no longer holds for the 600-cell. Here, we will use Proposition 2.9. Let

$$F(t) = (t+1)\prod_{i=2}^{m}(t+t_i)^2,$$

and let $\tilde{h}$ be the usual Hermite interpolation $H(a, F)$ of a (without requiring any ultraspherical coefficients to vanish). By Proposition 2.9,

$$\frac{a(t) - \tilde{h}(t)}{F(t)} = Q(a, F)(t)$$

is absolutely monotonic on $[-1, 1)$ (cfr. the remark at the end of 2.9). Let $q(t)$ be the quadratic Taylor polynomial for this quotient around $t = -1$. Then it follows from absolute monotonicity that

$$\frac{a(t) - \tilde{h}(t)}{F(t)} \geq q(t)$$

for all $t \in [-1, 1)$. Thus,

$$\frac{a(t) - h(t)}{F(t)} \geq q(t) + \frac{\tilde{h}(t) - h(t)}{F(t)}.$$

The right side of the inequality is a quadratic polynomial. If we verify that it is nonnegative over $[-1, 1)$, then $a(t) \geq h(t)$ over that interval, because $F(t) \geq 0$. To check this, it suffices to check that it is non-negative at $t = \pm 1$ and has non-positive leading coefficient. Each of these computations amounts to verifying that a certain explicit linear combination of $a(t_1), \dots, a(t_8), a'(t_1), \dots, a'(t_8)$, $a^{(2)}(-1)$ and $a^{(3)}(-1)$ is non-negative. This can be proved using the method from the previous subsection, with $l = 36$.

2.7.3 Proof of uniqueness

Finally, we must prove uniqueness when the potential function f is strictly completely monotonic, so that a is strictly absolutely monotonic. In that case, again by Proposition 2.9,

$$\frac{a(t) - \tilde{h}(t)}{F(t)}$$

is strictly absolutely monotonic on $(-1, 1)$, which implies that

$$\frac{a(t) - \tilde{h(t)}}{F(t)} > q(t)$$

for $t \in (-1, 1)$. Thus, $a(t) - h(t)$ has roots only at $t = t_i$ for some i. Uniqueness follows, because the vertices of the regular 600-cell are the only $(4, 120, (1 + \sqrt{5})/4)$ spherical code, as proved in [B78].

Chapter 3

Optimality in the Euclidean space

3.1 Periodic point configurations

The question of universally optimality can be posed in the same terms also in more general settings than a finite number of points on $\mathbb{S}^{d-1}$: for instance, definition (2.1) makes sense for any finite set in $\mathbb{R}^d$. However, if we want to deal with infinite and possibly unbounded discrete sets in $\mathbb{R}^d$, then the definition of potential energy could rise convergence problems in pathological cases, that is why we shall confine ourselves to periodic point configurations.

Definition 3.1. A discrete set $\mathcal{C} \subset \mathbb{R}^d$ is a *periodic configuration* if it is a union of finitely many translates of one given full-rank lattice of $\mathbb{R}^d$. More precisely, $\mathcal{C}$ is a N-periodic configuration if there exist a (full-rank Euclidean) lattice $\Lambda \subset \mathbb{R}^d$ and vectors $t_1, \ldots, t_N$ in $\mathbb{R}^d$, with $t_i - t_j \notin \Lambda$ for $i \neq j$, such that

$$\mathcal{C} = \bigcup_{i=1}^{N} (t_i + \Lambda).$$

The *point density* δ_p of such a $\mathcal{C}$ is the number of points per unit volume*, and if $\mathcal{C}$ is represented as an N-periodic configuration, then

$$\delta_p(\mathcal{C}) = \frac{N}{\mathrm{vol}(\mathbb{R}^d/\Lambda)}. \tag{3.1}$$

Given a potential function $f : (0, \infty) \to [0, \infty)$, define the f-potential energy of $\mathcal{C}$ to be

$$E_f(\mathcal{C}) = \frac{1}{N} \sum_{1 \leq i,j \leq N} \sum_{\substack{x \in \Lambda \\ x + t_i - t_j \neq 0}} f(|x + t_i - t_j|^2). \tag{3.2}$$

This is the average over all points in $\mathcal{C}$ of the sum over all distances to other points: of course summing over all pairs of points in $\mathcal{C}$ would give a divergent sum, and even thus the sum may be infinite, in which case we say that the

*We use this name and this notation to avoid confusion with the associated sphere packing.

f-energy of $\mathcal{C}$ is infinite. With this definition, it is also clear that the f-energy does not depend on the choice of Λ and $t_1, \ldots, t_N$ made to represent $\mathcal{C}$.

Let $\mathcal{C}_R$ denote the set $\mathcal{C} \cap B_R(0) = \{x \in \mathcal{C}, |x| \leq R\}$. The following lemma clarifies the link with the definition of f-energy for finite sets:

Lemma 3.2. *Let $\mathcal{C}$ be a periodic point configuration in $\mathbb{R}^d$. If the f-energy of $\mathcal{C}$ is finite, then it equals*

$$\lim_{R\to\infty} \frac{1}{|\mathcal{C}_R|} \sum_{\substack{x,y\in\mathcal{C}_R \\ x\neq y}} f(|x-y|^2).$$

The result holds even without assuming that f is non-negative, as long as $f(x) = O((1+|x|)^{-d/2-\delta})$ for some $\delta > 0$.

Proof. Suppose that $\mathcal{C} = \bigcup_{i=1}^N (t_i + \Lambda)$ as above, and say a point is of type j if it is in $t_j + \Lambda$. To each point $x \in \mathcal{C}$ we associate the sum

$$\sum_{\substack{y\in\mathcal{C} \\ y\neq x}} f(|x-y|^2). \tag{3.3}$$

This sum depends only on the type of x, and the definition of $E_f(\mathcal{C})$ equals the average over all types of this quantity.

All these sums must converge, either because we assume that $E_f(\mathcal{C})$ is finite, or else, if f is not assumed to be non-negative, by its bound. Let ε be small, and choose K such that for x of each type

$$\sum_{\substack{y\in\mathcal{C} \\ |x-y|>K}} \left|f(|x-y|^2)\right| \leq \varepsilon.$$

In particular, summing in (3.3) only over y such that $|x-y| \leq K$ yields a partial sum which differs from the total sum by less than ε.

In the sum

$$\sum_{\substack{x,y\in\mathcal{C}_R \\ x\neq y}} f(|x-y|^2)$$

we can concentrate on the points $x \in B_{R-K}(0)$, since the number in $B_R(0) \setminus B_{R-K}(0)$ is negligible compared to the number in $B_{R-K}(0)$ (the latter being $O(R^d)$ and the former $O(R^{d-1})$ as $R \to \infty$). Each point carries a bounded contribution into the sum, so omitting the points in $B_R(0) \setminus B_{R-K}(0)$ changes the sum by $O(R^{d-1})$.

For each $x \in \mathcal{C}_{R-K}$,

$$\sum_{y\in\mathcal{C}_R y\neq x} f(|x-y|^2)$$

is within ε of

$$\sum_{\substack{y\in\mathcal{C} \\ y\neq x}} f(|x-y|^2).$$

The number of points of each type in $\mathcal{C}_{R-K}$ are equal, up to a factor of $1 + O(1/R)$. Thus, for R large,

$$\frac{1}{|\mathcal{C}_R|} \sum_{\substack{x,y \in \mathcal{C}_R \\ x \neq y}} f(|x-y|^2)$$

is $O(1/R)$ pplus a quantity that differs from $E_f(\mathcal{C})$ by less of ε. Choosing ε arbitrarily small and R accordingly large completes the proof. □

Now we would be happy to determine whether there exist *universally optimal point configurations*, i.e. periodic configurations which minimise E_f for every completely monotonic function f. Unfortunately, at this time no such configuration is known, but some exceptional structures as the hexagonal lattice, the root lattice E_8 and the Leech lattice Λ_{24} are conjectured to be examples (cfr. Conjecture 3.5 below). Recent experiments show that also the root lattice D_4 and the periodical non-lattice configuration D_9^+ could be universally optimal (see [CKS09]).

3.2 A bound and a conjecture

We are ready to state the Euclidean analogue of Proposition 2.20, in terms of the Fourier transform of $\mathbb{R}^d$. We normalise the Fourier transform of an L^1 function $h : \mathbb{R}^n \to \mathbb{R}$ by

$$\widehat{h}(t) = \int_{\mathbb{R}^d} h(x) e^{2\pi i \langle x,t \rangle} dx$$

Proposition 3.3. *Let $f : (0,\infty) \to [0,\infty)$ be any function. Suppose $h : \mathbb{R}^d \to \mathbb{R}$ satisfies $h(x) \leq f(|x|^2)$ for all $x \in \mathbb{R}^d \setminus \{0\}$ and is the Fourier transform of a function $g \in L^1(\mathbb{R}^d)$ such that $g(t) \geq 0$ for all $t \in \mathbb{R}^d$. Then the f-potential energy of every periodic configuration in $\mathbb{R}^d$ with density δ_p satisfies*

$$E_f(\mathcal{C}) \geq \delta_p(\liminf_{t \to 0} g(t)) - h(0).$$

Without loss of generality we can assume that g and h are bot radial functions (replace g with the average of its rotations about the origin).

First we need the following Lemma:

Lemma 3.4. *Let $\mathcal{C}$ be a periodic point configuration in $\mathbb{R}^d$, with point density δ_p. If $\varepsilon > 0$ is sufficiently small (depending on $\mathcal{C}$), then*

$$\lim_{R \to \infty} \int_{B_\varepsilon(0)} \frac{|\sum_{x \in \mathcal{C}_R} e^{2\pi i \langle x,t \rangle}|^2}{|\mathcal{C}_R|} dt = \delta_p$$

Proof. We shall prove that for $\varepsilon > 0$ small enough, if g is any radial, smooth function, with support in $B_\varepsilon(0)$, then

$$\lim_{R \to \infty} \int_{\mathbb{R}^d} \frac{|\sum_{x \in \mathcal{C}_R} e^{2\pi i \langle x,t \rangle}|^2}{|\mathcal{C}_R|} g(t) dt = \delta_p g(0).$$

This will suffice to prove the lemma, because the characteristic function of a small ball can be bounded above and below by such functions. Using the identity

$$\left|\sum_{x\in\mathcal{C}_R} e^{2\pi i\langle x,t\rangle}\right|^2 = \sum_{x,y\in\mathcal{C}_R} e^{2\pi i\langle x-y,t\rangle}$$

we expand the numerator of the integrand, getting

$$\int_{\mathbb{R}^d} \frac{|\sum_{x\in\mathcal{C}_R} e^{2\pi i\langle x,t\rangle}|^2}{|\mathcal{C}_R|} g(t)dt = \frac{1}{|\mathcal{C}|}\sum_{x,y\in\mathcal{C}_R} \widehat{g}(x-y).$$

Now if $\mathcal{C}$ is the disjoint union of translates $t_1+\Lambda,\dots,t_N+\Lambda$ of the lattice Λ, then it follows from Lemma 3.2 that

$$\lim_{R\to\infty}\frac{1}{|\mathcal{C}_R|}\sum_{x,y\in\mathcal{C}_R}\widehat{g}(x-y) = \frac{1}{N}\sum_{j,k=1}^{N}\sum_{z\in\Lambda}\widehat{g}(z+t_j-t_k).$$

Notice that this quantity is not quite the same as that considered in Lemma 3.2, because here we allow $x=y$ or $z+t_j-t_k=0$ in the sum, but the extra terms amount to $\widehat{g}(0)$ on each side.

Now it suffices to use the Poisson summation formula, which states that for every Schwartz function $h:\mathbb{R}^d\to\mathbb{R}$ and every $v\in\mathbb{R}^d$,

$$\sum_{z\in\Lambda} h(z+v) = \frac{1}{\operatorname{vol}(\mathbb{R}^d/\Lambda)}\sum_{t\in\Lambda^*}\widehat{h}(t)e^{-2\pi i\langle v,t\rangle},$$

where as usual

$$\Lambda^* = \{t\in\mathbb{R}^d : \langle t,z\rangle\in\mathbb{Z} \text{ for all } z\in\Lambda\}$$

is the dual lattice of Λ. Taking $h=\widehat{g}$ yields

$$\frac{1}{N}\sum_{j,k=1}^{N}\sum_{z\in\Lambda}\widehat{g}(z+t_j-t_k) = \frac{1}{N\operatorname{vol}(\mathbb{R}^d/\Lambda)}\sum_{t\in\Lambda^*} g(t)\left|\sum_{i,j=1}^{N} e^{2\pi i\langle v_j,t\rangle}\right|^2.$$

If the support of g is sufficiently small, then only the $t=0$ term contributes to the right hand side, and it equals $\delta_p g(0)$, for $N/\operatorname{vol}(\mathbb{R}^d/\Lambda)=\delta_p$. ☐

Proof of Proposition 3.3. Define

$$\ell = \liminf \mathbb{R}^d \ni t\to 0 g(t).$$

Let $\varepsilon>0$, and choose $\eta>0$ such that $g(t)\geq \ell-\varepsilon$ whenever $|t|\leq\eta$. Given $\mathcal{C}$ with density δ_p, by Lemma 3.2, the f-potential energy of $\mathcal{C}$ is

$$E_f(\mathcal{C}) = \lim_{R\to\infty}\frac{1}{|\mathcal{C}_R|}\sum_{\substack{x,y\in\mathcal{C}_R\\ x\neq y}} f(|x-y|^2).$$

On one hand we have, since $h(x)\leq f(|x|^2)$ for all $x\neq 0$,

$$\frac{1}{|\mathcal{C}_R|}\sum_{\substack{x,y\in\mathcal{C}_R\\ x\neq y}} f(|x-y|^2) \geq -h(0) + \frac{1}{|\mathcal{C}_R|}\sum_{x,y\in\mathcal{C}} h(x-y);$$

on the other hand,

$$\begin{aligned}\frac{1}{|\mathcal{C}_R|}\sum_{x,y\in C} h(x-y) &= \frac{1}{|\mathcal{C}|}\sum_{x,y\in\mathcal{C}_R}\int_{\mathbb{R}^d} g(t)e^{2\pi i\langle x-y,t\rangle}dt \\ &= \int_{\mathbb{R}^d} g(t)\frac{|\sum_{x\in\mathcal{C}_R} e^{2\pi i\langle x,t\rangle}|^2}{|\mathcal{C}_R|}dt \\ &\geq \int_{B_\eta(0)} (\ell-\varepsilon)\frac{|\sum_{x\in\mathcal{C}_R} e^{2\pi i\langle x,t\rangle}|^2}{|\mathcal{C}_R|}dt.\end{aligned}$$

In the limit as $R\to\infty$, Lemma 3.4 implies that the potential energy is at least

$$-h(0)+\delta_p(\ell-\varepsilon),$$

if η is small enough, and since ε can be taken arbitrarily small, we have

$$E_f(\mathcal{C})\geq \delta_p\ell - h(0)$$

as desired. □

Now let Λ_2, Λ_8 and Λ_{24} denote the hexagonal lattice in $\mathbb{R}^2$, the E_8 root lattice in $\mathbb{R}^8$ and the Leech lattice in $\mathbb{R}^{24}$ respectively:

Conjecture 3.5. *Let $d\in\{2,8,24\}$ and let $f:(0,\infty)\to\mathbb{R}$ be completely monotonic and satisfy $f(x)=O(|x|^{-d/2-\varepsilon})$ as $|x|\to\infty$ for some $\varepsilon>0$. Then there exists a function h that satisfies the hypotheses of Proposition 3.3.*

As a result, Λ_d would have the least f-potential energy of any periodic configuration in $\mathbb{R}^d$ with the same density, i.e. the three lattices would be universally optimal.

3.3 Local optimality

As an attempt to prove universal optimality for the three lattices listed above, as well as for D_4 and any other periodic configuration, it seems reasonable to ask whether universal optimality holds at least *locally* (the exact meaning of locally here shall be explained later).

Among the completely monotonic potentials f, it is worthwile to put forward two families of functions, namely the *inverse power laws* $p_s(r)=r^{-s}$ and the *exponential laws* $f_c(r)=e^{-cr}$, which will play a considerable role later. Indeed, when $\mathcal{C}=\Lambda$ is a lattice, the p_s-energy ($s>d/2$) is

$$E_{p_s}(\Lambda)=\sum_{0\neq x\in\Lambda}|x|^{-2s}=\zeta(\Lambda,s),$$

the Epstein zeta function of Λ; similarly, the f_c-energy of Λ is

$$E_{f_c}(e^{-cr},\Lambda)=\sum_{0\neq x\in\Lambda}e^{-c|x|^2}=\theta_\Lambda(ic/\pi)-1,$$

where θ_Λ is the usual theta series of Λ.

Thus for lattices, optimality with respect to energy minimisation is reduced to optimality with respect to their zeta and theta series. Investigations on this subject have been conducted by Sarnak and Strömbergsson in [SS07] and by Coulangeon in [Cou06], in connection with the theory of spherical designs. In particular, one has the following criterion of local optimality *among lattices*:

Theorem 3.6 (Coulangeon [Cou06])**.** *Lattices for which all shells are* 4*-designs achieve a local minimum (among lattices) of the map*

$$\Lambda \mapsto E_{f_c}(\Lambda)$$

for big enough c*.*

The aim of the remaining part of this chapter is to prove a result of Coulangeon and Schürmann contained in [CS10], which states that lattices satisfying the conditions of Theorem 3.6 are locally universally optimal not only among lattices, but actually among all periodic configurations of points (see Theorem 3.17). Their proof combines ideas of previous papers of theirs, [Cou06] and [S10], with results due to Sarnak and Strömbergsson, [SS07], and applies in particular to the lattices A_2, D_4, E_8 and to the Leech lattice Λ_{24}: in other words, what we are going to prove in the next paragraphs is a local version of Cohn and Kumar's Conjecture 3.5.

3.3.1 A parametrisation of periodic configurations

Since most of the quantities we will handle, such as energy and point density, are invariant under isometries of $\mathbb{R}^d$, we may identify two isometric N-periodic configurations; in particular, the N-tuple $(t_1, \dots, t_N)$ can be defined up to translating all its components by a common vector.

Notation 3.7. In what follows, we denote by $\mathbb{R}^{Nd}_*$ the set of N-tuples $\mathbf{u} = (u_1, \dots, u_N)$ of vectors in $\mathbb{R}^d$ subject to the condition

$$u_i - u_j \notin \mathbb{Z}^d \text{ for } i \neq j$$

and by $\mathbb{R}^{Nd}_*/\mathbf{T}$ the same up to translation.

For any $\mathbf{u} = (u_i, \dots, u_N) \in \mathbb{R}^{Nd}_*$, we define a *standard periodic configuration*

$$\Omega_{\mathbf{u}} = \bigcup_{i=1}^{N} (u_i + \mathbb{Z}^d). \tag{3.4}$$

Hence, every N-periodic configuration can be written as $A\Omega_{\mathbf{u}}$ for some $A \in \mathrm{GL}_d(\mathbb{R})$ and $\mathbf{u} \in \mathbb{R}^{Nd}_*$. Moreover, the matrix A above is determined up to left multiplication by $\mathrm{O}(d)$ by its associated positive definite form $Q = A^t A$, and under this settings we have

$$|Ax|^2 = Q[x] := x^t Q x$$

(notice that we use column vectors.) Furthermore, we denote by $\mathcal{S}^d$ the set of $d \times d$ real symmetric matrices and by $\mathcal{S}^d_{>0}$ the cone of positive definite ones.

We thus get a parametrisation

$$\mathcal{S}_{>0}^{d,N} := \mathcal{S}_{>0}^{d} \times \mathbb{R}_{\mathbf{T}}^{Nd} \to \mathrm{O}(d)\backslash\mathcal{L}_N/\mathbf{T} \tag{3.5}$$

$$(Q, \mathbf{u}) \mapsto \mathcal{C} = A\Omega_{\mathbf{u}}, \quad A \text{ such that } A^tA = Q. \tag{3.6}$$

Finally, in order to make comparisons between the energy of different N-periodic sets, it is necessary to require the same point density, otherwise such a comparison would make no sense, for clearly, by shrinking or expanding a given periodic configuration with scaling factor, one can achieve any energy. Therefore we restrict to N-periodic configuration of point density N, which amounts, by (3.1) to consider the space $\mathcal{P}_{>0}^{d,N} := \mathcal{P}_{>0}^{d} \times \mathbb{R}_{*}^{Nd}/\mathbf{T}$, where $\mathcal{P}$ stands for the set of positive definite quadratic form of determinant 1.

By (3.2), the computation of $E_f(\mathcal{C})$ involves evaluating potential function over the set of non-zero elements in

$$\mathcal{C} - \mathcal{C} = \{x - y : x, y \in \mathcal{C}\};$$

here a problem is that a given element in $\mathcal{C} - \mathcal{C}$ admits several representations as a difference of two elements in $\mathcal{C}$. However, the situation can be controlled when $\mathcal{C}$ is actually a lattice, as we show in the following lemma:

Lemma 3.8. *Let $\mathcal{C} = \bigcup_{i=1}^{N} t_i + \Lambda$ be an N-periodic configuration in $\mathbb{R}^d$. For $x \in \mathcal{C}$, set*

$$\mathcal{C}_x = \{y - x : y \in \mathcal{C}\}.$$

The following are equivalent for $\mathcal{C}$:

(i) *$\mathcal{C}$ is a lattice;*

(ii) *$\mathcal{C} - \mathcal{C} = \mathcal{C}$;*

(iii) *$\mathcal{C}_x = \mathcal{C}$ for all $x \in \mathcal{C}$;*

(iv) *for any $k \in \{1, \dots, N\}$, there is a uniquely determined permutation σ_k of $\{1, \dots, N\}$ such that*

$$\forall i \in \{1, \dots, N\} \quad t_{\sigma_k(i)} \equiv t_i - t_k \mod \mathcal{C}.$$

Proof. The equivalence of *(i)*, *(ii)* and *(iii)* follows from the caracterisation of lattices as discrete additive subgroups of $\mathbb{R}^d$.

For *(iii)⇒(iv)*, we have that for fixed k, the difference $t_i - t_k$ lies in

$$\mathcal{C}_{t_k} = \mathcal{C} = \bigcup_{j=1}^{N} t_j + \Lambda,$$

so there exists a uniquely determined index $\sigma_k(i)$ such that $t_i - t_{\sigma_k(i)} \in t_{\sigma_k(i)} + \Lambda$. Moreover, $\sigma_k(i) = \sigma_k(j)$ if and only if $t_i - t_k \equiv t_j - t_k \mod \Lambda$, which means that $t_i - t_j \in \Lambda$, so that σ_k is a bijection. Finally, *(iv)* clearly implies that any pairwise difference of elements in $\mathcal{C}$ is still in $\mathcal{C}$, which shows that *(iv)⇒(ii)*. □

Before going on, we make a further assumption on the potential functions f that will appear in the following sections, besides being completely monotonic on $(0, \infty)$:

Assumption 3.9. *There exists $\varepsilon > 0$ such that $f(x) = O(x^{-\frac{d}{2}-\varepsilon})$ as x tends to infinity.*

This is meant to ensure that formula (3.2) converges, though not strictly necessary.

Remark 3.10 (Bernstein's Theorem). As in Chapter 2 we were able to restrict to functions of type $r \to (4-r)^k$ (see Remark 2.5), which turned out to be useful in the proof of Theorem 2.4 for the 600-cell, here we can use Bernstein's theorem (Theorem 12b in [W41]): any completely monotonic function on $(0,\infty)$ can be written as

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

(Stieltjes integral), for some weakly increasing function $\alpha : [0,\infty) \to \mathbb{R}$. This allows us to deal only with exponential laws $f_c(r) = e^{-cr}$, $c > 0$ (inequalities are preserved thanks to Fubini's theorem); we will consider separately the case of inverse power laws $p_s(r) = r^{-s}$, $s > 0$, which is interesting on its own.

3.3.2 Local study of f-potential energy

3.3.2.1 Local expression for the energy

The f-potential energy of an N-periodic configuration $\mathcal{C} = A\Omega_{\mathbf{u}}$ depends only on the associated periodic form $(Q, \mathbf{u})$, namely one has

$$E_f(\mathcal{C}) = E_f(Q, \mathbf{u}) = \frac{1}{N} \sum_{i=1}^{N} \sum_{\substack{x \in \Omega_{\mathbf{u}} \\ x \neq u_i}} f(Q[u_i - x]). \tag{3.7}$$

We want to do a local study of E_f, i.e. to expand it in a neighbourhood of a given N-periodic configuration

$$\mathcal{C}_0 = A_0 \Omega_{\mathbf{u}^0} = \bigcup_{i=1}^{N} (t_i^0 + \Lambda_0),$$

where we set $L_0 = A_0 \mathbb{Z}^d$ and $\mathbf{t}^0 = A_0 \mathbf{u}^0$, i.e. $t_i^0 = A u_i^0$ for $1 \leq i \leq N$. We also assume that $\mathcal{C}_0$ has point density $\delta_p(\mathcal{C}_0) = N$ (i.e. $\det \Lambda = 1$) and we let $X_0 = (Q_0, \mathbf{u}^0)$ be the corresponding periodic form, with $Q_0 = A_0^t A_0$.

The variety $\mathcal{P}_{>0}^{d,N} = \mathcal{P}_{>0}^{d} \times \mathbb{R}_*^{Nd}/\mathbf{T}$ is locally homeomorphic in a neighbourhood of $X_0 = (Q_0, \mathbf{u}^0)$ to its tangent space at X_0, which is identified with $\mathcal{T}_{Q_0} \times \mathbb{R}^{Nd}/\mathbf{T}$ where

$$\mathcal{T}_{Q_0} = \{K \in \mathcal{S}^d \colon \operatorname{Tr}(Q_0^{-1} K) = 0\}.$$

The isomorphism is obtained via the matrix exponential through the map

$$(K, \mathbf{u}) \mapsto (Q_0 \exp(Q_0^{-1} K), \mathbf{u}_0 + \mathbf{u}).$$

Notice that the tangent space

$$\mathcal{T}_{Q_0} \times \mathbb{R}^{Nd}/\mathbf{T}$$

at X_0 comes equipped with its standard $\mathrm{SL}_d(\mathbb{R})$-invariant scalar product

$$\langle (K,\mathbf{u}),(L,\mathbf{v})\rangle_{X_0} := \mathrm{Tr}(Q_0^{-1}KQ_0^{-1}L) + \sum_{i=1}^{N} u_i^t v_i \tag{3.8}$$

which defines the Riemannian structure of $\mathcal{P}^{d,N}_{>0}$. To study how E_f varies locally around X_0, it is sufficient to consider the f-energy of $(Q_0 \exp(Q_0^{-1}K), \mathbf{u}_0 + \mathbf{u})$ for small enough $H \in \mathcal{T}_{Q_0}$ and $\mathbf{u} \in \mathbb{R}^{Nd}/\mathbf{T}$. Thus (3.7) becomes

$$\frac{1}{N}\sum_{i=1}^{N} \sum_{\substack{x\in\Omega_{\mathbf{u}^0+\mathbf{u}}\\ x\neq u_i^0+u_i}} f\big(Q_0\exp(Q_0^{-1}K)[u_i^0+u_i-x]\big). \tag{3.9}$$

In the internal sum, each term $u_i^0+u_i-x$ can be written as $u_i^0-u_j^0+u_i-u_j$ for some $j\in\{1,\dots,N\}$ and some $v\in\mathbb{Z}^d$. The condition $u_i^0-u_j^0+u_i-u_j+v\neq 0$ is satisfied as soon as $u_i^0-u_j^0+v$ itself is non-zero, provided that the u_i are close enough to 0 (this is the case for instance if the u_i's satisfy $|u_i|<\rho_0/2$, where $\rho_0 := \min_{0\neq x\in\Omega_{\mathbf{u}^0}-\Omega_{\mathbf{u}^0}}|x|$). Thus, assuming that $\mathbf{u}$ lies in a suitable neighbourhood of 0, we can rewrite (3.9) as

$$\frac{1}{N}\sum_{i,j=1}^{N} \sum_{0\neq w\in u_i^0-u_j^0+\mathbb{Z}^d} f\big(Q_0\exp(Q_0^{-1}K)[w+u_i-u_j]\big). \tag{3.10}$$

Making a little change of coordinates in order to simplify notation, the above equation becomes

$$E_f(H,\mathbf{t}) := \frac{1}{N}\sum_{i,j=1}^{N} \sum_{0\neq w\in t_i^0-t_j^0+\Lambda_0} f\big(\exp(H)[w+t_i-t_j]\big) \tag{3.11}$$

where

- $\mathbf{t}=A_0\mathbf{u}$ and $\mathbf{t}^0=A_0\mathbf{u}^0$;
- $H\in\{H\in\mathcal{S}^d : \mathrm{Tr}(H)=0\}$;
- the scalar product (3.8) on $\mathcal{T}_{\mathrm{id}}$ takes the simpler form

$$\langle (K,\mathbf{u}),(L,\mathbf{v})\rangle = \mathrm{Tr}(KL) + \sum_{i=1}^{N} u_i^t v_i.$$

Remark 3.11. Notice that the definition of E_f depends on the representation of $\mathcal{C}_0$ as a periodic configuration, i.e. on the choice of A_0 and $\mathbf{u}^0$. Moreover, with this setting $E_f(\mathcal{C}) = E_f(0,\mathbf{0})$.

To go further in our simplification of the expression for E_f, the two main ingredients will be:

- using the additive structure of $\mathcal{C}_0$ (if any);
- using the translation invariance of energy.

These conditions are met in particular when $\mathcal{C}_0$ is a lattice, in which case we obtain the following lemma:

Lemma 3.12. *If* $\mathcal{C}_0 = \bigcup_{i=1}^N (t_i^0 + \Lambda_0)$ *is a lattice, then*

$$E_f(H, \mathbf{t}) = \frac{1}{N^2} \sum_{0 \neq w \in \mathcal{C}_0} \sum_{i,k=1}^N f\big(\exp(H)[w + t_i - t_{\sigma_k(i)}]\big), \tag{3.12}$$

where σ_k *is the bijection of Lemma 3.8.*

Proof. Since $\mathcal{C}_0 - \mathcal{C}_0 = \mathcal{C}_0$, any coset $t_i^0 - t_j^0$ in the inner sum of (3.11) can be written $t_k^0 + \Lambda_0$ for a uniquely defined k. More precisely, using Lemma 3.8(3), we obtain

$$E_f(H, \mathbf{t}) = \frac{1}{N} \sum_{k=1}^N \sum_{0 \neq w \in t_k^0 + \Lambda_0} \sum_{i=1}^N f\big(\exp(H)[w + t_i - t_{\sigma_k(i)}]\big), \tag{3.13}$$

where σ_k is the permutation defined by the condition that $t^0_{\sigma_k(i)} \equiv t_i^0 - t_k^0 \mod \Lambda_0$ for all $i \in \{1, \ldots, m\}$ (see Lemma 3.8). Notice that the t_j are replaced by $t_{\sigma_k(i)}$ and that the change from index j to k causes a reordering of terms.

Because of the translation invariance of energy, $E_f(H, \mathbf{t})$ is not modified if all the components of $\mathbf{t}^0$ are translated by a common vector $\alpha \in \mathbb{R}^d$; in particular, we can choose $\alpha = -t_j^0$ for some $j \in \{1, \ldots, m\}$. Applying this to (3.13), we get for any $j \in \{1, \ldots, m\}$ the expression

$$\begin{aligned} E_f(H, \mathbf{t}) &= \frac{1}{N} \sum_{k=1}^N \sum_{0 \neq w \in t_k^0 - t_j^0 + \Lambda_0} \sum_{i=1}^N f\big(\exp(H)[w + t_i - t_{\sigma_k(i)}]\big) \\ &= \frac{1}{N} \sum_{k=1}^N \sum_{0 \neq w \in -t^0_{\sigma_k(j)} + \Lambda_0} \sum_{i=1}^N f\big(\exp(H)[w + t_i - t_{\sigma_k(i)}]\big). \end{aligned} \tag{$\mathbf{E_j}$}$$

Adding up the $(\mathbf{E_j})$'s for $j = 1, \ldots, N$ and then averaging, together with noticing that

$$\bigcup_{j=1}^N -t^0_{\sigma_k(j)} + \Lambda_0 = \bigcup_{j=1}^N -t_j^0 + \Lambda_0 = \bigcup t_j^0 + \Lambda_0 = \mathcal{C}_0$$

we get the final expression

$$\begin{aligned} E_f(H, \mathbf{t}) &= \frac{1}{N^2} \sum_{k=1}^N \sum_{0 \neq w \in \mathcal{C}_0} \sum_{i=1}^N f\big(\exp(H)[w + t_i - t_{\sigma_k(i)}]\big) \\ &= \frac{1}{N^2} \sum_{0 \neq w \in \mathcal{C}_0} \sum_{i,k=1}^N f\big(\exp(H)[w + t_i - t_{\sigma_k(i)}]\big). \end{aligned}$$

□

3.3.2.2 Taylor expansion of E_f

We compute here the Taylor development of order 2 of (3.12), viewed as a function on the tangent space $\mathcal{T}_{\mathrm{id}} \times \mathbb{R}^{Nd}/\mathbf{T}$. To do that, we need to compute the gradient and the Hessian of E_f at the lattice $\mathcal{C}_0$, i.e. at $(0, \mathbf{0})$ in our notation, and then we will have

$$E_f(H, \mathbf{t}) = E_f(0, \mathbf{0}) + \langle \operatorname{grad} E_f(0, \mathbf{0}), (H, \mathbf{t})\rangle + \frac{1}{2} \operatorname{hess} E_f(0, \mathbf{0}[H, \mathbf{t}]) + o(|(H, \mathbf{t})|^2). \tag{3.14}$$

We do these computations in the following lemma: here f is either an inverse power law $p_s(r)$, or an exponential $f_c(r)$.

Lemma 3.13. *Assume as above that* $\mathcal{C}_0 = \bigcup_{i=1}^N t_i^0 + \Lambda_0$ *is a lattice in* $\mathbb{R}^d$. *Then*

(i) for an inverse power law $p_s(r) = r^{-s}$, *one has*

$$\langle \operatorname{grad} E_{p_s}(0, \mathbf{0}), (H, \mathbf{t})\rangle = -s \sum_{0 \neq w \in \mathcal{C}_0} H[w] |w|^{-2s-2}$$

$$\begin{aligned} \operatorname{hess} E_{p_s}(0, \mathbf{0})[H, \mathbf{t}] = s \sum_{0 \neq w \in \mathcal{C}_0} |w|^{-2s-4} \Big\{ &\frac{s+1}{2} (H[w])^2 - \frac{1}{2} H^2[w] |w|^2 \\ &+ \frac{1}{N^2} \sum_{i,k=1}^N \Big[2(s+1) \big(w^t (t_i - t_{\sigma_k(i)})\big)^2 - |w|^2 |t_i - t_{\sigma_k(i)}|^2 \Big] \Big\}; \end{aligned}$$

(ii) for an exponential law $f_c(r) = e^{-cr}$, *one has*

$$\langle \operatorname{grad} E_{f_c}(0, \mathbf{0}), (H, \mathbf{t})\rangle = -c \sum_{0 \neq w \in \mathcal{C}_0} H[w] e^{-c|w|^2}$$

$$\begin{aligned} \operatorname{hess} E_{f_c}(0, \mathbf{0})[H, \mathbf{t}] = c \sum_{0 \neq w \in \mathcal{C}_0} e^{-c|w|^2} \Big\{ &\frac{c}{2} (H[w])^2 - \frac{1}{2} H^2[w] \\ &+ \frac{1}{N^2} \sum_{i,k=1}^N \Big[2c \big(w^t (t_i - t_{\sigma_k(i)})\big)^2 - |t_i - t_{\sigma_k(i)}|^2 \Big] \Big\}. \end{aligned}$$

Proof. Using the Taylor expansion of the matrix exponential

$$\exp(H) = \sum_{k=0}^{\infty} \frac{H^k}{k!}$$

we write

$$\begin{aligned} &\exp(H)[w + t_i - t_{\sigma_k(i)}] = (\mathbb{I} + H + \frac{H^2}{2} + \text{hot})[w + t_i - t_{\sigma_k(i)}] \\ &= |w|^2 + \underbrace{H[w] + 2w^t (t_i - t_{\sigma_k(i)})}_{\mathcal{L}(H,\mathbf{t})} + \underbrace{|t_i - t_{\sigma_k(i)}|^2 + 2w^t H (t_i - t_{\sigma_k(i)}) + \frac{1}{2} H^2[w]}_{\mathcal{S}(H,\mathbf{t})} + o\big(|(H, \mathbf{t})|^2\big). \end{aligned}$$

Then, we expand the expressions for p_s and f_c, getting

$$\begin{aligned} \exp(H)[w + t_i - t_{\sigma_k(i)}]^{-s} &= |w|^{-2s} \left(1 + \frac{\mathcal{L}}{|w|^2} + \frac{\mathcal{S}}{|w|^2}\right)^{-s} + o\big(|(H, \mathbf{t})|^2\big) \\ &= |w|^{-2s} \left(1 - \frac{\mathcal{L} + \mathcal{S}}{|w|^2} + \frac{s(s+1)}{2} \frac{\mathcal{L}^2}{|w|^4}\right) + o\big(|(H, \mathbf{t})|^2\big) \end{aligned}$$

and

$$\begin{aligned} e^{-c\exp(H)[w+t_i-t_{\sigma_k(i)}]} &= e^{-c|w|^2} e^{-c\left(\mathcal{L}+\mathcal{S}+o\left(|(H,\mathbf{t})|^2\right)\right)} \\ &= e^{-c|w|^2}\left(1-c(\mathcal{L}+\mathcal{S})+\frac{c^2}{2}\mathcal{L}^2\right)+o\left(|(H,\mathbf{t})|^2\right). \end{aligned}$$

Finally, for a fixed $w \in \mathcal{C}_0$, we have to add the terms

$$\exp(H)[w+t_i-t_{\sigma_k(i)}]^{-s} \quad \text{resp. } e^{-c\exp(H)[w+t_i-t_{\sigma_k(i)}]},$$

corresponding to all pairs (i,k). Since σ_k is a permutation, the terms $2w^t(t_i - t_{\sigma_k(i)})$ appearing in $\mathcal{L}$ add up to zero, as do the terms $2w^tH(t_i-t_{\sigma_k(i)})$ in $\mathcal{S}$, and the terms $2w^t(t_i - t_{\sigma_k(i)})H[w]$ appearing in the expansion of $\mathcal{L}^2$. Altogether, this gives the formulae of the lemma. □

Remark 3.14. There are two important facts to underline in the previous calculations, that happen when $\mathcal{C}_0$ is a lattice:

- the gradient of the potential energy at $\mathcal{C}_0$, which is *a priori* a linear form in the variable $(H,\mathbf{t}) \in \mathcal{T}_{\text{id}} \times \mathbb{R}^{Nd}$, has actually a trivial component in the translational direction;
- the Hessian splits into the sum of a quadratic form in H and a quadratic form in $\mathbf{t}$.

In other words, when studying local perturbations of energy within the set of periodic configurations around a lattice, it is possible to separate *purely translational* moves (i.e. with $H = 0$) and *purely lattice* moves (i.e. with $\mathbf{t} = \mathbf{0}$). This observation will play an important role in the proof of Theorem 3.17.

3.3.3 Proof of the main result

In this section, we will state and prove the recent result of Coulangeon and Schürmann [CS10]. They have succeeded in showing that under some rather general conditions, a lattice which is locally optimal *among lattices* regarding energy minimisation, is actually locally optimal *among all periodic sets*.

One problem in giving a precise meaning to "optimal" or "critical point" for the energy is that a given periodic configuration admits infinitely many representations as $\mathcal{C} = \bigcup_{i=1}^N t_i + \Lambda$, for various N's and Λ's. To overcome this problem, we adopt the following definition:

Definition 3.15. Let f be a completely monotonic function.

(i) A periodic configuration $\mathcal{C}_0$ is said to be *f-critical* if it is a critical point of $E_f(\mathcal{C})$ on $\mathcal{P}^{d,N}_{>0}$ for any N.

(ii) A periodic configuration $\mathcal{C}_0$ is said to be *locally f-optimal* if it locally minimises $E_f(\mathcal{C})$ on $\mathcal{P}^{d,N}_{>0}$ for any N.

With this terminology, a periodic configuration is *locally universally optimal* if it is locally f-optimal for every complete monotonic function f, or equivalently, thanks to Bernstein's theorem, for every exponential function f_c, $c > 0$.

We need one more lemma, whose proof can be found in [V01], Theorem 3.2, which is a further characterisation of the spherical designs that enter in the main theorem:

Lemma 3.16. *Let $\mathcal{D}$ be a finite subset of the sphere $r\mathbb{S}^{d-1}$ of radius r in $\mathbb{R}^d$ and k an even positive integer. Assume that $\mathcal{D}$ is symmetric about the origin, i.e. $\mathcal{D} = -\mathcal{D}$. Then the following are equivalent:*

(i) $\mathcal{D}$ is a k-design[†]*;*

(ii) there exists a constant c_k, depending only on r, k and the cardinality of $\mathcal{D}$, such that for all $y \in \mathbb{R}^d$,

$$\sum_{x\in\mathcal{D}} (x \cdot y)^k = c_k (y \cdot y)^{k/2}. \tag{3.15}$$

Now we are ready to state the main result of this section:

Theorem 3.17. *(i) Let $\mathcal{C}_0$ be a lattice, all shells whereof are 2-designs. Then, viewed as a periodic configuration, $\mathcal{C}_0$ is f-critical for any completely monotonic function f.*

(ii) Let $\mathcal{C}_0$ be a lattice, all shells whereof are 4-designs. Then, viewed as a periodic set,

(a) $\mathcal{C}_0$ is locally p_s-optimal for every $s > \frac{d}{2}$;

(b) $\mathcal{C}_0$ is locally f_c-optimal for every big enough $c > 0$.

Proof. For any fixed positive integer N, write $\mathcal{C}_0$ as an N-periodic set $\bigcup_{i=1}^N t_i^0 + \Lambda_0$. We consider E_f (as in (3.11)) depending on the particular choice of Λ_0 and $\mathbf{t}^0$ to study locally the energy in a neighbourhood of $\mathcal{C}_0$ within $\mathcal{P}_>^{d,N}0$. In particular we use the Taylor expansion of E_f around $(0, \mathbf{0})$ obtained previously.

(i). We have to show that for every completely monotonic function f, the gradient of f at $(0, \mathbf{0})$ is orthogonal to $\mathcal{T}_{\mathrm{id}} \times \mathbb{R}^{Nd}$. Thanks to Bernstein's theorem, it is enough to show it for exponential functions f_c. For any $\alpha > 0$, set

$$\mathcal{C}_0(\alpha) = \{w \in \mathcal{C}_0 : |w|^2 = \alpha\}.$$

These shells of the lattice $\mathcal{C}_0$ are assumed to be 2-designs (if non-empty). Using Lemma 3.16*(ii)*, this is equivalent to the relation

$$\sum_{w\in\mathcal{C}_0(\alpha)} ww^t = \frac{\alpha|\mathcal{C}_0(\alpha)|}{d}\,\mathrm{id} \tag{3.16}$$

for any positive real number α, that is, the constant c_2 in Lemma 3.16*(ii)* equals $\frac{\alpha|\mathcal{C}_0(\alpha)|}{d}$ (this can be seen taking traces in (3.15)). Therefore, we have

$$\begin{aligned}
\langle \operatorname{grad} E_{f_c}(0, \mathbf{0}), (H, \mathbf{t})\rangle &= -c \sum_{0\neq w\in\mathcal{C}_0} H[w] e^{-c|w|^2} \\
&= -c \sum_{\alpha>0} \sum_{w\in\mathcal{C}_0(\alpha)} H[w] e^{-c\alpha} \\
&= -c \sum_{\alpha>0} e^{-c\alpha} \sum_{w\in\mathcal{C}_0(\alpha)} \mathrm{Tr}(ww^t H) \\
&= -c \sum_{\alpha>0} e^{-c\alpha}\, \mathrm{Tr}\left(\left(\frac{\alpha|\mathcal{C}_0(\alpha)|}{d}\,\mathrm{id}\right) H\right) = 0
\end{aligned}$$

[†] a spherical k-design on $r\mathbb{S}^{d-1}$ is defined the same way as a design on the unit sphere, i.e. every polynomial of degree $\leq k$ must have the same average on it as on the entire sphere.

since $\mathrm{Tr}(H) = 0$ for every $H \in \mathcal{T}_{\mathrm{id}}$.

(ii). Now to prove local optimality with respect to f it is enough to prove that the Hessian $E_f(0, \mathbf{0})$ is positive definite. By Proposition 1.2 in [Cou06] the hypothesis that all shells of $\mathcal{C}_0$ are 4-designs translates into

$$\forall H \in \mathcal{S}^d(\mathbb{R}), \qquad \sum_{0 \neq w \in \mathcal{C}_0(\alpha)} H[w]^2 = \frac{\alpha^2 |\mathcal{C}_0(\alpha)|}{d(d+2)} ((\mathrm{Tr}\, H)^2 + 2\,\mathrm{Tr}(H^2)), \tag{3.17}$$

provided that $\mathcal{C}_0(\alpha)$ is non-empty. But since all non-empty shells of $\mathcal{C}_0$ are also 2-designs, this implies that

$$\forall H \in \mathcal{S}^d(\mathbb{R}), \qquad \sum_{0 \neq w \in \mathcal{C}_0(\alpha)} H^2[w] = \frac{\alpha |\mathcal{C}_0(\alpha)|}{d}\, \mathrm{Tr}(H^2). \tag{3.18}$$

When $f = p_s$ is an inverse power function, putting (3.17) and (3.18) into the expression for $\mathrm{hess}\, E_{p_s}(0, \mathbf{0})$ obtained in Lemma 3.13*(i)* yields

$$\mathrm{hess}\, E_{p_s}(0, \mathbf{0})[H, \mathbf{t}] = \frac{s(s - d/2)}{d(d+2)} \zeta(\mathcal{C}_0, s)(\mathrm{Tr}\, H)^2 + \frac{s}{N^2} \Psi_s(\mathbf{t})$$

where

$$\Psi_s(\mathbf{t}) = \sum_{0 \neq w \in \mathcal{C}_0} \left\{ \sum_{i,k=1}^{N} \left[2(s+1)\big(w^t(t_i - t_{\sigma_k(i)})\big)^2 - |w|^2 |t_i - t_{\sigma_k(i)}|^2 \right] \right\} |w|^{-2s-4}.$$

Unless H is zero, the first term $\frac{s(s-d/2)}{d(d+2)} \zeta(\mathcal{C}_0, s)(\mathrm{Tr}\, H)^2$ is positive because $s > d/2$. As for $\Psi_s(\mathbf{t})$, we can rewrite it as

$$\Psi_s(\mathbf{t}) = \sum_{\alpha > 0} \sum_{0 \neq w \in \mathcal{C}_0(\alpha)} \left\{ \sum_{i,k=1}^{N} \left[2(s+1)\big(w^t(t_i - t_{\sigma_k(i)})\big)^2 - \alpha |t_i - t_{\sigma_k(i)}|^2 \right] \right\} \alpha^{-s-2}.$$

As each non-empty shell of $\mathcal{C}_0$ is a 2-design, we can further simplify to

$$\Psi_s(\mathbf{t}) = \sum_{\alpha > 0} \left(\frac{2(s+1)}{d} - 1 \right) |\mathcal{C}_0(\alpha)|^{-s-1} \sum_{i,k=1}^{N} |t_i - t_{\sigma_k(i)}|^2$$

which is clearly positive for $s > d/2$, unless $t_i = t_{\sigma_k(i)}$ for every $1 \leq i, k \leq N$; but since for every pair (i, j) with $1 \leq i, j \leq N$ there exists k such that $\sigma_k(i) = j$ (namely $k = \sigma_j(i)$), the last condition implies that $t_i = t_j$ for all (i, j) and consequently $\mathbf{t} \equiv \mathbf{0} \mod \mathbf{T}$. This proves *(ii)* in case *(a)*.

When $f = f_c$ is an exponential potential, then the same kind of computations as before yields

$$\mathrm{hess}\, E_{f_c}(0, \mathbf{0})[H, \mathbf{t}] = \frac{\mathrm{Tr}(H^2)}{d(d+2)} \sum_{0 \neq w \in \mathcal{C}_0} c|w|^2 \left(c|w|^2 - (d/2 + 1) \right) e^{-c|w|^2} + \frac{c}{N^2} \Upsilon_c(\mathbf{t})$$

where

$$\Upsilon_c(\mathbf{t}) = \sum_{0 \neq w \in \mathcal{C}_0} \left\{ \sum_{i,k=1}^{N} \left[2c\big(w^t(t_i - t_{\sigma_k(i)})\big)^2 - |t_i - t_{\sigma_k(i)}|^2 \right] \right\} e^{-c|w|^2}.$$

If $H \neq 0$, the first term

$$\frac{\mathrm{Tr}(H^2)}{d(d+2)} \sum_{0 \neq w \in \mathcal{C}_0} c|w|^2 \left(c|w|^2 - (d/2+1)\right) e^{-c|w|^2}$$

is positive as soon as c is strictly greater than $\frac{d+2}{2\min \mathcal{C}_0}$, where

$$\min \mathcal{C}_0 = \min_{0 \neq \mathcal{C}_0} |w|^2.$$

On the other hand, since all non-empty shells of $\mathcal{C}_0$ are 2-designs, the expression of $\Upsilon_c(\mathbf{t})$ reduces to

$$\Upsilon_c(\mathbf{t}) = \sum_{\alpha>0} \left(\frac{2c\alpha}{d} - 1\right) |\mathcal{C}_0(\alpha)| e^{-c\alpha} \sum_{i,k=1}^{N} |t_i - t_{\sigma_k(i)}|^2.$$

This quantity is positive for any $c > \frac{d}{2\min(\mathcal{C}_0)}$, for then it is a sum of positive terms. This proves *(ii)* in case *(b)*. □

Consequence. In the previous proof we have found that, when the 4-design condition is satisfied on every shell of $\mathcal{C}_0$, the Hessian of the f_c-potential energy splits into a sum

$$\operatorname{hess} E_{f_c}(0,\mathbf{0})[H,\mathbf{t}] = \frac{\mathrm{Tr}(H^2)}{d(d+2)} \sum_{0 \neq w \in \mathcal{C}_0} c|w|^2 \left(c|w|^2 - (d/2+1)\right) e^{-c|w|^2} + \\ + \frac{c}{N^2} \sum_{\alpha>0} \left(\frac{2c\alpha}{d} - 1\right) |\mathcal{C}_0(\alpha)| e^{-c\alpha} \sum_{i,k=1}^{N} |t_i - t_{\sigma_k(i)}|^2, \quad (3.19)$$

with the first term belonging to *purely lattice* moves and the second to *purely translational* ones. Setting $u = c/\pi$, we can rewrite (3.19) as

$$\operatorname{hess} E_{f_c}(0,\mathbf{0})[H,\mathbf{t}] = y \left[\frac{\mathrm{Tr}(H^2)}{d(d+2)} G(y) + \frac{2\pi}{N^2 d} F(y) \sum_{i,k=1}^{N} |t_i - t_{\sigma_k(i)}|^2\right] \quad (3.20)$$

where

$$F(y) = \sum_{\alpha>0} \left(\pi y\alpha - \frac{d}{2}\right) |\mathcal{C}_0(\alpha)| e^{-\pi y\alpha}$$
$$G(y) = \sum_{\alpha>0} \pi\alpha \left(\pi y\alpha - \left(\frac{d}{2} + 1\right)\right) |\mathcal{C}_0(\alpha)|.$$

In view of the next corollary, it is important to notice that

$$F'(y) = -G(y). \quad (3.21)$$

Corollary 3.18. *A lattice all shells whereof are* 4*-designs is locally universally optimal* among all periodic configurations *if and only if it is locally universally optimal* among lattices.

Proof. One implication is obvious; conversely, if $\mathcal{C}_0$ is locally universally optimal among lattices, then under the notation of (3.20) this means that $G(y) > 0$ for all $y > 0$. But then (3.21) implies that $F(y)$ is strictly decreasing on $(0, \infty)$; hence $F(y)$ is positive for every $y > 0$, since, as we have observed before, it is certainly positive for any big enough y, e.g. $y > \frac{d}{2\pi \min \mathcal{C}_0}$. Therefore also the translational component of $\operatorname{hess} E_f(0, \mathbf{0})$ is strictly positive unless $(H, \mathbf{t}) = (0, \mathbf{0})$, and that allows to conclude. □

This principle applies in particular to D_4, E_8 and to the Leech lattice Λ_{24}, for which the 4-design condition is well-known to hold (see for example [Cou06]). As a result, we have:

Theorem 3.19. *The root lattices D_4, E_8 and the Leech lattice Λ_{24} are locally universally optimal, i.e. they locally minimise the f-energy on $\mathcal{P}^{d,N}_{>0}$ for any N and for any completely monotonical potential function f.*

Proof. Applying Corollary 3.18, it is enough to prove that these lattices are locally universally optimal among lattices, and this has been done by Sarnak and Strömbergsson in their paper [SS07], Proposition 2. The computations on pages 138-139 show that the H-part of the Hessian

$$H \mapsto \frac{\operatorname{Tr}(H^2)}{d(d+2)} \sum_{0 \neq w \in \mathcal{C}_0} c|w|^2 \left(c|w|^2 - \left(\frac{d}{2} + 1 \right) \right) e^{-c|w|^2}.$$

is positive for any $c > 0$. □

Conclusion. What we have treated in the previous sections is undoubtedly a major advancement in the theory of universally optimal Euclidean configurations of points. Hopefully, in a not too distant future someone will be able to show whether *globally* universally optimal Euclidean configurations exist or not, and to provide a list of them.

FINIS OPERIS

Appendix A

Uniqueness of spherical codes

Uniqueness of the N-gon is trivial.

For the simplex, cross polytope, icosahedron, and the 600-cell, uniqueness can be proved via analysing the case of equality in the Bőrőczky bound (see [B78], p. 260, or [BD01] for another proof for the 600-cell).

For the $(24, 196560, 1/2)$, $(23, 4600, 1/3)$, $(8, 240, 1/2)$, and $(7, 56, 1/3)$ spherical codes, uniqueness was proved by Bannai and Sloane in [BS81], resumed in Chapter 14 of [CS99].

For the $(6, 27, 1/4)$, $(5, 16, 1/5)$, $(22, 275, 1/6)$, $(21, 162, 1/7)$, and $(22, 100, 1/11)$ codes, uniqueness follows from results in the theory of strongly regular graphs: in each case, there are only two distinct inner products other than 1, so one can construct a graph out of the vertices by making edges correspond to one particular inner product (one gets one of two complementary graphs, which encode the same information). Using Theorem Theorem 1.54 and Lemma 1.53 one shows that these graphs are strongly regular and determines their parameters. In each case, there are unique strongly regular graphs with these parameters (see [CGS78]). It follows that the Gram matrices of the corresponding configurations of points are uniquely determined, hence the configurations are themselves determined up to orthogonal transformations.

For the $(23, 552, 1/5)$ code, uniqueness follows from the uniqueness of the regular two-graph on 276 vertices. In any $(23, 552, 1/5)$ code, the linear programming bounds show that only the inner products -1 and $\pm 1/5$ occur. Such a code thus gives rise to an arrangement of 276 equiangular lines in $\mathbb{R}^{23}$, which corresponds to a regular two-graph on 276 vertices. Goethals and Seidel proved in [GS75] that it is unique, which implies the uniqueness of the $(23, 552, 1/5)$ code.

Finally, the last remaining case is the $(22, 891, 1/4)$ spherical code: a proof based on the techniques of Bannai and Sloane can be found in [CK04.2].

Bibliography

... Let us come to those references to authors which other books have, and you want for yours. The remedy for this is very simple: You have only to look out for some book that quotes them all, from A to Z as you say yourself, and then insert the very same alphabet in your book, and though the imposition may be plain to see, because you have so little need to borrow from them, that is no matter [...] At any rate, if it answers no other purpose, this long catalogue of authors will serve to give a surprising look of authority to your book ... (Cervantes, Don Quixote, Preface.)

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