Linear Programming Bounds for Periodic Energy Problems

By

Nathaniel Jay Tenpas

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Approved:

Douglas Hardin, Ph.D.

Edward Saff, Ph.D.

Alexander Powell, Ph.D.

Larry Rolen, Ph.D.

Piran Kidambi, Ph.D.

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Introduction

1.1 Background

In this thesis, we consider the fundamental problem of finding the 'best' way to arrange a finite number of points in some space. Here, 'best' can take a range of meanings; we might optimize the covering radius of a configuration, minimizing the maximal distance of a point in the space to the configuration. We can also optimize the packing radius, maximizing the minimal distance between two points in the configuration.

A third interpretation of 'best,' and our main focus, comes from the lens of discrete potential energy minimization. In this setting, we aim to minimize the potential energy arising from the pairwise interactions of particles in a configuration. The motivating physical example for this approach considers the particles as point charges constrained to the surface of some conductor. Configurations will tend to arrange on the surface so as to minimize their electrostatic potential energy, and so finding the mininizing arrangements, called 'ground states,' tells us about the long-term behavior of configurations. The study of these problems on the sphere dates back to at least 1904, when Nobel laureate JJ Thomson, recognized with discovering the electron, posed the question of minimizing the electrostatic potential energy arising from placing N unit charges on S^2.

Since then, much study, in a variety of spaces, has focused on both exact minimizers of potential energy for a fixed number of points and asymptotics as the number of points grows to infinity. Rigorous results for optimal configurations can often be quite delicate even for small cardinalities, though numerical experiments sometimes provide good candidates. For example, the century-old Thomson problem remains open for N as small as 7 and all $N > 12$, and minimizers for 5 points on S^2 with inverse power potentials have only recently been nearly completely characterized by Schwartz in a lengthy computer-assisted monograph [26]. These questions of exact minimizers

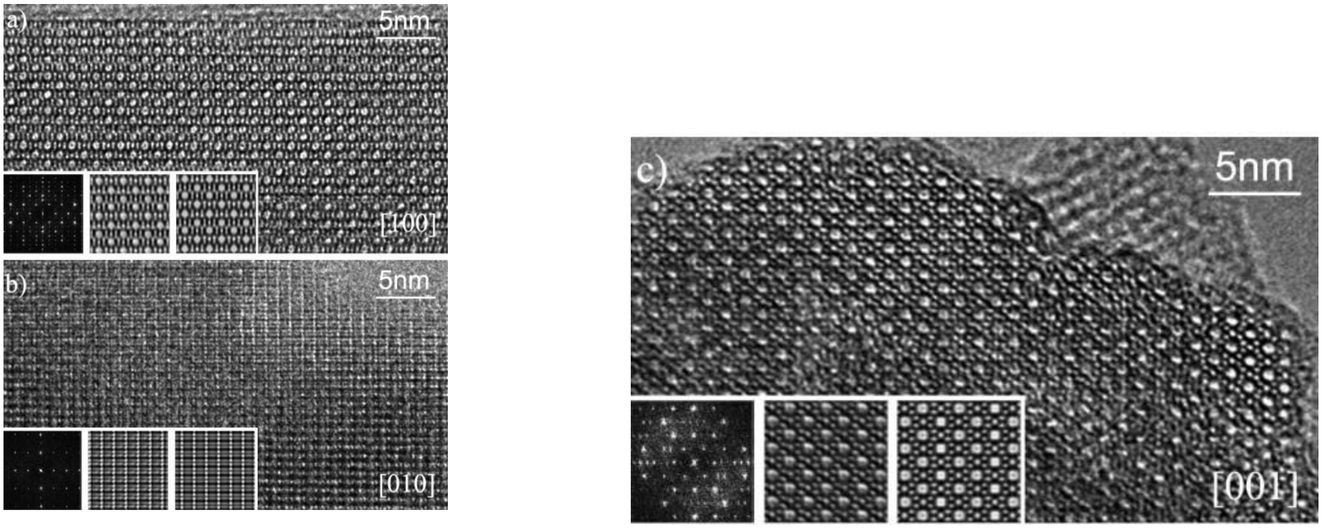

Figure 1.1: These TEM images from [29] show crystalline structure in crossections of the zeolite IM-5

tend to be geometric, and important geometric structures, like sharp codes on the sphere, often show up as minimizers. In contrast, asymptotic results tend to rely more on analytic tools.

One particularly important application of potential energy minimization is the study of crystallization. Chemists have long observed that at low temperatures, molecules arrange themselves in regular crystalline structures as opposed to random arrangements. The study of energy minimization for infinite configurations (a good approximation of a large crystal with many, many cells) helps to provide a rigorous justification for this phenomena. Since the energy of an infinite configuration equipped with a repulsive potential can always be decreased by taking points farther and farther apart, we need to fix the density of a configuration and take an average energy per point to obtain a meaningful model in this context of infinite, unbounded configurations.

Cohn and Kumar introduced the property of *universal optimality* for an infinite configuration $C \subseteq \mathbb{R}^d$ of density ρ, meaning that C minimizes potential energy among all configurations of density ρ for a very large class of repulsive potential functions. This class includes, in particular, the much-studied Riesz potentials: $|\cdot|^{-s}$, $s > d$. Universal optimality is a very strong property and it can be shown by taking Riesz potentials with $s \to \infty$ that a universally optimal periodic configuration in $\mathbb{R}^d$ must also solve the d-dimensional sphere packing problem. Cohn and Ku-

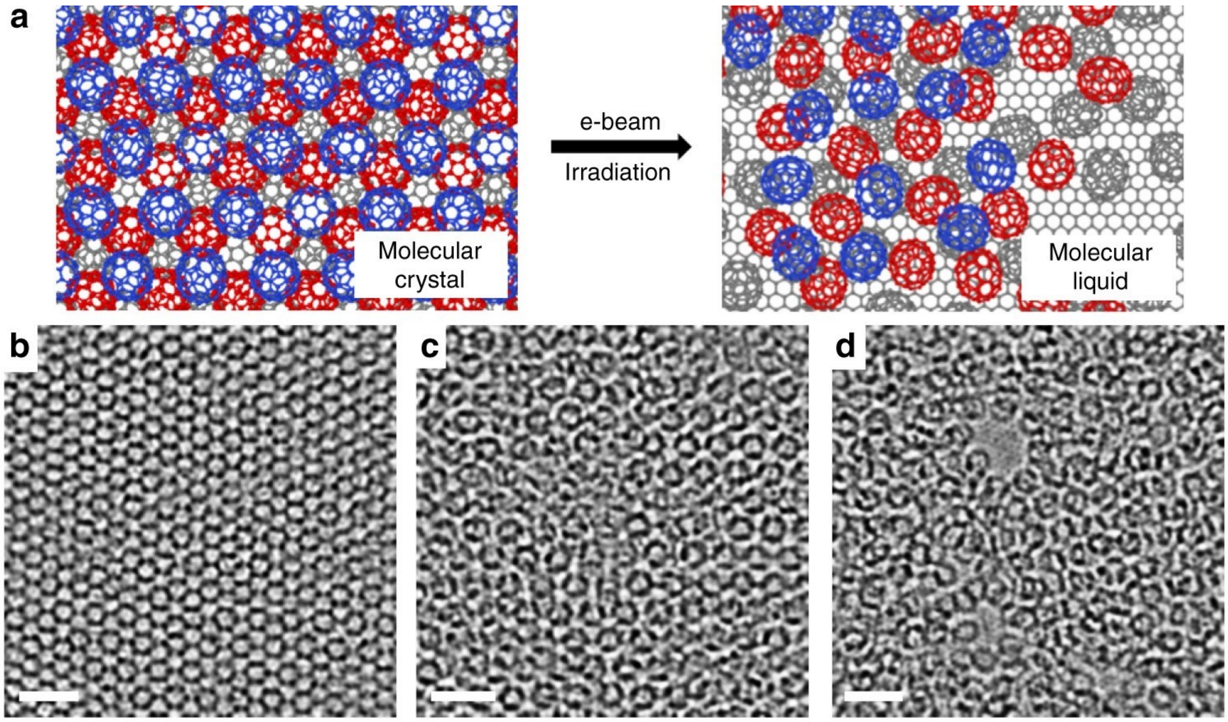

Figure 1.2: The TEM images b,c, and d from [5] show phase transition from crystal to liquid of the C_{70} molecular crystal as electron irradiation is applied.

mar proved that $\mathbb{Z}$ is universally optimal in $\mathbb{R}$, and further conjectured universal optimality of the hexagonal lattice $A_2 := \begin{bmatrix} 1 & 1/2 \\ 0 & \sqrt{3}/2 \end{bmatrix} \mathbb{Z}^2$, E_8, and the Leech lattice in dimensions 2, 8, and 24, respectively. This conjecture was natural for A_2 because similar conjectures of its optimality in numerous areas are long-standing, and it frequently appears as a ground state in the real-world study of 2-dimensional solids, as seen in our figures. Moreover, it is a classical result of Thue and Tóth that A_2 solves the circle packing problem in the plane [13]. For $d = 8, 24$, the Cohn-Kumar conjecture made sense because E_8 and the Leech Lattice have exceptional properties, and existing so-called *linear programming bounds* had proved that these lattices must be (at worst) very nearly optimal for sphere packing. Cohn and Kumar suspected these bounds could eventually be made sharp for the packing and universal optimality problems with $d = 2$[1]$, 8, 24$, as they had for $\mathbb{Z}$ in $\mathbb{R}$.

Between 2016 and 2019, remarkable work of Viazovska, Cohn, Kumar, Miller, and Radchenko

[1] In this case, since the packing result is known classically, a sharp linear programming packing bound would only serve as proof-of-concept for the method.

proved the sphere packing conjecture and subsequently, the universal optimality conjecture, for $d = 8, 24$. This work led to Viazovska receiving the 2022 Fields Medal, and their solutions used the linear programming bound approach conjectured by Cohn and Kumar. We should note that while Cohn, Kumar, and Elkies were first to apply linear programming bounds to configurations in $\mathbb{R}^d$ [6], linear programming bounds were originally developed in the context of coding theory for point configurations on the d-dimensional sphere (e.g., see [11], [19], [33]). The production of sharp energy bounds in $\mathbb{R}^d$ requires the existence of a function which, along with its Fourier transform, satisfies strict interpolation conditions.

1.2 High-Level Summary of Results

The main work of this thesis first extends the Cohn-Kumar linear programming bounds. The new bounds apply only to certain periodic configurations, rather than arbitrary configurations of fixed density. As compensation for being applicable to a narrower class of configurations, these new bounds are substantially easier to produce. Moreover, in certain situations, the production of sharp bounds boils down to solving a multivariate polynomial interpolation problem (as opposed to a Fourier interpolation problem in the Cohn/Kumar case).

By handling this polynomial interpolation, we produce several novel optimal configurations for a wide range of potential functions. Some of our optimality theorems would be necessary consequences of A_2's conjectured universal optimality, which (in light of solutions to the seemingly more complex cases of $d = 8, 24$) remarkably remains open.

Our first theorem shows the optimality of A_2 among two classes of periodic configurations:

Theorem A (Theorems 18 and 19)**.** *The lattice A_2 is universally optimal among all configurations of the form $\omega_4 + 2A_2$ and $\omega_6 + L'$, where L' is the rectangular sublattice pictured below.*

Utilizing classical results from statistical mechanics, we provide a sequence of bivariate interpolation problems whose solutions would imply the universal optimality of A_2. Thus, while our examples are necessary for the Cohn-Kumar conjecture to hold, they also provide the base cases of a path to sufficiency.

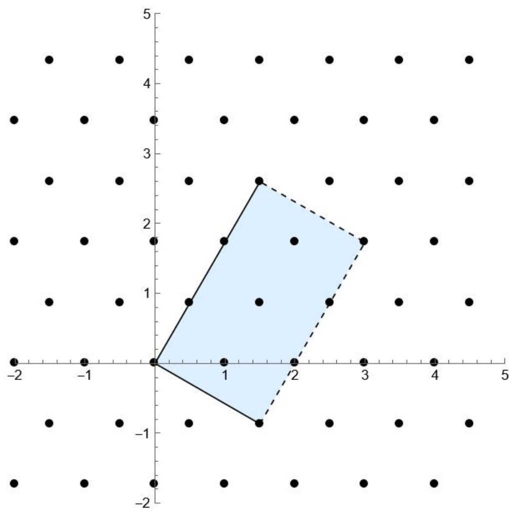

Figure 1.3: A_2 is shown with the fundamental domain of L shaded

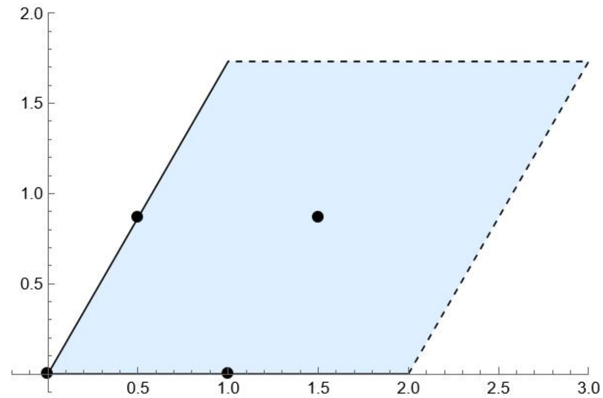

Figure 1.4: The 4 representatives of A_2 in $2A_2$ yield an optimal $2A_2$-periodic configuration

As we will detail, relatively few rigorous results exist about the optimality of A_2 for potential energy minimization, and in some sense, Theorem A is the most broad result of optimality for A_2 under Riesz or Gaussian interactions.

Next, we have claimed that our techniques make the construction of sharp bounds easier than the Cohn-Kumar bounds. One rigorous way to state this claim is via the following question:

Question 1. *Does there exist a lattice Λ and configuration $C^* := \omega_n^* + \Lambda$ such that C^* is universally optimal among configurations of the form $\Lambda + \omega_n$ but not among all configurations? If so, can the optimality of C^* among the configurations $\omega_n + \Lambda$ be proved with linear programming methods?*

An affirmative answer to both parts of the question would mean our bounds can be applied in a strictly wider context than the Cohn Kumar bounds. Prior to the work of this thesis, there were just two classes of configurations $\omega_n^* + \Lambda$ satisfying the first part of Question 1, each with $n = 2$. The proofs of these results don't use linear programming in a meaningful way, though they can be shoehorned into the framework we develop. Our final main theorem is again proved with our linear programming methods and gives a third class of examples addressing Question 1. For $\beta > 0$ and $m \in \mathbb{N}$, let $\Phi_\beta = \begin{bmatrix} 1 & 1/2 \\ 0 & \beta/2 \end{bmatrix} \mathbb{Z}^2$ and $\Lambda_{\beta,m} = \mathbb{Z} \times m\beta\mathbb{Z}$. We show:

Theorem B (Theorem 20)**.** *The configuration Φ_β is universally optimal among all configurations of the form $\omega_4 + \Lambda_{\beta,2}$ if and only if $\beta \geq \frac{1}{3}$.*

When $\beta = \sqrt{3}, 1/\sqrt{3}$, Φ_β is a scaling of the hexagonal lattice, and so the result is analogous to Theorem A. All other cases of β yield affirmative answers to both parts of Question 1. Our final contribution is the motivation and presentation of a conjecture generalizing Theorem B to arbitrary m.

Theorem A and the linear programming framework of Chapter 4 first appeared in joint work with Hardin [16], while Theorem B first appeared in [30].

1.3 Outline

In Chapter 2, we define energy minimization problems along with two related notions of universal optimality. We also summarize existing results in the area. We then introduce lattice and Fourier series basics in Chapter 3, along with the univariate Hermite interpolation framework, before proceeding to our linear programming bounds in Chapter 4. Once established, Chapter 5 states our main Theorems A and B rigorously and introduces families of interpolation problems whose solutions, put together, would prove more general theorems including a conjecture of this author. The proofs of our main theorems use the machinery from Chapter 4 and each require the production of a certificate function g which satisfies a number of interpolation and definiteness conditions. The verification of these conditions are the most technical portion of the work and are contained in Chapters 6, 7, and 8. These chapters reduces the proofs to the verification of inequalities evaluated at finitely many points. The appendix includes some technical bounds on theta functions and resulting computations, along with proofs for some of our key tools. The actual verification of the inequalities is carried out with interval arithmetic in the Mathematica notebooks [17] and [31].

Chapter 2

Energy Basics and Universal Optimality

2.1 Periodic and Euclidean Energy

Periodic energy of finite configurations. Let $F\colon \mathbb{R}^d \to (-\infty, \infty]$ be a lower-semicontinuous potential. For a finite multiset $\omega_n = \{x_1, ..., x_n\} \subseteq \mathbb{R}^d$ of cardinality n, we consider the F*-energy* of ω_n defined by

$$E_F(\omega_n) := \sum_{i=1}^{n} \sum_{\substack{j=1 \\ j\neq i}}^{n} F(x_i - x_j).$$

If for some lattice $\Lambda \subseteq \mathbb{R}^d$ (a lattice is a discrete, additive, rank d subgroup of $\mathbb{R}^d$, more on lattices in Chapter 3), F is Λ-periodic (i.e., $F(\cdot + v) = F$ for all $v \in \Lambda$), then we also refer to the F*-energy* as *periodic energy*. In this case, without loss of generality, we may assume that ω_n lies in the flat tori given by some specified fundamental domain $\Omega_\Lambda := \mathbb{R}^d/\Lambda$, since replacing a point $x \in \omega_n$ with any point in $x + \Lambda$ does not change $E_F(\omega_n)$.

The *minimal discrete* n*-point* F*-energy* is subsequently defined as

$$\mathcal{E}_F(n) := \inf\{E_F(\omega_n) \mid \omega_n \subseteq \mathbb{R}^d,\ |\omega_n| = n\}, \tag{2.1}$$

and an n-point configuration ω_n satisfying $E_F(\omega_n) = \mathcal{E}_F(n)$ is called F*-optimal*. We consider potentials F generated by various $f\colon [0,\infty) \to [0,\infty]$ with d-rapid decay (i.e. $f(r^2) \in \mathcal{O}(r^{-s}), r \to \infty$, for some $s > d$) using

$$F_{f,\Lambda}(x) := \sum_{v\in\Lambda} f(|x+v|^2). \tag{2.2}$$

Of special importance to us is the case when f is the exponential, mapping $t \to e^{-at}$, and we'll denote the resulting potential $F_{a,\Lambda}$.

Average energy of infinite configurations. The periodic energy of a finite configuration ω_n relates to the average energy of the infinite periodic configuration $\omega_n + \Lambda$. Following the conventions of [10], first take $B(x, r)$ be the ball of radius $r > 0$ centered at x. If C is an infinite multiset in $\mathbb{R}^d$ such that every ball intersects finitely many points, we call it an *infinite configuration*. Define $C_r : C \cap B(0, r)$ and the *density of* C as

$$\lim_{r\to\infty} \frac{|C_r|}{\mathrm{Vol}(B(0,r))},$$

assuming the limit exists and is finite. Then for a configuration C of density ρ, the *lower f-energy of C* is

$$E_f^l(C) := \liminf_{r\to\infty} \frac{E_f(C_r)}{|C_r|}.$$

If the limit exists, we'll write it as $E_f(C)$ and call it the *average f-energy of C* or *euclidean energy*. If $C' \subseteq \mathbb{R}^d$ has density ρ, we say C' is f-optimal if $E_f(C')$ exists and $E_f(C') \leq E_f^l(C)$ for all configurations $C \subseteq \mathbb{R}^d$ of density ρ. We will frequently abuse notation by identifying an $f\colon \mathbb{R} \to (-\infty, \infty]$ of d-rapid decay with the corresponding radial potential mapping $x \in \mathbb{R}^d$ to $f(|x|^2)$.

We have the following connection, which implies that if ν_n is $F_{f,\Lambda}$-optimal, then $\nu_n + \Lambda$ has minimal average f-energy among all configurations of the form $\omega_n + \Lambda$, called *n-point Λ-periodic configurations*. (cf. [8, Lemma 9.1] or [3, Chapter 10]).

Proposition 2. *Let $C = \omega_n + \Lambda$ and f have d-rapid decay. Then $E_f(C)$ exists and*

$$E_f(C) = \frac{1}{n}\left(E_{F_{f,\Lambda}}(\omega_n) + n \sum_{0\neq v\in\Lambda} f(v)\right).$$

2.2 Notions of Universal Optimality

Two notions of Universal optimality. As discussed in the introduction, much recent study on the energy of infinite configurations has focused on the concept of universal optimality, originally introduced in [6].

Definition 2.2.1. Let C be an infinite configuration, Λ be a lattice, and for each $a > 0$, let $f_a \colon x \to e^{-a|x|^2}$.

- We say C is *universally optimal* if C is f_a-optimal for every $a > 0$.
- We say that an n-point Λ-periodic configuration $\omega_n + \Lambda$ is Λ-*universally optimal* if for every $a > 0$, $\omega_n + \Lambda$ has minimal average f_a-energy among the set of n-point Λ-periodic configurations. In other words, $\omega_n + \Lambda$ is universally optimal among n-point Λ-periodic configurations.

Both properties are scale and rotation invariant. The phrasing of 'universal' is apt because of the scale invariance and also a theorem of Bernstein [2], which uses the Laplace transform to show that if Λ is universally optimal, then Λ minimizes f-energy for all f which are completely monotone [1] functions of distance squared with rapid decay and likewise for Λ-universally optimal configurations. This class of functions includes the much-studied Riesz potentials which map $x \to |x|^{-s/2}$, $s > d$) (cf. [3] and [20] for an overview). Note by Proposition 2 that $\omega_n^* + \Lambda$ is Λ-universally optimal if and only if ω_n^* is $F_{a,\Lambda}$-optimal for all $a > 0$, and so we will also call the finite configuration ω_n^* Λ-universally optimal. Universal optimality is a remarkable property for a configuration to possess because when the gaussian parameter a is large, energy is dominated by the contributions from each particle's nearest neighbors, and so local structure should dominate. In fact, taking $a \to \infty$ shows that a universally optimal periodic configuration must solve the d-dimensional packing problem. On the other hand, for small a, f_a is nearly constant on a large ball and so global structure comes into play.

Existing Results. As mentioned in the introduction, just three examples of universally optimal configurations are known: $\mathbb{Z}$, E_8, and the Leech lattice in dimensions 1,8, and 24, respectively. The hexagonal lattice in $\mathbb{R}^2$ is also conjectured to be universally optimal. In most other dimensions, it is likely that no configuration is universally optimal, and in certain dimensions ($d = 3, 5, 6, 7$) it

[1] f is completely monotone on an interval I if its derivatives satisfy $(-1)^n f^{(n)(x)} \geq 0$ for all $n \in \mathbb{N}$ and $x \in I$. Likewise f is absolutely monotone if $f^{(n)(x)} \geq 0$ for all $n \in \mathbb{N}$ and $x \in I$.

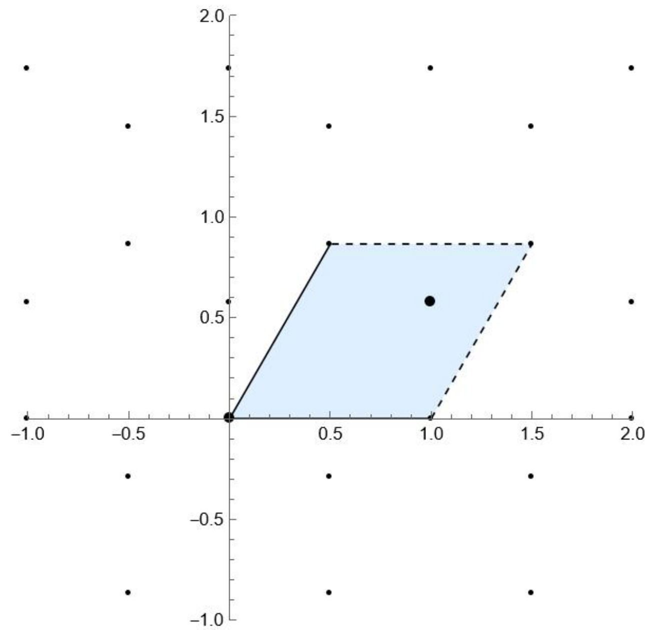

Figure 2.1: Example 1 is pictured. Filling in the center of each hexagon yields a scaling of A_2 and demonstrates the index 3 sublattice for which A_2 is known to be Λ-universally optimal.

has been proved that no *lattice* is universally optimal (though other configurations have not been ruled out).

Note that any universally optimal lattice Φ is Λ-universally optimal for any of its sublattices Λ (eg E_8 is $2E_8$-universally optimal). Indeed, Φ being universally optimal means it has minimal f_a-average energy over all configurations of fixed density, which of course includes all periodic configurations with the same density as Φ.

Thus, the conjectured universal optimality of A_2 would imply that A_2 is Λ-universally optimal for each of its sublattices. To this end, results on the minima of the A_2 lattice theta function were used to show that A_2 is Λ'-universally optimal for an index 3 sublattice Λ', which is a rotation and scaling of A_2 itself (see [1] for the key result on theta functions or [28] for a proof in the context of energy). Likewise, it can also be shown immediately from classical results on the $\mathbb{Z}$ lattice theta function that A_2 is Λ-universally optimal for an index 2 rectangular sublattice Λ (see Example 2). Every other sublattice remained open prior to this work.

These examples raise Question 1 from the introduction, which asks if there exist Λ-universally optimal configurations that are not universally optimal? We have just 2 known examples, each of the form $\omega_2 + \Lambda$.

Example 1. Set $\Lambda = A_2$ and $\omega_2^* = \{(0,0), (1/2, \sqrt{3}/6)\}$ or $\{(0,0), (1, \sqrt{3}/3)\}$, consisting of the origin and either of the wells of A_2, yielding a honeycomb structure (see [1] for the key result on theta functions or [28] for a proof in the context of energy).

Example 2. Let $\Lambda = \{r_1\mathbb{Z}\times\cdots r_d\mathbb{Z}\}$ be a rectangular lattice in $\mathbb{R}^d$ and $\omega_2^* = \{(0,0), 1/2(r_1, \ldots, r_d)\}$, consisting of the origin and the centroid of Λ's canonical fundamental domain.

Relation Between the Different Notions. We have already seen that universally optimal lattices Φ yield Λ-universally optimal configurations when Λ is a sublattice of Φ. Using classical physics results of [14], we show in Appendix A that the converse holds as well:

Theorem 3 (Proposition A)**.** *The following are equivalent:*

1. Λ *is universally optimal*
2. *For each sublattice* $\Phi \subseteq \Lambda$*,* Λ *is* Φ*-universally optimal.*
3. *There exists a sublattice* $\Phi \subseteq \Lambda$ *such that for infinitely many* $n \in \mathbb{N}$*,* Λ *is* $n\Phi$*-universally optimal.*

Thus, a universally optimal lattice yields infinitely many periodic energy problems for which we can find exact minimizers, and on the other hand, solutions to a particular sequence of periodic energy problems prove the universal optimality of a lattice. This second characterization is a main motivation for studying Λ-universal optimal in the context of the hexagonal lattice.

Other Optimality Results for A_2*.* Having discussed the current state of affairs for universal optimality, we find it convenient to mention notable optimality results for A_2 in other contexts: As mentioned, A_2 solves the circle packing problem in $\mathbb{R}^2$. Montgomery showed A_2 is universally optimal among lattices [23] and Theil showed optimality for a class of Lennard-Jones type potentials [32]. Part of why we find Theorem A of interest is that the class of 2-d lattices (up to scaling) is a 2-parameter family, while up to isometry, periodic configurations $\omega_4 + 2A_2$ and $\omega_6 + L$ form 6 and 10-dimensional families, respectively. So our optimality results are in some sense significantly more broad then the standard results for A_2 with a repulsive potential.

Chapter 3

Lattice Basics, Theta Functions, and Univariate Interpotlation

3.1 Preliminaries: Lattices and Fourier Series

We first gather some basic definitions and properties of lattices in $\mathbb{R}^d$, following the presentation of [10].

Definition 3.1.1. Let $\Lambda \subset \mathbb{R}^d$.

- Λ is a *lattice in* $\mathbb{R}^d$ if $\Lambda := V\mathbb{Z}^d = \left\{\sum_{i=1}^d a_i v_i \mid a_1, a_2, \ldots, a_d \in \mathbb{Z}\right\}$ for some nonsingular $d \times d$ matrix V with columns $v_1, \ldots v_d$. We refer to V as a *generator* or *generating matrix* for Λ.

- Once a choice of generator V is specified, we let $\Omega_\Lambda := V[0,1)^d$ denote the parallelepiped *fundamental domain* for Λ. The *co-volume of* Λ defined by $|\Lambda| := |\det V|$ is the volume of Ω_Λ which is, in fact, the same for any Lebesgue measurable fundamental domain[1] for $\mathbb{R}^d/\Lambda$ where Λ acts on $\mathbb{R}^d$ by translation. A lattice Λ' is an index k *sublattice* of Λ if $\Lambda' \subseteq \Lambda$ and $|\Lambda'|/|\Lambda'| = k$.

- The *dual lattice* Λ^* of a lattice Λ with generator V is the lattice generated by $V^{-T} = (V^T)^{-1}$ or, equivalently, $\Lambda^* := \{v \in \mathbb{R}^d \mid w \cdot v \in \mathbb{Z} \text{ for all } w \in \Lambda\}$.

- We denote by S_Λ the *symmetry group of* Λ consisting of isometries on $\mathbb{R}^d$ fixing Λ and denote by G_Λ the subgroup of S_Λ fixing the origin (and thus can be considered as elements of the orthogonal group $O(d)$). Note that $G_\Lambda = S_\Lambda/\Lambda$ where again we identify $v \in \Lambda$ with the translation $\cdot + v$. Further, note that $G_{\Lambda^*} = G_\Lambda$ since elements of $O(d)$ preserve inner products.

[1] A *fundamental domain* for a group G acting on a set X is a subset of X consisting of exactly one point from each G-orbit. Note that X/G will be used to denote both a fundamental domain and the set of G orbits in X.

Let Λ be a lattice in $\mathbb{R}^d$ with generator V and fundamental domain Ω_Λ. We let $L^2(\Omega_\Lambda)$ denote the Hilbert space of complex-valued Λ-periodic functions on $\mathbb{R}^d$ which are square integrable on Ω_Λ and have inner product $\langle f, g\rangle = \int_{\Omega_\Lambda} f(x)\overline{g(x)}\,dx$. Then $\{e^{2\pi i v\cdot x} \mid v \in \Lambda^*\}$ forms an orthogonal basis of $L^2(\Omega_\Lambda)$ yielding the Fourier expansion of a function $g \in L^2(\Omega_\Lambda)$:

$$g(x) = \sum_{v\in\Lambda^*} \hat{g}_v e^{2\pi i v\cdot x} \tag{3.1}$$

with Fourier coefficients $\hat{g}_v := \frac{1}{|\Lambda|}\int_{\Omega_\Lambda} g(x)$ for $v \in \Lambda^*$. Equality in (3.1) and the implied unconditional limit on the right hand side both hold in $L^2(\Omega_\Lambda)$. Of course, elements of $L^2(\Omega_\Lambda)$ are actually equivalence classes of functions. If $g \in L^2(\Omega_\Lambda)$ contains an element of $C(\mathbb{R}^d)$, then we identify g with its continuous representative and write $g \in L^2(\Omega_\Lambda) \cap C(\mathbb{R}^d)$. As will be the case in our applications, if $g \in L^2(\Omega_\Lambda)$ is such that $\sum_{v\in\Lambda^*} |\hat{g}_v| < \infty$, then the right-hand side of (3.1) converges uniformly and unconditionally to g and so $g \in L^2(\Omega_\Lambda) \cap C(\mathbb{R}^d)$ and (3.1) holds pointwise for every $x \in \mathbb{R}^d$.

We say that $g \in L^2(\Omega_\Lambda)$ is *conditionally positive semi-definite (CPSD)* if the Fourier coefficients $\hat{g}_v \geq 0$ for all $v \in \Lambda^* \setminus \{0\}$ and $\sum_{v\in\Lambda^*} \hat{g}_v < \infty$ and say that a CPSD g is *positive semi-definite (PSD)* if $\hat{g}_0 \geq 0$.[2] Note that the product of two PSD functions in $L^2(\Omega_\Lambda)$ is PSD.

3.2 Lattice symmetry, symmetrized basis functions, and polynomial structure

Let Λ be a lattice in $\mathbb{R}^d$, $f : [0,\infty) \to [0,\infty]$ have d-rapid decay, and $\sigma \in G_\Lambda$. Since $\sigma^{-1} \in G_\Lambda$ and σ is an isometry, we have

$$F_{f,\Lambda}(\sigma x) = \sum_{v\in\sigma^{-1}\Lambda} f(|\sigma x + \sigma v|^2) = \sum_{v\in\Lambda} f(|x+v|^2) = F_{f,\Lambda}(x).$$

Since $F_{f,\Lambda}$ is also Λ-periodic, we obtain (see [28]):

[2] If g is PSD in the above sense, then for any configuration $\omega_n = (x_1, \ldots, x_n)$ the matrix $G = (g(x_i - x_j))$ is positive semi-definite in the sense that $v^T G v \geq 0$ for any v whose components sum to 0. Conversely, Bochner's Theorem shows that any g with this property is PSD in our sense.

Proposition 4. *Suppose $f\colon [0,\infty) \to [0,\infty]$ has d-rapid decay and Λ is a lattice in $\mathbb{R}^d$. Then for all $\sigma \in G_\Lambda$, $v \in \Lambda$ and $x \in \mathbb{R}^2$, we have $F_{f,\Lambda}(\sigma x + v) = F_{f,\Lambda}(x)$ showing that $F_{f,\Lambda}$ is S_Λ-invariant.*

We next recall that $g \in L^2(\Omega_\Lambda)$ is σ-invariant for $\sigma \in G_\Lambda$ if and only if the Fourier coefficients of g are σ-invariant, as described in the next proposition, also proved in [28].

Proposition 5. *Suppose $g \in L^2(\Omega_\Lambda)$ and $\sigma \in G_\Lambda$. Then $g(\sigma x) = g(x)$ for a.e. $x \in \mathbb{R}^d$ if and only if $\hat{g}_{\sigma v} = \hat{g}_v$ for all $v \in \Lambda^*$.*

Proof. Since $\sigma^{-1} \in G_{\Lambda^*} = G_\Lambda$, we have

$$g(\sigma x) = \sum_{v \in \Lambda^*} \hat{g}_v e^{2\pi i v\cdot(\sigma x)} = \sum_{v \in \sigma^{-1}\Lambda^*} \hat{g}_v e^{2\pi i (\sigma v)\cdot(\sigma x)} = \sum_{v \in \Lambda^*} \hat{g}_{\sigma v} e^{2\pi i v \cdot x}.$$

The proposition then follows from uniqueness properties of the Fourier expansion. $\square$

Let Γ be a subgroup of G_Λ. For $v \in \Lambda^*$, let C_v^Γ be the Λ-periodic function defined by

$$C_v^\Gamma(x) := \frac{1}{|\Gamma|} \sum_{\sigma \in \Gamma} e^{2\pi i (\sigma v)\cdot x} = \frac{1}{|\Gamma(v)|} \sum_{v' \in \Gamma(v)} e^{2\pi i v' \cdot x}, \quad x \in \mathbb{R}^d. \tag{3.2}$$

where $\Gamma(v)$ denotes the orbit $\Gamma(v) = \{\sigma v \mid \sigma \in \Gamma\}$. We write C_v for C_v^Γ when Γ is unambiguous. If $g \in L^2(\Omega_\Lambda)$ and g is G_Λ-invariant (i.e., if $g(\sigma x) = g(x)$ for all $\sigma \in G_\Lambda$ and all x), then we may rewrite (3.1) as

$$g(x) = \sum_{v \in \Lambda^*/\Gamma} |\Gamma(v)|\, \hat{g}_v\, C_v^\Gamma(x). \tag{3.3}$$

We next consider the case of a *rectangular lattice* by which we mean a lattice of the form $\Lambda_R = (a_1\mathbb{Z}) \times \cdots \times (a_d\mathbb{Z})$ with $a_1, \ldots, a_d > 0$. The symmetry group of a rectangular lattice in $\mathbb{R}^d$ contains the subgroup H of order 2^d generated by the coordinate reflections

$$R_j(x_1, \ldots, x_j, \ldots, x_d) = (x_1, \ldots, -x_j, \ldots, x_d), \qquad j = 1, 2, \ldots, d. \tag{3.4}$$

Let $v \in \Lambda_R^* = (1/a_1)\mathbb{Z} \times \cdots \times (1/a_d)\mathbb{Z}$, and note that $v = (k_1/a_1, k_2/a_2, \ldots, k_d/a_d)$ for some

$k_1, \ldots, k_d \in \mathbb{Z}$. Recall the ℓ-th Chebyshev polynomial of the first kind defined by $\cos(\ell\theta) = T_\ell(\cos\theta)$ for $\ell = 0, 1, 2, \ldots$. A straightforward induction on d gives

$$C_v^H(x) = \prod_{i=1}^{d} \cos(2\pi k_i x_i / a_i) = \prod_{i=1}^{d} T_{|k_i|}(\cos(2\pi x_i/a_i)), \tag{3.5}$$

and so we have the following proposition:

Proposition 6. *Let $\Lambda_R = (a_1\mathbb{Z}) \times \cdots (a_d\mathbb{Z})$ with $a_1, \ldots, a_d > 0$. If $v \in \Lambda_R^*$, then $v = (k_1/a_1, k_2/a_2, \ldots, k_d/a_d)$ for some $k_1, \ldots, k_d \in \mathbb{Z}$ and*

$$C_v^H(x) = \prod_{i=1}^{d} T_{|k_i|}(t_i), \tag{3.6}$$

where $t_i = \cos(2\pi x_i/a_i) \in [-1, 1]$ for $i = 1, 2, \ldots, d$.

We next deduce a polynomial structure for C_v^Λ for lattices Λ that are invariant under the coordinate reflections R_j; i.e., such that $H \subseteq G_\Lambda$.

Proposition 7. *Let $\Lambda \subseteq \mathbb{R}^d$ be a lattice such that $H \subseteq G_\Lambda$. Then Λ contains a rectangular lattice $\Lambda_R = (a_1\mathbb{Z}) \times \cdots \times (a_d\mathbb{Z})$ and the function $C_v^{G_\Lambda}(x)$ is a polynomial in the variables $t_j = \cos(2\pi x_j/a_j)$ for $j = 1, 2, \ldots, d$ and any $v \in \Lambda^*$.*

Proof. We first show that Λ must contain some rectangular sublattice (i.e., of the form $\Lambda_R = (a_1\mathbb{Z}) \times \cdots \times (a_d\mathbb{Z})$). Since Λ is full-rank, for each $j = 1, 2, \ldots, d$, there is some $w^j \in \Lambda$ such that $a_j := 2w^j \cdot e^j \neq 0$ where e^j denotes the j-th coordinate unit vector. Then $a_j e^j = w^j - R_j w^j \in \Lambda$, and so the rectangular lattice $(a_1\mathbb{Z}) \times \cdots \times (a_d\mathbb{Z})$ is a sublattice of Λ.

Let $v \in \Lambda^*$. Since $\Lambda_R \subseteq \Lambda$, $\Lambda^* \subseteq \Lambda_R^*$, so $v \in \Lambda_R^*$. Let $C = \{\sigma_1, \ldots, \sigma_{[G_\lambda : H]}\}$ be a set of right coset representatives of H in G_Λ, so that $|C||H| = |G|$. Then we have

$$\begin{aligned} C_v^{G_\Lambda} &= \frac{1}{|G_\Lambda|} \sum_{g \in G_\Lambda} e^{2\pi i g v \cdot x} \\ &= \frac{1}{|C|} \sum_{\sigma \in C} \frac{1}{|H|} \sum_{h \in H} e^{2\pi i h \sigma v \cdot x} \\ &= \frac{1}{|C|} \sum_{\sigma \in C} C_{\sigma v}^H. \end{aligned} \tag{3.7}$$

Proposition 6 implies $C_{\sigma v}^H$ is polynomial in the variables $t_j = \cos(2\pi x_j / a_j)$ and thus so is $C_v^{G_\Lambda}$. □

With Λ and Λ_R as in Proposition 7, we consider the change of variables

$$t_i := \cos(2\pi x_i / a_i), \qquad i = 1, ..., d. \tag{3.8}$$

We then let $T_{a_1,\ldots,a_d} \colon \mathbb{R}^d \to \mathbb{R}^d$ be defined by

$$T_{a_1,\ldots,a_d}(x_1, ..., x_d) := (t_1, \ldots, t_d). \tag{3.9}$$

For any Λ_R-periodic function h with H-symmetry, $\tilde{h}$ will refer to the function defined on $[-1, 1]^d$ by

$$\tilde{h}(t) = h\left(\frac{a_1 \arccos t_1}{2\pi}, \ldots, \frac{a_d \arccos t_2}{2\pi}\right),$$

which ensures $\tilde{h}(t) = h(x)$. We say that $\tilde{h}$ is (C)PSD if h is (C)PSD.

By Proposition 7, the maps

$$P_v^\Lambda := \tilde{C}_v^{G_\Lambda}, \qquad v \in \Lambda^*, \tag{3.10}$$

are polynomials in the variables $t_1, \ldots, t_d$. It then follows that the collection of polynomials $\{P_v^\Lambda \mid v \in \Lambda^*/G_\Lambda\}$ is orthogonal with respect to the measure $(1-t_1^2)^{-1/2} \cdots (1-t_d^2)^{-1/2} dt_1 \cdots dt_d$ on $[-1, 1]^d$. Furthermore, $\tilde{h}$ is CPSD if and only if its expansion in terms of these polynomials has coefficients that are non-negative and summable.

We shall also write P_v when the choice of Λ is clear. Similarly, the $T_{a_1,\ldots,a_d}$ image of any subset

$D \subseteq \mathbb{R}^d$. In any case where we do so, the choice of rectangular lattice (and hence the choice of a_i's will be clear).

3.3 Divided differences and Univariate Interpolation

We review some basic results concerning one-dimensional polynomial interpolation (e.g., see [3, Section 5.6.2]). Let $f \in C^m[a,b]$ for some a, b be given along with some multiset

$$T = \{t_0, t_1, ..., t_m\} \subseteq [a,b].$$

Then there then exists a unique polynomial $H_T(f)(t)$ of degree at most m (called a *Hermite interpolant of* f) such that for each $\alpha \in T$, we have $H_T^{(\ell)}(f)(\alpha) = f^{(\ell)}(\alpha)$ for $0 \leq \ell < k_\alpha$ where k_α denotes the multiplicity of α in T. Let $f[t_0, ..., t_m]$ denote the coefficient of t^m in $H_T(f)(t)$. This coefficient is called the *m-th divided difference* of f for T. Then $H_T(f)$, may be expressed as

$$H_T(f)(t) = \sum_{k=0}^{m} f[t_0, t_1, ..., t_k] p_k(T; t) \tag{3.11}$$

where the *partial products* p_k are defined by

$$p_0(T;t) := 1 \text{ and } p_j(T;t) := \prod_{i<j}(t - t_i), \quad j = 1, 2, ..., m. \tag{3.12}$$

Then a generalization of the mean value theorem implies that there is some $\xi \in [a,b]$ such that

$$\frac{f^{(m)}(\xi)}{m!} = f[t_0, t_1, ..., t_m]. \tag{3.13}$$

Putting these together, we arrive at the classical *Hermite error formula*:

$$f(t) - H_T(f)(t) = f[t_0, t_1, ..., t_m, t] \prod_{i=0}^{m}(t - t_i) = \frac{f^{(m+1)}(\xi)}{(m+1)!} \prod_{i=0}^{m}(t - t_i). \tag{3.14}$$

In the case that f is absolutely monotone on $[a, b]$, such as with $\tilde{f}_1$ and $\tilde{f}_2$, then the sign of $f(t) - H_T(f)(t)$ equals the sign of $\prod_{i=0}^{m}(t - t_i)$.

Chapter 4

Linear Programming Bounds

We are now ready to carry out a computation that yields our linear programming bounds for the energy of an n-point Λ-periodic configuration. Upon proving them, we will examine conditions under which the bounds are sharp for a lattice configuration and compare the conditions to those from the Cohn-Kumar bounds for the energy of an arbitrary infinite configuration.

If $g \in L^2(\Omega_\Lambda)$ is CPSD and ω_n is an arbitrary n-point configuration in $\mathbb{R}^d$, then the following fundamental lower bound holds:

$$\begin{aligned} E_g(\omega_n) &= \sum_{x \neq y \in \omega_n} g(x-y) = -ng(0) + \sum_{x,y \in \omega_n} g(x-y) \\ &= -ng(0) + \sum_{v \in \Lambda^*} \hat{g}_v \sum_{x,y \in \omega_n} e^{2\pi i v \cdot x} e^{-2\pi i v \cdot y} \\ &= -ng(0) + \sum_{v \in \Lambda^*} \hat{g}_v \left| \sum_{x \in \omega_n} e^{2\pi i v \cdot x} \right|^2 \\ &\geq n^2 \hat{g}_0 - ng(0). \end{aligned} \tag{4.1}$$

For $v \in \mathbb{R}^d$ we refer to

$$M_v(\omega_n) := \sum_{x \in \omega_n} e^{2\pi i v \cdot x},$$

as the *v-moment of* ω_n. Note that equality holds in (4.1) if and only if $\hat{g}_v M_v(\omega_n) = 0$ for all $v \in \Lambda^* \setminus \{0\}$. This equality condition and (4.1) immediately yield the next proposition. The calculations in (4.1) are similar to the proof of the linear programming bounds for energy found in [8, Proposition 9.3] and are closely related to Delsarte-Yudin energy bounds for spherical codes (cf. [3, Chapters 5.5 and 10.4]).

Proposition 8. *Let $F\colon \mathbb{R}^d \to [0,\infty]$ be Λ-periodic, and suppose $g \in L^2(\Omega_\Lambda)$ is CPSD such that*

$g \leq F$ on Ω_Λ Then for any n-point configuration ω_n, we have

$$E_F(\omega_n) \geq E_g(\omega_n) \geq n^2\hat{g}_0 - ng(0) \tag{4.2}$$

with equality holding throughout (4.2) if and only if the following two conditions hold:

(a) $g(x-y) = F(x-y)$ *for all* $x \neq y \in \omega_n$,

(b) $\hat{g}_v M_v(\omega_n) = 0$ *for all* $v \in \Lambda^* \setminus \{0\}$.

If (a) and (b) hold, then $E_F(\omega_n) = \mathcal{E}_F(n)$.

While this proposition is phrased in terms of the F-energy of finite configurations for Λ-periodic potentials F, we emphasize that Proposition 2 implies such bounds are equivalent to bounds on average f-energy for Λ-periodic configurations.

Proposition 8 is the most general statement of our linear programming bounds, with minimal stipulations on F, Λ, and ω_n. Our attention now turns toward refining the conditions of the bounds when we have extra information on these objects. First, we consider the case where our configuration is obtained from an appropriate lattice and use this refinement to compare our bounds to the Cohn-Kumar bounds.

4.1 Moments for Lattice Configurations and Comparison with Cohn-Kumar Bounds

Let $\omega(\Phi, \Lambda) = \Phi/\Lambda$ where Λ is an index n sublattice of Φ. In other words, $\omega(\Phi, \Lambda)$ is a set of representatives of Φ in Λ. A first easy consequence of having $\omega_n = \omega(\Phi, \Lambda)$ in Proposition 8 is that the equality condition (a) becomes $g(x) = F(x)$ for all $x \in \omega(\Phi, \Lambda)$. We also characterize[1] when $M_v(\omega(\Phi, \Lambda)) = 0$ for $v \in \Lambda^*$.

[1] We are aware of similar lattice computations in discrete harmonic analysis (e.g., see [22]), but the authors could not find a reference for this exact result and so include a proof.

Theorem 9. *Suppose Λ is an index n sublattice of a lattice Φ in $\mathbb{R}^d$. Let $\omega(\Phi,\Lambda) = \Phi/\Lambda$ be a set of representatives of Λ in Φ. Then for $v \in \Phi^*$, we have*

$$M_v(\omega(\Phi,\Lambda)) = \begin{cases} n, & v \in \Phi^* \\ 0, & \textit{otherwise.} \end{cases} \tag{4.3}$$

Furthermore, if $G_\Lambda \subset G_\Phi$, then for any $v \in \Lambda^*$ and $\sigma \in G_\Lambda$, we have $M_{\sigma v}(\omega(\Phi,\Lambda)) = M_v(\omega(\Phi,\Lambda))$.

Proof. Let $\Phi = V\mathbb{Z}^d$; i.e., V is a generator for Φ. Since Λ is a sublattice of Φ, there is some integer $d \times d$ matrix W such that VW is a generator for Λ. Then W can be written in Smith Normal Form as $W = SDT$ where S and T are integer matrices with determinant ± 1 (equivalently, their inverses are also integer matrices) and D is a diagonal matrix with positive integer diagonal entries $\lambda_1, \ldots, \lambda_d$. It follows that $\widetilde{V} = VS$ is a generator for Φ and $U = \widetilde{V}D$ is a generator for Λ. Choosing the fundamental domains $\Omega_\Phi = \widetilde{V}[0,1)^d$ and $\Omega_\Lambda = U[0,1)^d$, we may assume without loss of generality that $\omega(\Phi,\Lambda) \subseteq \Omega_\Lambda$, and so we obtain

$$\omega(\Phi,\Lambda) = \{\widetilde{V}j \mid j \in [0..\lambda_1] \times \cdots \times [0..\lambda_d]\},$$

where $[0..p] := \{0,1,2,\ldots,p-1\}$ for positive integers p. Let $v \in \Lambda^*$ so that $v = U^{-T}k = \widetilde{V}^{-T}D^{-1}k$ for some $k = (k_1,k_2,\ldots,k_d) \in \mathbb{Z}^d$. Then $v \cdot (\widetilde{V}j) = j \cdot (D^{-1}k)$ and so

$$\begin{aligned} M_v(\omega(\Phi,\Lambda)) &= \sum_{j \in [0..\lambda_1] \times \cdots \times [0..\lambda_d]} e^{2\pi i j \cdot D^{-1}k} = \prod_{\ell=1}^{d} \left(\sum_{j_\ell=0}^{\lambda_\ell - 1} e^{2\pi i \frac{j_\ell k_\ell}{\lambda_\ell}} \right) \\ &= \begin{cases} \lambda_1 \cdots \lambda_d, & k \in D\mathbb{Z}^d, \\ 0, & \text{otherwise,} \end{cases} \end{aligned}$$

where we used the finite geometric sum formula in the last equality. Noting that $n = \lambda_1 \cdots \lambda_d$ and that $v \in \Phi^*$ if and only if $k \in D\mathbb{Z}^d$ establishes (4.3).

Finally, if $\sigma \in G_\Lambda$ and $G_\Lambda \subset G_\Phi$, then $\sigma v \in \Phi^*$ if and only if $v \in \Phi^*$ which completes the proof. $\square$

With these two observations, we are able to restate the equality conditions in Proposition 8 as:

(a) $g(x) = F(x)$ for all $x \in \omega(\Phi, \Lambda)$

(b) for all $0 \neq v \in \Phi^*$, $\hat{g}_v = 0$.

Defining the Fourier Transform in $\mathbb{R}^d$ as

$$\hat{h}(y) = \int_{\mathbb{R}^d} h(x) e^{-2\pi i x \cdot y} dx,$$

we now state the Cohn-Kumar linear programming bounds for comparison.

Proposition 10. *Let $f(|x|)\colon \mathbb{R}^d \to [0, \infty]$ be any positive, radial potential and suppose that $g(x)\colon \mathbb{R}^d \to \mathbb{R}$ is a radial Schwartz function, (ie there is some one-variable function h such that $g(x) = h(|x|)$ for all $x \in \mathbb{R}^d$). If $g(x) \leq f(|x|)$ for all $x \in \mathbb{R}^d$ and $\hat{g}(y) \geq 0$ for all $y \in \mathbb{R}^d$, then every infinite configuration in $\mathbb{R}^d$ with density ρ has lower f-energy at least $\rho\hat{g}(0) - g(0)$. Additionally, if Λ is a lattice such that*

1. *$g(x) = f(|x|)$ for all $x \in \Lambda \setminus \{0\}$ and*

2. *$\hat{g}(y) = 0$ for all $y \in \Lambda^* \setminus \{0\}$,*

then Λ is f-optimal.

So showing f-optimality of a lattice requires infinitely many equality conditions for both the candidate auxiliary function g and its Fourier transform $\hat{g}$. These conditions, along with the inequality conditions on g and $\hat{g}$, further yield equality conditions on the radial derivatives of g and $\hat{g}$:

1. $g'(x) = f'(|x|)$ for all $x \in \Lambda \setminus \{0\}$

2. $\hat{g}'(y) = 0$ for all $y \in \Lambda^* \setminus \{0\}$,

Thus, the Cohn-Kumar bounds require infinitely many equality conditions on each of $g, \hat{g}, g'$, and $\hat{g}'$ along with inequality conditions on all of $\mathbb{R}^d$ for g and $\hat{g}$. The problem of simultaneously controlling a function and its Fourier transform is fundamentally difficult and has been made rigorous with classical and modern uncertainty principles (eg. [15], [7]). In contrast, our linear programming bounds have finitely many equality conditions for g and its directional derivatives, the latter of which come, as in the Cohn-Kumar case, by combining the equality conditions on g with the inequality condition $g \leq F$. Moreover, we note that our inequality conditions only need to hold on the compact (in the flat torus topology) region Ω_Λ. Finally, unlike the Cohn-Kumar case, we have an orthogonal basis with which to construct g, and can characterize exactly which basis elements are available for the construction via Theorem 9 . In sum, there are strong reasons for thinking the Fourier interpolation problems used to obtain our bounds on periodic configurations should be easier to solve than those presented by the Cohn-Kumar bounds.

4.2 Using Lattice Symmetries for Polynomial Structure of Bounds

Our bounds can be further refined when Λ and F have appropriate symmetry. First, we can use such symmetry to reduce our search space for an auxiliary g and the resulting region on which we must check $g \leq F$.

Remark. If $F\colon \mathbb{R}^d \to [0, \infty]$ is Λ-periodic and G_Λ-invariant and $g \in L^2(\Omega_\Lambda)$ is CPSD such that $g \leq F$, then the S_Λ-invariant function

$$g^{\mathrm{sym}}(x) := \frac{1}{|G_\Lambda|} \sum_{\sigma \in G_\Lambda} g(\sigma x), \qquad x \in \mathbb{R}^d,$$

is also CPSD and satisfies $g^{\mathrm{sym}} \leq F$. Thus, we may restrict our search for functions g to use in Proposition 8 to those of the form

$$g(x) = \sum_{v \in \Lambda^*/G_\Lambda} |G_\Lambda(v)|\, \hat{g}_v\, C_v^{G_\Lambda}(x) \qquad \text{(see equation (3.3))},$$

in which case we only need verify the condition that $g \leq F$ on a fundamental domain of $\mathbb{R}^d/S_\Lambda$. For convenience, we shall write

$$W_\Lambda := \Lambda^*/G_\Lambda \text{ and } \Delta_\Lambda := \mathbb{R}^d/S_\Lambda, \tag{4.4}$$

In particular, when $\Lambda = A_2$, we will always choose the regions

$$\Delta_{A_2} := \{(x_1, x_2) \mid 0 \leq x_1 \leq \frac{1}{2}, 0 \leq x_2 \leq x_1/\sqrt{3}\} \tag{4.5}$$

$$W_{A_2} := \left\{ \begin{bmatrix} k_1 \\ k_2/\sqrt{3} \end{bmatrix} \in A_2^* \mid 0 \leq k_2 \leq k_1 \right\} \tag{4.6}$$

and when $\Lambda = (a_1\mathbb{Z}) \times \cdots \times (a_d\mathbb{Z})$, we'll consider the sets $\Delta_\Lambda := [0, a_1/2] \times \cdots \times [0, a_d/2]$,

$$W_\Lambda := \left\{ \begin{bmatrix} k_1 \\ k_2/\sqrt{3} \end{bmatrix} \mid k_1, k_2 \in \mathbb{Z} \text{ and } k_1, k_2 \geq 0 \right\}. \tag{4.7}$$

Recall that to prove configurations are Λ-universally optimal, we will be considering potentials of the form $F_{a,\Lambda}$ which, by Proposition 4.2, are both Λ and G_Λ-invariant. Thus, by the above remark, our auxiliary functions will be in the span of $\{C_v^{G_\Lambda} | v \in \Lambda^*\}$. This fact motivates us to apply the bounds to lattices Λ where the coordinate symmetry group H satisfies $H \subseteq G_\Lambda$, so that we may apply the change of variables in (3.9) and obtain a polynomial interpolation problem. We can restate our bounds in this case as:

Theorem 11. *Let $\Lambda \subset \mathbb{R}^d$ be such that $H \subseteq G_\Lambda$ where H is the coordinate symmetry group (see (3.4)) and suppose $F \colon \mathbb{R}^d \to (-\infty, \infty]$ is S_Λ invariant. By Proposition 7, Λ contains a rectangular sublattice*

$$a_1\mathbb{Z} \times \cdots \times a_d\mathbb{Z},$$

which induces the change of variables $T := T_{a_1,\ldots,a_d}$ defined in (3.9) and associated polynomials P_v^Λ defined in (3.10). Suppose $(c_v)_{v \in W_\Lambda}$ is such that (a) $c_v \geq 0$, for all nonzero $v \in W_\Lambda$, (b)

$\sum_{v\in W_\Lambda} c_v < \infty$, *and (c) the continuous function*

$$\tilde{g} := c_0 + \sum_{0\neq v\in W_\Lambda} c_v P_v^{G_\Lambda}.$$

satisfies $\tilde{g} \leq \tilde{F}$ *on* $\tilde{\Delta}_\Lambda$.

Then for any n-point configuration $\omega_n = \{x_1, \dots, x_n\} \subset \mathbb{R}^d$, *we have*

$$E_F(\omega_n) \geq E_g(\omega_n) = n^2 c_0 - n\tilde{g}(1, \dots, 1), \tag{4.8}$$

where equality holds if and only if

1. $\tilde{g}(t) = \tilde{F}(t)$ *for all* $t \in T(\{x_i - x_j \mid i \neq j \in \{1, \dots, n\}\})$ *and*

2. $c_v M_{\sigma v}(\omega_n) = 0$ *for all* $0 \neq v \in W_\Lambda$ *and* $\sigma \in G_\Lambda$.

If such a $\tilde{g}$ exists satisfying the conditions of Theorem 11, we refer to it as a 'magic' interpolant.

Remark. For simplicity, we have phrased Theorem 11 in terms of the polynomials $P_v^\Lambda := \tilde{C}_v^{G_\Lambda}$. We could just have easily done so for a subgroup of the symmetries G_Λ; that is, if $H \subseteq K \subseteq G_\Lambda$, then we could consider the polynomials $\tilde{C}_v^K$, which would result in $\tilde{g}$ of the form:

$$\tilde{g} := c_0 + \sum_{0\neq v\in \Lambda^*/K} c_v \tilde{C}_v^K. \tag{4.9}$$

Then we would show $\tilde{g} \leq \tilde{F}$ on $T(\mathbb{R}^d/K^*)$, where K^* is the group of isometries generated by K and Λ (considered as translation mappings).

Finally, we can simplify the equality conditions of Theorem 11 when our configuration is of the form $\omega(\Phi/\Lambda)$ for an appropriate Φ, as in Section 4.1:

Corollary 12. *Suppose* Λ, $T := T_{a_1,\dots,a_d}$, $\tilde{g}$, *and* F *are as in Theorem 11 and that* $\Lambda \subseteq \Phi$, *and* $G_\Lambda \subseteq G_\Phi$ *for some lattice* $\Phi \subset \mathbb{R}^d$. *Then the configuration* $\omega(\Phi, \Lambda)$ *defined in Prop. 9 is* F*-optimal if*

- $c_v = 0$ *for all* $0 \neq v \in \Phi^* \cap W_\Lambda$*, and*

- $\tilde{g}(t) = \tilde{F}(t)$ *for all* $t \in T(\Phi \cap \Delta_\Lambda) \setminus \{\mathbf{1}\}$ *where* $\mathbf{1} = (1, 1, \ldots, 1) \in \mathbb{R}^d$.

Proof. We must show these conditions imply g and $\omega(\Phi, \Lambda)$ satisfy the conditions of Proposition 8. Since $\tilde{g} \leq \tilde{F}$ on $\tilde{\Delta}_\Lambda$, certainly $g \leq F$ on Δ_Λ. Our definition of $\tilde{g}$ immediately makes g CPSD. It remains to show the two equality conditions hold. The condition $\tilde{g}(t) = \tilde{F}(t)$ for all $t \in T(\omega(\Phi/\Lambda) \cap \Delta_\Lambda) \setminus \{\mathbf{1}\}$ yields $g(x) = f(x)$ for all $x \in (\omega(\Phi/\Lambda) \cap \Delta_\Lambda) \setminus \{0\}$. Invoking the S_Λ-invariance of g, F, and Φ, we have $g(x) = f(x)$ for all $x \in \Phi \setminus \Lambda$, and every difference $x - y$ for $x \neq y \in \omega(\Phi, \Lambda)$ is contained in $\Phi \setminus \Lambda$. Thus, condition (a) of Proposition 8 is satisfied. For condition (b), since $c_v = 0$ for all $0 \neq v \in \Phi^* \cap W_\Lambda$, we have from our definition of $\tilde{g}$ that $\hat{g}_v = 0$ for all $0 \neq v \in \Phi^*$, and thus, by Theorem 9, $\hat{g}_v M_v(\omega(\Phi, \Lambda)) = 0$ for all $v \in \Lambda^* \setminus \{0\}$ as desired. $\square$

In attempting to apply Corollary 12 to show Λ-universal optimality of some configuration, and in particular, satisfying the condition $\tilde{g} \leq \tilde{F}$ on $\tilde{\Delta}_\Lambda$, it now becomes important to study the behavior of the polynomials P_v^Λ and the potentials $\tilde{F}_{a,\Lambda}$. We next show some properties of these functions in the case where Λ is rectangular or $\Lambda = A_2$, for which we need lattice theta functions.

4.3 Lattice theta functions

For $c > 0$, the classical Jacobi theta function of the third type, is defined by

$$\theta(c; x) := \sum_{k=-\infty}^{\infty} e^{-\pi k^2 c} e^{2\pi i k x}, \qquad x \in \mathbb{R}. \tag{4.10}$$

Via Poisson Summation on the integers, we have

$$\theta(c; x) = c^{-1/2} \sum_{k=-\infty}^{\infty} e^{-\frac{\pi(k+x)^2}{c}}, \tag{4.11}$$

and so, in terms of our earlier language for periodizing gaussians by lattices,

$$F_{a,\mathbb{Z}}(x) = (\pi/a)^{1/2}\theta(\frac{\pi}{a}; x). \tag{4.12}$$

We'll also use

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

It follows from the symmetries of $\theta(c,x)$ that for all $x \in \mathbb{R}$,

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

and moreover, as shown below, $\tilde{\theta}$ is absolutely monotone on $[-1,1]$. First, we recall the Jacobi triple product formula.

Theorem 13 (Jacobi triple product formula)**.** *Let $z, q \in \mathbb{C}$ with $|q| < 1$ and $z \neq 0$. Then*

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

Applying the Jacobi triple product with $q = e^{-\pi c}$ and $z = e^{\pi i x}$, gives

$$\tilde{\theta}(c;t) = \prod_{r=1}^{\infty}(1-e^{-2\pi r c})(1+2e^{-2\pi r c}t + e^{-2(2r-1)\pi c}). \tag{4.13}$$

It's elementary to verify that $\tilde{\theta}(c;\cdot)$ is entire, and that we may compute derivatives by applications of the product rule to (4.13). Hence, we arrive at the following proposition:

Proposition 14. *For any $c > 0$, the function $\tilde{\theta} = \tilde{\theta}(c;\cdot) : [-1,1] \to (0,\infty)$ is strictly absolutely monotone on $[-1,1]$ and its logarithmic derivative $\tilde{\theta}'/\tilde{\theta}$ is strictly completely monotone on $[-1,1]$.*

Proof. Our proposition is equivalent to showing that h' is strictly completely monotone, where

$h := \log \tilde{\theta}$. By Equation 4.13, Recall that $\tilde{\theta}$ can be expressed via the Jacobi triple product as

$$\tilde{\theta}(c;t) = \prod_{r=1}^{\infty}(1 - e^{-2\pi rc})(1 + 2e^{-2\pi rc}t + e^{-2(2r-1)\pi c}),$$

so

$$h = \sum_{r=1}^{\infty} \log\left[(1 - e^{-2\pi rc})(1 + 2e^{-2\pi rc}t + e^{-2(2r-1)\pi c})\right].$$

Let h_r be the rth term in this sum. It suffices to show that each h_r' is strictly completely monotone. Indeed, we have

$$h_r' = \frac{2e^{-2\pi rc}}{1 + 2e^{-2\pi rc}t + e^{-2(2r-1)\pi c}}$$

so

$$[h_r']^{(n)} = \frac{(-1)^n[2e^{-2\pi rc}]^{n+1}}{1 + 2e^{-2\pi rc}t + e^{-2(2r-1)\pi c}}$$

from which the claim follows since $1 + 2e^{-2\pi rc}t + e^{-2(2r-1)\pi c} \geq 0$ for all $r, c > 0$ and $t \geq -1$. □

If $\Lambda_R = (a_1\mathbb{Z}) \times \cdots \times (a_d\mathbb{Z})$ is a rectangular lattice, then $F_{a,\Lambda_R}(x)$ is a tensor product of such functions:

$$\begin{aligned} F_{a,\Lambda_R}(x) &= \sum_{v\in\Lambda_R} e^{-a\|x+v\|^2} = \sum_{k\in\mathbb{Z}^d}\prod_{i=1}^{d} e^{-aa_i^2(x_i/a_i+k_i)^2} \\ &= \prod_{i=1}^{d}\left(\sum_{k_i\in\mathbb{Z}} e^{-aa_i^2(\frac{x_i}{a_i}+k_i)^2}\right) = \prod_{i=1}^{d} F_{aa_i^2,\mathbb{Z}}(x_i/a_i). \end{aligned} \tag{4.14}$$

If Λ contains a rectangular sublattice Λ_R, then we may write F_Λ as a sum of such tensor products.

Proposition 15. *Suppose Λ is a lattice in $\mathbb{R}^d$ that contains a rectangular sublattice $\Lambda_R = (a_1\mathbb{Z}) \times \cdots \times (a_d\mathbb{Z})$ and let $\omega(\Lambda, \Lambda_R) = \Lambda/\Lambda_R$. Then*

$$F_{a,\Lambda}(x) = \sum_{y\in\omega(\Lambda,\Lambda_R)} F_{a,\Lambda_R}(x+y). \tag{4.15}$$

Proof. The formula follows immediately from $\Lambda = \omega(\Lambda, \Lambda_R) + \Lambda_R$. □

If $\Lambda = a_1\mathbb{Z} \times a_2\mathbb{Z}$, so that one choice of rectangular sublattice is Λ itself with resulting change of variables T, we obtain

$$F_{a,\Lambda}(x) = \frac{\pi}{a_1 a_2 a}\theta(\frac{\pi}{a_1^2 a}; \frac{x_1}{a_1})\theta(\frac{\pi}{a_2^2 a}; \frac{x_2}{a_2}), \tag{4.16}$$

and thus,

$$\begin{aligned}\tilde{F}_{a,\Lambda}(t_1, t_2) &:= F\left(\frac{a_1 \arccos(t_1)}{2\pi}, \frac{a_2 \arccos(t_2)}{2\pi}\right)\\ &= \frac{\pi}{a_1 a_2 a}\tilde{\theta}(\frac{\pi}{a_1 a}; t_1)\tilde{\theta}(\frac{\pi}{a_2 a}; t_2)\end{aligned}$$

for $t_1, t_2 \in [-1, 1]$. Thus, for fixed $t_1 \in [-1, 1]$, $\tilde{F}_{a,L}$ is strictly absolutely monotone as a function of t_2 and vice versa.

Similarly, when $\Lambda = A_2$, we consider the rectangular sublattice $\mathbb{Z} \times \sqrt{3}\mathbb{Z}$ with corresponding (t_1, t_2) change of variables and arrive at the following formulas, which also appear in [1] and [28]:

$$F(x) := F_{a,A_2}(x) = \frac{\pi}{\sqrt{3}a}\left(\theta(\frac{\pi}{a}; x_1)\theta(\frac{\pi}{3a}; \frac{x_2}{\sqrt{3}}) + \theta(\frac{\pi}{3a}; \frac{x_2}{\sqrt{3}} + \frac{1}{2})\theta(\frac{\pi}{a}; x_1 + \frac{1}{2})\right), \tag{4.17}$$

and

$$\begin{aligned}\tilde{F}(t) &:= F(\frac{\arccos t_1}{2\pi}, \frac{\sqrt{3}\arccos t_2}{2\pi})\\ &= \frac{\pi}{\sqrt{3}a}(\tilde{\theta}(\frac{\pi}{a}; t_1)\tilde{\theta}(\frac{\pi}{3a}; t_2) + \tilde{\theta}(\frac{\pi}{a}; -t_1)\tilde{\theta}(\frac{\pi}{3a}; -t_2)).\end{aligned} \tag{4.18}$$

The next corollary follows immediately from the absolute monotonicity of $\tilde{\theta}$ (see Proposition 14).

Corollary 16. *For any nonnegative integers l_1 and l_2 whose sum $l_1 + l_2$ is even, we have on all $[-1, 1]^2$ that*

$$\frac{\partial^{l_1+l_2}\tilde{F}}{\partial^{l_1}t_1\partial^{l_2}t_2} > 0.$$

Finally, we'll use the following lemma from [1] (also see [28]).

Lemma 17. *On all of* $[-1,1]\times[\frac{1}{2},1]$, *we have the inequalities*

$$\frac{\partial \tilde{F}}{\partial t_1} > 0, \frac{\partial \tilde{F}}{\partial t_2} \geq 0 \tag{4.19}$$

where the equality holds if and only if $t_1 = -1$, $t_2 = \frac{1}{2}$. *In particular, these inequalities hold on all* $\tilde{\Delta}_{A_2}$.

Proof. Since even partial deriviatives of $\tilde{F}$ are positive and every point $(t_1, t_2) \in \tilde{\Delta}_{A_2}$ satisfies $t_1 \geq -1$ and $t_2 \geq \frac{1}{2}$, it suffices to verify the inequalities

$$\frac{\partial \tilde{F}}{\partial t_1}(t_1, t_2) > 0, \frac{\partial \tilde{F}}{\partial t_2}(t_1, t_2) \geq 0$$

at $(-1, \frac{1}{2})$. See [1] or [28]. □

As observed in [28] (also see [3, Chapter 10] and [12]), Lemma 17 suffices to proves the A_2-universal optimality of the 2 and 3-point configurations discussed in Section 2.2. Indeed, it implies that for all $a > 0$, a global minimum of F_{a,A_2} occurs at $(1/2, \sqrt{3}/6)$, which is the only difference $x - y$ (up to S_{A_2} action) that occurs in either configuration, once they have been scaled so $\Lambda = A_2$. Thus, with ω_2^* as the configuration from Example 1, and ω_2 as an arbitrary 2-point configuration, we have

$$E_F(\omega_2) \geq 2F_{a,A_2}(1/2, \sqrt{3}/6) = E_F(\omega_2^*),$$

yielding the A_2-universal optimality of ω_2^* and similarly for the 3-point configuration. Moreover, by taking the constant function $g = F_{a,A_2}(1/2, \sqrt{3}/6)$, we can obtain the same result from a trivial application of our basic linear programming bound Proposition 8.

4.4 The Polynomials $P_v^{\Lambda_R}$ and $P_v^{A_2}$

When Λ is rectangular, we have already shown in Proposition 6 that the functions P_v^{Λ} are tensors of Chebyshev Polynomials. What can be said in the case when $\Lambda = A_2$? These polynomials have been studied extensively (see [21], [22], and references therein). Of particular importance to

$P_v^{A_2}$ are the polynomials $P_{v'}$ and $P_{v''}$, where $v' := [1, 1/\sqrt{3}]^T$ is the shortest non-zero vector in W_{A_2} (see (4.6) and $v'' := [2, 0]^T$ is the next shortest vector. We have

$$P_{v'} = \frac{1}{3}(-1 + 2t_2(t_1 + t_2)), \tag{4.20}$$

$$P_{v''} = \frac{1}{3}(-1 + 2t_1(t_1 - 3t_2 + 4t_2^3)). \tag{4.21}$$

Perhaps surprisingly, every other P_v can be expressed as a bivariate polynomial in $P_{v'}$ and $P_{v''}$, i.e. for any $v \in A_2^*$, there exist coefficients $c_{i,j}$ (with only finitely many nonzero) such that

$$P_v = \sum_{i,j \geq 0} c_{i,j}(-1 + 2t_2(t_1 + t_2))^i(-1 + 2t_1(t_1 - 3t_2 + 4t_2^3))^j$$

Note that since $P_{v'}$ and $P_{v''}$ contain only monomials of even total degree, the same is true of arbitrary P_v. To further understand these bivariate polynomials, we set $\alpha = P_{v'}$, $\beta = P_{v''}$ and introduce a notion of degree, first given in [25], on polynomials of the form $\alpha^{k_0}\beta^{k_1}, i, j \geq 0$.

Definition 4.4.1. The A_2-degree of $\alpha^{k_0}\beta^{k_1}$ is $2k_0 + 3k_1$.

If $v \in W_{A_2}$, then $v = k_0 v' + k_1 v''$ for some unique $k_0, k_1 \geq 0$, and so we can likewise introduce the notion of the A_2 degree of $v \in W_{A_2}$ as $2k_0 + 3k_1$. We will denote the degree function as $\mathcal{D}$ for both polynomials and elements of W_{A_2}. Now we can introduce an ordering on $\{\alpha^{k_0}\beta^{k_1} : k_0, k_1 \geq 0\}$ by A_2-degree and break ties via the power of α. Then the leading term (by A_2-degree) of P_v is $\alpha^{k_0}\beta^{k_1}$. Certainly, this is true for our first polynomials, $P_0 = 1$, $P_{v'} = \alpha$, and $P_{v''} = \beta$, and then an examination of the recursion generating the polynomials shows that the claim holds inductively (cf. [22]).

4.5 Polynomial Linear Programming in Action: The case of $\mathbb{Z}$

Before diving into our novel applications of Corollary 12, we find it instructive to review an alternate proof of the universal optimality of $\mathbb{Z}$ that proceeds through the periodic approach of Proposition 3. The main tool used here is the observation in Proposition 14 that the functions $\tilde{\theta}(c; t)$

are absolutely monotone. This proof is essentially from [28], but H. Cohn and A. Kumar were also aware of this approach [9]. The proof we give that equally spaced points are universally optimal on the unit interval is equivalent to that of [8] showing that the roots of unity are universally optimal on the unit circle. First, we note that by the scale invariance of Λ-universal optimality, showing the $2m\mathbb{Z}$-universal optimality of $\mathbb{Z}$ is equivalent to showing the $\mathbb{Z}$-universal optimality of $\frac{1}{2m}\mathbb{Z}$. This latter approach [2] with a fixed periodization lattice is preferable for our notation because the change of variables T and potentials $F_{a,\mathbb{Z}}$ are fixed with respect to m.

It's straightforward to check that the choices $\Lambda = \mathbb{Z}$, $\Phi = \frac{1}{2m}\mathbb{Z}$, and $\Lambda_r = \mathbb{Z}$ satisfy the conditions of Corollary 12. Then for our choice of representatives, let $\omega(\frac{1}{2m}\mathbb{Z}, \mathbb{Z}) = \{j/2m \mid j = 0, 1, \dots, 2m-1\}$ and $\Delta_{\mathbb{Z}} = [0, 1/2]$, so that $W_{\mathbb{Z}} = \mathbb{N} \cup \{0\}$ (see (4.7)). Then

- $t = \cos(2\pi x)$
- $P_k^{\mathbb{Z}}(t) = T_k(t)$ for $k = 0, 1, 2, \dots$
- We have $T(\frac{1}{2m}\mathbb{Z} \cap \Delta_{\mathbb{Z}}) = \{\cos(2\pi j/(2m)) \mid j = 0, 1, \dots, m\} = \{t_{j,m} \mid j = 0, 1, \dots, m\}$ where $t_{j,m} := \cos(\pi(m-j)/m)$.

Recall that the Chebyshev polynomials of the second kind are defined by the relation

$$U_k(\cos\theta)\sin\theta = \sin((k+1)\theta), \qquad k = 0, 1, 2, \dots$$

and form the family of monic orthogonal polynomials with respect to the measure $(1-t^2)dt$ on $[-1, 1]$. These polynomials can be related to Chebyshev polynomials of the first kind through the relations

$$U_k(t) = \begin{cases} 2\sum_{j=0}^{\ell} T_{2j+1} & k = 2\ell+1 \\ 1 + 2\sum_{j=1}^{\ell} T_{2j} & k = 2\ell, \end{cases}$$

[2] While we only consider even scalings of $\mathbb{Z}$, the same general approach with minor modifications could be applied to odd scalings as well, see [3]. Of course, the proof for the even scalings directly implies the result for the odd scalings by Proposition A.

showing that U_k is PSD for $k = 0, 1, 2, \ldots$. Observe that the points $-1 < t_{1,m} < \cdots < t_{m-1,m} < 1$ are also the roots of U_{m-1}. It then follows using the Christoffel-Darboux formula that the partial products $\prod_{j=1}^{k}(t - t_j)$ have expansions in $U_0, U_1, \ldots, U_k$ with positive coefficients for $j = 1, \ldots, m-2$ (see [8, Prop 3.2] or [3, Thm A.5.9]). Likewise, $\prod_{j=1}^{m-1}(t - t_j)$ is simply U_{m-1} and $(t+1) = (t - t_0)$, both of which are positive definite. Thus, such partial product is PSD as is any product of such partial products; in particular, with $T = \{t_0, t_0, t_1, t_1, \ldots, t_{m-1}, t_{m-1}\}$, the partial products $p_j(T; t)$ defined in (3.12) are PSD for $j \leq 2m$.

By Proposition 14, the function $\tilde{F}_{a,\mathbb{Z}}$ is absolutely monotone on $[-1, 1]$ and, since the divided differences of an absolutely monotone function are non-negative, it follows that the interpolant $H_T(\tilde{F}_{a,\mathbb{Z}})(t)$ defined in (3.11) is PSD. Moreover, $H_T(\tilde{F}_{a,\mathbb{Z}})(t)$ has degree at most $2m-1$, and the error formula (3.14) shows that $H_T(\tilde{F}_{a,\mathbb{Z}}) \leq \tilde{F}_{a,\mathbb{Z}}$ on [-1,1]. Thus, $H_T(\tilde{F}_{a,\mathbb{Z}})(t)$ is a magic function as desired.

Chapter 5

Main Results and Interesting Families of Interpolation Problems

We now turn our attention to applying Corollary 12 to configurations in the plane to obtain new optimality results. While our results are limited to small cardinality configurations (4 and 6 points), we also introduce sequences of increasing cardinality configurations whose base cases are our optimal configurations. Proofs of optimality for the families would yield the universal optimality of A_2 or the proof of a conjecture related to Question 1, though these famililes are not unique in this regard.

5.1 A Family of m^2-Point A_2-Periodic Configurations

Our first, and most natural, family of configurations is obtained by taking scalings of A_2 as sublattices of A_2. In the language of Corollary 12, we'll equivalently consider $\Lambda = A_2$, $\Phi_m = \frac{1}{m}A_2$, and $\Lambda_r = \mathbb{Z} \times \sqrt{3}\mathbb{Z}$. This family is natural because A_2 has the largest symmetry group of any lattice in $\mathbb{R}^2$, and so minimizes the number of nodes ($|\Phi_m \cap \Delta_\Lambda| - 1$) for our interpolation relative to the cardinality of the original configuration. Our choice of Λ_r yields the following change of variables to induce our polynomial structure, as described in Proposition 7:

$$(t_1, t_2) := \left(\cos(2\pi x_1), \cos\left(\frac{2\pi x_2}{\sqrt{3}}\right)\right). \tag{5.1}$$

We will use T to denote the change of variables $T(x) = (t_1(x_1), t_2(x_2))$.

Our main result for this family is the universal optimality of the base case:

Theorem 18. *A_2 is $2A_2$-universally optimal.*

We prove the $2A_2$-universal optimality of A_2 by constructing for each $a > 0$ a polynomial satisfying Corollary 11 of the form $\tilde{g}_a(t_1, t_2) := c_0 + c_1 P_{v'}(t_1, t_2)$ with $c_1 \geq 0$ such that $g_a \leq F_{a,A_2}$

on $\tilde{\Delta}_{A_2}$ with equality at $T(\frac{1}{2}A_2 \cap \Delta_{A_2}) = \{(-1, 1)\}$.

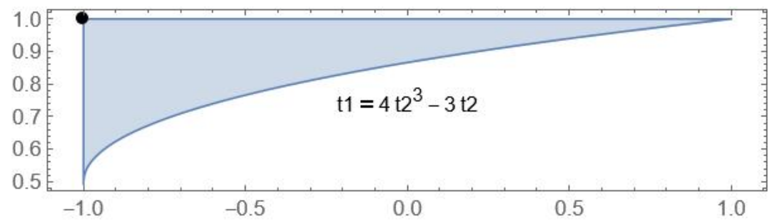

Figure 5.1: $\tilde{g}_a$ must stay below $\tilde{F}_a$ on $\tilde{\Delta}_{A_2}$ with equality at the corner point $(-1, 1)$.

For general m, recalling the background on G_2 polynomials in Sec. 4.4, we note that

$$\{v \in W_{A_2} \mid \mathcal{D}(v) < 2m\} \cap \left(\frac{1}{m}A_2\right)^* = \{0\},$$

and thus the polynomials $P_v^{A_2}$ for $v \in \{v \in W_{A_2} \mid \mathcal{D}(v) < 2m\}$ may be used in our construction of a magic $\tilde{g}$. The containment holds because if $v = k_0 v' + k_1 v''$ and $\mathcal{D}(v) < 2m$, then $k_0, k_1 < m$, and so $v \in mA_2^*$ implies $v = \vec{0}$. For the $m = 2$ base case already discussed, our interpolant $\tilde{g}_a$ satisfies

$$\tilde{g}_a \in \text{span}\{P_v : v \in W_{A_2}, \mathcal{D}(v) < 4\}$$

since it consists only of the degree 0 constant term and degree 2 term $P_{v'}(t_1, t_2)$. The remainder of the construction of $\tilde{g}_a$ and subsequent check of conditions of Corollary 11 are relegated to Section 6.

5.2 A family of $6m^2$-point periodic configurations

While the configurations $\omega(\frac{1}{m}A_2, A_2)$ optimize the number of interpolation nodes relative to the size of the configurations, the polynomials $P_v^{A_2}$ are relatively complex, and the natural spaces (we have found) of such polynomials arising from the condition $v \notin mA_2^*$, such as those $P_v^{A_2}$ with $\mathcal{D}(v) < 2m$, don't fit particularly well into existing bivariate interpolation theory. For example, the maps $P_v^{A_2}$ contain only monomials of even total degree, and so there is no way to obtain, say, the space of bivariate polynomials of total degree at most k.

This limitation motivates the family of $6m^2$-point configurations $\omega(\Phi_m, \Lambda)$ with $\Lambda = \Lambda_r = \mathbb{Z}\times\sqrt{3}\mathbb{Z} := L$ (thus yielding the same change of variables as in Section 5.1) and $\Phi_m = \frac{1}{m}\begin{bmatrix} 1/2 & 0 \\ \sqrt{3}/6 & \sqrt{3}/3 \end{bmatrix}\mathbb{Z}^2$. Our second main theorem is the proof of the base case for this family, which involves our most complex application of the linear programming bounds. As Φ_m is a rotation and scaling of A_2, this result can also be stated in terms of L'-universal optimality of A_2, where $L' := \begin{bmatrix} 1/2 & 3/2 \\ \sqrt{3}/2 & -\sqrt{3}/2 \end{bmatrix}\mathbb{Z}^2$

Theorem 19. *The lattice A_2 is L'-universally optimal, or equivalently $\frac{1}{m}\begin{bmatrix} 1/2 & 0 \\ \sqrt{3}/6 & \sqrt{3}/3 \end{bmatrix}\mathbb{Z}^2$ is L-universally optimal.*

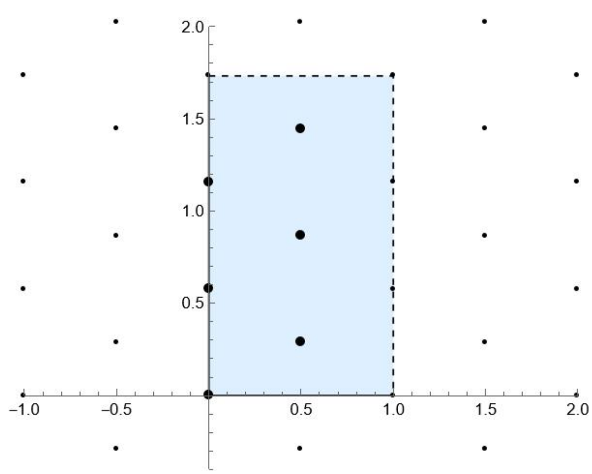

Figure 5.2: An optimal 6-point L-periodic configuration

In Chapter 7, we prove the L-universal optimality of $\omega(\Phi_m, L)$ by constructing for each $a > 0$ an interpolant of the form

$$g_a(t_1, t_2) = b_{0,0} + b_{1,0}t_1 + b_{0,1}t_2 + b_{1,1}t_1t_2 + b_{0,2}t_2^2$$

where $b_{i,j} \geq 0$ for $(i, j) \neq 0$. In that section, we will explain in greater detail why such a $\tilde{g}_a$ satisfies the conditions of Corollary 11.

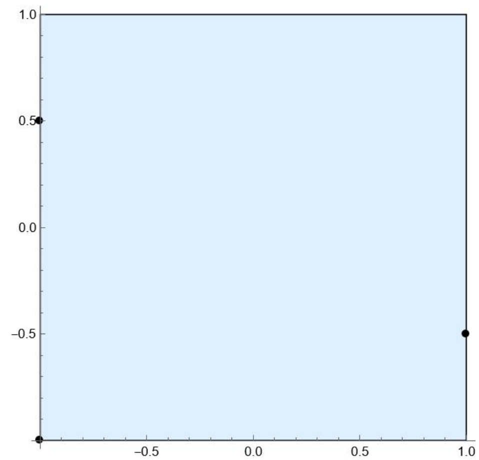

Figure 5.3: $\tilde{g}_a$ must stay below $\tilde{F}_a$ on $[-1,1]^2$ with equality at the three points shown

Finally, for arbitrary m, we propose a few nice subsets of $W_L \setminus \Phi_m^*$. First, we have the set

$$\{[k_1, k_2/\sqrt{3}]^T : 0 \le k_1 < 2m, 0 \le k_2 < 3m\} \subseteq W_L \setminus \Phi_m^*,$$

leading to the polynomial space

$$\text{span}\{P_v \mid v = [k_1, k_2/\sqrt{3}]^T : 0 \le k_1 < 2m, 0 \le k_2 < 3m\} = \mathcal{P}_{2m-1}(t_1) \times \mathcal{P}_{3m-1}(t_2).$$

Notably, our interpolant, $\tilde{g}_a$, for ω_6^* satisfies $\tilde{g}_a \in \mathcal{P}_1(t_1) \times \mathcal{P}_2(t_2)$. Working with such a tensor space of polynomials is natural due to the tensor product nature of

$$\tilde{F}_{a,L}(x) = \frac{\pi}{\sqrt{3}a}\tilde{\theta}(\frac{\pi}{a}; t_1)\tilde{\theta}(\frac{\pi}{3a}; t_2),$$

allowing us to leverage the one-dimensional interpolation theory (see Section 3.3).

5.3 A family of $2m$-point periodic configurations

Finally, we introduce a nearly one-dimensional family of configurations. For $\beta > 0$ and $m \in \mathbb{N}$, let $\Lambda_{\beta,m} = \mathbb{Z} \times m\beta\mathbb{Z}$ with $\Phi_\beta = \begin{bmatrix} 1 & 1/2 \\ 0 & \beta/2 \end{bmatrix} \mathbb{Z}^2$.

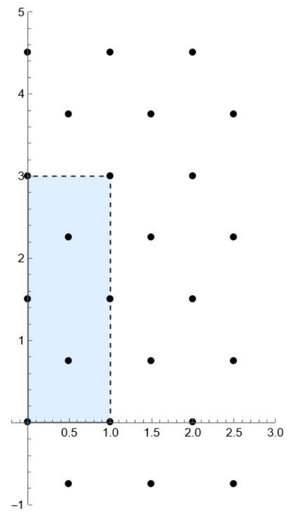

Figure 5.4: With $\beta = 3/2$ as shown, $\Phi_{\beta,2}$ is Λ_β, 2-universally optimal.

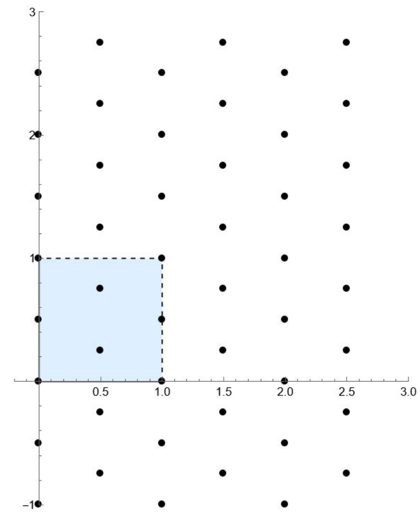

Figure 5.5: For $\beta = 1/2$, $\Phi_{\beta,2}$ is not $\Lambda_{\beta,2}$-universally optimal.

Our final main result characterizes the $\Lambda_{\beta,2}$-optimality of Φ_β:

Theorem 20. *The lattice Φ_β is $\Lambda_{\beta,2}$-universally optimal if and only if $\beta \geq \frac{1}{\sqrt{3}}$.*

To prove Theorem 20, we first note that analogous to the euclidean case, for a configuration to be Λ-universally optimal, it must be optimal for the sphere packing problem on the flat torus $\mathbb{R}^d/\Lambda$ (described below). A nice result in [18] shows that $\omega(\Phi_\beta, \Lambda_{\beta,2})$ is not optimal for sphere packing on the flat torus $\mathbb{R}^2/L_{\beta,2}$ when $\beta < 1/\sqrt{3}$ (in fact, they actually provide the optimal configuration). Thus, the reverse direction of Theorem 20 holds.

To prove the forward direction, we'll first set up the polynomial interpolation problem for arbitrary m and then propose an interpolant for the $m = 2$ case. For $m \geq 2$, let $T_{\beta,m}$ denote the change of variables

$$(t_1, t_2) := \left(\cos(2\pi x_1), \cos\left(\frac{2\pi x_2}{m\beta}\right)\right). \tag{5.2}$$

Note that for all $\beta \geq 1/\sqrt{3}$, we have $H \subseteq G^{\Phi_\beta}$ and

$$T_{\beta,m}(\Phi_\beta \cap \Delta_{\Lambda_{\beta,m}}) \setminus \{\mathbf{1}\} = \{((-1)^k, \cos(\frac{\pi k}{m}))|1 \leq k \leq m\}$$

In particular, $T_{\beta,2}(\Phi_\beta \cap \Delta_{\Lambda_{\beta,2}}) \setminus \{\mathbf{1}\} = \{(-1,0),(1,-1)\}$. The maps $\tilde{F}$ will be

$$\tilde{F}_{a_1,\Lambda_{\beta,m}} = \tilde{\theta}(\pi/a_1, t_1)\tilde{\theta}(\pi/(m^2\beta^2 a_1), t_2)$$

for each β and $a_1 > 0$ (the gaussian parameter). When a_1, m and β have been fixed, We will define $a_2 := m^2\beta^2 a_1 \geq m^2 a_1/3$, $\tilde{f}_1(t_1) := \tilde{\theta}(\pi/a_1, t_1)$, and $\tilde{f}_2(t_2) := \tilde{\theta}(\pi/a_2, t_2)$ so that

$$\tilde{F}(t_1, t_2) := \tilde{F}_{a_1,\Lambda_{\beta,m}}(t_1, t_2) = \tilde{f}_1(t_1)\tilde{f}_2(t_2).$$

Likewise, we compute $\Phi^* = \begin{bmatrix} 1 & 0 \\ 1/\beta & 2/\beta \end{bmatrix} \mathbb{Z}^2$, and so

$v = (k_1, k_2/(2\beta)) \in W_{\Lambda_{\beta,m}}$, $v \in \Lambda^*_{\beta,m} \setminus \{0\}$ if and only if $m|k_2$ and $k_2/m \equiv k_1 \pmod 2$. As a result, one available polynomial space consists of:

$$(\mathcal{P}_1(t_1) \times \mathcal{P}_{m-1}(t_2)) \bigoplus \mathcal{P}_{2m-1}(t_2)$$

When $m = 2$, $a_1 > 0$ and $\beta \geq 1/\sqrt{3}$ have been fixed, a priori, these restrictions still leave us with infinitely many degrees of freedom to construct our magic function $\tilde{g}$ [1], but we make the ansatz that a magic $\tilde{g}$ exists of the form:

$$\tilde{g} = c_{0,0} + c_{1,0}T_1(t_1) + c_{0,1}T_1(t_2) + c_{0,2}T_2(t_2). \tag{5.3}$$

In Chapter 8, we prove Theorem 20 by showing such a magic $\tilde{g}$ exists.

When $\beta \in \{1/\sqrt{3}, \sqrt{3}\}$, Φ_β is a rotated scaling of A_2 and thus Φ_β would necessarily be Λ_β, m-universally optimal for all $m \geq 2$ (in particular $m = 2$) if A_2 were to be universally optimal. As we have discussed, all $\beta \geq 1/\sqrt{3}$, except $\sqrt{3}, 1/\sqrt{3}$, in Theorem 20 yield the largest cardinality class of examples satisfying Question 1, and the first that use linear programming bounds in a

[1] The two equality conditions at $(-1,0)$ and $(1,-1)$ and $\tilde{F} \leq \tilde{g}$ imply that $\frac{\partial(f-g)}{\partial t_2}(-1,0) = 0$, and so we need at least a 3-dimensional space to find a magic $\tilde{g}$. We have verified that no magic $\tilde{g}$ exists in span$\{1, t_1, t_2\}$.

meaningful way.

Since the A_2 universal optimality conjecture would imply $\Phi_{1/\sqrt{3}}$ is $\Lambda_{1/\sqrt{3}}$, m-universally optimal for all m, we suspect that Theorem 20 can be generalized via the following conjecture:

Conjecture 21. *The lattice Φ_β is $\Lambda_{\beta,2}$-universally optimal for all $m \geq 2$ if and only if $\beta \geq \frac{1}{\sqrt{3}}$.*

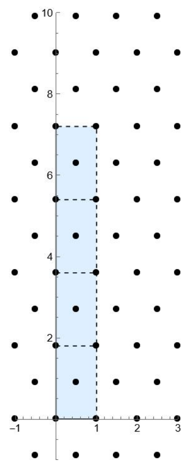

Figure 5.6: We conjecture that Φ_β remains universally optimal even as our periodization sublattice gets arbitrarily tall.

Example 2 shows the forward direction of Conjecture 21 holds for all $\beta > 0$ when $m = 1$, and we have proved the $m = 2$ case. One intuitive reason for thinking Conjecture 21 is true for larger m is that as $\beta \to \infty$, Φ_β converges pointwise to a scaling of $\mathbb{Z}$, where we know the corresponding $2m$-point periodic energy problems are solved by equally spaced points (see Section 4.5).

Connections to Periodic Sphere Packing

Periodic sphere packing provides further evidence for Conjecture 21. Given a lattice Λ and n-point configuration $\omega_n = x_1, \ldots, x_n$, we define the Λ-*periodic packing radius* of ω_n as

$$\delta_\Lambda(\omega_n) := \min\left(\{|x_i - x_j + v| : i \neq j, v \in \Lambda\}\right), \tag{5.4}$$

and the periodic packing problem asks us to find

$$\mathcal{P}(\Lambda, n) := \sup_{|\omega_n|=n} \delta_\Lambda(\omega_n) \tag{5.5}$$

and configurations attaining $\mathcal{P}(\Lambda, n)$. We note that that this definition of $\delta_\Lambda(\omega_n)$ means that the standard packing radius of the periodic configuration $C = \omega_n + \Lambda$, defined as $\delta(C) := \min_{x \neq y \in C}(|x-y|)$ satisfies

$$\delta(C) = \min\left(\delta_\Lambda(\omega_n), \min_{0 \neq v \in \Lambda}(|v|)\right),$$

and thus $\delta(C)$ and $\delta_\Lambda(\omega_n)$ may differ. This problem (sometimes including the vectors $0 \neq v \in \Lambda$) has been studied extensively (cf. [18], [24], [4],[27] and references therein).

In [18], a proof is given for $\beta \in [1/\sqrt{3}, \sqrt{3}]$ that the configurations $\delta_{\Lambda_{\beta,m}}(\omega(\Phi_\beta, \Lambda_{\beta,m})) = \mathcal{P}(\Lambda_{\beta,m}, 2m)$. We give a simple, alternative proof of the same result for all $\beta \geq 1/\sqrt{3}$ by reducing the dimension of the problem. First, using $\beta \geq 1/\sqrt{3}$, we check that $\delta_{\Lambda_{\beta,m}}(\omega(\Phi_\beta, \Lambda_{\beta,m})) = \frac{\sqrt{1+\beta^2}}{2}$, achieved for example by the difference of $\vec{0}$ and $(1/2, \beta/2)$ (this fails for $\beta < 1/\sqrt{3}$ as $(0, 2\beta)$ is shorter). Now take an arbitrary configuration $\omega_{2m} := x^1, \ldots, x^{2m}$ with $x^i = (x^i_1, x^i_2)$ for each i. With $d_{\mathbf{T_1}}$ as the flat torus metric from $\mathbb{R}/\mathbb{Z}$, we have for any x, y that $d_{\mathbf{T_1}}(x, y) \leq \frac{1}{2}$. Now let $d_{\mathbf{T_2}}$ be the flat torus metric from $\mathbb{R}/\beta\mathbb{Z}$. The minimal packing radius for $2m$ points in this metric is $\frac{1}{2m}$, achieved only by equally spaced points, so there must be two distinct points x^i, x^j such that $d_{\mathbf{T_2}}(x^i_2, x^j_2) \leq \frac{\beta}{2}$. Thus, there exists some $v \in \Lambda_{\beta,m}$ such that

$$|x^i - x^j + v| = \sqrt{d_{\mathbf{T_1}}(x^i_1, x^j_1)^2 + d_{\mathbf{T_2}}(x^i_2, x^j_2)^2} \leq \sqrt{(1/2^2)^2 + (\beta/2)^2} = \delta_{\Lambda_{\beta,m}}(\omega(\Phi_\beta, \Lambda_{\beta,m}))$$

as desired.

Chapter 6

Proof of Theorem 18

To prove A_2 is $2A_2$-universally optimal, it remains to show for each $a > 0$ that there are $c_0, c_1 \in \mathbb{R}$ with $c_1 \geq 0$ such that the resulting interpolant $\tilde{g}_a(t_1, t_2) := c_0 + c_1 P_{v'} = c_0 + c_1/3(-1 + t_2(t_1 + t_2))$ satisfies $\tilde{g}_a \leq \tilde{F}_a$ on $\tilde{\Delta}_{A_2}$ with equality at $(-1, 1)$ or, equivalently, finding such an interpolant of the form

$$\tilde{g}_a(t_1, t_2) := \tilde{F}_a(-1, 1) + b_1 t_2(t_1 + t_2) \tag{6.1}$$

for $b_1 \geq 0$.

Our formulas for $\tilde{g}_a$ are defined piecewise[1] in a. We set

$$b_1 = \begin{cases} 2\frac{\partial \tilde{F}}{\partial t_1}(-1, 1/2) & \text{if } 0 < a \leq 21 \\ \frac{\partial \tilde{F}}{\partial t_2}(-1, 1) & \text{if } a > 21. \end{cases} \tag{6.2}$$

Due to the different expansions used for θ (see (4.10) and (4.11)), we also find it convenient to rescale $\tilde{F}$ by a factor of $\sqrt{3}\pi/a$ for the small a case. Defining

$$\begin{aligned} \tilde{f}_1(t_1) &:= \begin{cases} \tilde{\theta}(\frac{\pi}{a}; t_1), & 0 < a \leq \pi^2 \\ \sqrt{\frac{\pi}{a}}\tilde{\theta}(\frac{\pi}{a}; t_1) & a > \pi^2, \end{cases} \\ \tilde{f}_2(t_2) &:= \begin{cases} \tilde{\theta}(\frac{\pi}{3a}; t_2), & 0 < a \leq \pi^2 \\ \sqrt{\frac{\pi}{3a}}\tilde{\theta}(\frac{\pi}{3a}; t_2) & a > \pi^2. \end{cases} \end{aligned} \tag{6.3}$$

[1] We suspect that b_1 need not be defined piecewise. In fact the choice $b_1 = \frac{\partial \tilde{F}}{\partial t_1}(-1, 1)$ numerically appears to lead to $\tilde{g}_a \leq \tilde{F}_a$ for all $a > 0$. But our most simple proofs come from this piecewise definition of b_1.

With this rescaling convention, it follows from (4.17) that

$$\tilde{F}(t_1, t_2) = \tilde{f}_1(t_1)\tilde{f}_2(t_2) + \tilde{f}_1(-t_1)\tilde{f}_2(-t_2). \tag{6.4}$$

6.1 Constructing a Magic $\tilde{g}_a$

For all $a > 0$, we will establish

Lemma 22. *For all points* $(t_1, t_2) \in \tilde{\Delta}_{A_2}$, $\dfrac{\partial^3 \tilde{F}}{\partial t_1 \partial t_2^2}(t_1, t_2) > 0$.

Proof. Since even partial derivatives of $\tilde{F}$ are positive, it suffices to check the inequality at the minimal t_1 and t_2 values, when $t_1 = -1$ and $t_2 = \frac{1}{2}$. This check is handled in Appendix C with large a and small a cases handled separately. □

Likewise, we have

Lemma 23. *Let* $\tilde{h}$ *be of the form* $\tilde{F}(-1, 1) + c_1 t_2(t_1 + t_2)$ *such that* $\tilde{h}(-1, 1/2) < \tilde{F}(-1, 1/2)$ *and* $\frac{\partial \tilde{F} - \tilde{h}}{\partial t_2}(-1, 1) \leq 0$. *Then for all* $t_2 \in [1/2, 1]$, $\tilde{F}(-1, t_2) \geq \tilde{h}(-1, t_2)$ *with equality only when* $t_2 = 1$.

Proof. We abuse notation here and use $\tilde{F}, \tilde{h}$ to refer to the one variable functions in t_2 obtained by fixing $t_1 = -1$. By assumption on the form of $\tilde{h}$, Lemma 17, and the two assumed inequalities, we have $\tilde{F}(1/2) \geq \tilde{h}(1/2)$, $\tilde{F}'(1/2) = \tilde{h}'(1/2) = 0$, $\tilde{F}(1) = \tilde{h}(1)$, and $\tilde{F}'(1) \leq \tilde{h}'(1)$. It follows that there are exists some point in $[1/2, 1]$ at which $\tilde{F}'' \leq \tilde{h}''$. Let $t_2' \leq t_2''$ be such that t_2' and t_2'' respectively are the minimal and maximal points in $[1/2, 1]$ at which $\tilde{F}'' \leq \tilde{h}''$. For $t_2 \geq t_2''$ we have $\tilde{F}'' \geq \tilde{h}''$ with equality only at t_2'' since $(\tilde{F} - \tilde{h})''$ is strictly convex (recall $\tilde{F}^{(4)} > 0$). Thus, we get $\tilde{F} \geq \tilde{h}$ by bounding $\tilde{F} - \tilde{h}$ below with a tangent line of $\tilde{F} - \tilde{h}$ at 1 and equality holds only if $t_2 = 1$. Similarly, for $t_2 \leq t_2'$, we get the desired inequality with tangent approximation from $\frac{1}{2}$. For $t_2 \in [t_2', t_2'']$, we note that $\tilde{F}'' = \tilde{h}''$ at the endpoints of the interval. Again using the strict convexity of $(\tilde{F} - \tilde{h})''$, we obtain $(\tilde{F} - \tilde{h})'' \leq 0$ for the whole interval. Thus, $\tilde{F}(t_2) \geq \tilde{h}(t_2)$ by bounding the difference below with its secant line (since we've already established $\tilde{F} \geq \tilde{h}$ at the endpoints t_2', t_2''), and equality can only hold at t_2'' if $t_2'' = 1$. □

6.1.1 Small a

Let $0 < a \leq 21$. We will refer to $\tilde{g}_a$ as simply $\tilde{g}$. We prove the following lemma[2] in Appendix C:

Lemma 24. *For* $0 < a \leq 21$*, we have*

$$\frac{\partial \tilde{F}}{\partial t_2}(-1,1), 4(\tilde{F}(-1,1) - \tilde{F}(-1,1/2)) \leq 2\frac{\partial \tilde{F}}{\partial t_1}(-1,1/2) \leq \frac{\partial^2(\tilde{F}-\tilde{g})}{\partial t_1 \partial t_2}(-1,1/2).$$

We handle the proof piecewise, splitting into 2 cases, $0 < a \leq \pi^2$ and $\pi^2 < a \leq 21$ depending on which formulas we use for $\tilde{f}_1$ and $\tilde{f}_2$. These 3 inequalities[3] suffice to show $\tilde{F} \leq \tilde{g}$. We certainly have $b_1 > 0$ since $b_1 = 2\frac{\partial \tilde{F}}{\partial t_1}(-1,1/2) > \frac{\partial \tilde{F}}{\partial t_2}(-1,1) > 0$ where the first inequality holds by assumption and the next by Lemma 17. Next, we have

$$(\tilde{F} - \tilde{g})(-1,1/2) = \tilde{F}(-1,1/2) - \tilde{F}(-1,1) + \frac{1}{4}b_1 > 0$$

and likewise

$$\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_2}(-1,1) = \frac{\partial \tilde{F}}{\partial t_2}(-1,1) - b_1 < 0.$$

Applying Lemma 23 and the previous two inequalities to $\tilde{g}$, we obtain $\tilde{F} \geq \tilde{g}$ for all points $(-1, t_2)$ with $t_2 \in [1/2, 1]$ with equality only at $(-1,1)$, and since $\tilde{F} - \tilde{g}$ is convex in t_1, it remains to show that $\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1} \geq 0$ for all points of the form $(-1, t_2)$, $t_2 \in [1/2, 1]$ (recall the picture of $\tilde{\Delta}_{A_2}$, Figure 5.1). By Lemma 22, $\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}$ is convex in t_2 in $\tilde{\Delta}_{A_2}$, so we just need to show

$$\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-1,1/2) \geq 0, \frac{\partial^2(\tilde{F}-\tilde{g})}{\partial t_1 \partial t_2}(-1,1/2) \geq 0.$$

[2]The reason we don't use this approach for all $a > 9.6$ is Lemma 24 fails at roughly $a = 22$. Namely, the terms $\frac{\partial \tilde{F}}{\partial t_2}(-1,1), 4(\tilde{F}(-1,1) - \tilde{F}(-1,1/2))$ both have lead exponential terms on the order of $e^{-a/4}$, while $\frac{\partial \tilde{F}}{\partial t_1}(-1,1/2)$ is on the order of $e^{-a/3}$.

[3]Though in the small a case, we have set $b_1 = 2\frac{\partial \tilde{F}}{\partial t_1}(-1,1/2)$ for simplicity, in fact, we could set b_1 to be any element of the (non-empty) interval $\left[\max\left\{\frac{\partial \tilde{F}}{\partial t_2}(-1,1), 4(\tilde{F}(-1,1) - \tilde{F}(-1,1/2))\right\}, 2\frac{\partial \tilde{F}}{\partial t_1}(-1,1/2)\right]$ and the exact same proof would work.

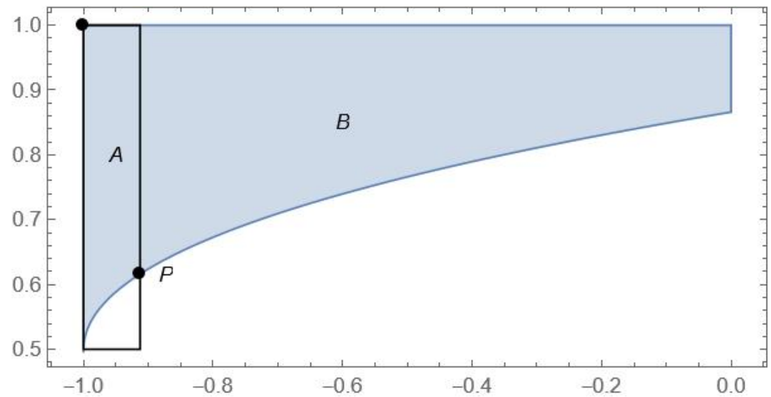

Figure 6.1: The figure depicts our strategy for showing $\tilde{F} \geq \tilde{g}$ in the large a case. We show $\tilde{F} \leq \tilde{g}$ on the rectangular region A (which includes points outside of $\tilde{\Delta}_{A_2}$) in Lemma 27. The remaining points of $\tilde{\Delta}_{A_2}$, in region B, are handled by Lemma 28.

But these follow directly from our assumptions on b_1. Indeed,

$$\frac{\partial(\tilde{F} - \tilde{g})}{\partial t_1}(-1, 1/2) = \frac{\partial \tilde{F}}{\partial t_1}(-1, 1/2) - \frac{b_1}{2} = 0 \tag{6.5}$$

$$\frac{\partial^2(\tilde{F} - \tilde{g})}{\partial t_1 \partial t_2}(-1, 1/2) = \frac{\partial^2 \tilde{F}}{\partial t_1 \partial t_2}(-1, 1/2) - b_1 > 0. \tag{6.6}$$

6.1.2 Large a

Throughout, we assume $a > 21$ and refer to $\tilde{g}_a$ as $\tilde{g}$. We begin by showing that $\tilde{F} \geq \tilde{g}$ on two segments of the boundary of $\tilde{\Delta}_{A_2}$.

Lemma 25. *We have $\tilde{F} \geq \tilde{g}$ on the set $\{(-1, t_2) : t_2 \in [1/2, 1]\} \cup \{(t_1, 1) : t_1 \in [-1, 1]\}$ with equality only at $(-1, 1)$.*

Proof. For the segment $\{(-1, t_2) : t_2 \in [1/2, 1]\}$, we prove in Appendix C.3 that for $a > 21$,

$$\frac{\partial \tilde{F}}{\partial t_1}(-1, 1) > \frac{\partial \tilde{F}}{\partial t_2}(-1, 1) \tag{6.7}$$

It also holds for $0 < a < 21$ as an immediate consequence of Lemma 24. We also show in

Appendix C.3 for $a > 21$ that $(\tilde{F} - \tilde{g})(-1, 1/2) > 0$, and so using the definition

$$b_1 = \frac{\partial \tilde{F}}{\partial t_2}(-1, 1),$$

for this range of a, we may apply Lemma 23 to obtain $\tilde{F} \geq \tilde{g}$ on $\{(-1, t_2) : t_2 \in [1/2, 1]\}$ with equality only at $(-1, 1)$. Now for the other segment, we simply apply (6.7), our definition of b_1, and the convexity of $\tilde{F} - \tilde{g}$ in t_1. $\square$

Next, we show that $\tilde{F}(t_1, t_2) \geq \tilde{g}(t_1, t_2)$ in $\tilde{\Delta}_{A_2}$ if $t_1 \leq \cos(2\pi\frac{\sqrt{3}}{4})$ with equality only at $(-1, 1)$, and in fact we'll show the stronger claim that $\tilde{F} \geq \tilde{g}$ on all of $A := [-1, \cos(2\pi\frac{\sqrt{3}}{4})] \times [1/2, 1]$ (see Figure 6.1) with equality only at $(-1, 1)$.

Let $H_{\tilde{F}}$ denote the Hessian matrix of $\tilde{F}$. It follows from the strict complete monotonicity of the log derivative of $\tilde{\theta}$ that $\tilde{f}_i''\tilde{f}_i < (\tilde{f}_i')^2$ for $i \in \{1, 2\}$ (see Proposition 14), and hence we have

$$\begin{aligned}\det(H_{\tilde{F}}(t_1, t_2)) = (\tilde{f_1}''(t_1)\tilde{f}_1(t_1))(\tilde{f_2}''(t_2)\tilde{f}_2(t_2)) - \tilde{f_1}'(t_1)^2\tilde{f_2}'(t_2)^2 +\\ (\tilde{f_1}''(-t_1)\tilde{f}_1(-t_1))(\tilde{f_2}''(-t_2)\tilde{f}_2(-t_2)) - \tilde{f_1}'(-t_1)^2\tilde{f_2}'(-t_2)^2 < 0\end{aligned}$$

for $t_1, t_2 \in [-1, 1]$.

To establish that $\tilde{F} \geq \tilde{g}$ on a rectangle $R \subset [-1, 1]^2$ with upper left corner point (c, d) (we subdivide the rectangle A into three such rectangles in the proof of Lemma 27), we introduce the following auxiliary function

$$\tilde{g}_{c,d}(t_1, t_2) := \tilde{g}(t_1, t_2) - b_1 t_1 t_2 + b_1(ct_2 + dt_1 - cd), \tag{6.8}$$

and observe that $t_1 t_2 \leq ct_2 + dt_1 - cd$ for $t_1 \geq c$, $t_2 \leq d$, and so

$$\tilde{g}(t_1, t_2) \leq \tilde{g}_{c,d}(t_1, t_2) \quad t_1 \geq c,\ t_2 \leq d \tag{6.9}$$

with equality if and only if $t_1 = c$ or $t_2 = d$. We further observe that

$$\det(H_{\tilde{F}-\tilde{g}_{c,d}}) = \det(H_{\tilde{F}}) - 2b_1 \tilde{f}_1''(t_1)\tilde{f}_2(t_2) < \det(H_{\tilde{F}}) < 0.$$

Hence, to verify $\tilde{F} \geq \tilde{g}$ on the rectangle R, it suffices to show $\tilde{F} \geq \tilde{g}_{c,d}$ on the boundary of the region by the second derivative test. For the two sides of the rectangle where $t_1 = c$ and $t_2 = d$, we will have already established $\tilde{F} \geq \tilde{g}$, and since $\tilde{g} = \tilde{g}_{c,d}$ on those sides, we immediately obtain $\tilde{F} \geq \tilde{g}_{c,d}$ there.

On the other two sides, we reduce the $a \geq 21$ case to just $a = 21$ in the following way. In each case, using truncated series approximations of θ and b_1 developed in Appendix B.2, we find an upper bound on $\tilde{g}^*_{c,d} \geq \tilde{g}_{c,d}$ with the key feature that $e^{a/4}\tilde{g}^*_{c,d}$ is linear in a. Meanwhile, as a lower bound for $\tilde{F}$, we truncate the expansions for f_1 and f_2 from (4.11) to obtain

$$\tilde{F}_T(t_1, t_2) := (e^{-ax^2} + e^{-a(x-1)^2})e^{-3au^2} + e^{-a((\frac{1}{2}-x)^2+3(\frac{1}{2}-u)^2)} < \tilde{F}(t_1, t_2), \qquad t_1, t_2 \in [-1, 1], \tag{6.10}$$

where

$$x = \frac{\arccos(t_1)}{2\pi}, \qquad u = \frac{\arccos(t_2)}{2\pi}. \tag{6.11}$$

It is straightforward to verify that $e^{a/4}\tilde{F}_T(t_1, t_2)$ is convex in a for any fixed (t_1, t_2) and so the difference $e^{a/4}(\tilde{F}_T - \tilde{g}^*_{c,d})$ is also (pointwise) convex in a. Thus, to establish $\tilde{F}_T \geq \tilde{g}^*_{c,d}$ at some point (t_1, t_2) for all $a \geq 21$ it suffices to show

$$\begin{aligned} (\tilde{F}_T - \tilde{g}^*_{c,d})(t_1, t_2)\Big|_{a=21} &\geq 0 \\ \frac{\partial\left[e^{a/4}(\tilde{F}_T - \tilde{g}^*_{c,d})(t_1, t_2)\right]}{\partial a}\Bigg|_{a=21} &\geq 0. \end{aligned} \tag{6.12}$$

In short, to establish $\tilde{F} \geq \tilde{g}$ on a rectangle R with upper left vertex (c, d) for which we have already established this inequality on the left and upper edges, it suffices to establish the inequalities (6.12) for (t_1, t_2) on the two bottom and right line segments bounding R. Moreover, since the above method actually establishes $\tilde{F} \geq \tilde{g}^*_{c,d}$, we have the strict inequality $\tilde{F} > \tilde{g}$ on the whole rectangle except for possibly points where $t_1 = c$ or $t_2 = d$. We summarize our discussion in the following lemma which will be helpful in the 6-point case.

Lemma 26. *Let $R\colon [c,c'] \times [d',d] \subseteq [-1,1]^2$ be a rectangle with upper left corner point (c,d), and further suppose that there exist functions $\tilde{g}, \tilde{g}_{c,d}, \tilde{g}^*_{c,d}, \tilde{F}_T$, and $\tilde{F}$ of the variables $(a,t_1,t_2) \in (0,\infty) \times [0,1]^2$ with continuous 2nd order partial derivatives which satisfy for all $a \geq a'$:*

1. *$\tilde{g} \leq \tilde{g}_{c,d} \leq \tilde{g}^*_{c,d}$ on R with $\tilde{g} = \tilde{g}_{c,d}$ if and only if $t_1 = c$ or $t_2 = d$*
2. *$\tilde{F}_T \leq \tilde{F}$ on R*
3. *$\det H_{\tilde{F}-\tilde{g}^*_{c,d}} < 0$ on R*
4. *For some m_1, $e^{a/m_1}(\tilde{F} - \tilde{g}_{c,d})$ is pointwise convex in the parameter a*

If there is some $a' > 0$ such that the inequalities

$$\begin{aligned} (\tilde{F}_T - \tilde{g}^*_{c,d})(t_1,t_2)\Big|_{a=a'} &\geq 0 \\ \frac{\partial\left[e^{a/m_1}(\tilde{F}_T - \tilde{g}^*_{c,d})(t_1,t_2)\right]}{\partial a}\Bigg|_{a=a'} &\geq 0 \end{aligned} \tag{6.13}$$

hold on ∂R, then $\tilde{F} > \tilde{g}$ on R for all $a \geq a'$. Further, if for all $a \geq a'$, $\tilde{F} \geq \tilde{g}$ on some $R' \subseteq \{(t_1,t_2) \in \partial R : t_1 = c \text{ or } t_2 = d\}$ and the inequalities (6.13) hold on $\partial R \backslash R'$, then $\tilde{F} \geq \tilde{g}$ on R for all $a \geq a'$, again with equality only possible if $t_1 = c$ or $t_2 = d$ and $(t_1,t_2) \in R'$.

Lemma 27. *The inequality $\tilde{F} \geq \tilde{g}$ holds on $A = [-1, \cos(2\pi\frac{\sqrt{3}}{4})] \times [\frac{1}{2}, 1]$ with equality only at $(-1,1)$.*

Proof. We partition $[-1, \cos(2\pi\frac{\sqrt{3}}{4})] \times [\frac{1}{2}, 1]$ into three subrectangles $R_k := [-1, \cos(2\pi\frac{\sqrt{3}}{4})] \times [d_{k-1}, d_k]$, $k = 1,2,3$ where $d_0 = 1/2$, $d_1 = 3/5$, $d_2 = 7/10$, and $d_3 = 1$ and aim to verify the inequality $\tilde{F} \geq \tilde{g}_{-1,d_k}$ on each R_k using Lemma 26, with $\tilde{g}_{-1,d_k}$ as in (6.8), $\tilde{F}_T$ as in (6.10), $m_1 = 4$, and $a' = 21$. The specific formulas for each g^*_{-1,d_k} are given in Appendix C.3. We begin by verifying inequalities (6.13) for $g^*_{-1,-1}$ on the line segments of R_1 with $t_1 = \cos(2\pi\sqrt{3}/4)$ or $t_2 = 7/10$, which combined with Lemma 26 implies $\tilde{F} \geq \tilde{g}$ on R_1. Now having established $\tilde{F} \geq \tilde{g}$ on the top side of R_2, we only need establish inequalities (6.13) for $g^*_{-1,-1}$ on the line segments of R_2 where $t_1 = \cos(2\pi\sqrt{3}/4)$ or $t_2 = 3/5$ to get $\tilde{F} \geq \tilde{g}$ on all R_2. In the same fashion, showing inequalities (6.13) on the sides of R_3 where $t_1 = \cos(2\pi\sqrt{3}/4)$ or $t_2 = 3/5$ completes the proof by yielding $\tilde{F} \geq \tilde{g}$ on R_3. The verification of these inequalities is carried out in the Appendix C.3 by reducing them to inequalities of the form $h_2(t) - h_1(t) > 0$ on an interval (α, β) where h_1 and h_2 are increasing functions and choose $\delta := (\beta - \alpha)/n$ with sufficiently large that we may rigorously verify the inequalities

$$h_1(\alpha + k\delta) < h_2(\alpha + (k-1)\delta), \qquad k = 1, 2, \ldots, n, \tag{6.14}$$

thereby reducing our check to a finite number of point evaluations. □

Finally, we show that $\tilde{F} - \tilde{g}$ increases in t_1 for every point in $\tilde{\Delta}_{A_2}$ with $t_1 \geq \cos(2\pi\frac{\sqrt{3}}{4})$, thus completing the proof for the $a > 21$ case and yielding $\tilde{F} \geq \tilde{g}$ on all $\tilde{\Delta}_{A_2}$ with equality only at $(-1, 1)$.

Lemma 28. *For all $a \geq 21$ and every $p = (t_1, t_2) \in \tilde{\Delta}_{A_2}$ with $t_1 \geq \cos(2\pi\frac{\sqrt{3}}{4})$, $\left.\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}\right|_p \geq 0$.*

Proof. Because of the convexity of the difference in t_1 and Lemma 22, it suffices to show that at $P = (\cos(2\pi\frac{\sqrt{3}}{4}), \cos(2\pi\frac{\sqrt{3}}{12}))$,

$$\left.\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}\right|_P \geq 0, \qquad \left.\frac{\partial^2(\tilde{F}-\tilde{g})}{\partial t_1 \partial t_2}\right|_P \geq 0 \tag{6.15}$$

which is handled in Appendix C.3. □

Chapter 7

Proof of Theorem 19

We consider the $m = 1$ case of the interpolation problem from Section 5.2 to prove Theorem 19. In this case, we need $\tilde{F}_a = \tilde{g}_a$ at the nodes $T(\Phi_1 \cap \Delta_L) \setminus \{\mathbf{1}\} = \{(-1,-1),(1,-\frac{1}{2}),(-1,\frac{1}{2})\}$. Using the same rescaling convention as Section 7, we have

$$\tilde{F}(t_1,t_2) = \tilde{f}_1(t_1)\tilde{f}_2(t_2),$$

where $\tilde{f}_1, \tilde{f}_2$ are as in (6.3). For $m = 1$, we may choose an interpolant $\tilde{g} := \tilde{g}_a \in \mathcal{P}_1(t_1) \times \mathcal{P}_2(t_2)$; i.e $\tilde{g}$ of the form

$$\tilde{g}(t_1,t_2) = \sum_{i=0}^{1}\sum_{j=0}^{2} b_{i,j} t_1^i t_2^j. \tag{7.1}$$

The equality requirement on $\{(-1,-1),(1,-\frac{1}{2}),(-1,\frac{1}{2})\}$ combined with the condition $\tilde{g} \leq \tilde{F}$ further yields the necessary conditions $\partial\tilde{g}/\partial t_2 = \partial\tilde{F}/\partial t_2$ at the points $(-1,1/2)$ and $(1,-1/2)$, giving a total of 5 linearly independent conditions on $\mathcal{P}_1(t_1) \times \mathcal{P}_2(t_2)$.

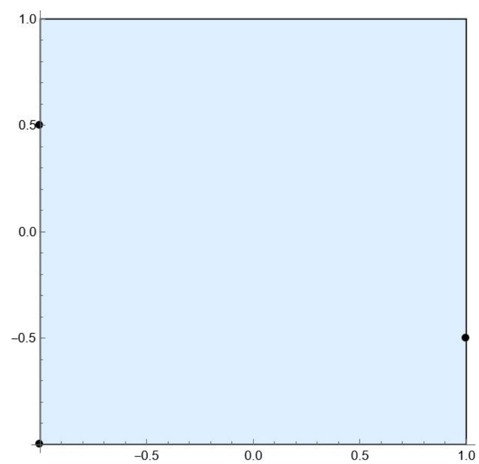

Figure 7.1: $\tilde{g}$ has 5 necessary equality interpolation conditions in order to provide a sharp bound, the 3 value conditions from $\tilde{\tau}_6$, plus two derivative conditions.

Note that $q(t_1,t_2) := (1+t_1)(t_2+1/2)^2$ vanishes on $\{(-1,-1),(1,-\frac{1}{2}),(-1,\frac{1}{2})\}$ and $\frac{\partial q}{\partial t_2}$

vanishes on $\{(-1,1/2),(1,-1/2)\}$. Thus, for any $\tilde{g}$ of the form (7.1) satisfying our interpolation conditions, there exists a c such that

$$\tilde{g}(t_1,t_2) = \frac{(1-t_1)}{2}\tilde{f}_1(-1)H_{\{-1,\frac{1}{2},\frac{1}{2}\}}(\tilde{f}_2)(t_2) + \frac{(1+t_1)}{2}\tilde{f}_1(1)H_{\{-\frac{1}{2},-\frac{1}{2}\}}(\tilde{f}_2)(t_2) + cq(t_1,t_2), \tag{7.2}$$

where $H_\tau(f)$ is the Hermite interpolant to f on the node set τ which can be expressed in terms of divided differences (see Section 3.3). In particular,

$$H_{\{-1,\frac{1}{2},\frac{1}{2}\}}(\tilde{f}_2)(t_2) = \tilde{f}_2(-1) + \tilde{f}_2[-1,\frac{1}{2}](t_2+1) + \tilde{f}_2[-1,\frac{1}{2},\frac{1}{2}](t_2+1)(t_2-\frac{1}{2}),$$

and $H_{\{-\frac{1}{2},-\frac{1}{2}\}}(\tilde{f}_2)(t_2) = \tilde{f}_2(-\frac{1}{2}) + \tilde{f}_2{}'(-\frac{1}{2})(t_2+\frac{1}{2})^2$.

7.1 $\tilde{g}$ is CPSD

Since $T_1(t) = t$ and $T_2(t) = 2t^2 - 1$, it easily follows that $\tilde{g}$ is CPSD if and only if $b_{i,j} \geq 0$ for $(i,j) \neq 0$. From (7.2), it follows that $b_{1,2} = -\frac{1}{2}\tilde{f}_1(-1)\tilde{f}_2[-1,\frac{1}{2},\frac{1}{2}] + c$. Observing that $q \geq 0$ on $[-1,1]^2$, we choose $c = \frac{1}{2}\tilde{f}_1(-1)\tilde{f}_2[-1,\frac{1}{2},\frac{1}{2}]$ as small as possible (to assist the requirement $\tilde{F} \geq \tilde{g}$) in which case $b_{1,2} = 0$.

In addition, the following derivative equality,

$$\tilde{f}_1(-1)\tilde{f}_2{}'(1/2) = \tilde{f}_1(1)\tilde{f}_2{}'(-1/2). \tag{7.3}$$

proved in [1] (also see [28]) implies that $b_{1,1} = b_{0,2}$. Hence we may express $\tilde{g}$ in the form

$$\tilde{g}(t_1,t_2) = a_{0,0} + a_{1,0}t_1 + a_{0,1}t_2 + a_{0,2}(t_1t_2 + t_2^2 + 1/4), \tag{7.4}$$

where $a_{0,0} = b_{0,0} - b_{0,2}/4$ and $a_{i,j} = b_{i,j}$ otherwise.

From (7.2), we then compute

$$
\begin{aligned}
a_{0,0} &= \frac{\tilde{f}_1(1)\tilde{f}_2(-1/2) + \tilde{f}_1(-1)\tilde{f}_2(1/2)}{2} \\
a_{0,1} &= \tilde{f}_1(-1)\tilde{f}_2{}'(-1/2) \\
a_{1,0} &= \frac{\tilde{f}_1(1)\tilde{f}_2(-1/2) - \tilde{f}_1(-1)\tilde{f}_2(1/2)}{2} + \frac{a_{0,1}}{2} \\
a_{0,2} &= \tilde{f}_1(-1)\tilde{f}_2[-1, \frac{1}{2}, \frac{1}{2}] = \frac{4}{9}(\tilde{f}_1(-1)\tilde{f}_2(-1) + a_{0,1} + a_{1,0} - a_{0,0}).
\end{aligned}
\tag{7.5}
$$

The strict absolute monotonicity and positivity of $\tilde{f}_2$ and $\tilde{f}_1$ show that the coefficients $a_{0,0}, a_{0,1}$, and $a_{0,2}$ in (7.5) are positive.

The next lemma which will be used to prove $a_{1,0} > 0$ as well as being a first step in establishing that $\tilde{g} \leq \tilde{F}$ on $[-1,1]^2$.

Lemma 29. *$\tilde{F}(-1,t_2) \geq \tilde{g}(-1,t_2)$ for all $t_2 \in [-1,1]$ with equality only if $t_2 \in \{-1, 1/2\}$.*

Proof. The result follows from the error formula (3.14) applied to the strictly absolute monotone function $\tilde{F}(-1,t_2) = \tilde{f}_1(-1)\tilde{f}_2(t_2)$ for t_2 on [-1,1]. □

It remains to show that $a_{1,0} > 0$.

Proposition 30. *The coefficients $a_{0,0}, a_{0,1}, a_{1,0}$, and $a_{0,2}$ are positive. Hence, $\tilde{g}$ is CPSD.*

Proof. By Lemma 29, $\tilde{g}(-1,-1/2) < \tilde{F}(-1,-1/2)$. Moreover, by definition, $\tilde{g}(1,-1/2) = \tilde{F}(1,-1/2)$. Since $(\tilde{F} - \tilde{g})(t_1,-1/2)$ is convex in t_1, we must have

$$
a_{1,0} - \frac{1}{2}a_{0,2} = \frac{\partial \tilde{g}}{\partial t_1}(-1,-1/2) \geq \frac{\partial \tilde{F}}{\partial t_1}(-1,-1/2) > 0. \tag{7.6}
$$

So $a_{1,0} - \frac{1}{2}a_{0,2} > 0$ which implies $a_{1,0} > 0$ since $a_{0,2} > 0$. □

As in the proof of Theorem 18, the most technical part of our proof is to verify $\tilde{g} \leq \tilde{F}$. In the remainder of Chapter 7, we reduce the proof of this inequality to a number of technical computations and estimates that are carried out in Appendix D.

7.2 $\tilde{F} \geq \tilde{g}$ on $[-1,1] \times ([-1,-1/2] \cup [1/2,1])$

The following lemma, proved in Appendix D, establishes several necessary inequality conditions for $\tilde{g} \leq \tilde{F}$. We next show the inequality holds on $[-1,1] \times ([-1,-1/2] \cup [1/2,1])$.

Lemma 31. *The following derivative conditions hold*

$$\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-1,-1) > 0, \tag{7.7}$$

$$\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-1,1/2) > 0, \tag{7.8}$$

$$\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(1,-1/2) < 0. \tag{7.9}$$

For fixed t_2, $\tilde{F}(t_1,t_2) - \tilde{g}(t_1,t_2)$ is strictly convex on $[-1,1]$ as a function of t_1 since $\tilde{g}(t_1,t_2)$ is linear in t_1 and $\tilde{f}_1$ is strictly absolutely monotone. The next proposition is an immediate consequence of this observation.

Lemma 32. *Let $t_2 \in [-1,1]$. If either condition*

(a) $\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-1,t_2) \geq 0$ *and* $\tilde{F}(-1,t_2) \geq \tilde{g}(-1,t_2)$ *or*

(b) $\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(1,t_2) \leq 0$ *and* $\tilde{F}(1,t_2) \geq \tilde{g}(1,t_2)$

holds, then

$$\tilde{F}(t_1,t_2) \geq \tilde{g}(t_1,t_2), \qquad t_1 \in [-1,1]. \tag{7.10}$$

If condition (a) holds, then we have strict inequality in (7.10) for $t_1 \neq -1$. If condition (b) holds, then we have strict inequality in (7.10) for $t_1 \neq 1$.

We use the above lemmas to obtain:

Lemma 33. *We have $\tilde{F} \geq \tilde{g}$ on $[-1,1] \times [1/2,1]$ with equality only at $(-1,1/2)$.*

Proof. We first note that $\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(t_1,t_2) = \tilde{f}_1{}'(t_1)\tilde{f}_2(t_2) - a_{1,0} - a_{0,2}t_2$ is (a) strictly increasing in t_1 for fixed t_2 and (b) strictly convex in t_2 for fixed t_1. Let $h(t_2) := \frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-1,t_2)$. The inequality (7.9) together with (a) implies $h(-1/2) < 0$. Hence, the strict convexity of h together with $h(1/2) > 0$ (from (7.8)) implies $h(t_2) = \frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-1, t_2) > 0$ for $t_2 \in [1/2, 1]$. Combining this fact with Lemma 29, we may invoke Lemma 32 part (a) to complete the proof. $\square$

Next, we establish that $\tilde{F} \geq \tilde{g}$ on the right-hand boundary $t_1 = 1$.

Lemma 34. *We have $\tilde{F}(1, t_2) \geq \tilde{g}(1, t_2)$ for all $t_2 \in [-1, 1]$ with equality only at $t_2 = -1/2$.*

Proof. Suppose by way of contradiction that there exists $t_2' \in [-1, 1]$ such that $t_2' \neq -\frac{1}{2}$ and $\tilde{F}(1, t_2') \leq \tilde{g}(1, t_2')$. Then there must be some point $-1/2 \neq p \in [-1, 1]$ such that $\tilde{f}_1(1)\tilde{f}_2(p) = \tilde{g}(1, p)$. Indeed, either t_2' is such a point, or $\tilde{F}(1, t_2') < \tilde{g}(1, t_2')$. We have from Lemmas 31, 32, and 33 that $\tilde{F}(1, \pm 1) > \tilde{g}(1, \pm 1)$, which yield two cases for t_2'. If $t_2' < -1/2$, then there exists $p \in (-1, t_2')$ such that $\tilde{F}(1, p) = \tilde{g}(1, p)$ by the intermediate value theorem. If $t_2' > -1/2$, instead apply the intermediate value theorem on the interval $[t_2', 1]$ to see that $p \in [1/2, 1]$.

Then $\tilde{g}(1, t_2)$ is the unique quadratic polynomial that interpolates the function $\tilde{F}(1, t_2)$ at $T = \{p, -1/2, -1/2\}$. Then the error formula (3.14) gives

$$\tilde{F}(1, t_2) - \tilde{g}(1, t_2) = \tilde{f}_1(1)\tilde{f}_2^{(3)}(\xi)(t_2 - p)(t_2 + 1/2)^2$$

for some $\xi \in [-1, 1]$. The positivity of $\tilde{f}_2^{(3)}$ then implies the contradiction $\tilde{F}(1, -1) = \tilde{f}_1(1)\tilde{f}_2(-1) < \tilde{g}(1, -1)$ completing the proof. $\square$

Lemma 35. *We have $\tilde{F} \geq \tilde{g}$ on $[-1, 1] \times [-1, -1/2]$ with equality only at $(-1, -1)$ and $(1, -1/2)$.*

Proof. From Lemma 29, we have $\tilde{F} \geq \tilde{g}$ for $t_1 = -1$. By Lemmas 31 and 32, we have the same inequality when $t_2 = -1/2$ or -1. Finally, by Lemma 34, we have the inequality for $t_1 = 1$. All of these inequalities are strict except for at $(-1, -1)$ and $(1, -1/2)$.

Let $p = (p_1, p_2)$ be an arbitrary point on the boundary of $[-1, 1] \times [-1, -1/2]$ such that $p_1 < 1$ and $p_2 < -1/2$, let $q = (1, -1/2)$, and let $l(s) := p + s(q - p)$, $0 \leq s \leq 1$, parametrize the line segment from p to q. Since $u_l := q - p$ has positive components, it follows that $\tilde{F}^l := \tilde{F} \circ l$

is strictly absolutely monotone on $[0,1]$. Also, let $\tilde{g}^l := \tilde{g} \circ l$ and note that $\tilde{g}^l$ is a polynomial of degree at most 2.

We claim that $(\tilde{F}^l - \tilde{g}^l)(\epsilon) > 0$ for all sufficiently small $\epsilon > 0$. Indeed, if $p \neq (-1,-1)$, then $(\tilde{F}^l - \tilde{g}^l)(0) > 0$ and the result follows by continuity. If $p = (-1,-1)$, then $\nabla(\tilde{F} - \tilde{g})(-1,-1) \cdot u_l > 0$ at (-1,-1) by Lemmas 31 and 29 which shows the result in this case. Similarly, the necessary derivative inequality and equality conditions at $(1,-1/2)$ imply $\nabla(\tilde{F} - \tilde{g})(-1,1/2) \cdot u_l < 0$. Together with the fact that $(\tilde{F}^l - \tilde{g}^l)(1) = 0$, we get $(\tilde{F}^l - \tilde{g}^l)(1-\epsilon) > 0$ for all ϵ sufficiently small.

Now supposing for a contradiction that $(\tilde{F}^l - \tilde{g}^l)(r') < 0$ for some $r' \in (0,1)$. By the intermediate value theorem there are points $0 < r_1 < r' < r_2 < 1$ such that $(\tilde{F}^l - \tilde{g}^l)(r_1) = (\tilde{F}^l - \tilde{g}^l)(r_2) = 0$. Then $\tilde{g}^l$ is a polynomial of degree at most 2 which interpolates $\tilde{F}^l$ for $T = \{r_1, r_2, 1\}$ and leads to a contradiction using the error formula (3.14). Since any point in $(-1,1) \times (-1,-1/2)$ must lie on such a line segment, we conclude that $\tilde{F} \geq \tilde{g}$ on $(-1,1) \times (-1,-1/2)$. Now to see the inequality must be strict, if $(\tilde{F}^l - \tilde{g}^l)(r') = 0$ for some $r' \in (0,1)$ $\tilde{g}^l$ is a polynomial of degree at most 2 which interpolates $\tilde{F}^l$ for $T = \{r', r', 1\}$, and again we obtain a contradiction with the error formula. □

Thus, we have proved $\tilde{F} \geq \tilde{g}$ on $[-1,1]^2$ whenever $t_2 \geq 1/2$ or $t_2 \leq -1/2$. Our proof of the inequality for the critical region $-1/2 \leq t_2 \leq 1/2$ is more delicate and requires different approaches for a small and a large.

7.3 The critical region for small a ($a < \pi^2$)

For $a < \pi^2$, we take a linear approximation approach. Let

$$L_{\pm 1}(t_1, t_2) := (\tilde{F} - \tilde{g})(\pm 1, t_2) + (t_1 \mp 1)\frac{\partial(\tilde{F} - \tilde{g})}{\partial t_1}(\pm 1, t_2)$$

denote the tangent approximation of $\tilde{F} - \tilde{g}$ for fixed t_2 about $t_1 = \pm 1$. Since $(\tilde{F} - \tilde{g})(t_1, t_2)$ is strictly convex in t_1 for fixed t_2, we have

$$(\tilde{F} - \tilde{g})(t_1, t_2) \geq \max\{L_{-1}(t_1, t_2), L_{-1}(t_1, t_2)\} \geq \min\{L_{-1}(-1, t_2), L_{-1}(0, t_2), L_1(0, t_2), L_1(1, t_2)\}, \tag{7.11}$$

where the second inequality uses that $L_{\pm 1}(t_1, t_2)$ is a linear polynomial in t_1 for fixed t_2. Note the first inequality in (7.11) is strict if $-1 < t_1 < 1$.

Now $L_{-1}(-1, t_2) = (\tilde{F} - \tilde{g})(-1, t_2) \geq 0$ by Lemma 29 and $L_1(1, t_2) = (\tilde{F} - \tilde{g})(1, t_2) \geq 0$ by Lemma 34. In fact, we shall next prove that $L_{-1}(0, t_2) \geq L_1(0, t_2)$ so that the minimum on the right-hand side of (7.11) is non-negative if $L_1(0, t_2)$ is non-negative.

Lemma 36. *If* $t_2 \in (-1, 1)$, *then* $L_{-1}(0, t_2) > L_1(0, t_2)$.

Proof. Since $\tilde{g}$ is affine in t_1, we have

$$L_{\pm 1}(0, t_2) := \tilde{F}(\pm 1, t_2) \mp \frac{\partial \tilde{F}}{\partial t_1}(\pm 1, t_2) - \tilde{g}(0, t_2). \tag{7.12}$$

Then, the error formula (3.14) applied to $\tilde{F}(\cdot, t_2)$ (or the Lagrange remainder formula) gives

$$\tilde{F}(0, t_2) = \tilde{F}(\pm 1, t_2) \mp \frac{\partial \tilde{F}}{\partial t_1}(\pm 1, t_2) + \frac{1}{2}\tilde{f}_1{}''(\chi_\pm)\tilde{f}_2(t_2),$$

where $-1 < \chi_- < 0 < \chi_+ < 1$ which with (7.12) and the absolute monotonicity of $\tilde{f}_1$ implies

$$L_{-1}(0, t_2) = \tilde{F}(0, t_2) - \frac{1}{2}\tilde{f}_1{}''(\chi_-)\tilde{f}_2(t_2) > \tilde{F}(0, t_2) - \frac{1}{2}\tilde{f}_1{}''(\chi_+)\tilde{f}_2(t_2) = L_1(0, t_2).$$

□

Hence, if

$$\phi(t_2) := L_1(0, t_2) \geq 0,$$

then (7.12) and Lemma 7.11 show $(\tilde{F} - \tilde{g})(t_1, t_2) > 0$ for all $-1 < t_1 < 1$. So it suffices to show

$\phi \geq 0$ on $[-1/2, 1/2]$ to prove that $\tilde{g} \leq \tilde{F}$ on the critical region. We can express $\phi(t_2)$ as

$$\phi(t_2) = (\tilde{f}_1(1) - \tilde{f}_1{}'(1))\tilde{f}_2(t_2) - a_{0,0} - a_{0,1}t_2 - a_{0,2}(t_2^2 + 1/4).$$

Using our technical bounds on $\tilde{\theta}$, we show the following lemma in Appendix D.1.2:

Lemma 37. *For $a < \pi^2$, $\tilde{f}_1(1) - \tilde{f}_1{}'(1) \geq 0$.*

Thus, $\phi^{(3)}(t_2) \geq 0$, and so its 2nd degree Taylor polynomial at $t_2 = -1/2$ yields the following lower bound for $t_2 \geq -1/2$:

$$\phi(t_2) \geq A + B(t_2 + 1/2) + \frac{C}{2}(t_2 + 1/2)^2$$

where $A = \phi(-1/2)$, $B = \phi'(-1/2)$, and $C = \phi''(-1/2)$. In Appendix D.1.2), we also prove

Lemma 38. *For $a < \pi^2$, $A, C > 0$. If $B < 0$, then $B^2 - 2AC < 0$.*

It follows from Lemma 38 that $A + B(t_2 + 1/2) + \frac{C}{2}(t_2 + 1/2)^2 > 0$ for $t_2 \geq -1/2$ completing the proof that $\tilde{g} \leq \tilde{F}$ in the case $a < \pi^2$, and moreover, showing that $\tilde{F} = \tilde{g}$ only at our interpolation points $(-1, 1), (-1, 1/2), (1, -1/2)$.

7.3.1 The critical region for $a \geq 9.6$

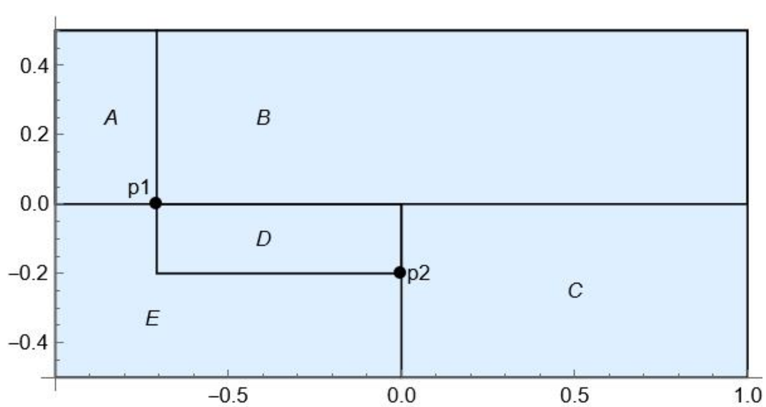

Figure 7.2: The figure depicts our proof strategy for showing $\tilde{F} \geq \tilde{g}$ on the critical region when a is large. The points p_1 and p_2 are located at $(-\sqrt{2}/2, 0), (0, -1/5)$, respectively.

To complete the proof of Theorem 19, it remains to show that $\tilde{F} \geq \tilde{g}$ on the critical region when $a > \pi^2$. In fact, we will show the inequality is strict on the interior of the critical region. We split the region into several subregions as in Figure 7.2. The inequality $\tilde{F} \geq \tilde{g}$ for Subregions A,B,C,D, and E from Figure 7.2 is handled in Lemmas 39, 40, 41, 42, and 43, respectively.

To prove $\tilde{F} \geq \tilde{g}$ on the regions A and D, we apply Lemma 26. Here we use

$$\tilde{g}_{c,d}(t_1, t_2) := \tilde{g}(t_1, t_2) + a_{0,2}(-t_1 t_2 + ct_2 + dt_1 - cd)$$

for $c, d \in [-1, 1]$. Approximating the coefficients $a_{i,j}$ for $a \geq a' := 9.6$, we obtain $\tilde{g}^*_{c,d}$ such that $\tilde{g}^*_{c,d} \geq \tilde{g}_{c,d}$ on the relevant subrectangle and $e^{a/3}\tilde{g}^*_{c,d}$ is linear in a. See Section D.2.3 for the construction of $\tilde{g}^*_{c,d}$ in the different subrectangles. As a lower bound for $\tilde{F}$, we use

$$\tilde{F}_T := (e^{-ax^2} + e^{-a(x-1)^2})e^{-3au^2} \tag{7.13}$$

where x and u are given in (6.11). Analogously to the 4-point case, it is straightforward to verify that these choices of $\tilde{F}_T$, $\tilde{g}_{c,d}$, and $\tilde{g}^*_{c,d}$ satisfy conditions 1–4 of Lemma 26 with $m_1 = 3$ and $a' = 9.6$.

Lemma 39. *We have $\tilde{F} \geq \tilde{g}$ on $A = [-1, -\sqrt{2}/2] \times [0, 1/2]$ with equality only at $(-1, 1/2)$.*

Proof. First, we show the inequality for $[-1, -\sqrt{2}/2] \times [1/4, 1/2]$. Since we already have $\tilde{F} \geq \tilde{g}$ when $t_2 = 1/2$ or $t_1 = -1$, it suffices by Lemma 26 to show inequalities (6.13) on the 2 segments when $t_2 = 1/4$ or $t_1 = -\sqrt{2}/2$, which we handle in Appendix D.2.3. Now having $\tilde{F} \geq \tilde{g}$ on the segment of $[-1, -\sqrt{2}/2] \times [0, 1/4]$ when $t_2 = 1/4$, we again show inequalities (6.13) with $\tilde{g}_{-1,1/4}$ on the segments when $t_2 = 0$ or $t_1 = -\sqrt{2}/2$ to complete the proof. ∎

Lemma 40. *We have $\tilde{F} > \tilde{g}$ on $B = [-\sqrt{2}/2, 1] \times [0, 1/2]$.*

Proof. By the convexity of $\tilde{F} - \tilde{g}$ in t_1, it suffices to show:

1. $\tilde{F}(-\sqrt{2}/2, t_2) \geq \tilde{g}(-\sqrt{2}/2, t_2)$ for all $t_2 \in [0, 1/2]$

2. $\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-\sqrt{2}/2, t_2) \geq 0$ for $t_2 \in [0, 1/2]$.

The first of these follows from Lemma 39. To prove the second, it actually suffices to just show that $\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-\sqrt{2}/2, 0) \geq 0$, which is handled in Appendix D.2.4. This sufficiency follows from the same reasoning as Lemma 33 and holds because $\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1} \geq 0$ is convex in t_2 and satisfies $\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-\sqrt{2}/2, -1/2) < 0$ (due to the necessary condition $\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(1, -1/2) < 0$). □

Lemma 41. *We have* $\tilde{F} \geq \tilde{g}$ *on* $C = [0, 1] \times [-1/2, 0]$ *with equality only at* $(1, -1/2)$.

Proof. We claim that for this portion of the critical region, it suffices to show at each point that

$$L_1(t_1, t_2) := \frac{\tilde{f}_2{}'(t_2)\tilde{f}_1(t_1)}{\tilde{f}_1{}'(t_1)\tilde{f}_2(t_2)} - \frac{\frac{\partial \tilde{g}}{\partial t_2}(t_1, t_2)}{\frac{\partial \tilde{g}}{\partial t_1}(t_1, t_2)} > 0,$$

since this would imply that $\tilde{g}$ increases along the level curves of $\tilde{F}$ as t_1 increases.

Thus, $\tilde{F} - \tilde{g}$ is minimized along the right and bottom boundaries of the region, where we have already showed $\tilde{F} - \tilde{g} \geq 0$ in the previous section with equality only at $(1, -1/2)$. The inequality $L_1(t_1, t_2) > 0$ for $(t_1, t_2) \in [0, 1] \times [-1/2, 0]$ is proved in Appendix D.2.5. □

Lemma 42. *We have* $\tilde{F} > \tilde{g}$ *on* $D = [-\sqrt{2}/2, 0] \times [\frac{1}{5}, 0]$.

Proof. We first show inequalities (6.13) hold for $\tilde{g}_{-\sqrt{2}/2,0}$ on each line segment on the boundary of $[-\sqrt{2}/2, 0 \times [-.1, 0]$ except the $t_2 = 0$ segment (where we already have $\tilde{F} > \tilde{g}$). Then we repeat the process with $\tilde{g}_{-\sqrt{2}/2,-.1}$ on each segment of $[-\sqrt{2}/2, 0] \times [-.2, -.1]$ except the $t_2 = -.1$ segment. The precise calculations are carried out in Appendix D.2.3.

□

Lemma 43. *We have* $\tilde{F} > \tilde{g}$ *on* $E = [-1, 0] \times [-.5, -.2] \cup [-1, -\sqrt{2}/2] \times [-.5, 0]$.

Proof. We extend the domain of the log function so that $\log(t) = \infty$ for $t \leq 0$. Note that this definition and the fact that $\tilde{F} > 0$ on all of $[-1, 1]^2$ imply $\log(\tilde{F}/\tilde{g}) > 0$ on E is equivalent to $\tilde{F} > \tilde{g}$ on E. Since we have already established that this inequality holds on ∂E, it suffices to show $\log(\tilde{F}/\tilde{g})$ takes no finite local minima on S, which we'll do by showing that

$$\frac{\partial}{\partial t_1} \log\left(\frac{\tilde{F}}{\tilde{g}}\right) < 0 \tag{7.14}$$

on all of E where $\tilde{g} > 0$, or equivalently, that if $\tilde{g}(t_1, t_2) > 0$, then

$$\frac{\tilde{f}_1(t_1)}{\tilde{f}_1{}'(t_1)} - \frac{\tilde{g}(t_1, t_2)}{\frac{\partial \tilde{g}(t_1,t_2)}{\partial t_1}} = \frac{\tilde{f}_1(t_1)}{\tilde{f}_1{}'(t_1)} - t_1 - \frac{\tilde{g}(0, t_2)}{a_{1,0} + a_{0,2}t_2} > 0$$

since each of $\tilde{f}_1, \tilde{f}_1{}', \frac{\partial \tilde{g}}{\partial t_1} > 0$ on E (see Equation 7.6). Notably, $\frac{\tilde{f}_1(t_1)}{\tilde{f}_1{}'(t_1)} - t_1$ is a function only in t_1, while $\frac{\tilde{g}(0,t_2)}{a_{1,0}+a_{0,2}t_2}$ depends only on t_2. Let

$$L_2(t_1, t_2) := \frac{\tilde{f}_1(t_1)}{\tilde{f}_1{}'(t_1)} - t_1 - \frac{\tilde{g}(0, t_2)}{a_{1,0} + a_{0,2}t_2}.$$

We will next establish that on all of E, L_2 is decreasing in t_1 and t_2. Thus to show $L_2 > 0$ on all of E, we need only check that $L_2(-\sqrt{2}/2, 0), L_2(0, -.2) > 0$, which is handled in Appendix D.2.6. To see that L_2 is decreasing in both t_1 and t_2, observe by Proposition 14 that

$$\frac{\partial L_2}{\partial t_1} = \left(\frac{\tilde{f}_1}{\tilde{f}_1{}'}\right)' - 1 = \frac{(\tilde{f}_1{}')^2 - \tilde{f}_1{}''\tilde{f}_1}{(\tilde{f}_1{}')^2} - 1 = -\frac{\tilde{f}_1{}''\tilde{f}_1}{(\tilde{f}_1{}')^2} - 1 < 0.$$

Similarly,

$$\frac{\partial L_2}{\partial t_2} = \frac{b_{0,0}a_{0,2} - a_{0,1}a_{1,0} - a_{0,2}t_2(2a_{1,0} + a_{0,2}t_2)}{(a_{1,0} + a_{0,2}t_2)^2}$$

whose sign depends only on $N_2(t_2) := b_{0,0}a_{0,2} - a_{0,1}a_{1,0} - a_{0,2}t_2(2a_{1,0} + a_{0,2}t_2)$. Now

$$N_2'(t_2) = -2a_{0,2}(a_{1,0} + a_{0,2}t_2) = -2a_{0,2}\left(\frac{\partial \tilde{g}}{\partial t_1}(t_1, t_2)\right) < 0$$

for $t_2 \geq -1/2$ (see Equation 7.6). So the negativity of $N_2(t_2)$ and (thus $\frac{\partial L_2}{\partial t_2}$) follows from checking $N_2(-1/2) < 0$, which we handle using our coefficient bounds. $\square$

Chapter 8

Proof of Theorem 20

Fix $a_1 > 0$ and $\beta \geq 1/\sqrt{3}$. It remains to construct a map

$$\tilde{g} = b_{0,0} + b_{1,0}t_1 + b_{0,1}t_2 + b_{0,2}t_2^2$$

such that $\tilde{g} \leq \tilde{F}$ on $[-1, 1]$ with equality at $(-1, 0)$ and $(1, -1)$ and $b_{1,0}, b_{0,1}, b_{0,2} \geq 0$. Our candidate for such a $\tilde{g}$ is

$$\tilde{g} = \tilde{f}_1{}'(1)\tilde{f}_2(-1) + \tilde{f}_1(-1)\tilde{f}_2(0) + \tilde{f}_1{}'(1)\tilde{f}_2(-1)t_1 + \tilde{f}_1(-1)\tilde{f}_2{}'(0)t_2 + \tag{8.1}$$

$$t_2^2\left[\tilde{f}_1(-1)(\tilde{f}_2{}'(0) - \tilde{f}_2(0)) - \tilde{f}_2(-1)(2\tilde{f}_1{}'(1) - \tilde{f}_1(1))\right] \tag{8.2}$$

$$= \tilde{f}_1(-1)H_{\{-1,0,0\}}[\tilde{f}_2](t_2) + (1 + t_1)\tilde{f}_1{}'(1)\tilde{f}_2(-1) - t_2^2\tilde{f}_2(-1)\left(\tilde{f}_1(-1) - \tilde{f}_1(1) + 2\tilde{f}_1{}'(1)\right), \tag{8.3}$$

where $H_\tau[h](t)$ is the unique Hermite interpolant of degree at most $|\tau| - 1$ to the function h on the node set τ (cf. Section 3.3). It is straightforward to check that such a $\tilde{g}$ satisfies the necessary value conditions at $(-1, 0)$ and $(1, -1)$, so it remains to verify the nonegativity of its exapnsion and the inequality $\tilde{F} \leq \tilde{g}$ on $[-1, 1]^2$.

Nonnegative Expansion

Positivity of $b_{0,1}$ and $b_{1,0}$ follow immediately from the absolute monotonicity of $\tilde{f}_1$ and $\tilde{f}_2$, so it remains to prove

Lemma 44. *For any $a_1 > 0$ and $a_2 \geq 4a_2/3$, we have $b_{0,2} > 0$.*

In Appendix E, we use our bounds on $\tilde{\theta}$ to construct bounds of

$$\frac{\tilde{f}_2{}'(0) - \tilde{f}_2(0)}{\tilde{f}_2(-1)} \text{ and } \frac{2\tilde{f}_1{}'(1) - \tilde{f}_1(1)}{\tilde{f}_1(-1)},$$

which are increasing in a_1 and a_2 and then use those bounds to show positivity of $b_{0,2}$ via the formula

$$\frac{b_{0,2}}{\tilde{f}_1(-1)\tilde{f}_2(-1)} = \frac{\tilde{f}_2{}'(0) - \tilde{f}_2(0)}{\tilde{f}_2(-1)} - \frac{2\tilde{f}_1{}'(1) - \tilde{f}_1(1)}{\tilde{f}_1(-1)}.$$

The positivity of $b_{0,2}$ is equivalent to the fact that for all choices of $a_1 > 0$ and $b \geq 1/\sqrt{3}$, tangent approximation of $\tilde{F}(-1,-1)$ from $(1,-1)$ is more accurate than from $(-1,0)$.

8.1 $\tilde{F} \geq \tilde{g}$ on $[-1,1]^2$

We begin with just one further technical computation:

Lemma 45. *For all $a_1 > 0$ and $a_2 \geq 4a_1/3$,*

$$\tilde{f}_1{}'(-1)\tilde{f}_2(1) > \tilde{f}_1{}'(1)\tilde{f}_2(-1).$$

As with the nonnegativity condition, in Appendix E, we construct monotone bounds on

$$\tilde{f}_1{}'(-1)/\tilde{f}_1{}'(1) \text{ and } \tilde{f}_2(-1)/\tilde{f}_2(1),$$

to subsequently prove the lemma. We now may show the desired $\tilde{F} \geq \tilde{g}$ inequality.

Lemma 46. *For all $a_1 > 0$, $a_2 \geq 4a_1/3$, $(t_1, t_2) \in [-1,1]^2$, we have $\tilde{F}(t_1,t_2) \geq \tilde{g}(t_1,t_2)$.*

Proof. We first show that the inequality $\tilde{F} \geq \tilde{g}$ reduces to a check on the boundary by the second derivative test. Our argument proceeds similarly to that proceeding Lemma 26. Let $H_{\tilde{F}}$ denote the Hessian matrix of $\tilde{F}$ and likewise for $H_{\tilde{F}-\tilde{g}}$ with $\tilde{F} - \tilde{g}$. By the strict complete monotonicity of $\tilde{\theta}$

(see Proposition 14), we have $\tilde{f}_i''\tilde{f}_i < (\tilde{f}_i')^2$ for $i \in \{1,2\}$, and thus

$$\det(H_{\tilde{F}}(t_1,t_2)) = (\tilde{f}_1{}''(t_1)\tilde{f}_1(t_1))(\tilde{f}_2{}''(t_2)\tilde{f}_2(t_2)) - \tilde{f}_1{}'(t_1)^2\tilde{f}_2{}'(t_2)^2 < 0$$

for $t_1, t_2 \in [-1,1]$. Then we use the positivity of $b_{0,2}$ to compute

$$\det H_{\tilde{F}-\tilde{g}}(t_1,t_2) = H_{\tilde{F}}(t_1,t_2) - 2\tilde{f}_1{}''(t_1)\tilde{f}_2(t_2)b_{0,2} < H_{\tilde{F}}(t_1,t_2) < 0.$$

Thus, it suffices to verify the difference $\tilde{F} - \tilde{g} \geq 0$ on the boundary. When $t_1 = -1$, we use the representation

$$\tilde{g}(-1,t_2) = \tilde{f}_1(-1)H_{\{-1,0,0\}}[\tilde{f}_2](t_2) - t_2^2\tilde{f}_2(-1)\left(\tilde{f}_1(-1) - \tilde{f}_1(1) + 2\tilde{f}_1{}'(1)\right) \tag{8.4}$$

$$\leq \tilde{f}_1(-1)H_{\{-1,0,0\}}[\tilde{f}_2](t_2) < \tilde{f}_1(-1)\tilde{f}_2(t_2), \tag{8.5}$$

where the first inequality follows from the fact that $(\tilde{f}_1(-1) - \tilde{f}_1(1) + 2\tilde{f}_1{}'(1)) > 0$ by the strict absolute monotonicity of $\tilde{f}_1$, and the second inequality follows from the classical Hermite error formula, which yields

$$\tilde{f}_2(t_2) - H_{\{-1,0,0\}}[\tilde{f}_2](t_2) = \frac{\tilde{f}_2{}^3(\xi)}{3!}(t_2+1)t_2^2 \geq 0, \tag{8.6}$$

for some $\xi \in [-1,1]$ depending on t_2. In particular, we have $(\tilde{F} - \tilde{g})(-1,1) > 0$. When $t_2 = 1$, we use the strict absolute monotonicity of $\tilde{f}_1$ and linearity of $\tilde{g}$ in t_1 to observe that the difference $(\tilde{F} - \tilde{g})(t_1,-1)$ is convex in t_1. Thus, the inequalities $(\tilde{F} - \tilde{g})(-1,1) > 0$ and $\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-1,1) > 0$ (from Lemma 45) immediately yield $(\tilde{F} - \tilde{g})(t_1,1) > 0$ for all $t_1 \in [-1,1]$. Likewise when $t_2 = -1$, the equalities $(\tilde{F}-\tilde{g})(1,-1) = \frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(1,-1) = 0$ immediately yield $(\tilde{F}-\tilde{g})(t_1,-1) \geq 0$ for all $t_1 \in [-1,1]$. Finally, we claim that the global minimum of $\tilde{F} - \tilde{g}$ on $[-1,1]^2$ cannot occur at a point of the form $(1,t_2)$ for $t_2 > 0$, which would complete the proof. Indeed, for every such point, we have

$$\frac{\partial(\tilde{F} - \tilde{g})}{\partial t_1}(1, t_2) = \tilde{f}_1{}'(1)(\tilde{f}_2(t_2) - \tilde{f}_2(-1)) > 0$$

by strict absolute monoticity of $\tilde{f}_2$, and so $\tilde{F} - \tilde{g}$ decreases locally as t_1 decreases. $\square$

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Appendices

Appendix A

Equivalence of Different Notions of Universal Optimality

In this section, we prove that the definition of a lattice Λ being universally optimal given in the introduction is equivalent to that given in [10]. We need the following classical result[1] from the statistical mechanics literature (cf. [14] or [20]).

Lemma 47. *Let $f : [0,\infty) \to [0,\infty]$ be a lower semi-continuous map of d-rapid decay and $\Omega \subset \mathbb{R}^d$ be a bounded, Jordan-measurable set. Then for any $\rho > 0$, $N_k \to \infty$ and $\ell_k \to \infty$ such that $\frac{N_k}{\ell_k^d Vol(\Omega)} \to \rho$, the limit*

$$\lim_{k\to\infty} \frac{\mathcal{E}_f(N_k, \ell_k\Omega)}{N_k} = C_{f,d,\rho}$$

exists and is independent of Ω.

The following proposition shows the equivalence of the different notions of universal optimality:

Proposition 48. *Let $\Lambda \subseteq \mathbb{R}^d$ be a lattice of some density $\rho > 0$. Fix $f\colon [0,\infty) \to [0,\infty]$ as a lower semi-continuous map of d-rapid decay. For an arbitrary sublattice $\Phi \subseteq \Lambda$, let $F_\Phi := F_{f,\Phi}$. Then the following are equivalent:*

(1) As an infinite configuration of density ρ, Λ is f-optimal.

(2) For every sublattice $\Phi \subseteq \Lambda$, the configuration $\Lambda \cap \Omega_\Phi$ is F_Φ-optimal.

(3) There is some sublattice $\Phi \subseteq \Lambda$ such that $\Lambda \cap \Omega_{m\Phi}$ is $F_{m\Phi}$-optimal for infinitely many $m \in \mathbb{N}$.

Proof. First, we'll prove (1) implies (2). Let Λ be a lattice of density ρ satisfying condition (1). If Φ is of index n, then for an arbitrary n-point configuration ω_n, we define $E_\Phi(\omega_n) := E_{F_\Phi}(\omega_n)$, and

[1] This result actually holds for a larger class of potentials that attain negative values. However, here we only really need this for nonnegative potentials such as f_a.

the n-point Φ-periodic configuration $C_n = \omega_n + \Phi$. Note that C_n has density ρ. By assumption $E_f(\Lambda) \leq E_f(C_n)$. Noting that Λ is also an n-point Φ-periodic configuration, we apply Proposition 2 to obtain

$$E_{F,\Phi}(\Lambda \cap \Omega_\Phi) = NE_f(\Lambda) - N \sum_{0 \neq v \in \Lambda} f(|v|^2) \leq NE_f(C_n) - N \sum_{0 \neq v \in \Lambda} f(|v|^2) = E_{F,\Phi}(\omega_n).$$

Since ω_n was arbitrary, we conclude $\Lambda \cap \Omega_\Phi$ is F_Φ-universally optimal as desired.

Clearly (2) implies (3) so it remains to show (3) implies (1). Assume Λ is generated by some matrix V_Λ. Let $\Phi \subseteq \Lambda$ be of index κ, generated by some matrix V_Φ and $\{N_k\} \to \infty$ be our increasing sequence of scalings for which Λ yields an $N_k\Phi$-universally optimal configuration. By Lemma 47, certainly $C_{f,d,\rho}$ is a lower bound for $E_f^l(C)$ for any C of density ρ, simply by the definition of average energy. Thus, we just have to show $E_f(\Lambda) \leq C_{f,d,\rho}$. To do so, we note that f satisfies the so-called *weakly tempered inequality* (cf. [14]), that is, there exist some $\epsilon, R_0, c > 0$, such that for any two N_1, N_2 point configurations $\mu_{N_1} = \{x_1, \ldots, x_{N_1}\}, \mu_{N_2} = \{x_1', \ldots, x_{N_2}'\}$, which are separated by distance at least $R \geq R_0$, we have

$$2\sum_{i=1}^{N_1}\sum_{j=1}^{N_2} f(|x_i - x_j'|^2) \leq \frac{N_1 N_2 c}{R^{d+\epsilon}}.$$

In other words, the interaction energy between the two sets decays like $R^{d+\epsilon}$. Now set

$$\alpha_k = \frac{1}{N_k^{\epsilon/(2(d+\epsilon))}},$$

and define for each $k \geq 1$, the configuration θ_k as a κN_k^d- point configuration which is f-optimal on the set $(1-\alpha_k)\bar{\Omega}_{N_k\Phi}$, Also define $\omega_{\kappa N_k^d} := \Lambda \cap \Omega_{N_k\Phi}$.

We claim the following inequality string holds, which would suffice to prove our desired result:

$$E_f(\Lambda) = \lim_{N_k \to \infty} \frac{E_{N_K\Phi}(\omega_{\kappa N_k^d})}{\kappa N_k^d} \leq \lim_{k \to \infty} \frac{E_{N_K\Phi}(\theta_k)}{\kappa N_k^d} \leq \lim_{k \to \infty} \frac{E_f(\theta_k)}{\kappa N_k^d} = C_{f,d,1}.$$

To obtain the first equality, we apply Proposition 2 to the lattices $N_k\Phi$ and the configurations $\omega_{\kappa N_k^d}$, yielding

$$E_f(\Lambda) = \frac{1}{\kappa N_k^d}\left(E_{N_K\Phi}(\omega_{\kappa N_k^d}) + \kappa N_k^d \sum_{0\neq v\in N_k\Phi} f(|v|^2)\right) \tag{A.1}$$

$$= \frac{E_{N_K\Phi}(\omega_{\kappa N_k^d})}{\kappa N_k^d} + \sum_{0\neq v\in N_k\Phi} f(|v|^2). \tag{A.2}$$

Since

$$\lim_{N_k\to\infty} \sum_{0\neq v\in N_k\Phi} f(|v|^2) = 0,$$

we have

$$E_f(\Lambda) = \lim_{N_k\to\infty} \frac{E_{f,N_K\Phi}(\omega_{\kappa N_k^d})}{\kappa N_k^d}$$

as needed. Our first inequality

$$\lim_{N_k\to\infty} \frac{E_{N_K\Phi}(\omega_{\kappa N_k^d})}{\kappa N_k^d} \leq \lim_{k\to\infty} \frac{E_{N_K\Phi}(\theta_k)}{\kappa N_k^d}$$

follows immediately from our assumption of condition (2).

To obtain our next inequality,

$$\lim_{k\to\infty} \frac{E_{N_K\Phi}(\theta_k)}{\kappa N_k^d} \leq \lim_{k\to\infty} \frac{E_f(\theta_k)}{\kappa N_k^d},$$

we first observe

$$E_{N_k\Phi}(\theta_k) = E_f(\theta_k) + \sum_{x\neq y\in\theta_k} \sum_{v\neq 0\in N_k\Phi} f(x-y+v),$$

so it suffices to show $\sum_{x\neq y\in\theta_k} \sum_{v\neq 0\in N_k\Phi} f(x-y+v) \in o(N_k^d)$ as $N_k \to \infty$. We claim that there exists some $m > 0$ such that for all $v \in N_k\Phi$,

$$d(\theta_k, \theta_k + v) \geq m\alpha_k|v|,$$

which is proved analogously to [3, Theorem 8.4.1].

Returning to $\sum_{x \neq y \in \theta_k} \sum_{v \neq 0 \in N_k\Phi} f(x - y + v)$ for k large enough, we can use the weakly tempered definition to obtain:

$$\begin{aligned}
\sum_{x \neq y \in \theta_k} \sum_{v \neq 0 \in N_k\Phi} f(|x - y + v|^2) &\leq \sum_{v \neq 0 \in N_k\Phi} \sum_{x \in \theta_k} \sum_{y \in \theta_k + v} f(|x - y|^2) \\
&\leq \sum_{v \neq 0 \in N_k\Phi} \frac{N_k^{2d} c}{d(\theta_k, \theta_k + v)^{d+\epsilon}} \\
&\leq \sum_{v \neq 0 \in N_k\Phi} \frac{N_k^{2d} c N_k^{\epsilon/2}}{(m|v|)^{d+\epsilon}} \\
&= \frac{c N_k^{(d-\epsilon/2)}}{m^{d+\epsilon}} \sum_{v \neq 0 \in \Phi} \frac{1}{|v|^{d+\epsilon}}
\end{aligned}$$

and this last quantity is of order $o(N_k^d)$ since the sum converges and no term but $N_k^{d-\epsilon/2}$ depends on k. We should note we treat $y \in \theta_k + v / \{x + v\}$ in the multiset sense, decreasing the cardinality of $x + v$ in $\theta_k + v$ by one.

The final equality $\lim_{k \to \infty} \frac{E_f(\theta_k)}{\kappa N_k^d} = C_{f,d,1}$ is immediate from Lemma 47, which we can apply by the definition of θ_k and the fact that $\alpha_k \to 0$. $\square$

Appendix B

Technical Estimates on Θ

B.1 Bounds for $a \leq \pi^2$

Recall that for $a < \pi^2$, we define $\tilde{f}_1(t_1) = \tilde{\theta}(\frac{\pi}{a}; t_1)$ and $\tilde{f}_2(t_2) = \tilde{\theta}(\frac{\pi}{3a}; t_2)$.

For $0 < a < \pi^2$, we use truncations of the formula

$$\theta(\frac{\pi}{a}; x) := \sum_{k=-\infty}^{\infty} e^{-dk^2} e^{2\pi ikx} = 1 + \sum_{k\geq 1} 2e^{-dk^2} \cos(2\pi kx).$$

where $d := \frac{\pi^2}{a} > 1$, to obtain bounds on θ. Thus, we will use

$$\tilde{f}_1(t_1, j) = f_1(x_1, j) := 1 + \sum_{k=1}^{j} 2e^{-dk^2} \cos(2\pi kx_1) \tag{B.1}$$

$$\tilde{f}_2(t_2, j) = f_2(\frac{x_2}{\sqrt{3}}, j) := 1 + \sum_{k=1}^{j} 2e^{\frac{-dk^2}{3}} \cos(\frac{2\pi kx_2}{\sqrt{3}}) \tag{B.2}$$

We first bound the tails of these series:

$$\begin{aligned} \left| \sum_{k\geq 3} 2e^{-dk^2} \cos(2\pi kx) \right| &\leq 2 \sum_{k\geq 0} e^{-d(k+3)^2} \leq 2e^{-4d} e^{-5} \sum_{k\geq 0} e^{-(k^2+6k)} \\ &\leq 2e^{-4d} e^{-5} \sum_{k\geq 0} e^{-(7k)} = e^{-4d} \frac{2}{e^5(1-e^{-7})} < \frac{e^{-4d}}{50}. \end{aligned} \tag{B.3}$$

Similarly, we have

$$\left| \sum_{k\geq 5} 2e^{-d/3k^2} \cos(2\pi kx) \right| \leq e^{-16d/3} \frac{2}{e^3(1-e^{-11/3})} < \frac{e^{-16d/3}}{5}. \tag{B.4}$$

Hence, for $t_1, t_2 \in [-1, 1]$, we have

$$\begin{aligned} \tilde{f}_1(t_1, 2) - \frac{e^{-4d}}{50} < \tilde{f}_1(t_1) < \tilde{f}_1(t_1, 2) + \frac{e^{-4d}}{50}, \\ \tilde{f}_2(t_2, 4) - \frac{e^{-16d/3}}{5} < \tilde{f}_2(t_2) < \tilde{f}_2(t_2, 4) + \frac{e^{-16d/3}}{5}. \end{aligned} \tag{B.5}$$

We also need bounds on the derivatives of $\tilde{f}_1$ and $\tilde{f}_2$. With $x = \frac{\arccos(t)}{2\pi}$, then $\tilde{\theta}(c, t) = \theta(c, x)$, and so by the chain rule

$$\tilde{\theta}'(t; \frac{\pi}{a}) = \left(-\sum_{k\geq 1} 2e^{-dk^2}(2\pi k)\sin(2\pi kx)\right)\frac{-1}{2\pi\sqrt{1-t^2}} = \frac{\sum_{k\geq 1} 2ke^{-dk^2}\sin(2\pi kx)}{\sin(2\pi x)}.$$

For $t = \pm 1$ ($x = 0, \frac{1}{2}$), we use L'Hopital's rule to obtain

$$\tilde{\theta}'(1; \frac{\pi}{a}) = \sum_{k\geq 1} 2k^2 e^{-dk^2}$$

and

$$\tilde{\theta}'(-1; \frac{\pi}{a}) = \sum_{k\geq 1}(-1)^{n+1} 2k^2 e^{-dk^2}.$$

Then we again bound the tails by comparison with geometric series. For example, using that $d > 1$ and for all $k \geq 0$, $(k+3)^2 \leq 9e^k$, we obtain

$$\begin{aligned} \sum_{k\geq 3} 2k^2 e^{-dk^2} = e^{-9d} 2\sum_{k\geq 0}(k+3)^2 e^{-d(k^2+6k)} &\leq e^{-4d} e^{-5} 2\sum_{k\geq 0} 9e^k e^{-(k^2+6k)} \\ &\leq e^{-4d} 18e^{-5}\sum_{k\geq 0} e^{-6k} = \frac{18e^{-4d}}{e^5(1-e^{-6})} < \frac{e^{-4d}}{8}. \end{aligned}$$

In the $d/3$ case, since $(k+6)^2 \leq 36e^{k/3}$, we analogously have

$$\sum_{k\geq 6} 2k^2 e^{-d/3k^2} = \sum_{k\geq 0} 2(k+6)^2 e^{-d/3(k+6)^2} < 2e^{-25d/3}.$$

When $t = \pm\frac{1}{2}$, we have $\sin 2\pi x = \sqrt{3}/2$ and so

$$\left|\frac{\sum_{k>j} 2ke^{-dk^2}\sin(2\pi kx)}{\sin(2\pi x)}\right| \leq \frac{4}{\sqrt{3}}\sum_{k>j}\left|ke^{-dk^2}\sin(2\pi kx)\right| \leq \sum_{k>j} 4ke^{-dk^2} \leq \sum_{k>j} 4k^2e^{-dk^2}$$

and we can apply the previous bounds for $\sum_{k\geq 6} 2k^2e^{-dk^2/3}$ Thus, we have the following bounds for $d > 1$, $t_1 = \pm 1$, and $t_2 \in \{-1, -\frac{1}{2}, \frac{1}{2}, 1\}$, where $\tilde{f_1}'(t_1, j)$ and $\tilde{f_2}'(t_2, j)$ indicate the truncation of the sums involved in $\tilde{f_1}'(t_1), \tilde{f_2}'(t_2)$ after j terms:

$$\begin{aligned} \tilde{f_1}'(t_1, 2) - \frac{e^{-4d}}{8} < \tilde{f_1}'(t_1) < \tilde{f_1}'(t_1, 2) + \frac{e^{-4d}}{8} \\ \tilde{f_2}'(t_2, 5) - 4e^{-25d/3} < \tilde{f_2}'(t_2) < \tilde{f_2}'(t_2, 5) + 4e^{-25d/3}. \end{aligned} \tag{B.6}$$

Finally, we need bounds for $\tilde{f}_2(\pm\frac{1}{2})$. Again, using the chain rule, we obtain

$$\tilde{\theta}''(d/3, -1/2) = \left(\sum_{k\geq 2} 2ke^{-\frac{d}{3}k^2}\frac{\cot(2\pi x)\sin(2\pi kx) - k\cos(2\pi kx)}{\sin^2(2\pi x)}\right)\Bigg|_{x=1/3} \tag{B.7}$$

$$= \sum_{k\geq 2} -8/3ke^{-\frac{d}{3}k^2}\left(k\cos(2\pi k/3) + \frac{1}{\sqrt{3}}\sin(2\pi k/3)\right). \tag{B.8}$$

Likewise,

$$\tilde{\theta}''(d/3, 1/2) = \sum_{k\geq 2} -8/3ke^{-\frac{d}{3}k^2}\left(k\cos(2\pi k/3) - \frac{1}{\sqrt{3}}\sin(2\pi k/3)\right).$$

Note

$$\left|-8/3ke^{-\frac{d}{3}k^2}\left(k\cos(2\pi k/3) + \frac{1}{\sqrt{3}}\sin(2\pi k/3)\right)\right| \leq \frac{8}{3}k(k+1)e^{-\frac{d}{3}k^2},$$

so using the fact that $(k+6)(k+7) \leq 42e^{k/3}$ for $k \geq 0$ yields

$$\left|\sum_{k\geq 6} -8/3ke^{-\frac{d}{3}k^2}\left(k\cos(2\pi k/3) + \frac{1}{\sqrt{3}}\sin(2\pi k/3)\right)\right| \leq \sum_{k\geq 6}\frac{8}{3}k(k+1)e^{-\frac{d}{3}k^2}$$

$$\leq e^{-25d/3}\frac{8}{3}e^{-11/3}\sum_{k\geq 0}(k+6)(k+7)e^{-\frac{d}{3}(k^2+12k)} \leq e^{-25d/3}\frac{8}{3}e^{-11/3}\sum_{k\geq 0} 42e^{-4k} < 5e^{-25d/3}.$$

Thus, we obtain our final bounds

$$\tilde{f}_2''(\pm\frac{1}{2},5) - 5e^{-25d/3} < \tilde{f}_2''(\pm\frac{1}{2}) < \tilde{f}_2''(\pm\frac{1}{2},5) + 5e^{-25d/3}. \tag{B.9}$$

As a final remark, it is straightforward to check that the leftmost lower bounds in (B.5), (B.6), and (B.9) are positive

B.2 Bounds for $a \geq \pi^2$

Throughout, assume that $a \geq 9.6$. We'll set $\epsilon = \frac{1}{1000}$ so that for all $a \geq 9.6$:

$$\epsilon > 2\sum_{n\geq 1} e^{-an} \text{ and } \epsilon > 5e^{-a}. \tag{B.10}$$

Then set $\epsilon_2 = \frac{1}{100} > 4(1+\epsilon)^2 \sum_{n\geq 1} e^{-2(9.6)n/3}$, $\epsilon_3 = \frac{1}{50}$, $\epsilon_4 = \frac{1}{40}$.

In the large a case, it is preferable to use the following formula for θ because of its rapid convergence:

$$\theta(c;x) = c^{-1/2} \sum_{k=-\infty}^{\infty} e^{-\frac{\pi(k+x)^2}{c}}.$$

Thus, we'll use the formulas

$$f_1(x_1) = \sqrt{\frac{a}{\pi}}\theta(\frac{\pi}{a};x_1) = \sum_{k=-\infty}^{\infty} e^{-a(k+x_1)^2}, \tag{B.11}$$

$$f_2(x_2) = \sqrt{\frac{3a}{\pi}}\theta(\frac{\pi}{3a},x_2) = \sum_{k=-\infty}^{\infty} e^{-3a(k+x_2)^2}. \tag{B.12}$$

B.2.1 Basic Lemmas and Other Estimates

We first establish a couple basic workhorse lemmas bounding θ and $\tilde{\theta}'$.

Lemma 49. *For* $x = \arccos(t)/(2\pi) \in [0, 1/2]$*,*

$$e^{-ax^2} + e^{-a(x-1)^2} < \theta(\frac{\pi}{a}; x) < (1+\epsilon)e^{-ax^2}(1 + e^{-a(1-2x)}) \leq 2(1+\epsilon)e^{-ax^2} \tag{B.13}$$

$$e^{-ax^2} < \theta(\frac{\pi}{a}; x) \leq e^{-ax^2}(1 + 2\sum_{n\geq 1} e^{-a(n^2-2nx)}). \tag{B.14}$$

Proof. Recall $\theta(\frac{\pi}{a}; x) = \sum_{n\in\mathbb{Z}} e^{-a(n+x)^2}$. The lower bounds follow from simply truncating the series. To obtain the first upper bound, observe

$$\sum_{n\in\mathbb{Z}} e^{-a(n+x)^2} = e^{-ax^2}\sum_{n\geq 0} e^{-a(n^2+2nx)} + e^{-a(x-1)^2}\sum_{n\geq 0} e^{-a(n^2+2(1-x)n)} \tag{B.15}$$

$$\leq (e^{-ax^2} + e^{-a(1-x)^2})\sum_{n\geq 0} e^{-an} < (1+\epsilon)(e^{-ax^2} + e^{-a(1-x)^2}). \tag{B.16}$$

The second upper bound follows in a similar fashion using the fact that for $n \geq 1$, the nth term is at least as large as the $-(n+1)$th term. $\square$

In the remainder of this section we shall use the dependent variables as in (6.11):

$$x = x_1 = \frac{\arccos(t_1)}{2\pi}, \qquad u = x_2/\sqrt{3} = \frac{\arccos(t_2)}{2\pi}. \tag{B.17}$$

Lemma 49 implies that for $t_2 \in [-\frac{1}{2}, 1]$, we have:

$$\begin{aligned} e^{-3au^2} &< \tilde{f}_2(t_2) < (1+\epsilon)e^{-3au^2} \\ 1 &< \tilde{f}_1(1), \tilde{f}_2(1) < 1+\epsilon \\ e^{-a/16} &< \tilde{f}_1(0) < (1+\epsilon_3)e^{-a/16}, \\ 2e^{-a/4} &< \tilde{f}_1(-1) < 2(1+\epsilon)e^{-a/4} \\ 2e^{-3a/4} &< \tilde{f}_2(-1) < 2(1+\epsilon)e^{-3a/4}. \end{aligned} \tag{B.18}$$

These particular bounds follow immediately except for the first, where we use that if $t_2 \in [-1/2, 1]$, then $u \in [0, 1/3]$ and so

$$2\sum_{n\geq 1} e^{-3a(n^2-2nx)} \leq 2\sum_{n\geq 1} e^{-3a(n-2n(1/3))} = 2\sum_{n\geq 1} e^{-a} < \epsilon.$$

Lemma 50. *For $x = \frac{\arccos(t_1)}{2\pi} \in (0, 1/2)$,*

$$\frac{ae^{-ax^2}(x-(1-x)e^{-a(1-2x)})}{\pi\sin(2\pi x)} \leq \tilde{\theta}'(\frac{\pi}{a}; t_1) \leq \frac{axe^{-ax^2}}{\pi\sin(2\pi x)}. \tag{B.19}$$

Proof. Using $t_1 = \cos(2\pi x)$, we have

$$\tilde{\theta}'(\frac{\pi}{a}; t_1) = \frac{\sum_{n\in\mathbb{Z}} -2a(n+x)e^{-a(n+x)^2}}{-2\pi\sin(2\pi x)} = \frac{a\sum_{n\in\mathbb{Z}}(n+x)e^{-a(n+x)^2}}{\pi\sin(2\pi x)}.$$

Let $s_n = (n+x)e^{-a(n+x)^2}$. Now to obtain the lower bound, we verify that for $n \geq 1$, $s_n + s_{-n-1} \geq 0$. Thus, $s_0 + s_{-1}$ yields a lower bound. Similarly, we check $s_n + s_{-n} \leq 0$, so s_0 yields an upper bound. It will be independently useful that $s_0 \geq s_{-1}$ for $\frac{1}{4} \leq x \leq \frac{1}{2}$. Indeed, in this case, taking $v = \frac{1}{2} - x$,

$$ae^{-ax^2}(x-(1-x)e^{-a(1-2x)} = ae^{-ax^2}(1/2 - v - (1/2+v)e^{-2av})$$

and $(1/2 - v - (1/2+v)e^{-2av})$ is concave in v for all $a \geq 9.6$, $v \in [0, \frac{1}{4}]$, and so it suffices to check the inequality for $v = 0, \frac{1}{4}$, which are both immediate. $\square$

As a consequence of Lemma 50, we obtain for $a \geq 9.6$ and $t_2 \in [-1/2, 1/2]$ that

$$\tilde{f_2}'(t_2) > \frac{3aue^{-3au^2}(1-\epsilon)}{\pi\sin(2\pi u)}. \tag{B.20}$$

Indeed, for such t_2, $u \in [1/6, 1/3]$, so $u - 1 \geq -5u$ and $1 - 2u \geq \frac{1}{3}$ which gives

$$\tilde{\theta}'(\frac{\pi}{3a}, t_2) \geq \frac{3ae^{-au^2}(u-(1-u)e^{-3a(1-2u)})}{\pi\sin(2\pi u)} \geq \frac{3aue^{-au^2}(1-5e^{-a})}{\pi\sin(2\pi u)} > \frac{3aue^{-au^2}(1-\epsilon)}{\pi\sin(2\pi u)}.$$

In particular,

$$\frac{(1-\epsilon)ae^{-a/12}}{\sqrt{3\pi}} < \tilde{f_2}'(\frac{1}{2}),$$
$$\frac{2(1-\epsilon)ae^{-a/3}}{\sqrt{3\pi}} < \tilde{f_2}'(-\frac{1}{2}). \tag{B.21}$$

A similar computation yields

$$\frac{ae^{-a/16}(1-\epsilon_4)}{4\pi} < \sqrt{\frac{a}{\pi}}\tilde{\theta}'(\frac{\pi}{a};0) < \frac{ae^{-a/16}}{4\pi}. \tag{B.22}$$

We also need to obtain bounds on $\tilde{\theta}'(\frac{\pi}{a};\pm 1)$. For $a \geq 9.6$,

$$\frac{a}{2\pi^2}(a-2)e^{-a/4} < \tilde{\theta}'(\frac{\pi}{a};-1) < \frac{a}{2\pi^2}(a-2+\epsilon)e^{-a/4}$$
$$\frac{(1-\epsilon_2)a}{2\pi^2} < \tilde{\theta}'(\frac{\pi}{a};1) < \frac{a}{2\pi^2}. \tag{B.23}$$

For $a \geq 21$,

$$\frac{(1-\epsilon)a}{2\pi^2} < \tilde{\theta}'(\frac{\pi}{a};1) < \frac{a}{2\pi^2}. \tag{B.24}$$

We first have

$$\tilde{\theta}'(\pi/a,-1) = \frac{a}{2\pi^2}\sum_{n\in\mathbb{Z}}\left[2a(n+1/2)^2-1\right]e^{-a(n+1/2)^2}.$$

We get an easy lower bound by just taking the $n = 0, -1$ terms. For an upper bound, we bound the tail:

$$2\sum_{n\geq 1}\left[2a(n+1/2)^2-1\right]e^{-a(n+1/2)^2} \leq e^{-a/4}4\sum_{n\geq 1}\left[a(2n)^2\right]e^{-a(n^2+n)} \tag{B.25}$$

$$\leq e^{-a/4}16\sum_{n\geq 1}an^2e^{-an^2}e^{-an} \leq e^{-a/4}16/1000\sum_{n\geq 1}e^{-an} \leq \epsilon e^{-a/4}, \tag{B.26}$$

where we have used that $an^2e^{-an^2} \leq \frac{1}{1000}$ since $be^{-b} \leq \frac{1}{1000}$ for $b \geq 9.6$. Thus, we obtain the bounds

$$\frac{a}{2\pi^2}(a-2)e^{-a/4} \leq \tilde{\theta}'(\pi/a,-1) \leq \frac{a}{2\pi^2}(a-2+\epsilon)e^{-a/4}.$$

Next,

$$\tilde{\theta}'(\pi/a,1) = \frac{a}{2\pi^2}\sum_{n\in\mathbb{Z}}\left[1-2an^2\right]e^{-an^2}.$$

By just using the $n=0$ term, we get an easy upper bound. Now bounding the tail, we have

$$\left|2\sum_{n\geq 1}\left[1-2an^2\right]e^{-an^2}\right| \leq 4\sum_{n\geq 1}an^2e^{-an^2} \leq 4\sum_{n\geq 1}e^{-2an^2/3} \leq 4\sum_{n\geq 1}e^{-2an/3} \leq 4\sum_{n\geq 1}e^{-2(9.6)n/3} \quad < \epsilon_2 \tag{B.27}$$

since $be^{-b} \leq e^{-2b/3}$ for $b \geq 9.6$ Thus, we have

$$\frac{(1-\epsilon_2)a}{2\pi^2} \leq \tilde{\theta}'(\frac{\pi}{a};1) \leq \frac{a}{2\pi^2} \tag{B.28}$$

and when $a \geq 21$, we obtain that the tail is at most $4\sum_{n\geq 1}e^{-14n} < \epsilon$ in the same manner, and so in this case,

$$\frac{(1-\epsilon)a}{2\pi^2} \leq \tilde{\theta}'(\frac{\pi}{a};1) \leq \frac{a}{2\pi^2},$$

as desired.

We finally need bounds on $\tilde{\theta}''(\frac{\pi}{3a},\pm\frac{1]}{2})$. First, we have

$$\tilde{\theta}''(\frac{\pi}{3a},t_2) = \frac{3a}{\pi^2\sin(2\pi u)^2}\sum_{n\in\mathbb{Z}}e^{-3a(n+u)^2}\left(-\frac{1}{2}+\pi\cot(2\pi u)(n+u)+3a(n+u)^2\right)$$

so that

$$\begin{aligned}\tilde{\theta}''(\frac{\pi}{3a},\frac{1}{2}) &= \frac{4a}{\pi^2}\sum_{n\in\mathbb{Z}}e^{-3a(n+\frac{1}{6})^2}\left(-\frac{1}{2}+\frac{\pi}{\sqrt{3}}(n+\frac{1}{6})+3a(n+\frac{1}{6})^2\right)\\ &\geq \frac{4a}{\pi^2}e^{-a/12}\left(-\frac{1}{2}+\frac{\pi}{6\sqrt{3}}+a/12\right)\end{aligned}$$

$$
\begin{aligned}
\tilde{\theta}''(\frac{\pi}{3a},-\frac{1}{2}) &= \frac{4a}{\pi^2}\sum_{n\in\mathbb{Z}} e^{-3a(n+\frac{1}{3})^2}\left(-\frac{1}{2}-\frac{\pi}{\sqrt{3}}(n+\frac{1}{3})+3a(n+\frac{1}{3})^2\right) \\
&\le \frac{4a}{\pi^2}e^{-a/3}\left(-\frac{1}{2}-\frac{\pi}{3\sqrt{3}}+a/3\right)+\frac{4a}{\pi^2}e^{-a/3}\sum_{n\neq 0} e^{-3a(n^2+2n)}\left(\left|-\frac{1}{2}\right|+\left|\frac{\pi}{\sqrt{3}}(n+\frac{1}{3})\right|+\left|3a(n+\frac{1}{3})^2\right|\right) \\
&\le \frac{4a}{\pi^2}e^{-a/3}\left(-\frac{1}{2}-\frac{\pi}{3\sqrt{3}}+a/3\right)+\frac{4a}{\pi^2}e^{-a/3}16\sum_{n\ge 1} e^{-an^2}an^2 \\
&\le \frac{4a}{\pi^2}e^{-a/3}\left(-\frac{1}{2}-\frac{\pi}{3\sqrt{3}}+a/3\right)+\frac{4a}{\pi^2}e^{-a/3}16\sum_{n\ge 1} e^{\frac{-an^2}{2}} \\
&\le \frac{4a}{\pi^2}e^{-a/3}\left(-\frac{1}{2}-\frac{\pi}{3\sqrt{3}}+a/3\right)+\frac{4a}{\pi^2}e^{-a/3} = \frac{4a}{\pi^2}e^{-a/3}\left(\frac{1}{2}-\frac{\pi}{3\sqrt{3}}+a/3\right),
\end{aligned}
$$

where for the first inequality we have just thrown away all the terms except for which $n = 0$ (these are certainly all positive), and for the second string of inequalities, we have used that $be^{-b} \le e^{-b/2}$ for $b \ge 9.6$ and then used a comparison with a geometric series to obtain $16\sum_{n\ge 1} e^{\frac{-an^2}{2}} \le 16\sum_{n\ge 1} e^{\frac{-an}{2}} \le 1$.

This leads to the bounds for $\tilde{f_2}''$:

$$
\begin{aligned}
\tilde{f_2}''(\frac{1}{2}) &\ge \frac{4a}{\pi^2}e^{-a/12}\left(-\frac{1}{2}+\frac{\pi}{6\sqrt{3}}+a/12\right) \\
\tilde{f_2}''(-\frac{1}{2}) &\le \frac{4a}{\pi^2}e^{-a/3}\left(\frac{1}{2}-\frac{\pi}{3\sqrt{3}}+a/3\right).
\end{aligned}
\tag{B.29}
$$

As in the case of $a \le 9.6$, we will use ${}_u\tilde{f}_1$ and ${}_l\tilde{f}_1$ to denote the bounds for $\tilde{f}_1$ produced in this section and likewise for $\tilde{f}_2$.

Appendix C

Computations for the Proof of Theorem 18

C.1 $\tilde{F} \geq \tilde{g}$ for small a and 4 points

First, we prove that $\frac{\partial^3 \tilde{F}}{\partial t_1 \partial t_2^2}(-1, 1/2) \geq 0$ to complete the proof of Lemma 22 for $a < \pi^2$. We'll use the notation ${}_u\tilde{f}_1(t_1), {}_l\tilde{f}_1(t_1)$ to denote the upper and lower bounds given in the previous section and likewise for $\tilde{f}_2$. We have

$$\begin{aligned} \frac{\partial^3 \tilde{F}}{\partial t_1 \partial t_2^2}(-1, 1/2) &\geq {}_l\tilde{f}_1{}'(-1)\, {}_l\tilde{f}_2{}''(1/2) - {}_u\tilde{f}_1{}'(1)\, {}_u\tilde{f}_2{}''(-1/2) \\ &= e^{-4d}\left[-440e^{-16d/3} - 130e^{-4d/3} + 96\right] > 0. \end{aligned} \tag{C.1}$$

To prove this final inequality, and several others later in the section, we use the following elementary lemma that reduces to verifying the inequality at $d = 1$ which is easily checked in the case above.

Lemma 51. *Let $h(d) = a_1 e^{c_1 d} + \cdots + a_n e^{c_n d}$, where the c_i's are increasing and there is some j such that $a_i \leq 0$ for $i < j$ and $a_i \geq 0$ for $i > j$. Then $h(d) > 0$ for all $d \geq 1$ if and only if $h(1) > 0$.*

Proof. Note $h(d) \geq 0$ if and only if $h(d)e^{-c_j d} \geq 0$, and we have

$$h(d)e^{-c_j d} = a_1 e^{(c_1 - c_j)d} + \cdots + a_{j-1} e^{(c_{j-1} - c_j)d} + a_j + \cdots + a_n e^{(c_n - c_j)d}.$$

By our assumptions on the a_i's and c_i's, for $i < j$, a_i and $c_i - c_j$ are both negative, so $a_i e^{(c_i - c_j)}$ is nondereasing. For $i > j$, both a_i and $c_i - c_j$ are nonnegative, and so again $a_i e^{(c_i - c_j)}$ is nondecreasing. Thus, $h(d)e^{-c_j d} > 0$ is nondecreasing, which suffices for the desired result. □

Next, we prove Lemma 24 for $a \leq \pi^2$.

Proof. First, we'll show

$$2\frac{\partial \tilde{F}}{\partial t_1}(-1,1/2) < \frac{\partial^2(\tilde{F}-\tilde{g})}{\partial t_1 \partial t_2}(-1,1/2).$$

Using the bounds from the previous section,

$$2\frac{\partial \tilde{F}}{\partial t_1}(-1,1/2) \leq 2\left[{}_u\tilde{f}_1{}'(-1)\,{}_u\tilde{f}_2(1/2) - {}_l\tilde{f}_1{}'(1)\,{}_l\tilde{f}_2(-1/2)\right], \tag{C.2}$$

$$\frac{\partial^2 \tilde{F}}{\partial t_1 \partial t_2}(-1,1/2) = \tilde{f}_1{}'(-1)\tilde{f}_2{}'(1/2) + \tilde{f}_1{}'(1)\tilde{f}_2{}'(-1/2) \tag{C.3}$$

$$\geq {}_l\tilde{f}_1{}'(-1)'\,{}_l\tilde{f}_2(1/2) + {}_l\tilde{f}_1{}'(1)\,{}_l\tilde{f}_2(-1/2), \tag{C.4}$$

from which we obtain

$$\frac{\partial^2 \tilde{F}}{\partial t_1 \partial t_2}(-1,1/2) - 2\frac{\partial \tilde{F}}{\partial t_1}(-1,1/2) \geq e^{-4d}\left[95/2 - 8/5e^{-7d/3} - 191/2e^{-4d/3} - e^{-d/3}/2\right] > 0$$

It remains to show

$$4(\tilde{F}(-1,1) - \tilde{F}(-1,1/2)), \frac{\partial \tilde{F}}{\partial t_2}(-1,1) < 2\frac{\partial \tilde{F}}{\partial t_1}(-1,1/2).$$

Just as above, we obtain

$$2\frac{\partial \tilde{F}}{\partial t_1}(-1,1/2) - 4(\tilde{F}(-1,1) - \tilde{F}(-1,1/2)) \geq$$

$$e^{-4d}\left[31/2 - 219/10e^{-16d/3} - (16e^{-3d})/25 - 8/5e^{-7d/3} - 427/10e^{-4d/3} - (4e^{-d/3})/25\right] > 0.$$

Similarly,

$$2\frac{\partial \tilde{F}}{\partial t_1}(-1,1/2) - \frac{\partial \tilde{F}}{\partial t_2}(-1,1) \geq$$

$$e^{-4d}\left[47/2 - 18e^{-25d/3} - 8e^{-13d/3} - (18e^{-3d})/25 - 8/5e^{-7d/3} - 127/2e^{-4d/3} - (2e^{-d/3})/25\right] > 0.$$

$\square$

C.2 Intermediate a and 4 points

C.2.1 Calculations for Lemma 22

First, we show Lemma 22 for $a \geq 9.6$

Proof. We need to show

$$\tilde{\theta}'(\frac{\pi}{a};-1)\tilde{\theta}''(\frac{\pi}{3a},\frac{1}{2})-\tilde{\theta}'(\frac{\pi}{a};1)\tilde{\theta}''(\frac{\pi}{3a},-\frac{1}{2})>0.$$

$\square$

Using the bounds of lemmas B.23 and B.29, we have:

$$\tilde{\theta}'(\frac{\pi}{a};-1)\tilde{\theta}''(\frac{\pi}{3a},\frac{1}{2})-\tilde{\theta}'(\frac{\pi}{a};1)\tilde{\theta}''(\frac{\pi}{3a},-\frac{1}{2})\geq \tag{C.5}$$

$$\frac{a(a-2)e^{-a/4}}{2\pi^2}\frac{4a}{\pi^2}e^{-a/12}\left(-\frac{1}{2}+\frac{\pi}{6\sqrt{3}}+a/12\right)-\frac{a}{2\pi^2}\frac{4a}{\pi^2}e^{-a/3}\left(\frac{1}{2}-\frac{\pi}{3\sqrt{3}}+a/3\right) \tag{C.6}$$

$$=\frac{a^2e^{-a/3}(18+3a^2+2a(-18+\sqrt{3}\pi))}{18\pi^4}. \tag{C.7}$$

The inner expression is quadratic in a. It is straightforward to check that it's positive with positive slope at $a = 9.6$ and convex.

C.2.2 Proof of Lemma 24

Next, we'll prove Lemma 24 for $9.6 < a \leq 21$.

Proof. To obtain

$$2\frac{\partial\tilde{F}}{\partial t_1}(-1,1/2)<\frac{\partial^2(\tilde{F}-\tilde{g})}{\partial t_1\partial t_2}(-1,1/2),$$

we apply the bounds from lemmas B.20, 49, B.23, we obtain

$$2\frac{\partial \tilde{F}}{\partial t_1}(-1,1/2) \leq 2\left[\frac{a}{2\pi^2}(a-2+\epsilon)e^{-a/4}(1+\epsilon)e^{-a/12} - (1-\epsilon_2)\frac{a}{2\pi^2}e^{-a/3}\right] \tag{C.8}$$

$$= \frac{e^{-a/3}}{\pi^2}\left[(a-2+\epsilon)(1+\epsilon) - (1-\epsilon_2)\right]. \tag{C.9}$$

$$\frac{\partial^2(\tilde{F}-\tilde{g})}{\partial t_1 \partial t_2}(-1,1/2) \geq \frac{a^2 e^{-a/3}(1-\epsilon)(a-2\epsilon_2)}{2\pi^3\sqrt{3}}. \tag{C.10}$$

Factoring out $\frac{ae^{-a/3}}{\pi^2}$ from each term, it suffices to show

$$\frac{a(1-\epsilon)(a-2\epsilon_2)}{\sqrt{3}\pi} - (2(a-2+\epsilon) - (1-\epsilon_2)) > 0$$

and this is certainly true by just checking the value and first derivative of this difference at $a = 9.6$ are positive since it is quadratic in a and convex.

Next we handle

$$4(\tilde{F}(-1,1) - \tilde{F}(-1,1/2)) < 2\frac{\partial \tilde{F}}{\partial t_1}(-1,1/2).$$

We have from Lemma 49 and B.23 that

$$4(\tilde{F}(-1,1) - \tilde{F}(-1,1/2)) \leq 4(2(1+\epsilon)^2(1+e^{-a/2})e^{-a/4} - 3e^{-a/3}) \tag{C.11}$$

$$2\frac{\partial \tilde{F}}{\partial t_1}(-1,1/2) \geq 2\left(\frac{a(a-2)e^{-a/4}}{2\pi^2}e^{-a/12} - \frac{a}{2\pi^2}(1+\epsilon)e^{-a/3}\right) \tag{C.12}$$

$$= \frac{ae^{-a/3}(a-3-\epsilon)}{\pi^2}. \tag{C.13}$$

Factoring out $e^{-a/4}$, it suffices to show

$$e^{-a/12}\left(12 + \frac{a(a-3-\epsilon)}{\pi^2}\right) - 8(1+\epsilon)^2(1+e^{-a/2}) \geq 0$$

which holds if

$$e^{-a/12}\left(12+\frac{a(a-3-\epsilon)}{\pi^2}\right)-8(1+\epsilon)^2(1+e^{-9.6/2})>0.$$

We can check that on $[9.6, 21]$, this final quantity is either increasing or concave, implying it doesn't have local minima, so it suffices to check the inequality at the endpoints $a = 9.6, 21$.

Finally, we need to show $\frac{\partial \tilde{F}}{\partial t_2}(-1,1) < 2\frac{\partial \tilde{F}}{\partial t_1}(-1,1/2)$. We already have a lower bound for $2\frac{\partial \tilde{F}}{\partial t_1}(-1,1/2)$, and from (B.23) and Lemma 49, we compute

$$\frac{\partial \tilde{F}}{\partial t_2}(-1,1) \leq \frac{3ae^{-a/4}}{2\pi^2}\left((2+2\epsilon)-(3a-2)e^{-a/2}\right). \tag{C.14}$$

Factoring $\frac{ae^{-a/4}}{2\pi^2}$, it suffices to show

$$2(a-3-\epsilon)e^{-a/12}-3(2+2\epsilon)+3(3a-2)e^{-a/2}>0,$$

and it's straightforward to check $2(a-3-\epsilon)e^{-a/12}$ is concave for $a \leq 21$. Since also for $a \in [9.6, 21]$ and any constant b satisfying $b \geq a$, we have

$$3(3a-2)e^{-b/2} \leq 3(3a-2)e^{-a/2},$$

it then suffices to check

$$\begin{aligned}
&2(a-3-\epsilon)e^{-a/12}-3(2+2\epsilon)+3(3a-2)e^{-21/2}>0 \qquad && a=21,11\\
&2(a-3-\epsilon)e^{-a/12}-3(2+2\epsilon)+3(3a-2)e^{-11/2}>0 \qquad && a=9.6,
\end{aligned}$$

which completes the proof. $\square$

C.3 Large a and 4 points

Now we assume $a \geq 21$, and first present the remaining bits of the proof of Lemma 25.

Proof. Using the bounds on $\tilde{\theta}$ given in (B.23) and Lemma 49, we obtain

$$0 \leq \frac{ae^{-a/4}}{2\pi^2}\left((a-2)-(2+2\epsilon)e^{-a/2}\right) \leq \frac{\partial \tilde{F}}{\partial t_1}(-1,1) \leq \frac{ae^{-a/4}}{2\pi^2}(a-2+\epsilon)(1+\epsilon) \tag{C.15}$$

$$0 \leq \frac{3(2-4\epsilon)ae^{-a/4}}{2\pi^2} \leq \frac{\partial \tilde{F}}{\partial t_2}(-1,1) \leq \frac{3ae^{-a/4}}{\pi^2}(1+\epsilon). \tag{C.16}$$

Thus,

$$\begin{aligned}\frac{\partial \tilde{F}}{\partial t_1}(-1,1) - \frac{\partial \tilde{F}}{\partial t_2}(-1,1) &\geq \frac{ae^{-a/4}}{2\pi^2}\left(a-2-3(2+2\epsilon)-e^{-a/2}(2+2\epsilon)\right)\\ &= \frac{ae^{-a/4}}{2\pi^2}\left(a-8-6\epsilon-e^{-a/2}(2+2\epsilon)\right)\end{aligned}$$

which is easily seen to be positive for $a \geq 21$.

Next, using Lemma 49 and equation (B.23),

$$\begin{aligned}(\tilde{F}-\tilde{g})(-1,1/2) &= \tilde{F}(-1,1/2) - \tilde{F}(-1,1) + \frac{b_1}{4}\\ &\geq 3e^{-a/3} - 2(1+\epsilon^2)e^{-a/4} - 2(1+\epsilon)^2 e^{-3a/4} + \frac{3(2-4\epsilon)ae^{-a/4}}{2\pi^2}\\ &= e^{-a/4}\left[3e^{-a/12} - 2(1+\epsilon)^2(1+e^{-a/2}) + \frac{3(2-4\epsilon)a}{2\pi^2}\right]\\ &\geq e^{-a/4}\left[3e^{-a/12} - 2(1+\epsilon)^3 + \frac{3(2-4\epsilon)a}{2\pi^2}\right] > 0.\end{aligned} \tag{C.17}$$

The quantity in the brackets is convex in a, so it suffices to verify the positivity of the value and derivative of this quantity at $a = 21$ which are straightforward computations. □

Now we present the remaining components of the proof of Lemma 27.

Proof. Recall we have

$$\tilde{F}_T := (e^{-ax^2} + e^{-a(x-1)^2})e^{-3au^2} + e^{-a((\frac{1}{2}-x)^2+3(\frac{1}{2}-u)^2)}$$

and note that for $c < t_1 < 0$, $0 < t_2 < d$, with $t_2 + c < 0$, we have the following upper bounds for

$\tilde{g}$

$$\begin{aligned}\tilde{g}(t_1,t_2) \leq \tilde{g}_{c,d}(t_1,t_2) &:= \tilde{F}(-1,1) + b_1 t_2^2 + b_1(dt_1 + ct_2 - cd)\\ &\leq {}_u\tilde{f}_1(-1)\,{}_u\tilde{f}_2(1) + {}_u\tilde{f}_1(1)\,{}_u\tilde{f}_2(-1) + b_1^l t_2(t_2+c) + b_1^l(dt_1) - cdb_1^u\\ &\leq 2(1+\epsilon)^3 e^{-a/4} + b_1^l t_2(t_2+c) + b_1^l(dt_1) - cdb_1^u =: \tilde{g}^*_{c,d}(t_1,t_2) \quad \text{(C.18)}\end{aligned}$$

where

$${}_u\tilde{f}_1(-1)\,{}_u\tilde{f}_2(1) + {}_u\tilde{f}_1(1)\,{}_u\tilde{f}_2(-1) = 2e^{-a/4}(1+\epsilon)^2(1+e^{-a/2}) \leq 2e^{-a/4}(1+\epsilon)^3,$$

and b_1^l and b_1^u are the bounds on $\frac{\partial \tilde{F}}{\partial t_2}(-1,1)$ given in (C.16).

We then show that inequalities (6.13) hold with the choices:

$$\tilde{g}^*_{-1,1} \text{ on the segments } \{(\cos(2\pi\sqrt{3}/4, t_2) : t_2 \in [.7,1]\} \text{ and } \{(t_1,.7) : t_1 \in (-1,\cos(2\pi\sqrt{3}/4)\} \quad \text{(C.19)}$$

$$\tilde{g}^*_{-1,.7} \text{ on the segments } \{(\cos(2\pi\sqrt{3}/4, t_2) : t_2 \in [.6,.7]\} \text{ and } \{(t_1,.6) : t_1 \in (-1,\cos(2\pi\sqrt{3}/4)\} \quad \text{(C.20)}$$

$$\tilde{g}^*_{-1,.6} \text{ on the segments } \{(\cos(2\pi\sqrt{3}/4, t_2) : t_2 \in [.5,.6]\} \text{ and } \{(t_1,.5) : t_1 \in (-1,\cos(2\pi\sqrt{3}/4)\}, \quad \text{(C.21)}$$

thus permitting the application of Lemma 26. Here, we'll handle the case of (C.19), and leave the other (similar) cases to the Mathematica notebook [17]. By definition, we have

$$\tilde{g}^*_{-1,1}(t_1,t_2) = 2(1+\epsilon)^3 e^{-a/4} + b_1^l t_2(t_2-1) + b_1^l t_1 + b_1^u.$$

Similarly, we have

$$\frac{\partial[e^{a/4}\tilde{g}^*_{-1,1}(t_1,t_2)]}{\partial a} = \frac{3(2-4\epsilon)}{2\pi^2} t_2(t_2-1) + \frac{3(2-4\epsilon)}{2\pi^2} t_1 + \frac{3}{\pi^2}(1+\epsilon),$$

and since $t_2 \geq 1/2$ on $\tilde{\Delta}_{A_2}$, it is immediate from the formulas that $\tilde{g}^*_{-1,1}$ and $\dfrac{\partial\left[e^{a/4}\tilde{g}^*_{c,d}(t_1,t_2)\right]}{\partial a}$ are increasing in t_1 and t_2 on the two line segments. $\square$

Likewise, we can decompose $\tilde{F}_T$ into

$$\begin{aligned}\tilde{F}_t(t_1,t_2) &= (e^{-ax^2}+e^{-a(x-1)^2})e^{-3au^2}+e^{-a[(\frac{1}{2}-x)^2-3(\frac{1}{2}-u)^2]}\\ &= e^{-a(x^2+3u^2)}+e^{-a\left[(\frac{1}{2}-x)^2+3(\frac{1}{2}-u)^2\right]}+e^{-a\left[(x-1)^2+3u^2\right]}.\end{aligned}$$

Since u decreases as t_2 increases on $[-1,1]$ with $u(1)=0$, $u(-1)=1/2$, we have $(e^{-ax^2}+e^{-a(x-1)^2})e^{-3au^2}$ increasing in t_2 and $e^{-a(\frac{1}{2}-x)^2}e^{-3a(\frac{1}{2}-u)^2}$ decreasing in t_2. By the same reasoning, $e^{-ax^2}e^{-3au^2}$ increases in t_1, while $e^{-a(\frac{1}{2}-x)^2}e^{-3a(\frac{1}{2}-u)^2}$ and $e^{-a(x-1)^2}e^{-3au^2}$ are decreasing in t_1. Finally,

$$\begin{aligned}\left.\frac{\partial[e^{a/4}\tilde{F}_T(t_1,t_2)]}{\partial a}\right|_{a=21} &= -(x^2+3u^2-1/4)e^{-21(x^2+3u^2-1/4)}\\ &\quad-\left[(\frac{1}{2}-x)^2+3(\frac{1}{2}-u)^2-1/4\right]e^{-21\left[(\frac{1}{2}-x)^2+3(\frac{1}{2}-u)^2-1/4\right]}\\ &\quad-\left[(x-1)^2+3u^2-1/4\right]e^{-21\left[(x-1)^2+3u^2-1/4\right]}.\end{aligned}$$

To break this function into a difference of increasing functions, we need the following elementary lemma, which can be proved by just checking the derivative:

Lemma 52. *Let n_1,n_2 be constants, and consider the function $\phi(\gamma) := (n_1+\gamma)e^{-21(n_2+\gamma)}$ for $\gamma\in\mathbb{R}$. Then ϕ is increasing as a function of γ for $\gamma \leq (1-21n_1)/21$.*

Now take $(x^2+3u^2-1/4-1/28)e^{-21(x^2+3u^2-1/4)}$ as a function of $3u^2$. Using the fact that $t_1<0$ and $t_2\geq 1/2$ on the whole rectangle A (so $1/4<x\leq 1/2$ and $0\leq 3u^2\leq 1/12$), we obtain

$$3u^2 \leq 1/12 = (1-21(1/4-1/4-1/28))/21 \leq (1-21(x^2-1/4-1/28))/21,$$

and so we may apply Lemma 52 to observe $(x^2+3u^2-1/4-1/28)e^{-21(x^2+3u^2-1/4)}$ is increasing as a function of $3u^2$. Since $3u^2$ is decreasing as a function of t_2, we finally apply the chain rule to see $-(x^2+3u^2-1/4-1/28)e^{-21(x^2+3u^2-1/4)}$ is increasing as a function of t_2 on all of A. In the same way, we can check that it is increasing as a function of t_1, along with the following, analogous claims:

- The quantity $-\left[(\frac{1}{2}-x)^2+3(\frac{1}{2}-u)^2-1/4-4/7\right]e^{-21\left[(\frac{1}{2}-x)^2+3(\frac{1}{2}-u)^2-1/4\right]}$ is decreasing in t_1 and t_2.
- The quantity $-\left[(x-1)^2+3u^2-1/4-2/5\right]e^{-21\left[(x-1)^2+3u^2-1/4\right]}$ is decreasing in t_1 and increasing in t_2.

In summary, we can take the decomposition

$$\begin{aligned}\left.\frac{\partial[e^{a/4}\tilde{F}_T(t_1,t_2)]}{\partial a}\right|_{a=21} &= -(x^2+3u^2-1/4-1/28)e^{-21(x^2+3u^2-1/4)}-\frac{1}{28}e^{-21(x^2+3u^2-1/4)}\\ &\quad-\left[(\frac{1}{2}-x)^2+3(\frac{1}{2}-u)^2-1/4-4/7\right]e^{-21\left[(\frac{1}{2}-x)^2+3(\frac{1}{2}-u)^2-1/4\right]}\\ &\quad-\frac{4}{7}e^{-21\left[(\frac{1}{2}-x)^2+3(\frac{1}{2}-u)^2-1/4\right]}\\ &\quad-\left[(x-1)^2+3u^2-1/4-2/5\right]e^{-21\left[(x-1)^2+3u^2-1/4\right]}-\frac{2}{5}e^{-21\left[(x-1)^2+3u^2-1/4\right]}.\end{aligned}$$

where each term is either increasing or decreasing in t_1 and t_2 on each of our line segments.

Finally, we present the proof of Lemma 28.

Proof. Recall it remains to show that at $P=(\cos(2\pi\frac{\sqrt{3}}{4}),\cos(2\pi\frac{\sqrt{3}}{12})):=(t_1',t_2')$,

$$\left.\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}\right|_P\geq 0,\qquad \left.\frac{\partial^2\tilde{F}-\tilde{g}}{\partial t_1\partial t_2}\right|_P\geq 0.$$

For the first inequality, we first compute using Lemmas 50 and 49, $x=\frac{\sqrt{3}}{4}$, and $u=\frac{\sqrt{3}}{12}$ that

$$\left.\frac{\partial\tilde{F}}{\partial t_1}\right|_P\geq\frac{a}{\pi\sin(2\pi x)}\left(e^{-ax^2}(x-(1-x)e^{-a(1-2x)})e^{-3au^2}-(\frac{1}{2}-x)e^{-a(\frac{1}{2}-x)^2}2(1+\epsilon)e^{-3a(1/2-u)^2}\right)\tag{C.22}$$

$$= \frac{ae^{-a/4}}{\pi \sin(2\pi x)} \left((x - (1-x)e^{-a(1-2x)}) - (\frac{1}{2} - x)2(1+\epsilon)e^{-a(1-x-3u)} \right) \tag{C.23}$$
$$\geq \frac{38ae^{-a/4}}{\pi 41} \tag{C.24}$$

using the fact that $x-(1-x)e^{-a(1-2x)} \geq \frac{39}{100}$, $(\frac{1}{2}-x)2(1+\epsilon)e^{-a(1-x-3u)} \leq \frac{1}{100}$, and $\sin(2\pi x) \leq \frac{41}{100}$ for $a \geq 21$. On the other hand, since $\cos(2\pi u) \leq \frac{62}{100}$,

$$\left.\frac{\partial \tilde{g}}{\partial t_1}\right|_P \leq .62b_1 \tag{C.25}$$
$$\leq \frac{ae^{-a/4}3(1+\epsilon).62}{\pi^2}. \tag{C.26}$$

Thus,

$$\left.\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}\right|_P \geq \frac{ae^{-a/4}}{\pi} \left(\frac{38}{41} - \frac{3(1+\epsilon)62}{100\pi} \right) > 0, \tag{C.27}$$

as the final inner quantity is positive.

It remains to show $\left.\frac{\partial^2 \tilde{F}-\tilde{g}}{\partial t_1 \partial t_2}\right|_P > 0$ in much the same fashion.

Using Lemma 50,

$$\left.\frac{\partial^2 \tilde{F}}{\partial t_1 \partial t_2}\right|_P \geq \tilde{f_1}'(\cos(2\pi\sqrt{3}/4))\tilde{f_2}'(\cos(2\pi\sqrt{3}/12)) \tag{C.28}$$
$$\geq \frac{39ae^{-ax^2}}{41\pi} \frac{3ae^{-3au^2}(u-(1-u)e^{-3a(1-2u)})}{\pi \sin(2\pi u)} \tag{C.29}$$
$$\geq \frac{5*3*39a^2e^{-a/4}}{4*41\pi^2}(u-(1-u)e^{-3a(1-2u)}) \tag{C.30}$$
$$\geq \frac{14*5*3*39a^2e^{-a/4}}{100*4*41\pi^2} \tag{C.31}$$

since $\sin(2\pi u) \leq \frac{4}{5}$ and $u-(1-u)e^{-3a(1-2u)} \geq \frac{14}{100}$. Thus,

$$\left.\frac{\partial^2 \tilde{F}-\tilde{g}}{\partial t_1 \partial t_2}\right|_P \geq \frac{14*5*3*39a^2e^{-a/4}}{100*4*41\pi^2} - \frac{ae^{-a/4}3(1+\epsilon)}{\pi^2} \tag{C.32}$$
$$= \frac{ae^{-a/4}}{\pi^2} \left(\frac{14*5*3*39a}{100*4*41} - 3(1+\epsilon) \right). \tag{C.33}$$

The inner quantity is increasing in a and so it suffices to check its positivity at $a = 21$. $\square$

Appendix D

Compuatations for the Proof of Theorem 19

D.1 $\tilde{F} \geq \tilde{g}$ for small a and 6 points

D.1.1 Satisfying Necessary Conditions

Recall we aim to show

$$\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-1,-1) > 0 \tag{D.1}$$

$$\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-1,1/2) > 0 \tag{D.2}$$

$$\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(1,-1/2) < 0. \tag{D.3}$$

Proof. First, we'll compute bounds for $a_{1,0}, a_{0,2}$. Recall

$$2a_{1,0} = \tilde{f}_1(1)\tilde{f}_2(-1/2) - \tilde{f}_1(-1)\tilde{f}_2(1/2) + \tilde{f}_1(-1)\tilde{f}_2{}'(1/2) \tag{D.4}$$

$$\frac{9}{4}a_{0,2} = \tilde{f}_1(-1)(\tilde{f}_2(-1) - \tilde{f}_2(\frac{1}{2}) + \frac{3}{2}\tilde{f}_2{}'(\frac{1}{2})). \tag{D.5}$$

Thus, using our bounds,

$${}_l\tilde{f}_1(1)\,{}_l\tilde{f}_2(-1/2) - {}_u\tilde{f}_1(-1)\,{}_u\tilde{f}_2(1/2) + {}_l\tilde{f}_1(-1)\,{}_l\tilde{f}_2{}'(1/2) < 2a_{1,0} \tag{D.6}$$

$$2a_{1,0} > {}_u\tilde{f}_1(1)\,{}_u\tilde{f}_2(-1/2) - {}_l\tilde{f}_1(-1)\,{}_l\tilde{f}_2(1/2) + {}_u\tilde{f}_1(-1)\,{}_u\tilde{f}_2{}'(1/2) \tag{D.7}$$

$${}_l\tilde{f}_1(-1)({}_l\tilde{f}_2(-1) - {}_u\tilde{f}_2(1/2) + \frac{3}{2}\,{}_l\tilde{f}_2{}'(1/2)) < \frac{9}{4}b_{0,2} < {}_u\tilde{f}_1(-1)({}_u\tilde{f}_2(-1) - {}_l\tilde{f}_2(1/2) + \frac{3}{2}\,{}_u\tilde{f}_2{}'(1/2)). \tag{D.8}$$

Call these upper and lower bounds $a^u_{i,j}, a^l_{i,j}$ respectively. Now using those bounds, we compute

$$\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-1,-1) = \tilde{f_1}'(-1)\tilde{f_2}(-1) - (a_{1,0} - a_{0,2}) \tag{D.9}$$

$$> {}_l\tilde{f_1}'(-1)\,{}_l\tilde{f_2}(-1) - a^u_{1,0} + a^l_{0,2} \tag{D.10}$$

$$\geq e^{-3d}\left[-2 + 1123/100e^{-4d/3} - (2429e^{-d})/200 + 2e^{2d/3}\right] > 0. \tag{D.11}$$

This final inequality is shown by checking that $-2 + 1123/100e^{-4d/3} - (2429e^{-d})/200 + 2e^{2d/3}$ is positive with positive derivative at $d = 1$ and then applying Lemma 51 to show its derivative is nonnegative for all $d > 1$.

The other conditions are similar. We must check the positivity of the lower bound

$$\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-1,1/2) \geq -(1629/200)e^{-13d/3} - (2429e^{-4d})/200 - 2e^{-3d} + 8e^{-7d/3} > 0 \tag{D.12}$$

by checking at $d = 1$ and applying Lemma 51. Finally, the negativity of the upper bound

$$\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(1,-1/2) \leq -e^{-3d}(2 + (7397e^{-7d/3})/1800 + 1621/200e^{-4d/3} - (2429e^{-d})/200) < 0 \tag{D.13}$$

follows from checking positivity of $2 + (7397e^{-7d/3})/1800 + 1621/200e^{-4d/3} - (2429e^{-d})/200$ and its derivative at $d = 1$, and then applying Lemma 51 to its derivative, $e^{-d}(2429/200 - (51779e^{-4d/3})/5400 - (1621e^{-d/3})/150)$, as we did with the bound of $\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-1,-1)$. □

D.1.2 Computations for the Linear Approximation Bound

We have the expansions

$$A = \phi(-1/2) = \left(\tilde{f_1}(1) - \tilde{f_1}'(1)\right)\tilde{f_2}(-1/2) - a_{0,0} + \frac{a_{0,1}}{2} - \frac{a_{0,2}}{2} \tag{D.14}$$

$$= \left(\frac{1}{2}\tilde{f}_1(1) - \tilde{f}_1{}'(1)\right)\tilde{f}_2(-1/2) + \frac{1}{6}\tilde{f}_1(-1)\tilde{f}_2{}'(1/2) - \tilde{f}_1(-1)\left(\frac{2}{9}\tilde{f}_2(-1) + \frac{5}{18}\tilde{f}_2(1/2)\right) \tag{D.15}$$

$$B = \phi'(-1/2) = (\tilde{f}_1(1) - \tilde{f}_1{}'(1))\tilde{f}_2{}'(-1/2) - a_{0,1} + a_{0,2} \tag{D.16}$$

$$= a_{0,2} - \tilde{f}_1{}'(1)\tilde{f}_2{}'(-1/2) \tag{D.17}$$

$$= \frac{4}{9}\tilde{f}_1(-1)\left(\tilde{f}_2(-1) - \tilde{f}_2(1/2) + \frac{3}{2}\tilde{f}_2{}'(1/2)\right) - \tilde{f}_1{}'(1)\tilde{f}_2{}'(1/2) \tag{D.18}$$

$$C = \phi''(-1/2) = \left(\tilde{f}_1(1) - \tilde{f}_1{}'(1)\right)\tilde{f}_2{}''(-1/2) - 2a_{0,2} \tag{D.19}$$

$$= \left(\tilde{f}_1(1) - \tilde{f}_1{}'(1)\right)\tilde{f}_2{}''(-1/2) - \frac{8}{9}\tilde{f}_1(-1)\left(\tilde{f}_2(-1) - \tilde{f}_2(1/2) + \frac{3}{2}\tilde{f}_2{}'(1/2)\right). \tag{D.20}$$

It remains to use these expansions to prove Lemmas 37 and 38.

Proof. To show Lemma 37, we prove the stronger statement $\tilde{f}_1(1) - 2\tilde{f}_1{}'(1) \geq 0$. From our aforementioned bounds,

$$\tilde{f}_1(1) - 2\tilde{f}_1{}'(1) \geq {}_l\tilde{f}_1(1) - {}_u\tilde{f}_1{}'(1) \geq 1 - (1427e^{-4d})/100 - 2e^{-d} > 0. \tag{D.21}$$

Onto Lemma 38, where we must first show $A, C > 0$. We have

$$2A = \left(\tilde{f}_1(1) - 2\tilde{f}_1{}'(1)\right)\tilde{f}_2(-1/2) + \frac{1}{3}\tilde{f}_1(-1)\tilde{f}_2{}'(1/2) - \tilde{f}_1(-1)\left(\frac{4}{9}\tilde{f}_2(-1) + \frac{5}{9}\tilde{f}_2(1/2)\right) \tag{D.22}$$

$$\geq \left({}_l\tilde{f}_1(1) - 2\,{}_u\tilde{f}_1{}'(1)\right){}_l\tilde{f}_2(-1/2) + \frac{1}{3}\,{}_l\tilde{f}_1(-1)\,{}_l\tilde{f}_2{}'(1/2) - {}_u\tilde{f}_1(-1)\left(\frac{4}{9}\,{}_u\tilde{f}_2(-1) + \frac{5}{9}\,{}_u\tilde{f}_2(1/2)\right) \tag{D.23}$$

$$\geq 2951/600e^{-16d/3} + 4879/600e^{-13d/3} - (2429e^{-4d})/200 + 2e^{-3d} > 0. \tag{D.24}$$

The final quantity, when multiplied by e^{4d} is convex in d, so we just check the value and derivative of this product at $d = 1$. Similarly, we calculate

$$C = \left(\tilde{f}_1(1) - \tilde{f}_1{}'(1)\right) \tilde{f}_2{}''(-1/2) - 2b_{0,2} \tag{D.25}$$
$$\geq \left({}_l\tilde{f}_1(1) - {}_u\tilde{f}_1{}'(1)\right) {}_l\tilde{f}_2{}''(-1/2) - 2a^u_{0,2} \tag{D.26}$$
$$\geq (3687e^{-7d})/25 - 688/45e^{-19d/3} - 9377/225e^{-16d/3} - 24e^{-3d} + 16e^{-7d/3} > 0 \tag{D.27}$$

by applying Lemma 51 to $-688/45e^{-19d/3} - 9377/225e^{-16d/3} - 24e^{-3d} + 16e^{-7d/3}$. Finally, with the additional assumption that $B < 0$, we must show $A^2 - BC < 0$. To bound B^2 above, we bound B below (since $B < 0$). We have

$$B = b_{0,2} - \tilde{f}_1{}'(1)\tilde{f}_2{}'(-1/2) \tag{D.28}$$
$$\geq 14309/450e^{-16d/3} - 65/4e^{-13d/3}. \tag{D.29}$$

We have arrived at the following lower bounds for A, B, C, with the A and C bounds shown to be positive:

$$A_l := 2951/600e^{-16d/3} + 4879/600e^{-13d/3} - 2429/200e^{-4d} + 2e^{-3d} \tag{D.30}$$
$$B_l := 14309/450e^{-16d/3} - 65/4e^{-13d/3} \tag{D.31}$$
$$C_l := 3687/25e^{-7d} - 688/45e^{-19d/3} - 9377/225e^{-16d/3} - 24e^{-3d} + 16e^{-7d/3}. \tag{D.32}$$

We now show $B_l^2 - 2A_lC_l < 0$, which is equivalent to $B_l/C_l - 2A_l/B_l > 0$. To do so, we plug in $d = 1$ and see the inequality holds there. Then, we claim B_l/C_l is increasing in d, while $2A_l/B_l$ is decreasing in d. The sign of the derivative of $B_l/C_l = \frac{e^{13d/3}}{e^{13d/3}C_l}$ depends only on the sign of

$$e^{3d}(B_le^{13d/3})'C_l - B_l(e^{13d/3}C_l)' \geq -520 + (400652e^{-d})/225 - (114472e^{-d/3})/75 + 520e^{2d/3} > 0$$

where we obtain the final inequality by checking positivity of $-520+(400652e^{-d})/225-(114472e^{-d/3})/75+520e^{2d/3}$ and its derivative at $d = 1$, and applying Lemma 51 to its derivative. Likewise, the derivative of $2A_l/B_l$ depends only on the sign of

$$e^{3d}(2e^{13d/3}(A_l e^{13d/3})' B_l - A_l(e^{13d/3}Bl)') \leq$$
$$-(130/3) + (182785597e^{-7d/3})/540000 - (34756561e^{-2d})/67500 + (4626181e^{-d})/21600 < 0,$$

and the final inequality depends on the same checks as with the previous case. All of these checks at $d = 1$ and algebraic simplifications are verified in [17]. □

D.2 Large a and 6 points

D.2.1 Coefficient Bounds

Again, we take $a \geq 9.6$. Our first task is using estimates on θ to bound the coefficients of $\tilde{g}$. We obtain

Lemma 53.

$$0 \leq \frac{2(1-\epsilon)a}{\sqrt{3}\pi} \leq e^{a/3}a_{0,1} \leq \frac{2(1+\epsilon)a}{\sqrt{3}\pi} \tag{D.33}$$
$$0 \leq 1/2(-1-6\epsilon) + \frac{(1-\epsilon)a}{\sqrt{3}\pi} \leq e^{a/3}a_{1,0} \leq 1/2(-1+3\epsilon) + \frac{(1+\epsilon)a}{\sqrt{3}\pi} \tag{D.34}$$
$$0 \leq \frac{3}{2} \leq e^{a/3}a_{0,0} \leq \frac{3}{2}(1+3\epsilon) \tag{D.35}$$
$$\frac{8}{9}\left(-(1+\epsilon) + \frac{\sqrt{3}a(1-\epsilon)}{2\pi}\right) \leq e^{a/3}a_{0,2} \leq \frac{8}{9}\left(\frac{9}{8}\epsilon_2 - (1+\epsilon) + \frac{\sqrt{3}a(1+\epsilon)}{2\pi}\right) \tag{D.36}$$
$$0 \leq \frac{3}{2} - \frac{2}{9}(1+\epsilon) + \frac{\sqrt{3}a(1-\epsilon)}{9\pi} \leq e^{a/3}b_{0,0} \leq \frac{3}{2}(1+3\epsilon) + \frac{1}{4}\epsilon_2 - \frac{2}{9}(1+\epsilon) + \frac{\sqrt{3}a(1+\epsilon)}{9\pi} \tag{D.37}$$

Proof. We begin by using lemmas 49 and B.20 to multiply our bounds on $\tilde{f}_1(1), \tilde{f}_2{}'(-\frac{1}{2})$ to obtain our bound on $a_{0,1}$.

Next, using this bound, combined with Lemma 49 and our definition

$$a_{1,0} := \frac{\tilde{f}_1(1)\tilde{f}_2(-1/2) - \tilde{f}_1(-1)\tilde{f}_2(1/2)}{2} + \frac{a_{0,1}}{2},$$

we obtain the bounds for $a_{1,0}$. We also use the fact that $e^2 < e$ so that $(1+\epsilon)^2 < 1 + 3\epsilon$.

The bounds for

$$a_{0,0} := \frac{\tilde{f}_1(1)\tilde{f}_2(-1/2) + \tilde{f}_1(-1)\tilde{f}_2(1/2)}{2}$$

follow in the same manner. For $a_{0,2}$, we next compute that

$$0 \leq \frac{4}{9}\tilde{f}_1(-1)\tilde{f}_2(-1) \leq \frac{4}{9}e^{-a}4(1+\epsilon)^2 \leq e^{-a/3}\epsilon_2.$$

Now using the definition,

$$a_{0,2} = \frac{4}{9}\tilde{f}_1(-1)(\tilde{f}_2(-1) - \tilde{f}_2(1/2) + \frac{3}{2}\tilde{f}_2{}'(1/2))$$

we obtain the bounds for $a_{0,2}$.

Finally, the $b_{0,0}$ bound follows immediately from previous bounds and the definition $b_{0,0} := a_{0,0} + a_{0,2}/4$. $\square$

We use the notation $a^u_{i,j}$ $a^l_{i,j}$ for the upper and lower bounds respectively, and we note that the bounds are linear in a with positive slope, up to a factor of $e^{-a/3}$, and so the nonnegativity follows from simply checking when $a = 9.6$.

D.2.2 Satisfying Necessary Conditions for large a

Recall we aim to show

$$\frac{\partial(\tilde{F} - \tilde{g})}{\partial t_1}(-1,-1) > 0 \tag{D.38}$$

$$\frac{\partial(\tilde{F} - \tilde{g})}{\partial t_1}(-1,1/2) > 0 \tag{D.39}$$

$$\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(1,-1/2) < 0. \tag{D.40}$$

Proof. For the first condition, using Lemma 53 and the absolute monotonicity of $\tilde{\theta}$, we have:

$$e^{a/3}\left(\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-1,-1)\right) \geq -e^{a/3}\left(\frac{\partial\tilde{g}}{\partial t_1}(-1,-1)\right) \geq e^{a/3}a^l_{0,2} - e^{a/3}a^u_{1,0} > 0, \tag{D.41}$$

and this last inequality is easy to check since $e^{a/3}a^l_{0,2} - e^{a/3}a^u_{1,0}$ is linear in a.

Now incorporating lemmas 50 and B.23,

$$e^{a/3}\left(\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-1,1/2)\right) \geq e^{a/3}\frac{a(a-2)}{2\pi^2}e^{-a/4}e^{-a/12} - (e^{a/3}a^u_{1,0} + \frac{e^{a/3}}{2}a^u_{0,2}) \tag{D.42}$$

$$= \frac{a(a-2)}{2\pi^2} - (e^{a/3}a^u_{1,0} + \frac{e^{a/3}}{2}a^u_{0,2}) > 0, \tag{D.43}$$

because this last quantity is quadratic in a and convex, so it suffices to check it is positive with positive slope at $a = 9.6$, Finally,

$$e^{a/3}\left(\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(1,-1/2)\right) \leq e^{a/3}\frac{a}{2\pi^2}e^{-a/3}(1+\epsilon) - (e^{a/3}a^l_{1,0} - \frac{e^{a/3}}{2}a^u_{0,2}) \tag{D.44}$$

$$= \frac{(1+\epsilon)a}{2\pi^2} - (e^{a/3}a^l_{1,0} - \frac{e^{a/3}}{2}a^u_{0,2}) < 0 \tag{D.45}$$

and this last quantity is linear in a, so again the final check is straightforward. □

D.2.3 Bounds for proofs of Lemmas 39 and 42

It remains to show that $\tilde{F}_T \geq \tilde{g}^*_{c,d}$ for various c, d and various line segments in the critical region $[-1,1]\times[-1/2,1/2]$, where $\tilde{g}^*_{c,d}$ is an upper bound for $\tilde{g}_{c,d}$ obtained by replacing $a_{i,j}$'s with upper and lower bounds from Lemma 53.

In particular, when $c < 0$ and $0 < d$, we define

$$\tilde{g}^*_{c,d}(t_1, t_2) := b^u_{0,0} + a^l_{1,0} t_1 a^u_{0,1} t_2 + a^u_{0,2} t_2^2 + a^l_{0,2}(dt_1 + ct_2 - cd), \tag{D.46}$$

and then $\tilde{g}_{c,d}(t_1, t_2) \leq \tilde{g}^*_{c,d}(t_1, t_2)$ if $c < t_1 < 0$ and $0 < t_2 < d$. For $c < 0$ and $d \leq 0$, we define

$$\tilde{g}^*_{c,d}(t_1, t_2) := b^u_{0,0} + a^l_{1,0} t_1 a^l_{0,1} t_2 + a^u_{0,2} t_2^2 + a^u_{0,2}(dt_1 + ct_2 - cd), \tag{D.47}$$

which gives $\tilde{g}_{c,d}(t_1, t_2) \leq \tilde{g}^*_{c,d}(t_1, t_2)$ if $c < t_1 < 0$ and $-1 \leq t_2 < d \leq 0$. To complete the proof of Lemmas 39 and 42 we show inequalities (6.13) hold with

1. $\tilde{g}^*_{-1,1/2}$ on the segments $\{(-\sqrt{2}/2, t_2) \mid t_2 \in [\frac{1}{4}, \frac{1}{2}]\} \cup \{(t_1, \frac{1}{4}) \mid t_1 \in [-1, -\sqrt{2}/2]\}$
2. $\tilde{g}^*_{-1,1/4}$ on the segments $\{(-\sqrt{2}/2, t_2) \mid t_2 \in [0, \frac{1}{4}]\} \cup \{(t_1, 0) \mid t_1 \in [-1, -\sqrt{2}/2]\}$
3. $\tilde{g}^*_{-\sqrt{2}/2,0}$ on the segments $\{(-\sqrt{2}/2, t_2) \mid t_2 \in [-.1, 0]\} \cup \{(0, t_2) \mid t_2 \in [-.1, 0]\} \cup \{(t_1, -.1) \mid t_1 \in [-\sqrt{2}/2, 0]\}$
4. $\tilde{g}^*_{-\sqrt{2}/2,-.1}$ on the segments $\{(-\sqrt{2}/2, t_2) \mid t_2 \in [-.2, -.1]\} \cup \{(0, t_2) \mid t_2 \in [-.2, -.1]\} \cup \{(t_1, -.2) \mid t_1 \in [-\sqrt{2}/2, 0]\}$,

in [17] with the same procedure as used in Section C.3.

D.2.4 Computations for proof of Lemma 40

Recall it remains to show $\frac{\partial(\tilde{F}-\tilde{g})}{\partial t_1}(-\sqrt{2}/2, 0) \geq 0$. By Lemma 50, (B.20), 49 and our coefficient estimates, we have

$$\frac{\partial(\tilde{F} - \tilde{g})}{\partial t_1}(-\sqrt{2}/2, 0) = \tilde{f_1}'(-\sqrt{2}/2)\tilde{f}_2(0) - a_{1,0} \tag{D.48}$$

$$\geq \frac{(ae^{-a(3/8)^2}(3/8 - 5/8e^{-a/4}))}{\pi(1/\sqrt{2})} e^{-3a/16} - e^{-a/3}(-1/2 + \frac{3}{2}\epsilon + \frac{(1+\epsilon)a}{\sqrt{3\pi}}) \tag{D.49}$$

$$= e^{-a/3}\left[\frac{\sqrt{2}ae^{a/192}(3-5e^{-a/4})}{8\pi} - (-1/2 + \frac{3}{2}\epsilon + \frac{(1+\epsilon)a}{\sqrt{3\pi}})\right]. \tag{D.50}$$

We claim that

$$\frac{\sqrt{2}ae^{a/192}(3-5e^{-a/4})}{8\pi} - (-1/2 + \frac{3}{2}\epsilon + \frac{(1+\epsilon)a}{\sqrt{3\pi}})$$

is positive for $a = 9.6$ and increasing in a for $a \geq 9.6$. The first of these conditions is a simple check. For the latter,

$$\frac{d}{da}\left[\frac{\sqrt{2}ae^{a/192}(3-5e^{-a/4})}{8\pi} - (-1/2 + 2\epsilon + \frac{(1+\epsilon)a}{\sqrt{3\pi}})\right] \tag{D.51}$$

$$= \frac{e^{-47a/192}(-960 + 235a + 576e^{a/4} + 3ae^{a/4})}{768\sqrt{2}\pi} - \frac{(1+\epsilon)}{\sqrt{3\pi}} \tag{D.52}$$

$$> \frac{e^{-47a/192}(576e^{a/4} + 3ae^{a/4})}{768\sqrt{2}\pi} - \frac{(1+\epsilon)}{\sqrt{3\pi}} \tag{D.53}$$

$$= \frac{(576e^{a/192} + 3ae^{a/192})}{768\sqrt{2}\pi} - \frac{(1+\epsilon)}{\sqrt{3\pi}} > 0 \tag{D.54}$$

where this last quantity is greater than 0 because it's true for $a = 9.6$ and clearly increasing in a.

D.2.5 Positivity of L_1 for Proposition 41

Recall to prove Lemma 41, it suffices to show that

$$L_1(t_1, t_2) := \frac{\tilde{f}_2{}'\tilde{f}_1}{\tilde{f}_1{}'\tilde{f}_2} - \frac{\frac{\partial \tilde{g}}{\partial t_2}}{\frac{\partial \tilde{g}}{\partial t_1}} > 0$$

on $[0,1] \times [-1/2, 0]$. We first bound $\frac{\tilde{f}_1\tilde{f}_2{}'}{\tilde{f}_1{}'\tilde{f}_2}$below. Using the Lemma 49, $\tilde{f}_1 \geq e^{-ax^2}$. Since $|t_2| \leq \frac{1}{2}$, by (B.18) it follows that

$$\tilde{f}_2 < e^{-3au^2}(1+\epsilon). \tag{D.55}$$

With Lemma 50, ${\tilde{f}_1}' \leq \frac{axe^{-ax^2}}{\pi\sin(2\pi x)}$. Finally, with $u \in [1/4, 1/3]$, we have by (B.20),

$$
{\tilde{f}_2}' \geq \frac{3aue^{-3au^2}(1-\epsilon)}{\pi\sin(2\pi u)}. \tag{D.56}
$$

Combining these bounds, we obtain:

$$
\frac{\tilde{f}_1 {\tilde{f}_2}'}{{\tilde{f}_1}' \tilde{f}_2} \geq \frac{e^{-3ax^2} 3ae^{-3au^2} u(1-\epsilon)}{\pi\sin(2\pi u)} \cdot \frac{\pi\sin(2\pi x)}{axe^{-ax^2}e^{-3au^2}(1+\epsilon)} = \frac{3u(1-\epsilon)\sin(2\pi x)}{(1+\epsilon)x\sin(2\pi u)}. \tag{D.57}
$$

Next, a couple of observations:

Lemma 54. $\frac{\sin(2\pi x)}{x} = \frac{2\pi\sqrt{1-t_1^2}}{\arccos(t_1)}$ *is concave in* t_1 *for* $t_1 \in (-1,1)$. *Also,* $\frac{u}{\sin(2\pi u)}$ *is decreasing in* t_2 *for* $t_2 \in (-1,1)$.

Proof. Let $\phi(t) = \frac{\sqrt{1-t^2}}{\arccos t_1}$. Then

$$
\phi''(t) = -\frac{(-2 + 2t^2 + t\sqrt{1-t^2}\arccos(t) + \arccos(t)^2)}{((1-t^2)^{3/2}\arccos(t)^3)}.
$$

Since the denominator is positive, it suffices to show positivity of the numerator for $t \in [-1,1]$. Equivalently, letting $y = \arccos[t]$, $y \in [0,\pi]$, we'll show positivity of

$$
N_1(y) := -2\sin(y)^2 + \cos(y)\sin(y)y + y^2.
$$

Now $N_1(0) = 0$, $N_1'(0) = 0$ and $N_1''(y) = 4\sin(y)(-y\cos(y) + \sin(y)) \geq 0$ since $1 \geq y\cot(y)$ for $y \in (0,\pi]$ as $y \leq \tan(y)$ for $y \in (0,\pi/2)$ and $y\cot(y) \leq 0$ for $y \in (\pi/2,\pi)$. Now for the second part of the lemma, it suffices to show $\frac{u}{\sin(2\pi u)}$ is increasing in u for $u \in [0,1/2]$. We have

$$
\left(\frac{u}{\sin(u)}\right)' = (1 - u\cot(u))\csc(u) \geq 0
$$

since $1 \geq y\cot(y)$ for $y \in (0,\pi)$ as shown above. $\square$

Returning to the proof, we have

$$L_1 \geq \frac{3u(1-\epsilon)\sin(2\pi x)}{(1+\epsilon)x\sin(2\pi u)} - \frac{\frac{\partial \tilde{g}}{\partial t_2}}{\frac{\partial \tilde{g}}{\partial t_1}} \tag{D.58}$$

$$= \frac{3u(1-\epsilon)\sin(2\pi x)}{(1+\epsilon)x\sin(2\pi u)} - \frac{a_{0,1} + a_{0,2}(t_1 + 2t_2)}{a_{1,0} + a_{0,2}t_2} \tag{D.59}$$

$$= \frac{3u(1-\epsilon)\sin(2\pi x)}{(1+\epsilon)x\sin(2\pi u)} - \left(2 + \frac{\tilde{f}_1(-1)\tilde{f}_2(1/2) - \tilde{f}_1(1)\tilde{f}_2(-1/2) + a_{0,2}t_1}{a_{1,0} + a_{0,2}t_2}\right). \tag{D.60}$$

By Lemma 54 and the linearity of $\frac{\frac{\partial \tilde{g}}{\partial t_2}}{\frac{\partial \tilde{g}}{\partial t_1}}$ in t_1 for fixed t_1, if $L_1(0, t_2), L_1(1, t_2) \geq 0$, then $L_1(t_1, t_2) \geq 0$ for all $t_1 \in [-1, 1]$. We'll also be using the bound developed in the proof of bounding $a_{1,0}$ in Lemma 53 that

$$e^{-a/3}(1 - 3\epsilon) \leq \tilde{f}_1(-1)\tilde{f}_2(1/2) - \tilde{f}_1(1)\tilde{f}_2(-1/2) \leq e^{-a/3}(1 + 6\epsilon)$$

If $t_1 = 1$, then for $t_2 \in [-1/2, 0]$, we obtain

$$\frac{\tilde{f}_1(-1)\tilde{f}_2(1/2) - \tilde{f}_1(1)\tilde{f}_2(-1/2) + a_{0,2}t_1}{a_{1,0} + a_{0,2}t_2} = \frac{\tilde{f}_1(-1)\tilde{f}_2(1/2) - \tilde{f}_1(1)\tilde{f}_2(-1/2) + a_{0,2}}{a_{1,0} + a_{0,2}t_2} \tag{D.61}$$

$$\leq \frac{1 + 6\epsilon + e^{a/3}a^u_{0,2}}{e^{a/3}(a^l_{1,0} + t_2 a^u_{0,2})} \tag{D.62}$$

Technically, this lower bound requires that $e^{a/3}(a^l_{1,0} + t_2 a^u_{0,2}) > 0$ for all $t_2 \in [-\frac{1}{2}, 0]$, but this quantity is linear in a so it's easy to check. Thus, for $t_2 \in [-1/2, 0]$,

$$L_1 \geq \frac{3u(1-\epsilon)2\pi}{(1+\epsilon)\sin(2\pi u)} - 2 - \frac{1 + 6\epsilon + e^{a/3}a^u_{0,2}}{e^{a/3}(a^l_{1,0} + t_2 a^u_{0,2})}$$

and we claim $\frac{1 + 6\epsilon + e^{a/3}a^u_{0,2}}{e^{a/3}(a^l_{1,0} + t_2 a^u_{0,2})}$ is decreasing in a, from which it would follow that it suffices to check that the bound is at least 0 only when $a = 9.6$ (as the other terms have no dependence on a).

To that end, note that as a function of a

$$\frac{1+6\epsilon+e^{a/3}a^u_{0,2}}{e^{a/3}(a^l_{1,0}+t_2a^u_{0,2})}$$

is rational (with numerator and denominator both linear) and so the sign of its derivative is independent of a. Thus, checking it is negative for all a is simple.

In summary, for any $a \geq 9.6$, we have $L_1(1,t_2) > 0$ when $t_2 \in [-1/2, 0]$ if

$$\frac{3u(1-\epsilon)2\pi}{(1+\epsilon)\sin(2\pi u)} - 2 - \frac{1+6\epsilon+e^{a/3}a^u_{0,2}}{e^{a/3}(a^l_{1,0}+t_2a^u_{0,2})} > 0$$

holds for $a = 9.6$. The x terms have disappeared as we took the limit $x \to 0$. As we have shown this inequality is a difference of two increasing functions in u, this inequality is verified in [17] using the same interval partition approach described in Section C.3 which reduces our check to a finite number of point evaluations.

The case where $t_1 = 0$ is more simple. Here we again use (D.60) with $t_1 = 0$ to obtain

$$L(0,t_2) \geq \frac{12u(1-\epsilon)}{(1+\epsilon)\sin(2\pi u)} - \left(2 + \frac{\tilde{f}_1(-1)\tilde{f}_2(1/2) - \tilde{f}_1(1)\tilde{f}_2(-1/2)}{a_{1,0}+a_{0,2}t_2}\right) \tag{D.63}$$

$$\geq \frac{12u(1-\epsilon)}{(1+\epsilon)\sin(2\pi u)} - \left(2 + \frac{1+6\epsilon}{e^{a/3}(a^l_{1,0}+a^u_{0,2}t_2)}\right) \tag{D.64}$$

and with the definitions of $a^l_{1,0}$ and $a^u_{0,2}$ this quantity is clearly increasing in a and so it suffices to check when $a = 9.6$ (the denominator is positive and increasing in a). Again, this inequality is handled in Mathematica with finitely many point evaluations as we have a difference of increasing functions in u.

D.2.6 Log Derivative Estimates for the proof of Lemma 43

It remains to show:

1. $N(-1/2) < 0$

2. $L_2(0, -\frac{1}{5}) > 0$ 1/12-1/4-1/

3. $L_2(-\frac{\sqrt{2}}{2}, 0) > 0$

First,

$$\begin{aligned} N(-1/2) &= b_{0,0}a_{0,2} - a_{0,1}a_{1,0} + \frac{a_{0,2}}{2}(2a_{1,0} - \frac{1}{2}a_{0,2}) \\ &= a_{0,2}(a_{0,0} + a_{1,0}) - a_{0,1}a_{1,0} \\ &\leq a^u_{0,2}(a^u_{0,0} + a^u_{1,0}) - a^l_{0,1}a^l_{1,0} \end{aligned}$$

Now this last quantity (up to a factor of $e^{2a/3}$) is quadratic in a, concave down, along with negative and decreasing for a, as shown in the notebook.

Next, we show $L_2(t_1, t_2) := \frac{\tilde{f}_1(t_1)}{\tilde{f}_1{}'(t_1)} - t_1 - \frac{b_{0,0}+a_{0,1}t_2+a_{0,2}t_2^2}{a_{1,0}+a_{0,2}t_2} \geq 0$ at $(0, -1/5)$, or equivalently that

$$e^{a/3+a/16}\left[\tilde{f}_1(t_1)(a_{1,0} + a_{0,2}(-1/5)) - \tilde{f}_1{}'(t_1)(b_{0,0} + a_{0,1}(-1/5) + a_{0,2}(-1/5)^2)\right] \geq 0$$

Using lemmas 50 and 49, we have

$$e^{a/3+a/16}\left[\tilde{f}_1(t_1)(a_{1,0} + a_{0,2}(-1/5)) - \tilde{f}_1{}'(t_1)(b_{0,0} + a_{0,1}(-1/5) + a_{0,2}(-1/5)^2)\right] \geq \quad \text{(D.65)}$$

$$e^{a/3+a/16}\left[e^{-a/16}(a^l_{1,0} + a^u_{0,2}(-1/5)) - ae^{-a/16}/(4\pi)(b^u_{0,0} + a^l_{0,1}(-1/5) + a^u_{0,2}(-1/5)^2)\right] \quad \text{(D.66)}$$

$$= e^{a/3}(a^l_{1,0} + a^u_{0,2}(-1/5)) - a/(4\pi)e^{a/3}(b^u_{0,0} + a^l_{0,1}(-1/5) + a^u_{0,2}(-1/5)^2) \geq 0, \quad \text{(D.67)}$$

and this last inequality is easy to show because the lower bound is quadratic and convex in a with positive value and derivative, at $a = 9.6$.

The case where $t_1 = -\sqrt{2}/2, t_2 = 0$ is similar but requires a little more care. Unfortunately, the bounds

$$\tilde{f}_1(t_1) \geq e^{-ax^2}, \quad \tilde{f}_1{}'(t_1) \leq axe^{-ax^2}/(\pi \sin(2\pi x)$$

are too coarse to work for all $a \geq 9.6$. Instead, we must truncate one fewer term to get our lower bound for $\tilde{f}_1$ and use two more terms for our upper bound of $\tilde{f}_1{}'$ (see the proof of Lemma 50), to obtain

$$\frac{\tilde{f}_1(t_1)}{\tilde{f}_1{}'(t_1)} \geq (e^{-ax^2} + e^{-a(x-1)^2}) \frac{\pi \sin(2\pi x)}{a\,(xe^{-ax^2} + (x-1)e^{-ax^2} + (x+1)e^{-a(x+1)^2})} \tag{D.68}$$

$$= \frac{\pi \sin(2\pi x)}{a} \frac{1 + e^{-a(1-2x)}}{x - (1-x)e^{-a(1-2x)} + (x+1)e^{-a(1+2x)}}. \tag{D.69}$$

So for $t_1 = -\sqrt{2}/2$, we obtain

$$\frac{\tilde{f}_1(-\sqrt{2}/2)}{\tilde{f}_1{}'(-\sqrt{2}/2)} \geq \frac{\pi\sqrt{2}}{2a} \frac{1 + e^{-a/4}}{\frac{3}{8} - \frac{5}{8}e^{-a/4} + \frac{11}{8}e^{-7a/4}} \tag{D.70}$$

$$= \frac{4\pi\sqrt{2}}{a} \frac{1 + e^{-a/4}}{3 - e^{-a/4}(5 - 11e^{-3a/2})} \tag{D.71}$$

$$\geq \frac{4\pi\sqrt{2}}{a} \frac{1 + e^{-a/4}}{3 - (5-\epsilon)e^{-a/4}}. \tag{D.72}$$

Thus,

$$L_2(-\sqrt{2}/2, 0) \geq \frac{4\pi\sqrt{2}}{a} \frac{1 + e^{-a/4}}{3 - (5-\epsilon)e^{-a/4}} + \sqrt{2}/2 - \frac{e^{a/3} b^u_{0,0}}{e^{a/3} a^l_{1,0}}$$

which is nonnegative if and only if

$$4\pi\sqrt{2}(e^{a/3}a^l_{1,0}) \frac{1 + e^{-a/4}}{3 - (5-\epsilon)e^{-a/4}} + \sqrt{2}/2a(e^{a/3}a^l_{1,0}) - a(e^{a/3}b^u_{0,0}) \geq 0$$

Now if $9.6 \leq a \leq c$, then we have the inequality

$$4\pi\sqrt{2}(e^{a/3}a^l_{1,0}) \frac{1 + e^{-c/4}}{3 - (5-\epsilon)e^{-c/4}} \leq 4\pi\sqrt{2}(e^{a/3}a^l_{1,0}) \frac{1 + e^{-a/4}}{3 - (5-\epsilon)e^{-a/4}} \tag{D.73}$$

since

$$\frac{1+e^{-c/4}}{3-(5-\epsilon)e^{-c/4}}$$

is decreasing in c for $c \geq 9.6$. So it remains to show in the accompanying Mathematica document that for every $a \in \mathbb{R}$, there is some choice of $c \geq a$ such that

$$L_3(a,c) := 4\pi\sqrt{2}(e^{a/3}a_{1,0}^l)\frac{1+e^{-c/4}}{3-(5-\epsilon)e^{-c/4}} + \sqrt{2}/2a(e^{a/3}a_{1,0}^l) - a(e^{a/3}b_{0,0}^u) > 0$$

In particular, we do so by showing that for each $i = 1, \ldots, 6$ and the sequence $a_0 = 9.6, 9.8, 10, 10.2, 11, 12, \infty = a_6$, we have $L_3(a, a_i) \geq 0$ for $a \geq a_{i-1}$. Each of these checks is easy since $L_3(a,c)$ is quadratic in a for fixed c. As with the $a \leq \pi^2$ case, all of these checks and algebraic simplifications are verified in [17].

Appendix E

Computations for the Proof of Theorem 20

E.1 Positivity of $b_{0,2}$

To show $b_{0,2} > 0$, it suffices to show for all $a_1 > 0$ and $a_1 \geq 4a_2/3$ that

$$\frac{\tilde{f}_2{}'(0) - \tilde{f}_2(0)}{\tilde{f}_2(-1)} - \frac{2\tilde{f}_1{}'(1) - \tilde{f}_1(1)}{\tilde{f}_1(-1)} > 0.$$

Lemma 55. *For $a_1 \geq \pi^2$, $a_2 \geq 272\pi/65$, respectively we have*

$$\frac{2\tilde{f}_1{}'(1) - \tilde{f}_1(1)}{\tilde{f}_1(-1)} < \frac{e^{a_1/4}(a_1 - \pi^2)}{2\pi^2}, \quad \frac{\tilde{f}_2{}'(0) - \tilde{f}_2(0)}{\tilde{f}_2(-1)} > \frac{15e^{3a_2/16}(65a_2 - 272\pi)}{8008\pi} > 0. \tag{E.1}$$

If $\pi^2 \leq a_2 < 272\pi/65$, then

$$\frac{\tilde{f}_2{}'(0) - \tilde{f}_2(0)}{\tilde{f}_2(-1)} > \frac{3e^{3a_2/16}(65a_2 - 272\pi)}{1600\pi}. \tag{E.2}$$

Moreover, each of the bounds is increasing for a_1 and a_2 at least π^2, respectively.

Proof. The bounds follow immediately from combining the bounds in B.2 and monotonicity comes via differentiation. For example,

$$\frac{d}{da_2}\left[\frac{15e^{3a_2/16}(65a_2 - 272\pi)}{8008\pi}\right] = \frac{15e^{3a_2/16}(1040 + 195a_2 - 816\pi)}{128128\pi},$$

whose sign only depends on $1040 + 195a_2 - 816\pi$, which is positive for $a_2 \geq \pi^2$. The other proofs are similarly straightforward and contained in an accompanying Mathematica notebook [31]. □

Lemma 56. *If $a_i \leq \pi^2$, with $d_i := \pi^2/a_1$, $i = 1, 2$, we have*

$$\frac{2\tilde{f}_1{}'(1) - \tilde{f}_1(1)}{\tilde{f}_1(-1)} < \frac{-1 + 1427e^{-4d_1}/100 + 2e^{-d_1}}{1 + 101e^{-4d_1}/50 - 2e^{-d_1}}, \quad \frac{\tilde{f}_2{}'(0) - \tilde{f}_2(0)}{\tilde{f}_2(-1)} > \frac{-1 + 371e^{-4d_2}/200 + 2e^{-d_2}}{1 + 99e^{-4d_2}/50 - 2e^{-d_2}}, \tag{E.3}$$

both of which are increasing in a_i.

Proof. The bounds follow immediately from combining the bounds in 4.10, and their monotonicity comes from differentiation. For example, to show the first bound in (E.3) is increasing in a_1, we show it's decreasing in d_1. Its derivative with respect to d_1 depends only on the sign of

$$\begin{aligned}
&(-1 + 1427e^{-4d_1}/100 + 2e^{-d_1})'(1 + 101e^{-4d_1}/50 - 2e^{-d_1}) - \\
&(-1 + 1427e^{-4d_1}/100 + 2e^{-d_1})'(1 + 101e^{-4d_1}/50 - 2e^{-d_1})' \\
&= 4887e^{-5d_1}/50 - 1629e^{-4d_1}/25 < 0,
\end{aligned}$$

where the last inequality follows simply by checking at $d_1 = 1$ by Lemma 51. $\square$

Now we are ready to show the desired inequality with $b_{0,2}$. If $a_1 \geq \pi^2$ (and so also $a_2 \geq 4\pi^2/3$, which we note yields the inequality string $a_2 \geq 4\pi^2/3 > 272\pi/65$), then using the fact that $a_2 \geq 4a_1/3$, we have the inequalities

$$\begin{aligned}
\frac{\tilde{f}_2{}'(0) - \tilde{f}_2(0)}{\tilde{f}_2(-1)} - \frac{2\tilde{f}_1{}'(1) - \tilde{f}_1(1)}{\tilde{f}_1(-1)} &> \frac{15e^{3a_2/16}(65a_2 - 272\pi)}{8008\pi} - \frac{e^{a_1/4}(a_1 - \pi^2)}{2\pi^2} \\
&\geq \frac{15e^{3(4a_1/3)/16}(65(4a_1/3) - 272\pi)}{8008\pi} - \frac{e^{a_1/4}(a_1 - \pi^2)}{2\pi^2} \\
&= e^{a_1/4}\frac{-19\pi^2 + 13a_1(-77 + 25\pi)}{2002\pi^2} > 0,
\end{aligned}$$

with the final inequality following by simply by checking $-19\pi^2 + 13a_1(-77 + 25\pi) > 0$ for $a_1 = \pi^2$. This point evaluation and others like it are verified in [31].

Now we proceed to an intermediate region, where $a_2 \geq \pi^2$, and $a_1 \leq \pi^2$. We have for this region that if $a_2 \geq 272\pi/65$, then using monotonicity of the bounds, we obtain

$$\begin{aligned}\frac{\tilde{f}_2{}'(0)-\tilde{f}_2(0)}{\tilde{f}_2(-1)}-\frac{2\tilde{f}_1{}'(1)-\tilde{f}_1(1)}{\tilde{f}_1(-1)} &> 0-\frac{-1+1427e^{-4d_1}/100+2e^{-d_1}}{1+101e^{-4d_1}/50-2e^{-d_1}}\\ &\geq -\frac{-1+1427e^{-4}/100+2e^{-1}}{1+101e^{-4}/50-2e^{-1}}>0.\end{aligned}$$

When $a_2 \in [\pi^2, 4\pi^2/3]$, things are more delicate. In that case, if $a_2 \in [\pi^2, 272\pi/65]$, since $d_1 \geq 4\pi^2/(3a_2)$, we use the inequality

$$\begin{aligned}\frac{\tilde{f}_2{}'(0)-\tilde{f}_2(0)}{\tilde{f}_2(-1)}-\frac{2\tilde{f}_1{}'(1)-\tilde{f}_1(1)}{\tilde{f}_1(-1)} &> \frac{15e^{3a_2/16}(65a_2-272\pi)}{8008\pi}-\frac{-1+1427e^{-4d_1}/100+2e^{-d_1}}{1+101e^{-4d_1}/50-2e^{-d_1}}\\ &\geq \frac{15e^{3a_2/16}(65a_2-272\pi)}{8008\pi}-\frac{-1+1427e^{-4(4\pi^2/(3a_2))}/100+2e^{-4\pi^2/(3a_2)}}{1+101e^{-4d_1}/50-2e^{-4\pi^2/(3a_2)}}>0\end{aligned}$$

We have a difference of increasing functions in a_2, allowing us to verify the final inequality using interval arithmetic in [31].

Finally, for $a_2 \leq \pi^2$, we have $d_1 \geq 4d_2/3$, so using monotonoicity of the bounds, we obtain

$$\frac{\tilde{f}_2{}'(0)-\tilde{f}_2(0)}{\tilde{f}_2(-1)}-\frac{2\tilde{f}_1{}'(1)-\tilde{f}_1(1)}{\tilde{f}_1(-1)} > \frac{-1+371e^{-4d_2}/200+2e^{-d_2}}{1+99e^{-4d_2}/50-2e^{-d_2}}-\frac{-1+1427e^{-4d_1}/100+2e^{-d_1}}{1+101e^{-4d_1}/50-2e^{-d_1}} \tag{E.4}$$

$$> \frac{-1+371e^{-4d_2}/200+2e^{-d_2}}{1+99e^{-4d_2}/50-2e^{-d_2}}-\frac{-1+1427e^{-16d_2/3}/100+2e^{-4d_2/3}}{1+101e^{-16d_2/3}/50-2e^{-4d_2/3}}. \tag{E.5}$$

To verify the positivity of (E.5), we rearrange terms and show

$$(-1+371e^{-4d_2}/200+2e^{-d_2})(1+101e^{-16d_2/3}/50-2e^{-4d_2/3}) \tag{E.6}$$

$$-(-1+1427e^{-16d_2/3}/100+2e^{-4d_2/3})(1+99e^{-4d_2}/50-2e^{-d_2}) \tag{E.7}$$

$$=-(9803/400)e^{-28d_2/3}+1629/50e^{-19d_2/3}-599/25e^{-16d_2/3}+767e^{-4c}/200 \tag{E.8}$$

$$> e^{-16d_2/3}\left[1529/50e^{-d_2}-599/25+767e^{4d_2/3}/200\right]>0 \tag{E.9}$$

where in (E.8), we have used Lemma 51 to check $-(9803/400)e^{-28d_2/3}+2e^{-19d_2/3} > 0$ for $d_2 \geq 1$, and we have checked that $1529/50e^{-d_2} - 599/25 + (767e^{4d_2/3}/200$ is positive for $d_2 = 1$ and has positive derivative for all $d_2 \geq 1$ again using Lemma 51, thus completing the check that $b_{0,2} > 0$.

E.2 Proof of Lemma 45

We need to show for all $a_1 > 0$ and $a_2 \geq 4a_1/3$ that

$$\tilde{f}_1{}'(-1)/\tilde{f}_1{}'(1) > \tilde{f}_2(-1)/\tilde{f}_2(1)$$

We have the following basic bounds:

Lemma 57. *For $a_1, a_2 \geq \pi^2$, respectively we have*

$$\tilde{f}_1{}'(-1)/\tilde{f}_1{}'(1) > (a_1 - 2)e^{-a_1/4},\ \tilde{f}_2(-1)/\tilde{f}_2(1) < 2(1+\epsilon)e^{-a_2/4}. \tag{E.10}$$

For $a_1, a_2 \leq \pi^2$, respectively we have

$$\tilde{f}_1{}'(-1)/\tilde{f}_1{}'(1) > \frac{-65/8e^{-4d_1} + 2e^{-d_1}}{65e^{-4d_1}/8 + 2e^{-d_1}},\ \tilde{f}_2(-1)/\tilde{f}_2(1) > \frac{1 + 101e^{-4d_2}/50 - 2e^{-d_2}}{1 + 99e^{-4d_2}/50 + 2e^{-d_2}}, \tag{E.11}$$

and all of these bounds are decreasing in a_1 and a_2, respectively.

For $a_1 \geq \pi^2$, using monotonicity, we compute

$$\begin{aligned}
\tilde{f}_1{}'(-1)/\tilde{f}_1{}'(1) - \tilde{f}_2(-1)/\tilde{f}_2(1) &> (a_1 - 2)e^{-a_1/4} - 2(1+\epsilon)e^{-a_2/4} \\
&\geq (a_1 - 2)e^{-a_1/4} - 2(1+\epsilon)e^{-(4a_1/3)/4} \\
&= e^{-a_1/4}(a_1 - 2 - 2(1+\epsilon)e^{-a_1/12}) \\
&> e^{-a_1/4}(a_1 - 4) > 0.
\end{aligned}$$

If $a_2 \geq \pi^2$ and $a_1 \leq \pi^2$,

$$\begin{aligned}\tilde{f_1}'(-1)/\tilde{f_1}'(1) - \tilde{f}_2(-1)/\tilde{f}_2(1) &> \frac{-(65/8)e^{-4d_1} + 2e^{-d_1}}{65e^{-4d_1}/8 + 2e^{-d}} - 2(1+\epsilon)e^{-a_2/4} \\ &> \frac{-(65/8)e^{-4} + 2e^{-1}}{(65e^{-4})/8 + 2e^{-1}} - 2(1+\epsilon)e^{-\pi^2/4} > 0.\end{aligned}$$

Finally, for $a_2 \leq \pi^2$, we have

$$\tilde{f_1}'(-1)/\tilde{f_1}'(1) - \tilde{f}_2(-1)/\tilde{f}_2(1) > \frac{-(65/8)e^{-4d_1} + 2e^{-d_1}}{65e^{-4d_1}/8 + 2e^{-d_1}} - \frac{1 + 101e^{-4d_2}/50 - e^{-d_2}}{1 + 99e^{-4d_2}/50 + 2e^{-d_2}} \tag{E.12}$$

$$> \frac{-(65/8)e^{-4(4d_2/3)} + 2e^{-(4d_2/3)}}{65e^{-4(4d_2/3)}/8 + 2e^{-(4d_2/3)}} - \frac{1 + 101e^{-4d_2}/50 - 2e^{-d_2}}{1 + 99e^{-4d_2}/50 + 2e^{-d_2}}. \tag{E.13}$$

To prove the positivity of (E.13), as before we rearrange terms to show

$$\begin{aligned}&(-(65/8)e^{-4(4d_2/3)} + 2e^{-(4d_2/3)})(1 + 99e^{-4d_2}/50 + 2e^{-d_2}) \\ &-(1 + 101e^{-4d_2}/50 - 2e^{-d_2})(65e^{-4(4d_2/3)} + 2e^{-(4d_2/3)}) \\ &= -(65/2)e^{-28d_2/3} - 1633/100e^{-16d_2/3} + 8e^{-7d_2/3} > 0\end{aligned}$$

where the last inequality follows from applying Lemma 51 and checking positivity at $d_2 = 1$.