AN UPPER BOUND ON GROTHENDIECK'S CONSTANT

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Abstract. We show that Grothendieck's real constant K_G can be upper bounded by projecting vectors onto a random plane through the origin and thresholding a degree five Hermite polynomial. This resolves a conjecture of Braverman-Makarychev-Makarychev-Naor from 2011, who required an extra randomization step in their rounding scheme and proved $K_G < \frac{\pi}{2\log(1+\sqrt{2})} - 10^{-500}$. As a corollary of our result, we prove the bound $K_G < \frac{\pi}{2\log(1+\sqrt{2})} - 10^{-217}$ by thresholding degree three Hermite polynomials in the plane. We finally give a rigorous computer-assisted proof that $K_G < \frac{\pi}{2\log(1+\sqrt{2})} - 10^{-5}$ using interval arithmetic and degree three Hermite polynomial thresholding.

1. Introduction

Grothendieck's real constant K_G is the infimum over all $K \in (0, \infty)$ such that, for all positive integers m, n and for every real $m \times n$ matrix (a_{ij}), we have

$$\max_{\substack{x_1,\ldots,x_m \\ y_1,\ldots,y_n \in S^{m+n-1}}} \sum_{i=1}^{m}\sum_{j=1}^{n} a_{ij}\langle x_i, y_j\rangle \leq K \cdot \max_{\substack{\epsilon_1,\ldots,\epsilon_m \\ \delta_1,\ldots,\delta_n \in\{-1,1\}}} \sum_{i=1}^{m}\sum_{j=1}^{n} a_{ij}\epsilon_i\delta_j, \tag{1}$$

where $\langle x, y\rangle = \sum_{i=1}^{d} x_i y_i$ for all $x, y \in \mathbb{R}^d$ and $S^{d-1} = \{x \in \mathbb{R}^d \colon \langle x, x\rangle = 1\}$ for any $d \geq 1$.

Inequality (1) was originally stated as an inequality of two different tensor norms [G53] (see also [P12, Section 3]), though the discretized formulation (1) was proven in [LP68].

Determining the exact value of K_G remains a significant open problem since it was first posited in [G53]. We can rephrase the problem of finding the constant K_G as: what is the "best" way to "round" the vectors $x_1, \ldots, x_m, y_1, \ldots, y_n$ to ± 1? There are many good references on (1) and its connections to combinatorics, functional analysis, Banach space theory, operator algebras, the Connes embedding problem, theoretical computer science, and quantum mechanics; see, for example, [P12, KN12]. Note also that Grothendieck's constant is the maximal quantum violation in Bell's inequality from quantum mechanics [T87]. Also, assuming the Unique Games Conjecture [K02], it is NP-hard to approximate the right side of (1) within any constant smaller than Grothendieck's constant K_G [RS09].

Grothendieck [G53] originally proved that $K_G \leq \sinh(\pi/2) \approx 2.3013$. In [K77], Krivine improved this bound to $K_G \leq \frac{\pi}{2\log(1+\sqrt{2})} \approx 1.78221397819$ (see Example 1.4 below), and it was generally believed that this inequality should be an equality [K01]. However, it was then

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shown in [BMMN13] that there is a $c' > 0$ such that

$$K_G < \frac{\pi}{2\log(1+\sqrt{2})} - c'. \tag{2}$$

An effective c' was proven but not specified in [BMMN13]; an inspection of the argument seems to give $c' = 10^{-500}$. Krivine's argument [K77] shows that, after "preprocessing" the vectors $x_1, \ldots, x_m, y_1, \ldots, y_n$ by nonlinearly mapping them to a different Hilbert space (Fock space), we can then map those vectors to ± 1 by projecting them onto a Gaussian random vector, and taking the sign of this projected value. (The nonlinear preprocessing removes the nonlinearity that appears after projecting onto the Gaussian.) The argument of [BMMN13] instead projects the preprocessed vectors onto a random plane through the origin, and then (with probability $0 < p < 1$) applies a perturbation of the sign function on this two-dimensional plane to "round" the vectors to ± 1 (and with probability $1 - p$ applies the sign function). This perturbation uses a degree 5 Hermite polynomial.

Also, rounding schemes of this form (projecting onto a random hyperplane through the origin and then thresholding, possibly with additional randomness) can obtain arbitrarily good approximations of K_G [RN14]. In other words, finding the exact value of K_G reduces to finding the best "rounding scheme" for vectors $x_1, \ldots, x_m, y_1, \ldots, y_n$ in (1) (where the rounding scheme itself might need additional randomness).

The best known lower bounds for K_G were recently shown in [H26, JM26] to be around 1.6769. In particular, [JM26] showed a 10^{-12} improvement over the bound from [D84, R91].

1.1. **Krivine Rounding Schemes.**

We now describe the rounding scheme we will use to prove the best known constant in Grothendieck's inequality.

Definition 1.1 (**Krivine rounding scheme**, [BMMN13])**.** Fix $k \in \mathbb{N}$ and let $f, g \colon \mathbb{R}^k \to \{-1, 1\}$ be odd measurable functions. Let $G_1, G_2 \in \mathbb{R}^k$ be independent standard Gaussian random vectors, so that G_1 has density $x \mapsto (2\pi)^{-k/2} e^{-\|x\|_2^2/2}$. For any $t \in (-1, 1)$, define the (complex correlation parameter) noise stability

$$\begin{aligned} H_{f,g}(t) &:= \mathbb{E}\left[f\left(\frac{1}{\sqrt{2}} G_1\right) g\left(\frac{t}{\sqrt{2}} G_1 + \frac{\sqrt{1-t^2}}{\sqrt{2}} G_2\right)\right] \\ &= \frac{1}{\pi^k (1-t^2)^{k/2}} \int_{\mathbb{R}^k} \int_{\mathbb{R}^k} f(x) g(y) \exp\left(\frac{-\|x\|_2^2 - \|y\|_2^2 + 2t\langle x, y\rangle}{1-t^2}\right) dx\, dy. \end{aligned} \tag{3}$$

Then $H_{f,g}$ extends to an analytic function on the strip $\{z \in \mathbb{C} \colon \Re(z) \in (-1, 1)\}$. We shall call $\{f, g\}$ a **Krivine rounding scheme** if $H_{f,g}$ is invertible on a neighborhood of the origin, and if we consider the Taylor expansion

$$H_{f,g}^{-1}(z) = \sum_{j=0}^{\infty} \widehat{a}_{2j+1} z^{2j+1}, \tag{4}$$

then there exists $c = c(f, g) \in (0, \infty)$ satisfying

$$\sum_{j=0}^{\infty} |\widehat{a}_{2j+1}| c^{2j+1} = 1. \tag{5}$$

Only odd Taylor coefficients appear in (4) since $H_{f,g}$, and therefore also $H_{f,g}^{-1}$, is odd.

A Krivine rounding scheme yields an algorithmic proof of Grothendieck's inequality in the following way.

Algorithm 1.2 (**Krivine rounding algorithm**, [BMMN13])**.**
Input: Vectors $\{x_r\}_{r=1}^m, \{y_s\}_{s=1}^n \subseteq S^{m+n-1}$, and $f,g\colon \mathbb{R}^k \to \{-1,1\}$, which define coefficients $\{\widehat{a}_{2j+1}\}_{j=0}^{\infty}$ by (4) and a constant $c := c(f,g)$ by (5).
Output: Random signs $\{\sigma_r\}_{r=1}^m, \{\tau_s\}_{s=1}^n \subseteq \{-1,1\}$.
Step 0 (Notation). Consider the Hilbert space

$$\mathcal{H} = \bigoplus_{j=0}^{\infty} \left(\mathbb{R}^{m+n}\right)^{\otimes(2j+1)}.$$

For any $x \in S^{m+n-1}$ we can then define two vectors $I(x), J(x) \in \mathcal{H}$ by

$$\begin{aligned} I(x) &:= \sum_{j=0}^{\infty} |\widehat{a}_{2j+1}|^{1/2} c^{(2j+1)/2} x^{\otimes(2j+1)} \\ J(x) &:= \sum_{j=0}^{\infty} \operatorname{sign}(\widehat{a}_{2j+1})|\widehat{a}_{2j+1}|^{1/2} c^{(2j+1)/2} x^{\otimes(2j+1)}, \end{aligned} \tag{6}$$

The choice of c was made in order to ensure that $I(x)$ and $J(x)$ are unit vectors in $\mathcal{H}$. Moreover, the definitions (6) were made so that the following identity holds:

$$\forall x,y \in S^{m+n-1}, \qquad \langle I(x), J(y)\rangle_{\mathcal{H}} \overset{(4)}{=} H_{f,g}^{-1}\big(c\langle x,y\rangle\big). \tag{7}$$

Step 1 (Preprocessing the vectors). Transform the initial unit vectors

$$\{x_r\}_{r=1}^m, \{y_s\}_{s=1}^n \subseteq S^{m+n-1}$$

to vectors

$$\{u_r\}_{r=1}^m, \{v_s\}_{s=1}^n \subseteq S^{m+n-1}$$

satisfying the identities

$$\forall\,(r,s) \in \{1,\ldots,m\} \times \{1,\ldots,n\}, \qquad \langle u_r, v_s\rangle = \langle I(x_r), J(y_s)\rangle_{\mathcal{H}} \overset{(7)}{=} H_{f,g}^{-1}\big(c\langle x_r,y_s\rangle\big). \tag{8}$$

As explained in [AN04], these new vectors can be computed efficiently provided $H_{f,g}^{-1}$ can be computed efficiently; this simply amounts to computing a Cholesky decomposition.
Step 2 (Random projection). Let $G\colon \mathbb{R}^{m+n} \to \mathbb{R}^k$ be a random $k \times (m+n)$ matrix whose entries are i.i.d. standard Gaussian random variables. Let $\sigma_1,\ldots,\sigma_m,\tau_1,\ldots,\tau_n \in \{-1,1\}$ be random signs defined by

$$\forall\,(r,s) \in \{1,\ldots,m\} \times \{1,\ldots,n\}, \qquad \sigma_r := f\left(\frac{1}{\sqrt{2}}Gu_r\right) \quad \text{and} \quad \tau_s := g\left(\frac{1}{\sqrt{2}}Gv_s\right). \tag{9}$$

A Krivine rounding scheme automatically upper bounds K_G via the constant c from (5).

Corollary 1.3 ([BMMN13])**.** Let $f,g\colon \mathbb{R}^k \to \{-1,1\}$ be a Krivine rounding scheme. Then

$$K_G \le \frac{1}{c(f,g)}.$$

Proof, [BMMN13]. Having obtained the random signs $\sigma_1, \ldots, \sigma_m, \tau_1, \ldots, \tau_n \in \{-1, 1\}$ as in (9), for every $m \times n$ matrix (a_{rs}) we have

$$\max_{\varepsilon_1,\ldots,\varepsilon_m,\delta_1,\ldots,\delta_n \in \{-1,1\}} \sum_{r=1}^{m}\sum_{s=1}^{n} a_{rs}\varepsilon_r\delta_s \geq \mathbb{E}\left[\sum_{r=1}^{m}\sum_{s=1}^{n} a_{rs}\sigma_r\tau_s\right]$$
$$\overset{(*)}{=} \mathbb{E}\left[\sum_{r=1}^{m}\sum_{s=1}^{n} a_{rs}H_{f,g}(\langle u_r, v_s\rangle)\right] \overset{(8)}{=} c(f,g)\sum_{r=1}^{m}\sum_{s=1}^{n} a_{rs}\langle x_r, y_s\rangle,$$

where $(*)$ follows by rotational invariance from (9) and (3). $\square$

Example 1.4. Let $k = 1$ and let $f(x) = g(x) = \text{sign}(x)$ for all $x \in \mathbb{R}$. Then $H_{f,g}(z) = \frac{2}{\pi}\arcsin(z)$, $H_{f,g}^{-1}(z) = \sin(\pi z/2)$, $\widehat{a}_{2j+1} = (-1)^j(\pi/2)^{2j+1}/(2j+1)!$, so $c = c(f,g)$ satisfies

$$1 = \sum_{j=0}^{\infty} |\widehat{a}_{2j+1}| c^{2j+1} = \sum_{j=0}^{\infty} \frac{(\pi/2)^{2j+1}}{(2j+1)!} c^{2j+1} = \sinh(\pi c/2).$$

So, $c = \frac{2}{\pi}\sinh^{-1}(1) = \frac{2}{\pi}\log(1+\sqrt{2})$, and Corollary 1.3 gives Krivine's bound $K_G \leq \frac{\pi}{2\log(1+\sqrt{2})}$.

1.2. **The Proof of** [BMMN13]**.** The main result of [BMMN13] is (2). The proof of (2) in [BMMN13] did not directly use Corollary 1.3 or Algorithm 1.2. Instead, they fix $k = 2$ and some small $0 < p < 1$ and they modify (9) so that, with probability $1 - p$, (9) is used to define $\sigma_1, \ldots, \sigma_m, \tau_1, \ldots, \tau_n$ with $f(x) = g(x) = \text{sign}(x_2)\ \forall\ x \in \mathbb{R}^2$, and with probability p (9) is used with $f(x) = g(x) = \text{sign}(x_2 - \eta h_5(x_1))\ \forall\ x \in \mathbb{R}^2$ where $\eta > 0$ is small and h_5 denotes a fifth degree Hermite polynomial, defined in (14).

In other words, the proof of (2) requires an extra randomization step. This randomization and extra parameter p are needed for technical reasons, to control the inverse of $H_{f,g}$.

However, this extra randomization step should be unnecessary to prove (2), due to Corollary 1.3. Krivine rounding schemes themselves are in fact sufficient to prove Grothendieck's inequality (1) with its sharp constant (for $k \to \infty$ [RN14], with possibly additional randomness), but finding an explicit example of a Krivine rounding scheme that yields an explicit bound such as (2) remained an open problem. Consequently, [BMMN13] conjectured the existence of the following specific Krivine rounding scheme.

Conjecture 1.5 ([BMMN13, Conjecture 5.5])**.** $\exists\ \eta > 0$ such that the functions $f_\eta(x) = g_\eta(x) = \text{sign}(x_2 - \eta h_5(x_1))\ \forall\ x \in \mathbb{R}^2$ form a Krivine rounding scheme with $c(f_\eta, f_\eta) > \frac{2}{\pi}\log(1+\sqrt{2})$. That is, (2) can be proven without the auxiliary randomization step and parameter $0 < p < 1$.

Conjecture 1.5 could be rephrased as asking: does there exist a Krivine rounding scheme $f, g \colon \mathbb{R}^2 \to \{-1, 1\}$ with $c(f,g) > \frac{2}{\pi}\log(1+\sqrt{2})$? Note that [BMMN13] did not find such a Krivine rounding scheme, nor did [RN14]. (Note also that the Krivine rounding schemes of [RN14] may require additional randomness beyond the definition of Krivine rounding scheme, as in the main result of [BMMN13].) Moreover, [BMMN13] showed in [BMMN13, Lemma 2.4] that every Krivine rounding scheme $f, g \colon \mathbb{R} \to \{-1, 1\}$ satisfies $c(f,g) \leq \frac{2}{\pi}\log(1+\sqrt{2})$ (with equality well known from Example 1.4). So, a k-dimensional domain with $k \geq 2$ is necessary in order to find $f, g \colon \mathbb{R}^k \to \{-1, 1\}$ with $c(f,g) > \frac{2}{\pi}\log(1+\sqrt{2})$.

1.3. **Our Contribution.** Our first main result is to prove Conjecture 1.5.

Theorem 1.6 (Main). *Conjecture 1.5 holds.*

Although an exact constant $c' > 0$ is not specified for (2) in [BMMN13], it seems that they showed $K_G < \frac{\pi}{2\log(1+\sqrt{2})} - 10^{-500}$. In removing their unnecessary extra parameter p, we then deduce an improved bound on K_G using $f_\eta(x) = g_\eta(x) = \mathrm{sign}(x_2 - \eta h_5(x_1))\ \forall\ x \in \mathbb{R}^2$ in Definition 1.1 with $\eta > 0$ small. That is, we show:

$$K_G < \frac{\pi}{2\log(1+\sqrt{2})} - 10^{-389}. \tag{10}$$

As suggested in [BMMN13], if we use instead $f_\eta(x) = \mathrm{sign}(x_2 - \eta h_3(x_1))$ and $g_\eta(x) = \mathrm{sign}(x_2 + \eta h_3(x_1))\ \forall\ x \in \mathbb{R}^2$, we obtain a better bound

$$K_G < \frac{\pi}{2\log(1+\sqrt{2})} - 10^{-217}. \tag{11}$$

The bounds (11) and (10) are proven in Section 8.

Although the upper bound (11) is certainly far from the true constant K_G, it indicates that the true value of K_G should be well-approximated by two-dimensional Krivine rounding schemes. In other words, the main advance of Theorem 1.6 is conceptual, since it was previously unclear what explicit bounds Krivine rounding schemes could produce.

As in [BMMN13], the proof of (10) and (11) is perturbative, relying on taking a small η parameter such that various Taylor approximation errors are small. It is unlikely such a perturbative approach could reveal the first few decimal places of K_G, due to the large approximation errors and small η values. It is therefore natural to try to directly (numerically) search for Krivine rounding schemes with reasonable constants, leading to improved K_G bounds in Corollary 1.3.

This approach was already considered in [BMMN13]:

Question 1.7 ([BMMN13, Question 3.2]). *Are the optimizers of König's bilinear functional (109) an alternating Krivine rounding scheme (is $\mathrm{sign}(\widehat{a}_{2j+1}) = (-1)^j$ for all $j \geq 0$ in (4))?*

If Question 1.7 were true, then these optimizers would yield optimal estimates of K_G by [BMMN13, Equation (22)]. However, our numerical simulations answer this question in the negative. The purported optimizer of König's bilinear functional, nicknamed the "tiger partition" (see Figures 1 and 2 below), appears to not be an alternating Krivine rounding scheme, as defined in [BMMN13, Definition 2.2].

Answer 1.8. *We observe numerically that Question 1.7 seems to be false in dimension $k = 2$, since the tiger partition's fifth coefficient $\widehat{a}_5$ appears to be negative.*

In other words, optimizers of König's functional may be irrelevant for producing good rounding schemes (with improved bounds on K_G). We discuss this numerical observation in Section 15. Since the tiger partition itself is not defined rigorously in [BMMN13] (in fact finding an analytic description of it is mentioned as a question in [BMMN13, Question 3.1]), it is unclear how to formalize Answer 1.8 using e.g. interval arithmetic, so we instead use floating-point numerical operations in Answer 1.8. In summary, the tiger partition of [BMMN13] might be a red herring for improved K_G bounds. It could still occur that optimizers of König's bilinear functional in $\mathbb{R}^k$ for $k > 2$ are alternating Krivine rounding schemes, though we find no evidence of this from numerical calculations when $k = 3, 4$.

But if the tiger partition is not a good rounding scheme, what Krivine rounding scheme is good? Using rigorous interval arithmetic, we prove that $f_\eta(x) = \mathrm{sign}(x_2 - \eta h_3(x_1))$ and $g_\eta(x) = \mathrm{sign}(x_2 + \eta h_3(x_1))$ does lead to reasonably good bounds on K_G when $k = 2$. That is, we replace the perturbative approach of (11) by numerically computing a high degree Taylor expansion of $H_{f,g}$ in (120) (and its inverse) together with a high degree tail error bound. Since f_η, g_η are defined with Hermite polynomials, the coefficients in the Taylor expansion have relatively simple expressions in terms of one-dimensional integrals that allow precise estimation. Accurately computing these high degree Taylor expansions avoids the losses inherent from purely low degree expansions used to prove (10) and (11). We therefore find the following.

Theorem 1.9. *Using rigorous interval arithmetic, we show*

$$K_G < \frac{\pi}{2\log(1+\sqrt{2})} - 10^{-5}.$$

We discuss the numerics used to verify Theorem 1.9 further in Section 16. Supporting numerical codes appear at the following URL:

GitHub Link 1. `https://github.com/sheilman77/grothendieck_upper_bounds`

In fact, by perturbing the Hermite polynomial h_3 in the definition of f, g, we found numerical evidence that K_G is at most

$$\frac{\pi}{2\log(1+\sqrt{2})} - 3\cdot 10^{-5}.$$

However, to keep the length of this paper and the resulting codes more manageable, we leave the certification of this result to future work.

In light of the main result of [RN14], one might naturally ask if higher-dimensional ($k > 2$) Krivine rounding schemes could be found numerically, that improve upon our observed K_G bounds. The larger k is, the more difficult the numerical calculations would become, so again we leave this investigation for future work. We simply note that our computations suggest that good Krivine rounding schemes could result from relatively simple choices of f, g, rather than a complicated choice of tiger partitions as put forward in [BMMN13].

1.4. **Contrast with Previous Approaches.** How does our approach differ from that of [BMMN13]? Our approach to Theorem 1.6 is broadly similar to the corresponding bound from [BMMN13]. The main technical difference from [BMMN13] is in the treatment of the inverse of the H function. Instead of using an auxiliary parameter p to control the inverse of H, we work directly with this inverse function itself. We prove a direct inverse expansion for H in terms of η in Section 4 (after defining $q = \eta^2$), and then control the absolute inverse-coefficient sum with two different pieces, using an index cutoff $\log(1/\eta)$ in Section 5. In contrast, [BMMN13] uses a fixed index cutoff. In essence, the variable index cutoff supplants the auxiliary rounding parameter p used in [BMMN13].

However, we reiterate the conceptual difference between our result and [BMMN13]. The main suggestion of [BMMN13] is that optimizers of König's bilinear functional should lead to good bounds on K_G. Such optimizers seemed so complicated that perhaps finding the exact value of K_G could be a hopeless endeavor. We instead advocate for a different path forward.

Theorem 1.6 and the resolution of Conjecture 1.5 suggest instead that relatively simple choices of Krivine rounding schemes f, g do lead to good bounds on K_G. This realization then led to the successful rigorous computer-assisted proof of Theorem 1.9 as detailed in Section 16. So, perhaps K_G can be found after all.

2. Some Notation and Definitions

Let $\Re z$ denote the real part of $z \in \mathbb{C}$. Let

$$S := \{z \in \mathbb{C}\colon\ |\Re z| < 1\}, \qquad L := \log(1+\sqrt{2}). \tag{12}$$

Thus $L = \operatorname{arsinh}(1)$, so $\sinh L = 1$. We use the Hermite normalization of [BMMN13]: the polynomials h_m are orthonormal for the weight $e^{-x^2}\,dx$, i.e.

$$\int_{\mathbb{R}} h_m(x)h_n(x)e^{-x^2}\,dx = \delta_{mn}. \tag{13}$$

In particular,

$$h_5(x) = \frac{4x^5 - 20x^3 + 15x}{2\pi^{1/4}\sqrt{15}}, \qquad h_3(x) = \frac{2x^3 - 3x}{\pi^{1/4}\sqrt{3}}, \qquad \forall\, x \in \mathbb{R}. \tag{14}$$

For $\eta \in (0,1)$ and $d \in \{3,5\}$, define

$$f_\eta(x_1,x_2) = f_\eta^{(d)}(x_1,x_2) \begin{cases} 1, & x_2 \geq \eta h_d(x_1), \\ -1, & x_2 < \eta h_d(x_1). \end{cases}. \tag{15}$$

Since h_d is odd for $d \in \{3,5\}$, f_η is odd almost everywhere. As in [BMMN13, Equation (41)], we use a different normalization for the function (3) denoted $\forall\ z \in S$ as

$$H_\eta(z) := \frac{1}{2\pi(1-z^2)} \int_{\mathbb{R}^2\times\mathbb{R}^2} f_\eta(x)f_\eta(y)\exp\left(\frac{-\|x\|_2^2 - \|y\|_2^2 + 2z\langle x,y\rangle}{1-z^2}\right)dx\,dy. \tag{16}$$

When $d=3$, we use $f_\eta^{(3)}(x)(f_{-\eta}^{(3)}(y))$ in the integrand (16). By [BMMN13, Lemma 4.3],

$$H_0(z) = \arcsin z \qquad \forall\, z \in S. \tag{17}$$

The function (3) when applied to the pair (f_η, f_η) in dimension $k=2$ with $d=5$ differs from (16) by a scalar:

$$H_{f_\eta,f_\eta}(z) = \frac{2}{\pi}H_\eta(z). \tag{18}$$

Indeed, (3) has prefactor $\pi^{-2}(1-z^2)^{-1}$, whereas (16) has prefactor $(2\pi)^{-1}(1-z^2)^{-1}$. Let

$$q := \eta^2, \qquad \widetilde{H}_q(z) := H_{\sqrt{q}}(z). \tag{19}$$

When the local inverse of $\widetilde{H}_q$ at the origin is defined, denote it by $B_q = \widetilde{H}_q^{-1}$, and write

$$B_q(z) = \sum_{m=0}^{\infty} a_{2m+1}(q)z^{2m+1}, \tag{20}$$

for all z near 0. (For small q, this inverse will be shown to exist and be analytic in a neighborhood of the origin in Lemma 4.1 below.) The even coefficients vanish because $\widetilde{H}_q$ is odd, and the coefficients are real since $\widetilde{H}_q$ has real Taylor coefficients at the origin.

3. The first perturbation term of H

For any $z \in S$ and $u, v \in \mathbb{R}$, define the two-dimensional Gaussian kernel

$$p_z(u,v) = \frac{1}{\pi\sqrt{1-z^2}} \exp\left(-\frac{u^2+v^2-2zuv}{1-z^2}\right). \tag{21}$$

For real $z = t \in (-1,1)$, this is the joint density of a centered Gaussian pair (U,V) with $\mathbb{E}U^2 = \mathbb{E}V^2 = 1/2$ and $\mathbb{E}UV = t/2$. To justify the estimates below, note that

$$\frac{u^2+v^2-2zuv}{1-z^2} = \frac{(u+v)^2}{2(1+z)} + \frac{(u-v)^2}{2(1-z)}.$$

Since $\Re(1/(1+z)) > 0$ and $\Re(1/(1-z)) > 0$ for $z \in S$, for every compact set $K \subset S$ there are constants $c_K, C_K > 0$ such that

$$\left|\partial_u^\alpha \partial_v^\beta p_z(u,v)\right| \le C_{K,\alpha,\beta}(1+|u|+|v|)^{\alpha+\beta} e^{-c_K(u^2+v^2)} \tag{22}$$

for all $z \in K$, $u, v \in \mathbb{R}$, $\alpha, \beta \ge 0$. In particular, the Gaussian integrals and the threshold differentiations used below are locally uniform in $z \in S$.

The following identities are well known, but we include their proofs for completeness.

Lemma 3.1 (Hermite covariance)**.** *For every $m, n \ge 0$ and every $z \in S$,*

$$\iint_{\mathbb{R}^2} h_m(u)h_n(v)p_z(u,v)\,du\,dv = \frac{z^n}{\sqrt{\pi}}\delta_{mn}. \tag{23}$$

In particular, for $d \in \{3,5\}$

$$\iint_{\mathbb{R}^2} h_d(u)h_d(v)p_z(u,v)\,du\,dv = \frac{z^d}{\sqrt{\pi}}. \tag{24}$$

Also,

$$\iint_{\mathbb{R}^2} h_d(u)^2 p_z(u,v)\,du\,dv = \frac{1}{\sqrt{\pi}}. \tag{25}$$

Proof. We first prove (23). It suffices to prove the identity for real $z = t \in (-1,1)$; the identity for all $z \in S$ follows by analyticity and the estimate (22). We use the Hermite generating function in the normalization of [BMMN13], namely

$$\sum_{n=0}^{\infty} h_n(x)\frac{s^n}{\sqrt{n!}} = \pi^{-1/4}\exp\left(\sqrt{2}sx - \frac{s^2}{2}\right). \tag{26}$$

If (U,V) has density p_t, then $\mathbb{E}U^2 = \mathbb{E}V^2 = 1/2$ and $\mathbb{E}UV = t/2$. Hence

$$\begin{aligned}\mathbb{E}&\left[\left(\sum_{m=0}^{\infty} h_m(U)\frac{s^m}{\sqrt{m!}}\right)\left(\sum_{n=0}^{\infty} h_n(V)\frac{r^n}{\sqrt{n!}}\right)\right] \\ &= \pi^{-1/2}\exp\left(-\frac{s^2+r^2}{2}\right)\mathbb{E}e^{\sqrt{2}sU+\sqrt{2}rV} = \pi^{-1/2}e^{tsr}.\end{aligned}$$

The last equality follows from the known formula for the moment generating function of (U,V). Comparing the coefficient of $s^m r^n$ gives (23) for real t, and then analytic continuation gives the general case.

Having proved (23) (which then implies (24)), we now prove (25). For real $z = t \in (-1, 1)$, completing the square gives

$$\int_{\mathbb{R}} p_t(u,v)\,dv \overset{(21)}{=} \frac{e^{-u^2}}{\sqrt{\pi}}.$$

Hence

$$\iint_{\mathbb{R}^2} h_d(u)^2 p_t(u,v)\,du\,dv = \frac{1}{\sqrt{\pi}}\int_{\mathbb{R}} h_d(u)^2 e^{-u^2}\,du \overset{(13)}{=} \frac{1}{\sqrt{\pi}}.$$

The identity extends to all $z \in S$ by analytic continuation. □

The following Lemma could be considered a routine extension of [BMMN13, Theorem 4.4], which used an expansion only for $z = i$.

Lemma 3.2 (Expansion of $\widetilde{H}_q$). *Uniformly for z on compact subsets of S, as $q \downarrow 0$,*

$$\widetilde{H}_q(z) = \arcsin z + qQ(z) + O(q^2), \tag{27}$$

where $\sigma := 1$ for $d = 5$, $\sigma := -1$ for $d = 3$, and for $d \in \{3, 5\}$, we have

$$Q(z) = Q_d(z) = \frac{2(\sigma z^d - z)}{\sqrt{\pi}\sqrt{1-z^2}}. \tag{28}$$

The expansion (27) may be differentiated once with respect to z, locally uniformly on S.

Remark 3.3. *We make the constants from Lemma 3.2 explicit in Sections 10 and 11. When $d = 5$, we have by (90), (91), (92) and (95) that*

$$\sup_{z\in\sin(1.08\cdot\mathbb{D})} |\widetilde{H}_q(z) - (\arcsin z + qQ(z))| \le q^2 e^{23.6}.$$

$$\sup_{z\in\sin(1.08\cdot\mathbb{D})} \left|\frac{d}{dz}\left[\widetilde{H}_q(z) - (\arcsin z + qQ(z))\right]\right| \le \frac{100}{\cos(1.08)} q^2 e^{24.58}.$$

When $d = 3$, we have by (90), (93), (94) and (95)

$$\sup_{z\in\sin(1.08\cdot\mathbb{D})} |\widetilde{H}_q(z) - (\arcsin z + qQ(z))| \le q^2 e^{14.5}.$$

$$\sup_{z\in\sin(1.08\cdot\mathbb{D})} \left|\frac{d}{dz}\left[\widetilde{H}_q(z) - (\arcsin z + qQ(z))\right]\right| \le \frac{100}{\cos(1.08)} q^2 e^{15}.$$

Proof. For any $z \in S$, define

$$G_z(a,b) := \iint_{\mathbb{R}^2} \operatorname{sign}(u-a)\operatorname{sign}(v-b) p_z(u,v)\,du\,dv, \qquad \forall\, a, b \in \mathbb{R}. \tag{29}$$

By (22), G_z is C^4 in the threshold variables (a, b), with bounds that are uniform for z in a fixed compact subset of S. Direct differentiation then gives

$$\partial_a G_z(a,b) = -2\int_{\mathbb{R}} \operatorname{sign}(v-b) p_z(a,v)\,dv, \qquad \partial_b G_z(a,b) = -2\int_{\mathbb{R}} \operatorname{sign}(u-a) p_z(u,b)\,du. \tag{30}$$

At $(a, b) = (0, 0)$ these derivatives vanish, because the integrands are odd. A second threshold differentiation gives

$$\partial_{aa} G_z(0,0) = \partial_{bb} G_z(0,0) = -\frac{4z}{\pi\sqrt{1-z^2}}, \qquad \partial_{ab} G_z(0,0) = \frac{4}{\pi\sqrt{1-z^2}}. \tag{31}$$

For instance,

$$\begin{aligned}\partial_{aa}G_z(0,0) &= -2\int_{\mathbb{R}} \operatorname{sign}(v)\partial_u p_z(0,v)\,dv \\ &= -\frac{4z}{1-z^2}\int_{\mathbb{R}} |v|\frac{\exp(-v^2/(1-z^2))}{\pi\sqrt{1-z^2}}\,dv = -\frac{4z}{\pi\sqrt{1-z^2}},\end{aligned}$$

where $\Re(1/(1-z^2)) > 0$ on S. Also $\partial_{ab}G_z(a,b) = 4p_z(a,b)$, which yields the displayed formula for $\partial_{ab}G_z(0,0)$.

Let (X_1, Y_1) be distributed according to the kernel p_z. From (16) and (21), or first for real z and then by analyticity, we have

$$\widetilde{H}_q(z) \overset{(19)}{=} H_{\sqrt{q}}(z) \overset{(16)}{=} \frac{\pi}{2}\,\mathbb{E}\left[G_z\big(\sqrt{q}\,h_d(X_1), \sqrt{q}\,\sigma h_d(Y_1)\big)\right], \tag{32}$$

where $\sigma = 1$ for $d = 5$ and $\sigma = -1$ for $d = 3$. (Since (16) has an absolutely convergent integrand, $H_{\sqrt{q}}(z)$ is analytic in the strip S.) Write $A = h_d(X_1)$ and $B = \sigma h_d(Y_1)$. Taylor expansion of G_z at $(0,0)$ to third order, with integral remainder, gives

$$\begin{aligned}G_z(\sqrt{q}A, \sqrt{q}B) = G_z(0,0) &\\ &+ \frac{q}{2}\Big(\partial_{aa}G_z(0,0)A^2 + 2\partial_{ab}G_z(0,0)AB + \partial_{bb}G_z(0,0)B^2\Big) \\ &+ \frac{q^{3/2}}{6}\Big(\partial_{aaa}G_z(0,0)A^3 + 3\partial_{aab}G_z(0,0)A^2B \\ &\qquad + 3\partial_{abb}G_z(0,0)AB^2 + \partial_{bbb}G_z(0,0)B^3\Big) \\ &+ O_K\big(q^2(|A|+|B|)^4\big),\end{aligned}$$

uniformly for z in a compact subset of S. The cubic expectation is zero: the kernel $p_z(x,y)\,dx\,dy$ is invariant under $(x,y) \mapsto (-x,-y)$, and each of A^3, A^2B, AB^2, B^3 is odd under this simultaneous sign change. Since h_d is a polynomial, the fourth moment in the remainder is finite and locally uniformly bounded in z. Hence by (32)

$$\widetilde{H}_q(z) = \widetilde{H}_0(z) + \frac{\pi}{2}q\left(\partial_{aa}G_z(0,0)\mathbb{E}A^2 + \partial_{ab}G_z(0,0)\mathbb{E}AB\right) + O_K(q^2). \tag{33}$$

Here we used $\partial_{aa}G_z = \partial_{bb}G_z$ by (31) and $\mathbb{E}A^2 = \mathbb{E}B^2$. By Lemma 3.1, $\mathbb{E}A^2 = 1/\sqrt{\pi}$ and $\mathbb{E}AB = \sigma z^d/\sqrt{\pi}$. Substituting (31) into (33) yields

$$\widetilde{H}_q(z) = \widetilde{H}_0(z) + q\frac{2(\sigma z^d - z)}{\sqrt{\pi}\sqrt{1-z^2}} + O_K(q^2).$$

Together with (17), this is (27). The locally uniform expansion of the derivative follows from Cauchy's integral formula, applied on a slightly larger compact subset of S. □

4. The inverse function and its coefficients

In this Section we modify and extend [BMMN13, Lemmas 5.3 and 5.4].

Lemma 4.1 (Inverse perturbation). *Fix $0 < r \le 1.08$. For all sufficiently small $q > 0$, the inverse branch $B_q = \widetilde{H}_q^{-1}$ is analytic on $r\mathbb{D}$. Uniformly for $z \in r\mathbb{D}$,*

$$B_q(z) = \sin z + q\Psi(z) + O_r(q^2), \tag{34}$$

where for $d = 5$, we have

$$\Psi(z) = -Q(\sin z)\cos z \overset{(28)}{=} \frac{2}{\sqrt{\pi}}\big(\sin z - \sin^5 z\big) = \frac{6\sin z + 5\sin(3z) - \sin(5z)}{8\sqrt{\pi}}. \tag{35}$$

Consequently, if

$$\sin z = \sum_{\substack{n\geq 1\\ n \text{ odd}}} b_n z^n, \qquad \Psi(z) = \sum_{\substack{n\geq 1\\ n \text{ odd}}} c_n z^n,$$

then, for $n = 2m+1$,

$$b_n = \frac{(-1)^m}{n!}, \qquad c_n = \frac{(-1)^m}{8\sqrt{\pi}\,n!}\big(6 + 5\cdot 3^n - 5^n\big). \tag{36}$$

In particular, there is an absolute constant C_0 such that

$$|c_n| \leq C_0\frac{5^n}{n!} \qquad \forall \text{ odd } n \geq 1. \tag{37}$$

Moreover, for every $0 < \rho \leq 1.08$ there are constants $q_\rho > 0$ and $C_\rho < \infty$ such that, for all $0 < q < q_\rho$ and all odd $n \geq 1$, the Taylor coefficients $a_n(q)$ of B_q (20) satisfy

$$|a_n(q) - b_n - qc_n| \leq C_\rho q^2 \rho^{-n}. \tag{38}$$

Remark 4.2. *In the $d = 3$ case, we have instead*

$$\Psi(z) = \frac{2}{\sqrt{\pi}}(\sin(z) + \sin^3(z)) = \frac{7\sin z - \sin(3z)}{2\sqrt{\pi}}, \qquad b_n = \frac{(-1)^m}{n!}, \qquad c_n = \frac{(-1)^m}{2\sqrt{\pi}n!}(7 - 3^n), \tag{39}$$

$$|c_n| \leq C_0\frac{3^n}{n!}, \qquad |a_n(q) - b_n - qc_n| \leq C_\rho q^2\rho^{-n} \tag{40}$$

Proof. Let $K_r = \sin(\overline{r\mathbb{D}})$. Since $r < \pi/2$, $\arcsin(\sin z) = z$ for $|z| \leq r$, and $\cos z$ is bounded away from zero on $\overline{r\mathbb{D}}$.

We need to check that $K_R = \{\sin\zeta\colon\ |\zeta| \leq R\}$ is contained compactly in the strip $S = \{w \in \mathbb{C}\colon\ |\Re w| < 1\}$. We shall use $R = 27/25$. Write $\zeta = x + iy$. Then

$$|\Re(\sin\zeta)| = |\sin x\cosh y| = |\sin x|\cosh y.$$

We use the elementary inequalities

$$\cosh y \leq e^{y^2/2}, \quad \forall\, y \in \mathbb{R}, \qquad \sin x \leq xe^{-x^2/6}, \quad \forall\, 0 \leq x < \pi$$

Now if $|\zeta| \leq R$, then $x^2 + y^2 \leq R^2$, so

$$|\Re(\sin\zeta)| \leq |x|e^{-x^2/6}e^{y^2/2} \leq |x|\exp\left(\frac{R^2}{2} - \frac{2x^2}{3}\right).$$

The right-hand side is maximized at $x = \sqrt{3}/2$, so plugging this in and using $R = 27/25$,

$$|\Re(\sin\zeta)| \leq \frac{\sqrt{3}}{2}\exp\left(\frac{R^2 - 1}{2}\right) \leq \frac{\sqrt{3}}{2}e^{\frac{104}{2\cdot 625}} < \frac{19}{20}.$$

In particular $K_{27/25} \subset S$. Choose s with $r < s < \pi/2$, and choose an open set U such that

$$K_r \subset K_s \subset U \subset S.$$

Then choose $0 < \rho_0 \le \rho_{r,s}$, so that the disk $D(w_0, \rho_0)$ satisfies $D(w_0, \rho_0) \subset K_s$ for every $w_0 \in K_r$. On U, the derivative

$$H_0'(w) = (\arcsin)'(w) = \frac{1}{\sqrt{1-w^2}}$$

is bounded away from zero since $U \subset S$. Then Lemma 12.1 below implies that, for any w with $|w - w_0| \le \rho_0$, we have

$$|H_0(w) - H_0(w_0)| \ge \frac{1}{\cosh s} |w - w_0| . \tag{41}$$

Lemma 3.2 gives some $C_U > 0$ such that, for all sufficiently small q,

$$\sup_{w \in U} |\widetilde{H}_q(w) - H_0(w)| \le C_U q. \tag{42}$$

On the circle $\{w \in \mathbb{C} \colon |w - \sin z| = \rho_0\} \subset U$, the lower bound (41) gives

$$|H_0(w) - z| = |H_0(w) - H_0(\sin z)| \ge \frac{1}{\cosh s}\rho_0.$$

So, for q small enough such that $C_U q < \frac{1}{\cosh s}\rho_0$, Rouché's theorem implies that the function

$$w \mapsto \widetilde{H}_q(w) - z = \widetilde{H}_q(w) - H_0(w) + H_0(w) - z$$

has exactly one zero in $D(\sin z, \rho_0)$. Denote it by $w_q = B_q(z)$. Since $\widetilde{H}_q'(w_q) = H_0'(w_q) + O(q)$ by Lemma 3.2 and H_0' is bounded away from zero on U, the implicit function theorem shows that B_q depends analytically on z. This is the inverse branch of $\widetilde{H}_q$ on $r\mathbb{D}$.

We now prove the sharper estimate $B_q(z) = \sin z + O_r(q)$. Put

$$w_0 = \sin z, \qquad w_q = B_q(z). \tag{43}$$

Since $\widetilde{H}_q(w_q) = z = H_0(w_0)$, (42) gives

$$|H_0(w_q) - H_0(w_0)| = |H_0(w_q) - \widetilde{H}_q(w_q)| \le C_U q.$$

Using (41) with $w = w_q$,

$$|w_q - w_0| \le \cosh(s) C_U q. \tag{44}$$

Therefore, $B_q(z) = \sin z + O_r(q)$ by (43), uniformly for $z \in r\mathbb{D}$.

Next write the expansion from Lemma 3.2 on U in the form

$$\widetilde{H}_q(w) = H_0(w) + qQ(w) + q^2 R_q(w), \qquad \sup_{w \in U} |R_q(w)| \le \widetilde{C}_U. \tag{45}$$

Since $H_0(w_q) = H_0(w_0) + H_0'(w_0)(w_q - w_0) + O_r(|w_q - w_0|^2)$, and since (44) gives $|w_q - w_0| = O_r(q)$, we have

$$H_0(w_q) - H_0(w_0) = H_0'(w_0)(w_q - w_0) + O_r(q^2). \tag{46}$$

Similarly, Q is analytic on U, hence

$$qQ(w_q) = qQ(w_0) + qO_r(|w_q - w_0|) = qQ(w_0) + O_r(q^2). \tag{47}$$

Finally, $q^2 R_q(w_q) = O_r(q^2)$. Substituting (45) (with $w = w_q$), (46) and (47) into

$$0 = \widetilde{H}_q(w_q) - H_0(w_0)$$

which follows from $\widetilde{H}_q(w_q) = z = H_0(w_0)$, gives

$$0 = H_0'(w_0)(w_q - w_0) + qQ(w_0) + O_r(q^2). \tag{48}$$

That is,

$$0 = (\arcsin)'(w_0)(w_q - w_0) + qQ(w_0) + O_r(q^2).$$

On $r\mathbb{D}$, $(\arcsin)'(\sin z) = 1/\cos z$ and $\sqrt{1-\sin^2 z} = \cos z$. Hence

$$w_q - w_0 = -qQ(\sin z)\cos z + O_r(q^2) \overset{(28)}{=} \frac{2q}{\sqrt{\pi}}(\sin z - \sin^5 z) + O_r(q^2),$$

which proves (34). The trigonometric identity in (35) follows from

$$\sin^5 z = \frac{10\sin z - 5\sin(3z) + \sin(5z)}{16}.$$

Expanding the sine functions gives (36), and (37) is immediate. Finally, applying Cauchy's integral formula to the remainder in (34) on the circle $|z| = \rho$ gives (38). □

Remark 4.3. *In the above proof we may take $C_0 = 1/4$ in (37) and we take C_ρ to be the same constant from (38) as in (34). Then Lemma 12.1 gives $|H_0(w) - H_0(w_0)| \geq \frac{1}{\cosh(s)}|w - w_0|$.*

Also (42) can be written as, for all $w \in U$,

$$|\widetilde{H}_q(w) - H_0(w)| \leq q|Q(w)| + O(q^2) \leq 5q + q^2 e^{24.6},$$

by numerics in Section 10, i.e. (90) and (92), so we can use (for $d = 5$)

$$C_U := 5 + qe^{24.6}.$$

Then after (45) the $O_r(|w_q - w_0|^2)$ is bounded by $9|w_q - w_0|^2$ by upper bounding the second derivative of arcsin *by (99). Then the implied constant $O_r(q^2)$ in (46) is at most $9(C_U \cosh(s))^2 q^2$. Then denoting C_Q as the first implied constant in (47), the $O_r(q^2)$ term in (47) is at most $C_Q(C_U \cosh(s))q^2$, with $C_Q \leq 8.5$ by (101) below.*

And then $q^2 R_q(w_q)$ is bounded by $\widetilde{C}_U q^2$ by (45), and we may take $\widetilde{C}_U = e^{24.6}$. Next, the $O_r(q^2)$ term in (48) is at most q^2 times

$$\widetilde{C}_U + 9(C_U\cosh(s))^2 + C_Q(C_U\cosh(s))$$

the same implied constant bounds then carry through to the next displayed equations, after also multiplying by 1.643 to account for the $O_r(q^2)$ term being multiplied by $\cos(z)$ on the set $|z| \leq 1.08$.

When $d = 5$, we may choose $r = 1.08$, $s = 1.09$, $\cosh(s) = \cosh(1.09) < 5/3$, $\widetilde{C}_U = e^{24.6}$, $C_0 = 1/4$, so the $O_r(q^2)$ term in (48) can be bounded by q^2 times

$$e^{24.6} + 9([5 + qe^{24.6}] \cdot (5/3))^2 + 8.5([5 + qe^{24.6}] \cdot (5/3)) \leq q^2 e^{63} + qe^{31} + e^{25}.$$

Likewise, we can use $C_\rho = q^2 e^{63} + qe^{31} + e^{25}$. When $d = 3$, we can choose $\widetilde{C}_U := e^{15}$, $C_0 = 1/2$, $C_Q = 23$ by (94) and (100), so the $O_r(q^2)$ term in (48) can be bounded by q^2 times

$$e^{15} + 9([3 + qe^{15}] \cdot (5/3))^2 + 23([3 + qe^{15}] \cdot (5/3)) \leq q^2 e^{42} + qe^{29} + e^{15.5}.$$

5. The absolute coefficient sum at L

Let $a_n(q)$ be the Taylor coefficients of B_q, as in (20). For $t \geq 0$, define

$$A_q(t) = \sum_{\substack{n \geq 1 \\ n \text{ odd}}} |a_n(q)|\, t^n, \tag{49}$$

whenever this series converges. Recalling (5) and Corollary 1.3, an upper bound on K_G results from understanding where A_q takes the value 1. Since we anticipate $A_q(t)$ taking the value 1 at some $t > L$, we will eventually show that $A_q(L)$ is less than 1 for small q in Section 8. To prepare for that result, we compare the absolute coefficient sum $A_q(L)$ with the same alternating sum without absolute values, i.e. $B_q(iL)/i$. A similar strategy with different details was used in [BMMN13, Theorem 5.1], which required an auxiliary parameter p.

Lemma 5.1. *As $q \downarrow 0$,*

$$A_q(L) = \frac{B_q(iL)}{i} + o(q^2). \tag{50}$$

The $o(q^2)$ term is bounded by $6C_\rho q^2 q^{\frac{0.3537}{\log\log(1/q)}} + q^{2.01}$, if $q < e^{-390}$ and $d = 5$. If $d = 3$, the $o(q^2)$ term is at most $6C_\rho q^2 q^{\frac{0.3537}{\log\log(1/q)}} + q^{2.01}$, if $q < \min(e^{-81}, (4C_\rho)^{-5})$.

Proof. We first prove the case $d = 5$, saving $d = 3$ for Remark 5.2. Fix $\rho := 1.08$. By (12)

$$L < .89 < 1 < \rho. \tag{51}$$

All coefficient estimates below use Lemma 4.1 with this value of ρ. For odd n, put

$$s_n := (-1)^{(n-1)/2}, \qquad d_n(q) := b_n + qc_n, \qquad e_n(q) := a_n(q) - d_n(q). \tag{52}$$

Thus $b_n = s_n/n!$. By (36),

$$s_n d_n(q) = \frac{1 + q\delta_n}{n!}, \qquad \delta_n := \frac{6 + 5 \cdot 3^n - 5^n}{8\sqrt{\pi}}, \tag{53}$$

and $|\delta_n| \leq C5^n$ with $C = 1/4$. Also, by (38),

$$|e_n(q)| \leq C_\rho q^2 \rho^{-n}. \tag{54}$$

Let $T := \log(1/q)$, and define

$$N_1 := \left\lfloor 1.75 \frac{T}{\log T} \right\rfloor, \qquad N_0 := \left\lfloor 3.7 \frac{T}{\log T} \right\rfloor. \tag{55}$$

We first prove that $a_n(q)$ has the alternating sign s_n for every odd $n \leq N_1$, when q is small enough. Indeed, by definition of T and N_1

$$\max_{n \leq N_1} q\,|\delta_n| \leq Cq5^{N_1} \leq C \exp\big(-T + (3.5\log 5)T/(2\log T)\big) = o(1),$$

so $s_n d_n(q) \geq \frac{1}{2} n!^{-1}$ for all odd $n \leq N_1$ and small q (since $-T + (3.5\log 5)T/(2\log T) < -(1/3)\cdot T$ when $T > 69$, it suffices to choose $q < \min(e^{-70}, 2^{-6}C^{-3})$.)

On the other hand, Stirling's formula and (54) give

$$\max_{n \leq N_1} n!\,|e_n(q)| \leq C_\rho q^2 \max_{n \leq N_1} n! \rho^{-n},$$

$$\log\left(q^2 N_1! \rho^{-N_1}\right) \leq -2T + N_1 \log N_1 - N_1 \log \rho = -\frac{1}{4}T + o(T),$$

which tends to $-\infty$. (It is bounded by $-.2T$ when $T \geq 70$). Hence $|e_n(q)| \leq \frac{1}{4}n!^{-1}$ for all odd $n \leq N_1$, and therefore $s_n a_n(q) > 0$ for every such n, by (52) using also $s_n d_n(q) \geq \frac{1}{2}n!^{-1}$. (It suffices to choose $q < \min(e^{-6}, (4C_\rho)^{-5})$.) Since $B_q(iL)/i = \sum_{\substack{n\geq 1 \\ n \text{ odd}}} s_n a_n(q) L^n$ by (20),

$$0 \leq A_q(L) - \frac{B_q(iL)}{i} = \sum_{\substack{n\geq 1 \\ n \text{ odd}}} \big(|a_n(q)| - s_n a_n(q)\big) L^n. \tag{56}$$

Since $s_n a_n(q) > 0$ for all $n \leq N_1$, those terms vanish in the right sum of (56). For $n > N_1$, use the elementary inequality

$$|d + e| - s(d + e) \leq |d| - sd + 2\,|e|\,, \qquad s \in \{-1, 1\}, \quad d, e \in \mathbb{R}. \tag{57}$$

It then follows from (56) that

$$A_q(L) - \frac{B_q(iL)}{i} \leq \sum_{\substack{n>N_1 \\ n \text{ odd}}} \big(|d_n(q)| - s_n d_n(q)\big) L^n + 2 \sum_{\substack{n>N_1 \\ n \text{ odd}}} |e_n(q)|\, L^n. \tag{58}$$

The error tail is $o(q^2)$, since $L = \log(1 + \sqrt{2}) < \rho = 1.08$, $L/\rho < .817$ and (54) imply

$$\begin{aligned}\sum_{n>N_1} |e_n(q)|\, L^n &\leq C_\rho q^2 \sum_{n>N_1,\text{ odd}} \left(\frac{L}{\rho}\right)^n = C_\rho q^2 \frac{(L/\rho)^{N_1+1}}{1-(L/\rho)^2} \\ &\leq 3C_\rho q^2 .817^{N_1} \leq 3C_\rho q^2 q^{\frac{3.5\log(1/.817)}{2\log\log(1/q)}} \leq 3C_\rho q^2 q^{\frac{0.3537}{\log\log(1/q)}} = o(q^2).\end{aligned} \tag{59}$$

It remains to bound the d_n-tail. Since

$$\max_{n\leq N_0} q\,|\delta_n| \leq Cq5^{N_0} \leq Cq^{1-\frac{3.7\log 5}{\log\log(1/q)}} < 1, \text{ if } q < e^{-390} \tag{60}$$

we have by (53) that $s_n d_n(q) > 0$ for all odd $n \leq N_0$ and for all $q < e^{-390}$. Therefore, due to the terms $N_1 < n \leq N_0$ being zero in the following sum,

$$\begin{aligned}\sum_{\substack{n>N_1 \\ n \text{ odd}}} \big(|d_n(q)| - s_n d_n(q)\big) L^n &= \sum_{\substack{n>N_0 \\ n \text{ odd}}} \big(|d_n(q)| - s_n d_n(q)\big) L^n \\ &\overset{(52)}{\leq} 2 \sum_{n>N_0,\text{ odd}} \big(|b_n| + q\,|c_n|\,\big) L^n \\ &\overset{(36)}{\leq} 2 \sum_{n>N_0,\text{ odd}} \frac{L^n}{n!} + \frac{2}{7} q \sum_{n>N_0,\text{ odd}} \frac{(5L)^n}{n!}.\end{aligned} \tag{61}$$

For every fixed $\lambda > 0$ and every sufficiently large N,

$$\sum_{n>N} \frac{\lambda^n}{n!} \leq 2\frac{\lambda^{N+1}}{(N+1)!} \leq 2\left(\frac{e\lambda}{N+1}\right)^{N+1}. \tag{62}$$

With $N = N_0$, the right-hand side is $\exp(-3.7T + o(T)) = o(q^2)$, because $N_0 \log N_0 = 3.7T + o(T)$. More specifically,

$$\sum_{n>N_0} \frac{L^n}{n!} \leq q^{2.1}, \qquad \sum_{n>N_0} \frac{(5L)^n}{n!} < q^{1.01}, \text{ if } q < e^{-390}$$

So, the right side of (61) is $o(q^2)$. With (59), (56), (58), this proves (50) when $d = 5$. $\square$

Remark 5.2. *In the $d = 3$ case, we let $N_0 := \lfloor 4T/\log T \rfloor$, and (53) becomes*

$$\delta_n = \frac{7 - 3^n}{2\sqrt{\pi}}.$$

with $|\delta_n| \leq C3^n$ with $C = 1/2$, and $-T + 3.5(\log 3)T/(2\log T) < -.4T$ when $T > 27$, so it suffices to choose $q < \min(e^{-27}, 2^{-2}C^{-2})$, then (60) becomes

$$\max_{n \leq N_0} Cq3^{N_0} = Cq^{1 - \frac{4\log 3}{\log\log(1/q)}} < 1, \text{ if } q < e^{-81},$$

Then (61) becomes

$$\sum_{\substack{n > N_1 \\ n \text{ odd}}} \big(|d_n(q)| - s_n d_n(q)\big)L^n \leq 2 \sum_{n > N_0, \text{ odd}} \frac{L^n}{n!} + q \sum_{n > N_0, \text{ odd}} \frac{(3L)^n}{n!}.$$

and the inequalities after that become

$$\sum_{n > N_0} \frac{L^n}{n!} \leq q^{2.1}, \qquad \sum_{n > N_0} \frac{(3L)^n}{n!} < q^{1.01}, \text{ if } q < e^{-65}$$

6. Evaluation of $B_q(iL)$

Lemma 5.1 reduces the problem of understanding $A_q(L)$ to instead understanding $B_q(iL)$. In this section, we therefore write a power series expansion for $B_q(iL)$. As we will see below, this reduces to understanding $H_\eta(i)$ or equivalently $\widetilde{H}_q(i)$.

For these reasons, the proof of Theorem 4.4 in [BMMN13] gives the following $d = 5$ expansion, albeit without explicit error bound

$$4\pi \frac{H_\eta(i)}{i} = 4\pi L + 1600\sqrt{2}\,\eta^4 + O(\eta^6). \tag{63}$$

In Section 14 and (107), we show that the $O(\eta^6)$ term is bounded by $2.3 \cdot 10^{13}|\eta|^6$. In terms of $q = \eta^2$, this is

$$\frac{\widetilde{H}_q(i)}{i} \overset{(18)\wedge(19)}{=} L + \frac{400\sqrt{2}}{\pi} q^2 + O(q^3), \tag{64}$$

and the $O(q^3)$ term can be taken to be $2 \cdot 10^{12} q^3$. Also, (28) gives $Q(i) = 0$, because $i^5 = i$, explaining the lack of linear term in q in (64). Likewise when $d = 3$, we obtain in (108)

$$\left|4\pi \frac{H_\eta(i)}{i} - 4\pi L - 48\sqrt{2}\,\eta^4\right| \leq 2.7 \cdot 10^7 |\eta|^6. \qquad \left|\frac{\widetilde{H}_q(i)}{i} - L - \frac{12\sqrt{2}}{\pi} q^2\right| \leq 2.7 \cdot 10^7 |q|^3.$$

Lemma 6.1. *Let $d = 5$. Then as $q \downarrow 0$,*

$$B_q(iL) = i - \frac{800i}{\pi} q^2 + O(q^3), \tag{65}$$

where $O(q^3)$ is bounded by $e^{9.4}q^3 + e^{36}q^4 + e^{59}q^5$.

Proof. Recall that $\sin(iL) = i\sinh L \overset{(12)}{=} i$, so $\Psi(iL) \overset{(35)}{=} 0$. Then Lemma 4.1 applies at iL since $|iL| \overset{(12)}{<} .89$. That is, if we define

$$\delta_q := B_q(iL) - i. \tag{66}$$

Then $|\delta_q| \le q^2(q^2e^{63} + qe^{31} + e^{25})$ by Remark 4.3. Using that B_q is the inverse of $\widetilde{H}_q$ then Taylor expanding $\widetilde{H}_q$ at i, using analyticity on S, gives

$$iL = \widetilde{H}_q(B_q(iL)) \overset{(66)}{=} \widetilde{H}_q(i + \delta_q) = \widetilde{H}_q(i) + \widetilde{H}_q'(i)\delta_q + O(\delta_q^2). \tag{67}$$

By Lemma 3.2, differentiated once in z, (i.e. Remark 3.3, using $\arcsin'(i) = 1/\sqrt{2}$ and $Q'(i) = 4\sqrt{2/\pi}$)

$$\widetilde{H}_q'(i) = \widetilde{H}_0'(i) + [4\sqrt{2/\pi}]q + O(q^2) = \frac{1}{\sqrt{2}} + q4\sqrt{2/\pi} + O(q^2),$$

where $O(q^2) \le 213q^2e^{24.6}$. Equation (64) says

$$\widetilde{H}_q(i) = iL + i\frac{400\sqrt{2}}{\pi}q^2 + O(q^3),$$

where $O(q^3)$ is at most $2 \cdot 10^{12}q^3$. Substituting this and the $\delta_q = O(q^2)$ bound back into (67),

$$\delta_q = -\frac{i(400\sqrt{2}/\pi)q^2 + O(q^3)}{1/\sqrt{2} + q4\sqrt{2/\pi} + O(q^2)} = -\frac{800i}{\pi}q^2 + O(q^3),$$

where $O(q^3)$ is at most

$$11494q^3 + 76710e^{24.6}q^4 + 1.2 \cdot 10^{13}q^4 + 852 \cdot 10^{12}e^{24.6}q^5,$$

which proves the lemma. □

Combining Lemma 5.1 with Lemma 6.1, we obtain, for $d = 5$,

$$A_q(L) = 1 - \frac{800}{\pi}q^2 + o(q^2) < 1 \tag{68}$$

for all sufficiently small $q > 0$, i.e. $o(q^2)$ term is at most

$$e^{9.4}q^3 + e^{36}q^4 + e^{59}q^5 + 6C_\rho q^2 q^{\frac{0.3537}{\log\log(1/q)}} + q^{2.01},$$

if $q < \min(e^{-390}, C_\rho^{-1/.185})$. That is, we found our desired upper bound on $A_q(L)$.

Remark 6.2. *In the $d = 3$ case, we have $|\delta_q| \le q^2(q^2e^{42} + qe^{29} + e^{15.5})$ by Remark 4.3, $Q'(i) = 2\sqrt{2/\pi}$, $\widetilde{H}_q(i) = iL + q^2 i12\sqrt{2}/\pi + O(q^3)$ with $O(q^3)$ bounded by $2.7 \cdot 10^7|q|^3$, and the $\widetilde{H}_q'(i)$ expansion has error term bounded by $213e^{15}$ by Remark 3.3, so we get*

$$\delta_q = -\frac{i(12\sqrt{2}/\pi)q^2 + O(q^3)}{1/\sqrt{2} + q2\sqrt{2/\pi} + O(q^2)} = -\frac{24i}{\pi}q^2 + O(q^3),$$

with $O(q^3)$ term bounded by $13q^3 + e^{24}q^4 + e^{39}q^5$. Combining Lemma 5.1 with this analogue of Lemma 6.1, we obtain, for $d = 3$,

$$A_q(L) = 1 - \frac{24}{\pi}q^2 + o(q^2), \tag{69}$$

with $o(q^2)$ term bounded from Remark 5.2 by

$$13q^3 + e^{24}q^4 + e^{39}q^5 + 6C_\rho q^2 q^{\frac{0.3537}{\log\log(1/q)}} + q^{2.01}, \qquad \forall\, 0 < q < \min(e^{-81}, C_\rho^{-1/.29})$$

7. Qualitative Proof Completion

Since we obtained our desired quantitative estimates that $A_q(L) < 1$ for small q (with $d = 5$ in (68) and $d = 3$ in (69)), we can now conclude the proof of Theorem 1.6. We will postpone the computation of explicit constants in Theorem 1.6 to Section 8.

Proof of Theorem 1.6. We first show the absolute coefficient sum A_q exceeds 1 slightly to the right of L. Since $L = \operatorname{arsinh}(1) < 0.9$, choose a radius $r \in (0.9, 1)$. Lemma 4.1 gives, for all small q, coefficient bounds that are summable at $t = 0.9$. Therefore, by dominated convergence,

$$\lim_{q \downarrow 0} A_q(0.9) = \sum_{\substack{n \geq 1 \\ n \text{ odd}}} \frac{0.9^n}{n!} = \sinh(0.9) > 1. \tag{70}$$

Together with (68), this implies that, for every sufficiently small $q > 0$, there exists $\gamma_q \in (L, 0.9)$ such that

$$A_q(\gamma_q) = 1. \tag{71}$$

Indeed, $A_q(t)$ is continuous on $[0, 0.9]$, since its defining series converges uniformly there.

It remains to translate (71) to the normalization in Definition 1.1. By (18),

$$H_{f_{\sqrt{q}}, f_{\sqrt{q}}}(z) = \frac{2}{\pi} \widetilde{H}_q(z),$$

and hence the inverse in Definition 1.1 is

$$H^{-1}_{f_{\sqrt{q}}, f_{\sqrt{q}}}(z) = B_q\left(\frac{\pi}{2} z\right) = \sum_{\substack{n \geq 1 \\ n \text{ odd}}} a_n(q) \left(\frac{\pi}{2}\right)^n z^n. \tag{72}$$

Thus by (49), (71) is exactly

$$\sum_{\substack{n \geq 1 \\ n \text{ odd}}} \left| a_n(q) \left(\frac{\pi}{2}\right)^n \right| \left(\frac{2\gamma_q}{\pi}\right)^n = 1. \tag{73}$$

This is condition (5) for $H_{f_{\sqrt{q}}, f_{\sqrt{q}}}$ with $\widehat{a}_n = a_n(q)(\pi/2)^n$ for all $n \geq 1$ odd by (72). Therefore, when $d = 5$, $(f_{\sqrt{q}}, f_{\sqrt{q}})$ is a Krivine rounding scheme with

$$c(f_{\sqrt{q}}, f_{\sqrt{q}}) \overset{(73)}{=} \frac{2\gamma_q}{\pi} > \frac{2}{\pi} L = \frac{2}{\pi} \log(1 + \sqrt{2}). \tag{74}$$

Since $q = \eta^2$, Theorem 1.6 follows. Similarly, when $d = 3$, we replace (68) with (69) and deduce $c(f_{\sqrt{q}}, f_{-\sqrt{q}}) > \frac{2}{\pi} \log(1 + \sqrt{2})$ for sufficiently small $q > 0$.

□

8. Quantitative Proof Completion

In this section, we make the argument from Section 7 quantitative, in order to prove explicit upper bounds on K_G. The Krivine parameter γ_q is the unique positive solution of

$$A_q(\gamma_q) = 1.$$

At $q = 0$, one has $B_0(z) = \sin z$, and therefore

$$A_0(t) = \sum_{\substack{n \geq 1 \\ n \text{ odd}}} \frac{t^n}{n!} = \sinh t.$$

Since $L \overset{(12)}{=} \operatorname{arsinh}(1)$,

$$A_0(L) = 1, \qquad A_0'(L) = \cosh L = \sqrt{2}.$$

By the mean-value theorem, for some ξ_q between L and γ_q,

$$1 - A_q(L) = A_q(\gamma_q) - A_q(L) = A_q'(\xi_q)(\gamma_q - L). \tag{75}$$

Proof of (10). Let $d = 5$. Since $.88 < \gamma_q < .9$, $.88 < \xi_q < .9$, so Lemma 9.1 with $\rho = 1$ and $\cosh(L) = \sqrt{2}$ imply

$$\begin{aligned} |A_q'(\xi_q) - \sqrt{2}| &\leq |A_q'(\xi_q) - \cosh(\xi_q)| + |\cosh(\xi_q) - \cosh(L)| \\ &\leq 38q + q^2[q^2e^{63} + qe^{31} + e^{25}](100) + .02. \end{aligned}$$

Using (68),

$$1 - A_q(L) = \frac{800}{\pi}q^2 + o(q^2),$$

with $o(q^2)$ term bounded by $e^{9.4}q^3 + e^{36}q^4 + e^{59}q^5 + 6C_\rho q^2 q^{\frac{0.3537}{\log\log(1/q)}} + q^{2.01}$. Therefore

$$\gamma_q - L \overset{(75)}{=} \frac{\frac{800}{\pi}q^2 + o(q^2)}{\sqrt{2} + o(1)} \geq \frac{\frac{800}{\pi}q^2 - (e^{9.4}q^3 + e^{36}q^4 + e^{59}q^5 + 6C_\rho q^2 q^{\frac{0.3537}{\log\log(1/q)}} + q^{2.01})}{\sqrt{2} + .02 + 38q + 100q^2[q^2e^{63} + qe^{31} + e^{25}]}.$$

That is,

$$\gamma_q \geq L + q^2 \frac{\frac{800}{\pi} - (e^{9.4}q + e^{36}q^2 + e^{59}q^3 + 6C_\rho q^{\frac{0.3537}{\log\log(1/q)}} + q^{0.01})}{\sqrt{2} + .02 + 38q + 100q^2[q^2e^{63} + qe^{31} + e^{25}]},$$

if $q < e^{-390}$. So, choosing $q = e^{-450}$, we get

$$\gamma_q \geq \log(1+\sqrt{2}) + e^{-900}\frac{250}{1.435} \geq \log(1+\sqrt{2}) + e^{-895}.$$

Corollary 1.3 then yields

$$\boxed{K_G \leq \frac{1}{c(f_{\sqrt{q}}, f_{\sqrt{q}})} \overset{(74)}{=} \frac{\pi}{2\gamma_q} \leq \frac{\pi}{2(\log(1+\sqrt{2}) + e^{-895})} \leq \frac{\pi}{2\log(1+\sqrt{2})} - e^{-895}.}$$

□

Proof of (11). Let $d = 3$. In this case, we have by Lemma 9.1

$$\begin{aligned} |A_q'(\xi_q) - \sqrt{2}| &\leq |A_q'(\xi_q) - \cosh(\xi_q)| + |\cosh(\xi_q) - \cosh(L)| \\ &\leq 12q + q^2[q^2e^{42} + qe^{29} + e^{15.5}](100) + .02. \end{aligned}$$

From Remark 6.2,

$$1 - A_q(L) = \frac{24}{\pi}q^2 + o(q^2),$$

with $o(q^2)$ term bounded by

$$13q^3 + e^{24}q^4 + e^{39}q^5 + 6C_\rho q^2 q^{\frac{0.3537}{\log\log(1/q)}} + q^{2.01}, \qquad \forall\, 0 < q < \min(e^{-81}, C_\rho^{-1/.29}).$$

Therefore

$$\gamma_q - L \overset{(75)}{=} \frac{\frac{24}{\pi}q^2 + o(q^2)}{\sqrt{2}+o(1)} \geq \frac{\frac{24}{\pi}q^2 - (13q^3 + e^{24}q^4 + e^{39}q^5 + 6C_\rho q^2 q^{\frac{0.3537}{\log\log(1/q)}} + q^{2.01})}{\sqrt{2} + .02 + 12q + 100q^2[q^2e^{42} + qe^{29} + e^{15.5}]}.$$

That is,

$$\gamma_q \geq L + q^2 \frac{\frac{24}{\pi} - (13q + e^{24}q^2 + e^{39}q^3 + 6C_\rho q^{\frac{0.3537}{\log\log(1/q)}} + q^{0.01})}{\sqrt{2} + .02 + 12q + 100q^2[q^2e^{42} + qe^{29} + e^{15.5}]}.$$

$q < e^{-81}$. So, choosing $q = e^{-250}$, we get

$$\gamma_q \geq \log(1+\sqrt{2}) + 2.768e^{-500}.$$

Corollary 1.3 then yields

$$\boxed{K_G \leq \frac{1}{c(f_{\sqrt{q}}, f_{-\sqrt{q}})} \overset{(74)}{=} \frac{\pi}{2\gamma_q} \leq \frac{\pi}{2(\log(1+\sqrt{2}) + 2.768e^{-500})} \leq \frac{\pi}{2\log(1+\sqrt{2})} - 3.56e^{-500}.}$$

□

9. Absolute Inverse Bound

Lemma 9.1 (Quantitative control of A_q')**.** *For any* $0 \leq t < \rho$*,*

$$|A_q'(t) - \cosh t| \leq qM_{d,1}(\rho) + q^2[q^2e^{63} + qe^{31} + e^{25}]\frac{\rho}{(\rho-t)^2}, \text{ if } d = 5$$

$$|A_q'(t) - \cosh t| \leq qM_{d,1}(\rho) + q^2[q^2e^{42} + qe^{29} + e^{15.5}]\frac{\rho}{(\rho-t)^2}, \text{ if } d = 3$$

Here

$$M_{3,1}(\rho) = \frac{7\cosh\rho + 3\cosh(3\rho)}{2\sqrt{\pi}}, \qquad M_{5,1}(\rho) = \frac{6\cosh\rho + 15\cosh(3\rho) + 5\cosh(5\rho)}{8\sqrt{\pi}}.$$

Proof. Define d_n, e_n as in (52) and Lemma 4.1. Then

$$a_n(q) = d_n(q) + e_n(q) = b_n + qc_n + e_n(q).$$

Since

$$\big||a_n(q)| - |b_n|\big| \leq |a_n(q) - b_n| \leq q|c_n| + |e_n(q)|,$$

where b_n is the coefficient of $\sin z$ and c_n is the coefficient of Ψ_d, we get

$$|A_q(t) - \sinh t| \leq q \sum_{\substack{n\geq 1\\ n \text{ odd}}} |c_n|t^n + \sum_{\substack{n\geq 1\\ n \text{ odd}}} |e_n(q)|t^n.$$

We similarly bound A_q' as follows.

$$|A_q'(t) - \cosh t| \leq q \sum_{\substack{n\geq 1\\ n \text{ odd}}} n|c_n|t^{n-1} + \sum_{\substack{n\geq 1\\ n \text{ odd}}} n|e_n(q)|t^{n-1}.$$

The first sum is bounded by $M_{d,1}(\rho)$, and the second satisfies

$$\sum_{n\geq 1} n|e_n(q)|t^{n-1} \leq C_\rho q^2 \sum_{n\geq 1} n\rho^{-n}t^{n-1} = C_\rho q^2 \frac{\rho}{(\rho-t)^2}$$

This proves the derivative bound, via (35), (36), (38) and Remark 4.3.

□

10. Numerical Bounds

This section records the numerical input used to make explicit estimates of C_R. The main results are (90) together with the numerically verified (91), (92), (93), (94). For any $z \in \mathbb{C}$, denote $\mathrm{erf}(z) := \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt$ as the line integral in $\mathbb{C}$. For any $0 < R \leq 1.1$, let

$$K_R := \{\sin z\colon\ |z| \leq R\} \subset S := \{z \in \mathbb{C}\colon |\Re(z)| < 1\}. \tag{76}$$

For any $w \in K_R$, write

$$T_w := \frac{1}{1-w^2}, \qquad \Phi_w(a,b) := T_w(a^2+b^2-2wab), \qquad \forall\, a,b \in \mathbb{R},$$

and define $p_z(u,v)$ as in (21). Let $G_z(a,b)$ be defined as in (29). For mixed derivatives,

$$\partial_a^r \partial_b^s G_w(a,b) = 4\partial_a^{r-1}\partial_b^{s-1} p_w(a,b), \qquad \forall\, r,s \geq 1.$$

Thus, for example,

$$\partial_a^3\partial_b G_w = 4(\Phi_a^2 - \Phi_{aa})p_w, \qquad \partial_a^2\partial_b^2 G_w = 4(\Phi_a\Phi_b - \Phi_{ab})p_w, \qquad \partial_a\partial_b^3 G_w = 4(\Phi_b^2 - \Phi_{bb})p_w.$$

The pure fourth derivatives are evaluated from the one-dimensional formula

$$\int_{\mathbb{R}} \mathrm{sgn}(v-b) p_w(a,v)\, dv = \frac{e^{-a^2}}{\sqrt{\pi}} \mathrm{erf}\left(\frac{wa-b}{\sqrt{1-w^2}}\right), \tag{77}$$

which implies

$$\partial_a G_w(a,b) = -\frac{2e^{-a^2}}{\sqrt{\pi}} \mathrm{erf}\left(\frac{wa-b}{\sqrt{1-w^2}}\right). \tag{78}$$

Put

$$s := 1-w^2, \qquad \lambda := \frac{w}{\sqrt{s}}, \qquad \tau_a := \frac{wa-b}{\sqrt{s}}, \qquad \tau_b := \frac{wb-a}{\sqrt{s}}.$$

Differentiating (78) three more times gives the explicit pure fourth derivative

$$\begin{aligned}\partial_a^4 G_w(a,b) = -\frac{2e^{-a^2}}{\sqrt{\pi}} \Bigg[&(12a - 8a^3)\,\mathrm{erf}(\tau_a) \\ &+ \frac{e^{-\tau_a^2}}{\sqrt{\pi}} \left(6\lambda(4a^2-2) + 24a\lambda^2\tau_a + 4\lambda^3(2\tau_a^2 - 1)\right)\Bigg].\end{aligned} \tag{79}$$

The formula for $\partial_b^4 G_w(a,b)$ is obtained from (79) by interchanging a and b, i.e. by replacing a, τ_a with b, τ_b. The mixed fourth derivatives have the simpler density forms

$$\begin{aligned}\partial_a^3\partial_b G_w(a,b) &= 4p_w(a,b)\left[\frac{4(a-wb)^2}{s^2} - \frac{2}{s}\right], \\ \partial_a^2\partial_b^2 G_w(a,b) &= 4p_w(a,b)\left[\frac{4(a-wb)(b-wa)}{s^2} + \frac{2w}{s}\right], \\ \partial_a\partial_b^3 G_w(a,b) &= 4p_w(a,b)\left[\frac{4(b-wa)^2}{s^2} - \frac{2}{s}\right].\end{aligned} \tag{80}$$

Equations (79) and (80) are the formulas used in the numerical supremum computations below.

We now record the precise fourth-order Taylor remainder that is used to bound the $O(q^2)$ term. Fix real numbers A, B, and define the one-variable function

$$\phi(t) = G_w(tA, tB), \qquad 0 \le t \le \sqrt{q}.$$

The integral Taylor formula gives, for complex-valued G_w,

$$\begin{aligned} G_w(\sqrt{q}A, \sqrt{q}B) = G_w(0,0) + \sqrt{q}\,\phi'(0) + \frac{q}{2}\phi''(0) + \frac{q^{3/2}}{6}\phi'''(0) \\ + \frac{q^2}{6}\int_0^1 (1-\theta)^3 \phi^{(4)}(\theta\sqrt{q})\, d\theta. \end{aligned} \tag{81}$$

Here

$$\begin{aligned} \phi^{(4)}(t) &= \mathcal{D}_{4,w}(tA, tB; A, B), \\ \mathcal{D}_{4,w}(a,b;A,B) &= A^4 G_{aaaa}(a,b) + 4A^3 B G_{aaab}(a,b) + 6A^2B^2 G_{aabb}(a,b) \\ &\quad + 4AB^3 G_{abbb}(a,b) + B^4 G_{bbbb}(a,b). \end{aligned} \tag{82}$$

Let $d \in \{3,5\}$, let $\sigma \in \{-1,1\}$, and set

$$A = h_d(u), \qquad B = \sigma h_d(v).$$

Write $\widetilde{H}_q^{(d,\sigma)}$ for the analogue of $\widetilde{H}_q$ obtained from these two perturbations, and write

$$Q_{d,\sigma}(w) = \frac{2(\sigma w^d - w)}{\sqrt{\pi}\sqrt{1-w^2}}. \tag{83}$$

Thus the symmetric construction is $(d,\sigma) = (5,1)$, while the asymmetric $h_3, -h_3$ construction is $(d,\sigma) = (3,-1)$. After multiplying (81) by $(\pi/2)p_w(u,v)$ and integrating in (u,v), the linear term vanishes and the cubic term vanishes by antisymmetry. The quadratic term is the already computed $qQ_{d,\sigma}(w)$. Therefore

$$\begin{aligned} \widetilde{H}_q^{(d,\sigma)}(w) \overset{(82)}{=} \arcsin w + qQ_{d,\sigma}(w) \\ + \frac{\pi q^2}{12}\int_0^1 (1-\theta)^3 \iint_{\mathbb{R}^2} \mathcal{D}_{4,w}\big(\theta\sqrt{q}A, \theta\sqrt{q}B; A, B\big) p_w(u,v)\, du\, dv\, d\theta. \end{aligned} \tag{84}$$

Consequently the desired fourth-order bound is

$$\left| \widetilde{H}_q^{(d,\sigma)}(w) - \arcsin w - qQ_{d,\sigma}(w) \right| \le \frac{\pi q^2}{48}\Lambda_{d,\sigma}(w), \tag{85}$$

where

$$\Lambda_{d,\sigma}(w) = \iint_{\mathbb{R}^2} \sup_{a,b\in\mathbb{R}} \left|\mathcal{D}_{4,w}\big(a,b; h_d(u), \sigma h_d(v)\big)\right| |p_w(u,v)|\, du\, dv. \tag{86}$$

We further bound $\Lambda_{d,\sigma}$ by derivative-by-derivative suprema. Define for any $w \in S$

$$\begin{aligned} m_{j,d}(w) &:= \sup_{a,b\in\mathbb{R}} \left|\partial_a^{4-j}\partial_b^j G_w(a,b)\right|, \qquad 0 \le j \le 4, \\ J_{j,d}(w) &:= \iint_{\mathbb{R}^2} |h_d(u)|^{4-j} |h_d(v)|^j |p_w(u,v)|\, du\, dv. \end{aligned} \tag{87}$$

Then for all $w \in S$

$$\Lambda_{d,\sigma}(w) \overset{(86)}{\le} \sum_{j=0}^{4} \binom{4}{j} m_{j,d}(w) J_{j,d}(w). \tag{88}$$

Further, set

$$\mathcal{J}_d(w) := \iint_{\mathbb{R}^2} (|h_d(u)| + |h_d(v)|)^4 |p_w(u,v)| \, du \, dv,$$

which gives

$$\Lambda_{d,\sigma}(w) \le M_{4,d}(w)\mathcal{J}_d(w), \tag{89}$$

where for any $w \in S$

$$M_{4,d}(w) := \sup_{a,b\in\mathbb{R}} \max_{r+s=4} \left|\partial_a^r \partial_b^s G_w(a,b)\right|,$$

The fourth-order Taylor formula (85) gives: for any $w \in S$

$$\boxed{\left|\widetilde{H}_q(w) - \arcsin w - qQ(w)\right| \overset{(85)\wedge(89)}{\le} q^2 \frac{\pi}{48} M_{4,d}(w)\mathcal{J}_d(w),} \tag{90}$$

where $\sigma := -1$ if $d = 3$, $\sigma := 1$ if $d = 5$, and

$$Q(w) = Q_d(w) := \frac{2(\sigma w^d - w)}{\sqrt{\pi}\sqrt{1-w^2}}.$$

Direct numerical maximization (available at Link 1) gives

$$\sup_{w\in K_{1.08}} \log\left(\frac{\pi}{48} M_{4,d}(w)\mathcal{J}_d(w)\right) < 23.58, \text{ if } d = 5 \tag{91}$$

$$\sup_{w\in K_{1.09}} \log\left(\frac{\pi}{48} M_{4,d}(w)\mathcal{J}_d(w)\right) < 24.58, \text{ if } d = 5 \tag{92}$$

$$\sup_{w\in K_{1.08}} \log\left(\frac{\pi}{48} M_{4,d}(w)\mathcal{J}_d(w)\right) < 14.5, \text{ if } d = 3 \tag{93}$$

$$\sup_{w\in K_{1.09}} \log\left(\frac{\pi}{48} M_{4,d}(w)\mathcal{J}_d(w)\right) < 15, \text{ if } d = 3 \tag{94}$$

11. Derivative Bounds

We shall also need the differentiated version of the error bound (90). Let $0 < R_- < R_+ < 1.1$, and define

$$\mathcal{E}_q(\zeta) = \widetilde{H}_q(\sin\zeta) - \zeta - qQ(\sin\zeta).$$

Assume that

$$\sup_{|\zeta|\le R_+} |\mathcal{E}_q(\zeta)| \le C_{R_+} q^2.$$

Since $\mathcal{E}_q$ is holomorphic on $|\zeta| < R_+$, Cauchy's estimate gives

$$\sup_{|\zeta|\le R_-} |\mathcal{E}_q'(\zeta)| \le \frac{C_{R_+}}{R_+ - R_-} q^2.$$

Equivalently,

$$\sup_{|\zeta|\le R_-} \left|(\widetilde{H}_q \circ \sin)'(\zeta) - 1 - q(Q\circ\sin)'(\zeta)\right| \le \frac{C_{R_+}}{R_+ - R_-} q^2.$$

If one wants the derivative in the original variable $w = \sin\zeta$, then

$$\mathcal{E}_q'(\zeta) = \left[\widetilde{H}_q'(w) - (\arcsin)'(w) - qQ'(w)\right]\cos\zeta.$$

Since

$$\min_{|\zeta|\le R_-} |\cos\zeta| = \cos R_-,$$

we therefore obtain the differentiated version of (90):

$$\boxed{\sup_{w\in K_{R_-}} \left|\widetilde{H}_q'(w) - (\arcsin)'(w) - qQ'(w)\right| \le \frac{C_{R_+}}{(R_+ - R_-)\cos R_-} q^2,} \tag{95}$$

12. Lower Lipschitz bound for arcsin

Lemma 12.1 (Explicit lower Lipschitz bound for arcsin). *Let $0 < r < s < 1.1$, define K_t as in (76). For any $w_0 \in K_r$ and $w \in K_s$ we have*

$$|H_0(w) - H_0(w_0)| \ge \frac{1}{\cosh s}|w - w_0|. \tag{96}$$

Inequality (96) also holds under the following assumptions. Let

$$a := \frac{r+s}{2}, \qquad \rho_{r,s} := \frac{s-r}{2}\cos a\,\frac{\sin a}{a}.$$

If $w_0 \in K_r$ and $|w - w_0| \le \rho_{r,s}$, then $w \in K_s$, so (96) holds.

Proof. Let $w_0 = \sin\zeta_0 \in K_r$ and $w = \sin\zeta \in \sin(s\mathbb{D})$. Then $H_0(w_0) = \zeta_0$ and $H_0(w) = \zeta$ and

$$\sin\zeta - \sin\zeta_0 = (\zeta - \zeta_0)\int_0^1 \cos\big((1-t)\zeta_0 + t\zeta\big)\,dt.$$

For any $\xi \in \mathbb{C}$ with $|\xi| \le s$,

$$|\cos\xi|^2 = \cos^2(\Re\xi) + \sinh^2(\Im\xi) \le 1 + \sinh^2 s = \cosh^2 s.$$

Hence

$$|w - w_0| \le \cosh s\,|\zeta - \zeta_0| = \cosh s\,|H_0(w) - H_0(w_0)|.$$

That is,

$$|H_0(w) - H_0(w_0)| \ge \frac{1}{\cosh s}|w - w_0|.$$

Therefore, (96) holds. Now, since $s < \pi/2$, the map sin is injective on $\overline{s\mathbb{D}}$. Indeed, if $\sin\zeta = \sin\xi$, then

$$2\cos\left(\frac{\zeta+\xi}{2}\right)\sin\left(\frac{\zeta-\xi}{2}\right) = 0.$$

But $|(\zeta+\xi)/2| \le s < \pi/2$, so the cosine factor cannot vanish, and $|(\zeta-\xi)/2| \le s < \pi/2$, so the sine factor vanishes only if $\zeta = \xi$.

We first lower-bound the distance from K_r to $\partial\sin(s\mathbb{D})$. Let

$$|\zeta_0| \le r, \qquad |\zeta_*| = s.$$

Then

$$\sin\zeta_* - \sin\zeta_0 = 2\cos\left(\frac{\zeta_*+\zeta_0}{2}\right)\sin\left(\frac{\zeta_*-\zeta_0}{2}\right).$$

Since

$$\left|\frac{\zeta_*+\zeta_0}{2}\right| \le a,$$

we have

$$\left|\cos\left(\frac{\zeta_* + \zeta_0}{2}\right)\right| \geq \cos a.$$

Also, if $|u| \leq a < \pi/2$, then

$$|\sin u| \geq \frac{\sin a}{a}|u|.$$

Indeed, writing $u = x + iy$, and using $\sin u = \sin x \cosh y + i \cos x \sinh y$, together with $\cosh^2 y = 1 + \sinh^2 y$, $\sin x/x$ is decreasing for $x > 0$ and $\sinh y \geq y$ for $y > 0$,

$$|\sin u|^2 = \sin^2 x + \sinh^2 y \geq \left(\frac{\sin a}{a}\right)^2 (x^2 + y^2).$$

Applying this to $u = (\zeta_* - \zeta_0)/2$, and using

$$|\zeta_* - \zeta_0| \geq s - r,$$

gives

$$|\sin \zeta_* - \sin \zeta_0| \geq (s - r) \cos a \, \frac{\sin a}{a}.$$

Thus every point within distance $\rho_{r,s}$ of K_r lies inside $\sin(s\mathbb{D})$.

□

13. Polynomial Bounds

In this section, we record some numerical bounds for the Q and Q' terms appearing in (90) and (95). Let $r := \frac{43}{40}$. All bounds in this section are on the disk $|z| \leq r$. Write $z = x + iy$. Since $r < \pi/2$, the disk $\{|z| \leq r\}$ contains no zero of $\cos z$. Hence the functions below are holomorphic on a neighborhood of $\{|z| \leq r\}$, and the maximum modulus principle reduces the estimates to the boundary $|z| = r$.

For $d = 3$, we use

$$\Psi_3(z) = \frac{2}{\sqrt{\pi}}\big(\sin z + \sin^3 z\big) = \frac{7 \sin z - \sin(3z)}{2\sqrt{\pi}},$$

and

$$Q_3(w) = -\frac{2(w + w^3)}{\sqrt{\pi}\sqrt{1 - w^2}}.$$

Since, on $|z| < \pi/2$, the chosen branch satisfies

$$\sqrt{1 - \sin^2 z} = \cos z,$$

we have

$$Q_3'(\sin z) = -\frac{2}{\sqrt{\pi}} \frac{1 + 3\sin^2 z - 2\sin^4 z}{\cos^3 z}.$$

Also

$$(\arcsin)''(\sin z) = \frac{\sin z}{\cos^3 z}.$$

For $d = 5$, we use

$$\Psi_5(z) = \frac{2}{\sqrt{\pi}}\big(\sin z - \sin^5 z\big) = \frac{6 \sin z + 5\sin(3z) - \sin(5z)}{8\sqrt{\pi}},$$

and

$$Q_5(w) = \frac{2(w^5 - w)}{\sqrt{\pi}\sqrt{1-w^2}}.$$

Thus

$$Q_5'(\sin z) = \frac{2}{\sqrt{\pi}} \frac{-1 + 5\sin^4 z - 4\sin^6 z}{\cos^3 z}.$$

We numerically verify (with details at Link 1) that

$$\sup_{|z|\le 1.075} |\Psi_3(z)| \le 2.22. \tag{97}$$

$$\sup_{|z|\le 1.075} |\Psi_5(z)| \le 4.1. \tag{98}$$

$$\sup_{|z|\le 1.075} |(\arcsin)''(\sin z)| \le 8.2. \tag{99}$$

$$\sup_{|z|\le 1.075} |Q_3'(\sin z)| \le 22.3. \tag{100}$$

$$\sup_{|z|\le 1.075} |Q_5'(\sin z)| \le 8.21. \tag{101}$$

14. Sixth Order Perturbation Bound

In this section, we record an explicit form of the error term of the expansion (63) both in the $d = 5$ and $d = 3$ cases, culminating in (107) and (108). Define

$$\varphi_d(\eta) := 4\pi \frac{H_\eta^{(d,\sigma)}(i)}{i}, \tag{102}$$

where $d = 5, \sigma = 1$ denotes the symmetric h_5, h_5 perturbation of the sign function and $d = 3, \sigma = -1$ denotes the asymmetric $h_3, -h_3$ perturbation. Thus

$$A := h_d(U), \qquad B := \sigma h_d(V),$$

with

$$h_3(x) := \frac{2x^3 - 3x}{\sqrt{3}\,\pi^{1/4}}, \qquad \text{and} \qquad h_5(x) := \frac{4x^5 - 20x^3 + 15x}{2\pi^{1/4}\sqrt{15}}.$$

At $z = i$, write, for all $a, b \in \mathbb{R}$,

$$p_i(a,b) \overset{(21)}{=} \frac{1}{\pi\sqrt{2}} \exp\left(-\frac{a^2+b^2}{2} + iab\right).$$

$$G_i(a,b) \overset{(29)}{=} \mathbb{E}\big[\operatorname{sign}(X-a)\operatorname{sign}(Y-b)\big],$$

where the expectation is with respect to the complex Gaussian density p_i. $\forall\ 0 \le j \le 6$, let

$$m_j := \sup_{a,b\in\mathbb{R}} \left|\partial_a^{6-j}\partial_b^j G_i(a,b)\right|.$$

As in Section 10, we can compute derivatives of G as follows: The mixed derivatives are computed from

$$\partial_a^m \partial_b^n G_i(a,b) = 4\,\partial_a^{m-1}\partial_b^{n-1} p_i(a,b), \qquad m, n \ge 1.$$

Thus, for $1 \le j \le 5$,

$$\partial_a^{6-j}\partial_b^j G_i(a,b) = 4\,\partial_a^{5-j}\partial_b^{j-1} p_i(a,b).$$

For the two pure derivatives we use

$$\partial_a G_i(a,b) = -\frac{2e^{-a^2}}{\sqrt{\pi}}\,\mathrm{erf}\left(\frac{ia-b}{\sqrt{2}}\right), \qquad \partial_b G_i(a,b) = -\frac{2e^{-b^2}}{\sqrt{\pi}}\,\mathrm{erf}\left(\frac{ib-a}{\sqrt{2}}\right).$$

Therefore

$$\partial_a^6 G_i(a,b) = \partial_a^5\left[-\frac{2e^{-a^2}}{\sqrt{\pi}}\,\mathrm{erf}\left(\frac{ia-b}{\sqrt{2}}\right)\right], \qquad \partial_b^6 G_i(a,b) = \partial_b^5\left[-\frac{2e^{-b^2}}{\sqrt{\pi}}\,\mathrm{erf}\left(\frac{ib-a}{\sqrt{2}}\right)\right].$$

A numerical maximization of these explicit functions (for details see Link 1) gives

j	numerical value of m_j	bound used
0	38.713601595 . . .	39
1	6.306143426 . . .	6.4
2	2.700948949 . . .	2.8
3	1.731970161 . . .	1.8
4	2.700948949 . . .	2.8
5	6.306143426 . . .	6.4
6	38.713601595 . . .	39.

Thus we shall use

$$(m_0, m_1, m_2, m_3, m_4, m_5, m_6) \le (39, 6.4, 2.8, 1.8, 2.8, 6.4, 39). \tag{103}$$

Next define the one-dimensional standard-normal moments

$$N_{d,k} := \mathbb{E}_{Z\sim N(0,1)}|h_d(Z)|^k.$$

The numerical values, rounded upward, are

k	0	1	2	3	4	5	6
$N_{3,k}$	1	0.962	6.207	112.21	3370	$1.466\cdot 10^5$	$8.575\cdot 10^6$
$N_{5,k}$	1	1.04	42.74	9680	$4.952\cdot 10^6$	$4.689\cdot 10^9$	$7.289\cdot 10^{12}$.

We now bound the sixth derivative of φ_d from (102). Since

$$H_\eta^{(d,\sigma)}(i) \overset{(3)}{=} \frac{\pi}{2}\iint_{\mathbb{R}^2} G_i(\eta A, \eta B)p_i(u,v)\,du\,dv,$$

we have

$$\varphi_d(\eta) \overset{(102)}{=} \frac{2\pi^2}{i}\iint_{\mathbb{R}^2} G_i(\eta A, \eta B)p_i(u,v)\,du\,dv.$$

Also, for all $u, v \in \mathbb{R}$

$$|p_i(u,v)| = \frac{1}{\pi\sqrt{2}}e^{-(u^2+v^2)/2} = \sqrt{2}\,\gamma(u)\gamma(v),$$

where γ is the standard normal density. Hence

$$\left|\varphi_d^{(6)}(\eta)\right| \le 2\pi^2\sum_{j=0}^{6}\binom{6}{j}m_j\iint_{\mathbb{R}^2}|h_d(u)|^{6-j}|h_d(v)|^j|p_i(u,v)|\,du\,dv$$
$$= 2\pi^2\sqrt{2}\sum_{j=0}^{6}\binom{6}{j}m_j N_{d,6-j}N_{d,j}.$$

Therefore

$$\sup_{\eta\in\mathbb{R}} \left|\varphi_d^{(6)}(\eta)\right| \le 2\pi^2\sqrt{2}\sum_{j=0}^{6}\binom{6}{j} m_j N_{d,6-j} N_{d,j}. \tag{104}$$

By Taylor's theorem with integral remainder,

$$\varphi_d(\eta) = \varphi_d(0) + \frac{\varphi_d^{(4)}(0)}{24}\eta^4 + \frac{\eta^6}{5!}\int_0^1 (1-t)^5 \varphi_d^{(6)}(t\eta)\,dt,$$

because the odd derivatives vanish and the second derivative vanishes for the admissible perturbations. Hence

$$\left|\varphi_d(\eta) - \varphi_d(0) - \frac{\varphi_d^{(4)}(0)}{24}\eta^4\right| \overset{(104)}{\le} C_d|\eta|^6, \tag{105}$$

where

$$C_d := \frac{\pi^2\sqrt{2}}{360}\sum_{j=0}^{6}\binom{6}{j} m_j N_{d,6-j} N_{d,j}.$$

Using the displayed numerical bounds (103) gives

$$C_3 < 2.7\cdot 10^7, \qquad C_5 < 2.3\cdot 10^{13}. \tag{106}$$

For the $d=5$ case, [BMMN13] compute

$$\frac{\varphi_5^{(4)}(0)}{24} = 1600\sqrt{2}.$$

Thus, for $|\eta| \le 10^{-2}$,

$$\boxed{\left|\varphi_5(\eta) - \varphi_5(0) - 1600\sqrt{2}\,\eta^4\right| \overset{(105)\wedge(106)}{\le} 2.3\cdot 10^{13}|\eta|^6.} \tag{107}$$

The same estimate in fact holds for all real η, since the bound above uses a global supremum over a, b. For the $d=3$ case corresponding to the $f_\eta, f_{-\eta}$ perturbation,

$$\frac{\varphi_3^{(4)}(0)}{24} = 48\sqrt{2}.$$

Therefore, for $|\eta| \le 10^{-2}$,

$$\boxed{\left|\varphi_3(\eta) - \varphi_3(0) - 48\sqrt{2}\,\eta^4\right| \overset{(105)\wedge(106)}{\le} 2.7\cdot 10^{7}|\eta|^6.} \tag{108}$$

15. Numerical optimization of the planar König functional

In this section, we provide more detail for Answer 1.8. That is, we provide numerical evidence that the planar optimizer of König's bilinear functional is not an alternating Krivine rounding scheme. König's bilinear functional is

$$B_K(f,g) := \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} f(x)g(y)e^{-(\|x\|_2^2+\|y\|_2^2)/2}\sin\langle x,y\rangle\,dx\,dy, \tag{109}$$

defined for measurable odd ±1-valued functions

$$f, g\colon \mathbb{R}^2 \to \{-1,1\}.$$

15.1. **Discretization and coordinate ascent.** Let $x, y \in \mathbb{R}^2$. Write $x = (r\cos\theta, r\sin\theta)$ and $y = (s\cos\phi, s\sin\phi)$ in polar coordinates. For the radial integrals we use the substitution

$$u = \frac{r^2}{2}, \qquad v = \frac{s^2}{2},$$

so that the Gaussian factor becomes $e^{-u}e^{-v}$ and the radial integration is naturally approximated by Gauss–Laguerre quadrature. For the angular variables we use the trapezoidal rule on a uniform grid. Thus f and g are represented by sign arrays on a polar grid with variables

$$(r_i, \theta_a), \qquad (s_j, \phi_b),$$

and the discretized integrated kernel is

$$K_{(i,a),(j,b)} = w_i w_j \,(\theta_a - \theta_{a-1})\,(\phi_b - \phi_{b-1})\, \sin\big(r_i s_j \cos(\theta_a - \phi_b)\big),$$

where w_i, w_j are the Gauss–Laguerre weights (including the Jacobian factors).

We then perform alternating best-response updates. For any $m \geq 0$, define

$$g^{(m+1)} := \mathrm{sign}(Tf^{(m)}), \qquad f^{(m+1)} := \mathrm{sign}(Tg^{(m+1)}),$$

where, as in [BMMN13, Section 3] we have

$$(Tf)(y) := \int_{\mathbb{R}^2} f(x) e^{-\|x\|_2^2/2} \sin\langle x, y\rangle \, dx.$$

Each update is optimal with the other function held fixed, so this is a coordinate-ascent procedure for the discretized B_K functional, as noted in [BMMN13].

15.2. **Best refined run.** Our best refined candidate used an optimization grid of size

$$160 \times 4096$$

in radial versus angular coordinates. The resulting non-hyperplane fixed point (f, g) resembles the tiger partition from [BMMN13] and satisfies the discrete fixed-point equations exactly on the grid:

$$f = \mathrm{sign}(Tg), \qquad g = \mathrm{sign}(Tf),$$

with zero sign mismatches. The optimized value was

$$B_K(f, g) \approx 11.094573248978.$$

For comparison, two sign functions in the plane have value

$$B_K(\mathrm{sign}(x_1), \mathrm{sign}(x_1)) \overset{(109)}{=} 4\pi \ \mathrm{arsinh}(1) \approx 11.075667144195.$$

Hence the numerical tiger candidate improves the hyperplane benchmark by ≈ 0.0189061047.

15.3. **Pictures of the optimized functions f and g.** Figure 1 shows the optimized function f, and Figure 2 shows the corresponding optimized function g.

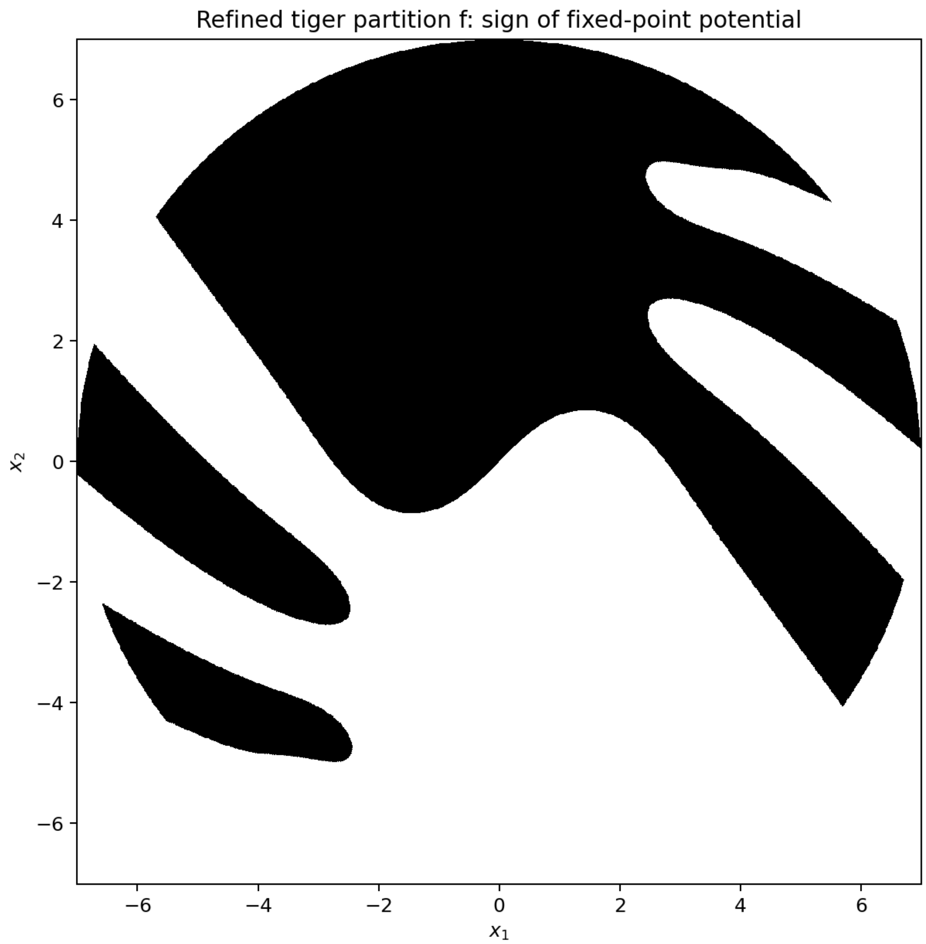

FIGURE 1. Refined numerical tiger partition f. The black region is $\{x : f(x) = 1\}$ and the white region is $\{x : f(x) = -1\}$.

15.4. **Coefficients of H and H^{-1}.** Let (f, g) denote the optimized pair from Figures 1 and 2. As in (3), (4) and (5), we examine the Taylor coefficients of $H_{f,g}(t)$ and its inverse.

Using a finer coefficient grid of size 320×16384, we obtained the following coefficients:

degree	coefficient of $H_{f,g}$	coefficient of $H_{f,g}^{-1}$
1	0.6271552605725179	1.594501494075198
3	0.09456848251227919	−0.6112883827335565
5	0.04449372752246313	**−0.028166647067356606**
7	0.025141713405143495	0.11401753102956447
9	0.017053623803116084	−0.12414815588752107
11	0.012245521324230563	0.13002877790599687
13	0.00923026485410719	−0.05335404389331977

Thus (3) has the approximation for any t near 0 as

$$H_{f,g}(t) \approx 0.6271552606\,t + 0.0945684825\,t^3 + 0.0444937275\,t^5 + 0.0251417134\,t^7 + 0.0170536238\,t^9 + \cdots$$

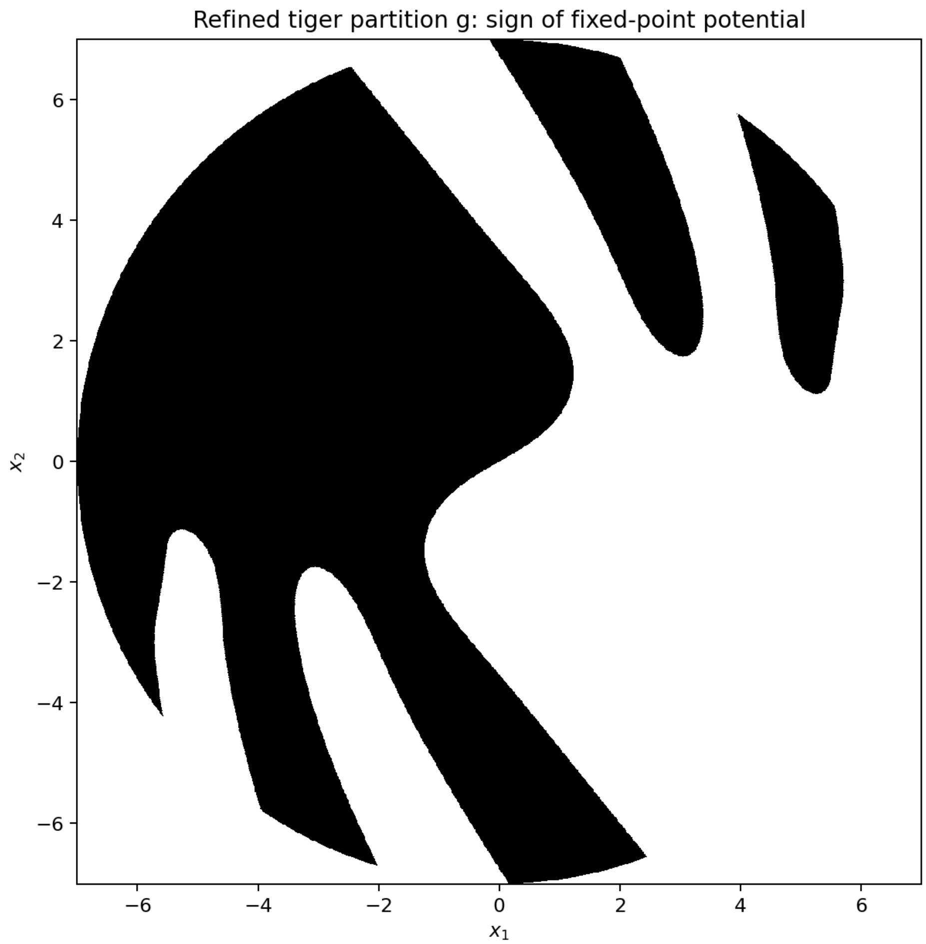

FIGURE 2. Refined numerical tiger partition g. The black region is $\{x : g(x) = 1\}$ and the white region is $\{x : g(x) = -1\}$.

and (4) has the approximation for any t near 0 as

$$H_{f,g}^{-1}(z) \approx 1.5945014941\, z - 0.6112883827\, z^3 - \mathbf{0.0281666471}\, z^5 \\ + 0.1140175310\, z^7 - 0.1241481559\, z^9 + \cdots .$$

In particular, the coefficient of z^5 in $H_{f,g}^{-1}$ is negative:

$$\widehat{a}_5 \approx -0.0281666471.$$

Since an alternating Krivine scheme would require

$$\operatorname{sign}(\widehat{a}_{2j+1}) = (-1)^j,$$

the sign of $\widehat{a}_5$ violates the definition of alternating Krivine rounding scheme. That is, it appears that the answer to Question 1.7 is: No.

15.5. **More detail on the fifth coefficient.** Denote the coefficients of $H_{f,g}$ as

$$H_{f,g}(t) := \widehat{\beta}_1 t + \widehat{\beta}_3 t^3 + \widehat{\beta}_5 t^5 + \cdots .$$

Then series reversion gives

$$a_5 = \frac{3\widehat{\beta}_3^2 - \widehat{\beta}_1\widehat{\beta}_5}{\beta_1^7}.$$

Using the numerical values above,

$$3\widehat{\beta}_3^2 - \widehat{\beta}_1\widehat{\beta}_5 \approx -0.00107488162417 < 0,$$

hence

$$\widehat{a}_5 < 0.$$

16. Explicit Degree 3 Hermite Perturbation

In this section we give a rigorous computer-assisted proof using Sage that

$$K_G < \frac{\pi}{2\log(1+\sqrt{2})} - 10^{-5}, \tag{110}$$

using interval arithmetic. That is, we prove Theorem 1.9. Define

$$\eta := 0.04249900400783211,$$

and define $f, g\colon \mathbb{R}^2 \to \{-1,1\}$ by

$$f(x_1,x_2) = \mathrm{sign}(x_2 - \eta h_3(x_1)), \qquad g(x_1,x_2) = \mathrm{sign}(x_2 + \eta h_3(x_1)), \qquad \forall\,(x_1,x_2) \in \mathbb{R}^2. \tag{111}$$

Let $H_{f,g}$ be defined by (3). As in (18) and (16), define

$$H_\eta(z) = \frac{\pi}{2} H_{f,g}(z), \qquad \forall\,|\Re(z)| < 1.$$

As in (20) and (49), define

$$B(z) := H_\eta^{-1}(z) =: \sum_{n\ge 1} a_n z^n \tag{112}$$

$$A(t) := \sum_{n\ge 1} |a_n| t^n.$$

Recall from Section 8 and (74) that if $\gamma > 0$ satisfies $A(\gamma) = 1$, and if $A(L) < 1 < A(0.9)$, then γ lies in $(L, 0.9)$, and the corresponding Grothendieck bound is

$$K_G \le \frac{\pi}{2\gamma}. \tag{113}$$

16.1. Exact coefficient formula used in the certificate.

$\forall\, m \ge 0$, denote

$$h_m(x) := \frac{(-1)^m}{\sqrt{2^m m! \sqrt{\pi}}} e^{x^2}\left(\frac{d}{dx}\right)^m e^{-x^2}, \qquad \psi_m(x) := \pi^{1/4} h_m(x), \quad \forall\, x \in \mathbb{R}. \tag{114}$$

Then $(\psi_m)_{m\ge 0}$ is orthonormal in $L_2(\mu)$, where

$$d\mu(x) = \pi^{-1/2} e^{-x^2}\, dx. \tag{115}$$

Note that $\int_{\mathbb{R}} d\mu(x) = 1$. Also $(\Psi_{m,n})_{m,n\ge 0}$ is an orthonormal basis of $L_2(\mu \otimes \mu)$, where

$$\Psi_{m,n}(x_1,x_2) := \psi_m(x_1)\psi_n(x_2), \qquad \forall\, m,n \ge 0$$

For any $n \ge 0$, $w \in \mathbb{R}$, define

$$I_n(w) := \int_{\mathbb{R}} \mathrm{sign}(x-w)\psi_n(x)\, d\mu(x). \tag{116}$$

Then

$$I_0(w) = -\operatorname{erf}(w),$$

and integration by parts with (114) shows, for $n \geq 1$ and $w \in \mathbb{R}$,

$$I_n(w) = \sqrt{\frac{2}{\pi n}} e^{-w^2} \psi_{n-1}(w). \tag{117}$$

For the two sign functions f, g, define their Hermite coefficients by

$$\begin{aligned} \widehat{f}(m,n) &:= \int_{\mathbb{R}^2} f(x_1,x_2) \Psi_{m,n}(x_1,x_2)\, d\mu(x_1) d\mu(x_2) \\ &\overset{(111)}{=} \int_{\mathbb{R}^2} \operatorname{sign}(x_2 - \eta h_3(x_1)) \psi_m(x_1) \psi_n(x_2) d\mu(x_1) d\mu(x_2) \\ &\overset{(116)}{=} \int_{\mathbb{R}} \psi_m(x_1) I_n(\eta h_3(x_1)) d\mu(x_1), \qquad \forall\, m,n \geq 0, \end{aligned}$$

where (117) allows $\widehat{f}(m,n)$ to be written as a one-dimensional integral, which is a much simpler task to estimate on a computer than a two-dimensional integral. Similarly,

$$\widehat{g}(m,n) := \int_{\mathbb{R}^2} g(y_1,y_2) \Psi_{m,n}(y_1,y_2)\, d\mu(y_1) d\mu(y_2) = \int_{\mathbb{R}} \psi_m(x_1) I_n(-\eta h_3(x_1)) d\mu(x_1).$$

Thus, in $L_2(\mu \otimes \mu)$,

$$f = \sum_{m,n \geq 0} \widehat{f}(m,n) \Psi_{m,n}, \qquad g = \sum_{m,n \geq 0} \widehat{g}(m,n) \Psi_{m,n}. \tag{118}$$

Define

$$\beta_k := \frac{\pi}{2} \sum_{m=0}^{k} \widehat{f}(m,k-m) \widehat{g}(m,k-m). \tag{119}$$

Then the Taylor coefficients of H_η are

$$\begin{aligned} H_\eta(z) &\overset{(18)\wedge(16)\wedge(21)}{=} \frac{\pi}{2} \int_{\mathbb{R}^2 \times \mathbb{R}^2} f(x) g(y) p_z(x_1,y_1) p_z(x_2,y_2) dx dy \\ &\overset{(118)\wedge(23)\wedge(114)}{=} \frac{\pi}{2} \sum_{m,n \geq 0} \widehat{f}(m,n) \widehat{g}(m,n) z^{m+n} \overset{(119)}{=} \sum_{k \geq 1} \beta_k z^k, \end{aligned} \tag{120}$$

The inverse coefficients from (112) are computed by the finite recursion

$$a_1 = \frac{1}{\beta_1},$$

and for $n \geq 2$,

$$a_n = -\frac{1}{\beta_1} \sum_{k=2}^{n} \beta_k [z^n] \left(\sum_{j=1}^{n-1} a_j z^j \right)^k. \tag{121}$$

Indeed, for any $n \geq 2$,

$$0 = [z^n] H_\eta(H_\eta^{-1}(z)) \overset{(120)}{=} \sum_{k \geq 1} [z^n] \beta_k (H_\eta^{-1}(z))^k \overset{(112)}{=} \beta_1 a_n + \sum_{k=2}^{n} [z^n] \beta_k (H_\eta^{-1}(z))^k$$
$$\overset{(112)}{=} \beta_1 a_n + \sum_{k=2}^{n} [z^n] \beta_k \Big(\sum_{j=1}^{n-1} a_j z^j \Big)^k,$$

since the terms $j \geq n$ have no contribution to the $[z^n]$ coefficient in the sum where $k \geq 2$. Solving for a_n proves (121) which gives an algorithm for computing the coefficients of H_η^{-1} when given the coefficients β_k of H_η from (120).

16.2. **The inverse-tail/Rouché condition.** The Sage code gives rigorous enclosures for

$$\sum_{n=1}^{201} |a_n| L^n.$$

To pass from this finite sum to the full infinite sum

$$A(L) = \sum_{n \geq 1} |a_n| L^n, \tag{122}$$

one must also justify that $B = H_\eta^{-1}$ is analytic on a disk of radius strictly larger than L, and one needs a bound on B on that disk. The latter is supplied by a Rouché-type inverse-domain check. It is convenient to work in the ζ-coordinate and therefore define

$$\mathcal{H}_\eta(\zeta) := H_\eta(\sin \zeta), \qquad \forall\, \zeta \in \mathbb{C}. \tag{123}$$

As we will describe below, the Sage code will verify the following for some $0 < r < s < \pi/2$:

$$\sup_{|\zeta| = s} |\mathcal{H}_\eta(\zeta) - \zeta| < s - r. \tag{124}$$

In particular, we will use $s = 1.05$, $r = 1.05 - .08113$. The following lemma then uses (124) to prove a tail bound.

Lemma 16.1 (Rouché inverse-tail certificate)**.** *Let $0 < r < s < \pi/2$. Assume (124) holds. Then $B = H_\eta^{-1}$ is holomorphic on $|w| < r$. Moreover,*

$$\sup_{|w| \leq r} |B(w)| \leq \sinh s.$$

Consequently, for every $N \geq 1$,

$$\sum_{n > N} |a_n| L^n \leq \sinh(s) \frac{(L/r)^{N+1}}{1 - L/r}.$$

Proof. Fix $w \in \mathbb{C}$ with $|w| \leq r$. Suppose $|\zeta| = s$. By the triangle inequality

$$|\zeta - w| \geq s - r.$$

By (124),

$$|\mathcal{H}_\eta(\zeta) - \zeta| < s - r \leq |\zeta - w|.$$

Hence the function $\zeta \mapsto \mathcal{H}_\eta(\zeta) - w = H_\eta(\zeta) - \zeta + \zeta - w$ and the function $\zeta \mapsto \zeta - w$ have the same number of zeros in $|\zeta| < s$, namely one, by Rouché's theorem. Thus $\mathcal{H}_\eta^{-1}$ is holomorphic on $|w| < r$, with values in $|\zeta| < s$. Therefore

$$B(w) \overset{(112)\wedge(123)}{=} \sin(\mathcal{H}_\eta^{-1}(w))$$

is holomorphic on $|w| < r$, and

$$|B(w)| \leq \sup_{|\zeta| \leq s} |\sin \zeta| \leq \sinh s.$$

Cauchy's estimate gives $|a_n| \leq \sinh(s) r^{-n}$. Summing the geometric tail proves the claim. □

The numerical output quoted below will use

$$r = 1.05 - \delta, \qquad s = 1.05,$$

where $\delta := 0.08113$, so by Lemma 16.1 with $N = 201$, we get

$$\sum_{n>N} |a_n| L^n \leq \sinh(1.05) \frac{(L/(1.05 - \delta))^{202}}{1 - L/(1.05 - \delta)} \leq 7 \cdot 10^{-8}. \tag{125}$$

This tail is valid since the inequality

$$\sup_{|\zeta|=1.05} |\mathcal{H}_\eta(\zeta) - \zeta| < \delta$$

is verified by our Sage code `rouche_v9.sage`, which took about 54 hours to run. Since the tail bound (125) is small, it remains to accurately estimate the finite sum to index 201.

16.3. **Certifying $A(L) < 1$.** The successful Sage run of `groth_series_verify` gave the following rigorous ball enclosures for the finite part of the sum:

$$\sum_{n=1}^{201} |a_n| L^n \leq 0.99999268092473327272958431689612741992831340719675 09 + 4.27 \cdot 10^{-58},$$

with (a_n) computed via (121) and (119). Combining this estimate with (122) and (125) gives

$$A(L) \leq 0.999992680924733272729584 31 + 7 \cdot 10^{-8} \leq 0.999992750924734.$$

In particular,

$$A(L) < 1 - 7.249 \cdot 10^{-6}. \tag{126}$$

The same run also certified the derivative, using term-by-term differentiation

$$\sup_{L \leq t \leq 0.9} A'(t) \leq 1.4459221948078752122929593376044317888266688361343087 + 5.71 \cdot 10^{-58}.$$

In particular,

$$\sup_{L \leq t \leq 0.9} A'(t) < 1.446. \tag{127}$$

16.4. **Certifying $A(.9)$ and Sage integration compatibility.** Below we will apply the intermediate value theorem to the function A. We verified $A(L) < 1$, so it remains to check

$$A(0.9) > 1.$$

Since all terms in $A(t)$ are nonnegative, it is enough to use only the first two odd inverse coefficients:

$$A(0.9) \geq |a_1|(0.9) + |a_3|(0.9)^3.$$

The included file `arb_h3_A09_certificate_panel.sage` computes rigorous ball enclosures for a_1 and a_3, then proves

$$|a_1|(0.9) + |a_3|(0.9)^3 > 1.02.$$

This proves $A(0.9) > 1$.

The Sage code performs a rigorous interval-ball subdivision integral on $[-M, M]$: on each subinterval I, the integrand is evaluated on a real ball enclosing I, so the range of the integrand on I is enclosed, and multiplying by the interval width encloses the integral over I. The tails outside $[-M, M]$ are bounded by the Cauchy-Schwarz inequality as

$$\int_{|x|>M} |\psi_m(x) I_n(\pm\eta h_3(x))| \, d\mu(x) \leq \sqrt{\mu(|x| > M)},$$

(using also $|I_n(w)| \leq 1$ for all $w \in \mathbb{R}$ by Cauchy-Schwarz), and for any $M > 0$

$$\mu(|x| > M) \overset{(115)}{=} \operatorname{erfc}(M) \leq \frac{e^{-M^2}}{\sqrt{\pi} M}.$$

Thus the $A(0.9) > 1$ check is self-contained and does not rely on a Sage-provided integration method.

16.5. **Concluding the K_G Bound.**

Proof of Theorem 1.9. Since all above inequalities are certified by Sage, the inequalities

$$A(L) < 1 < A(0.9)$$

imply that there exists $\gamma \in (L, 0.9)$ with $A(\gamma) = 1$ by the Intermediate Value Theorem. Moreover, by the Mean Value Theorem,

$$1 - A(L) = A(\gamma) - A(L) \leq \left(\sup_{L \leq t \leq 0.9} A'(t) \right) (\gamma - L). \tag{128}$$

Using the certified values above from (126) and (127)

$$1 - A(L) \geq 7.249 \cdot 10^{-6}, \qquad \sup_{L \leq t \leq 0.9} A'(t) \leq 1.446.$$

Thus

$$\gamma - L \overset{(128)}{\geq} 5.013 \cdot 10^{-6}.$$

$$K_G \overset{(113)}{\leq} \frac{\pi}{2\gamma} \leq \frac{\pi}{2(L + 5.013 \cdot 10^{-6})}.$$

That is,

$$\boxed{K_G < \frac{\pi}{2\log(1+\sqrt{2})} - 1.013 \cdot 10^{-5}.}$$

□

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