MULTIPLICITY OF NONTRIVIAL ZEROS OF PRIMITIVE L-FUNCTIONS VIA HIGHER-LEVEL CORRELATIONS

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ABSTRACT. We give universal bounds on the fraction of nontrivial zeros having given multiplicity for L-functions attached to a cuspidal automorphic representation of $\mathrm{GL}_m/\mathbb{Q}$. For this, we apply the higher-level correlation asymptotic of Hejhal, Rudnick, and Sarnak in conjunction with semidefinite programming bounds.

1. INTRODUCTION

Let $m \geq 1$ and let π be an irreducible cuspidal automorphic representation of $\mathrm{GL}_m/\mathbb{Q}$. Let $L(s, \pi)$ be its attached L-function (see [23] for theoretical background). Such functions generalize the classical Dirichlet L-functions (the case $m = 1$). Let $\rho_j = 1/2 + i\gamma_j$, with $j \in \mathbb{Z}$, be an enumeration of the nontrivial zeros of $L(s, \pi)$ repeated according to multiplicity. The Generalized Riemann Hypothesis (GRH) for $L(s, \pi)$ states that all its nontrivial zeros are aligned in the line $\mathrm{Re}\, s = 1/2$; that is, $\gamma_j \in \mathbb{R}$ for all j. Assuming GRH, we can enumerate the ordinates of the zeros in a nondecreasing fashion

$$\ldots \leq \gamma_{-2} \leq \gamma_{-1} < 0 \leq \gamma_1 \leq \gamma_2 \leq \ldots$$

and we have

$$N(T) := \sum_{\substack{j \geq 1 \\ \gamma_j \leq T}} 1 \sim \frac{m}{2\pi} T \log T.$$

Hejhal [22] and later on Rudnick and Sarnak [29, 30] investigated the n-level correlation distribution of the zeros of $L(s, \pi)$ guided by the relationship with Gaussian ensemble models in random matrix theory, pointed out by the breakthrough work of Montgomery [26]. This area has a long history, and we recommend [30], and the references therein, for more information.

Let $a_\pi(n)$ be the coefficients such that

$$L(s, \pi) = \sum_{n \geq 1} \frac{a_\pi(n)}{n^s}.$$

The results of Rudnick and Sarnack hold under the hypotheses that GRH holds for $L(s, \pi)$ and that

$$\sum_p \frac{|a_\pi(p^k) \log p|^2}{p^k} < \infty$$

for all $k \geq 2$. This second condition holds whenever $m \leq 3$ [30, Proposition 2.4]. They then show that

$$(1) \qquad \frac{1}{N(T)} \sum_{\substack{j_1,\ldots,j_n \geq 1 \text{ distinct} \\ \gamma_{j_1},\ldots,\gamma_{j_n} \leq T}} f\left(\tfrac{m \log T}{2\pi}\gamma_{j_1},\ldots,\tfrac{m \log T}{2\pi}\gamma_{j_n}\right)$$

$$\to \int_{\mathbb{R}^n} f(x)W_n(x)\delta\left(\frac{x_1 + \ldots + x_n}{n}\right)dx_1 \cdots dx_n$$

as $T \to \infty$, where

$$W_n(x) = \det\left[\frac{\sin(\pi(x_i - x_j))}{\pi(x_i - x_j)}\right]_{i,j=1,\ldots,n}$$

is Dyson's limiting n-level correlation density for the Gaussian Unitary Ensemble (GUE) model, and f is any *admissible* test function satisfying

- $f \in C^\infty(\mathbb{R}^n)$, f is symmetric, and $f(x + t(1,\ldots,1)) = f(x)$ for $t \in \mathbb{R}$;
- $\overline{\text{supp}}(\widehat{f}) \subseteq \{x \in \mathbb{R}^n : |x_1| + \ldots + |x_n| < 2/m\}$ (in the distributional sense);
- $f(x) \to 0$ rapidly as $|x| \to \infty$ in the hyperplane $\sum_j x_j = 0$.

Let m_ρ denote the multiplicity of ρ, and define

$$N^*(T) := \sum_{\substack{j \geq 1 \\ \gamma_j \leq T}} m_{\rho_j}.$$

Montgomery's pair correlation approach has been used to obtain bounds of the form

$$(2) \qquad N^*(T) \leq (c + o(1))N(T),$$

where for $m = 1$ the current smallest known value for c assuming the Riemann hypothesis is 1.3208 [8, 9, 26, 27]. Let $Z_n(T)$ count the number of nontrivial zeros of $L(s,\pi)$ with multiplicity at most $n - 1$ up to height T:

$$Z_n(T) = \sum_{\substack{j \geq 1 \\ \gamma_j \leq T, \, m_{\rho_j} \leq n-1}} 1.$$

Then $Z_2(T) \geq 2N(T) - N^*(T)$, so (2) can for instance be used to give a lower bound on the fraction of simple zeros, although the current best known bound is obtained using different techniques [5, 8, 9, 13, 19].

The goal of this paper is to use the n-level correlations by Hejhal, Rudnick, and Sarnak to obtain bounds analogous to (2), and use this to obtain universal bounds on the fraction of nontrivial zeros of $L(s,\pi)$ having multiplicity at most $n - 1$.

Theorem 1. *Let $L(s,\pi)$ be the L-function attached to an irreducible cuspidal automorphic representation π of $\mathrm{GL}_m/\mathbb{Q}$. Assuming GRH for $L(s,\pi)$ we have*

$$\liminf_{T\to\infty} \frac{Z_n(T)}{N(T)} \geq \begin{cases} 0.9614 & \text{if } n = 3 \text{ and } m = 1, \\ 0.2997 & \text{if } n = 3 \text{ and } m = 2, \\ 0.9787 & \text{if } n = 4 \text{ and } m = 1, \end{cases}$$

where the results for $(n,m) = (3,2),(4,1)$ hold under the additional assumption that certain series of rational functions are summed correctly using Maple; see Section 6.

As far as we know, the bounds in Theorem 1 are all new. Using a different method, it has been shown that at least 95.5% of the nontrivial zeros of the zeta function are simple or double zeros [12]. Our $(n, m) = (3, 1)$ case improves on this result. The case $m = 2$ is of special interest, since for this there are no previous effective bounds in the literature. For $(n, m) = (2, 2)$ we show in Section 3 our method does not produce a positive lower bound, but as shown above for $(n, m) = (3, 2)$ it does. Proving a positive proportion of zeros are simple in the case $(n, m) = (2, 2)$ is a notoriously difficult problem [17], and no positive lower bounds for $Z_2(T)/N(T)$ are known (in general), but there has been a great deal of interesting work on simple zeros for GL_2 L-functions (via Ω-results, for instance) [1–3, 7, 14, 25, 32].

Montgomery's approach to finding a good value for c in (2) leads to an optimization problem that is similar to the one-dimensional version of the Cohn-Elkies bound [11] for the sphere packing problem. Interestingly, however, the higher-order correlation approach in this paper is very different from the higher-order correlation approach for the sphere packing problem recently introduced in [10].

In Section 2 we set up the optimization problem to compute the above bounds, and we show how the optimal solution connects to reproducing kernels, inspired by the approach from [6]. In Section 3 we give a simpler analytical derivation of the known optimal solution for the case $n = 2$.

For larger values of n we use a computational approach to obtain rigorous bounds, whereas in Section 4 we use the symmetry and the rank-1 structure to find the bounds by solving linear systems. We then give two approaches for finding good solutions to the optimization problem. In Section 5 we use a parametrization using polynomials to find a good value for the case $(n, m) = (3, 1)$ and explain why this approach becomes problematic for $n > 3$. In Section 6 we give an alternative parametrization based on lattice shifts and use this to compute bounds for $(n, m) = (3, 2), (4, 1)$.

2. Derivation of the optimization problem

Let

$$M_n(T) = \sum_{\substack{j_1,\ldots,j_n \geq 1 \text{ distinct} \\ \gamma_{j_1} = \ldots = \gamma_{j_n} \leq T}} 1 = \sum_{\substack{j \geq 1 \\ \gamma_j \leq T}} (m_{\rho_j} - 1) \cdots (m_{\rho_j} - n + 1).$$

Then $M_1(T) = N(T)$ and $M_2(T) = N^*(T) - N(T)$. For a nonnegative admissible test function f, we have that

$$\frac{M_n(T)}{N(T)} f(1,\ldots,1) \leq \frac{1}{N(T)} \sum_{\substack{j_1,\ldots,j_n \geq 1 \text{ distinct} \\ \gamma_{j_1},\ldots,\gamma_{j_n} \leq T}} f\big(\tfrac{m \log T}{2\pi} \gamma_{j_1}, \ldots, \tfrac{m \log T}{2\pi} \gamma_{j_n}\big),$$

where we use that

$$f(1,\ldots,1) = f\big(\tfrac{m \log T}{2\pi} \gamma_{j_1}, \ldots, \tfrac{m \log T}{2\pi} \gamma_{j_n}\big)$$

whenever $\gamma_{j_1} = \ldots = \gamma_{j_n}$. Dividing by $f(1,\ldots,1)$ and applying (1) therefore gives

$$\limsup_{T \to \infty} \frac{M_n(T)}{N(T)} \leq c_{n,m},$$

where
$$c_{n,m} := \inf \frac{1}{f(1,\ldots,1)} \int_{\mathbb{R}^n} f(x)W_n(x)\delta\Big(\frac{x_1+\ldots+x_n}{n}\Big)\,dx$$
and where the infimum is taken over nonnegative admissible test functions f.

We have
$$\int_{\mathbb{R}^n} f(x)W_n(x)\delta\Big(\frac{x_1+\ldots+x_n}{n}\Big)\,dx$$
$$= \int_{\mathbb{R}^{n-1}} \int_{\mathbb{R}} f(x+(x_n,\ldots,x_n,0))W_n(x+(x_n,\ldots,x_n,0))$$
$$\cdot\, \delta\Big(\frac{x_1+\ldots+x_{n-1}}{n}+x_n\Big)\,dx_n dx_1\cdots dx_{n-1}$$
$$= \int_{\mathbb{R}^{n-1}} f(x_1,\ldots,x_{n-1},0)W_n(x_1,\ldots,x_{n-1},0)\,dx_1\cdots dx_{n-1}.$$

With $g(x_1,\ldots,x_{n-1}) = f(x_1,\ldots,x_{n-1},0)$, we see that $\overline{\operatorname{supp}}(\widehat{g})$ is now contained in the interior of $\frac{2}{m}H_{n-1}$, where
$$H_{n-1} = \{x \in \mathbb{R}^{n-1} : |x_1|+\ldots+|x_{n-1}|+|x_1+\ldots+x_{n-1}| \le 1\}.$$

Note that $H_{n-1} \subseteq [-1/2,1/2]^{n-1}$. Now let
$$\nu_n(g) := \int_{\mathbb{R}^{n-1}} g(x)W_n(x,0)\,dx$$

for any $g \in L^1(\mathbb{R}^{n-1})$ satisfying
  (i) $\overline{\operatorname{supp}}(\widehat{g}) \subseteq \frac{2}{m}H_{n-1}$;
  (ii) g is nonnegative;
  (iii) $g(0) = 1$.

It is now obvious that $c_{n,m} \ge \inf_g \nu_n(g)$, where the infimum is taken over functions g satisfying (i), (ii) and (iii). We show that $c_{n,m} = \inf_g \nu_n(g)$. Let $g \in L^1(\mathbb{R}^{n-1})$ satisfy the conditions above and assume further that g is invariant under the group G generated by
$$F_i g(x) = g(x-x_i(1,\ldots,1)-x_i e_i),$$

for $i = 1,\ldots,n-1$. Note that $F_i^2 = \operatorname{Id}$ and $F_i F_j F_i$ simply flips x_i by x_j. In particular, G is a finite group. Let $\varphi_\epsilon \in C^\infty(\mathbb{R}^{n-1})$ be a radial approximate identity as $\epsilon \to 0$, such that $\operatorname{supp}(\varphi_\epsilon) \subset \epsilon H_{n-1}$, $\int \varphi_\epsilon = 1$ and $\varphi_\epsilon \ge 0$. Let $g_\epsilon = g\widehat{\varphi_\epsilon}$, and observe that since $\widehat{g_\epsilon} = \widehat{g} * \varphi_\epsilon$, we then have that $g_\epsilon \in \mathcal{S}(\mathbb{R}^{n-1})$ and
$$\operatorname{supp}(\widehat{g_\epsilon}) \subset \Big(\frac{2}{m}+\epsilon\Big)H_{n-1}.$$

In particular, the function $f_\epsilon(x_1,\ldots,x_n) = g_\epsilon(a(x_1-x_n),\ldots,a(x_{n-1}-x_n))$, with $a = 1/(1+m\epsilon/2)$, is now an admissible test function for (1) and we obtain
$$c_{n,m} \le \int_{\mathbb{R}^n} f_\epsilon(x)W_n(x)\delta\Big(\frac{x_1+\ldots+x_n}{n}\Big)\,dx = \nu_n(g_\epsilon(a\cdot)) \le \nu_n(g(a\cdot)).$$

Taking $\epsilon \to 0$ we conclude that $c_{n,m} \le \inf_g \nu_n(g)$ over functions g satisfying (i), (ii), (iii) and invariant under G. Assume now g is not invariant under G. Since $W_n(x_1,\ldots,x_{n-1},0)$ is G-invariant, is it clear that $\nu_n(g) = \nu_n(\widetilde{g})$, where
$$\widetilde{g}(x) = \frac{1}{|G|}\sum_{\rho \in G} \rho g(x),$$

and so $\nu_n(g) \geq c_{n,m}$.

Let $\mathrm{PW}(\Omega)$ be the Paley-Wiener space of functions $g \in L^2(\mathbb{R}^{n-1})$ whose Fourier transform is supported in Ω. Given a finite-dimensional subspace F of $\mathrm{PW}(\frac{1}{m}H_{n-1})$ and a basis $\{g_i\}$ of F, we can optimize over functions of the form

$$(3) \qquad g(x) = \sum_{i,i'} X_{i,i'} g_i(x) g_{i'}(x),$$

where X is a positive semidefinite matrix. These are integrable functions satisfying conditions (i) and (ii). Since $\nu_n(g)$ and $g(0)$ are linear in the entries of X, this reduces the optimization problem to the semidefinite program

$$(4) \qquad \begin{aligned} \text{minimize} \quad & \nu_n(g) \\ \text{subject to} \quad & g(0) = 1, \\ & X \succeq 0. \end{aligned}$$

Here $X \succeq 0$ means X is a positive semidefinite matrix of appropriate size. Since we optimize a linear functional over positive semidefinite matrices with affine constraints, this is a semidefinite program, which can be solved efficiently in practice.

We have that

$$\sum_{\substack{j \geq 1 \\ \gamma_j \leq T,\, m_{\rho_j} \geq n}} 1 \leq \frac{M_n(T)}{(n-1)!},$$

and therefore

$$\frac{Z_n(T)}{N(T)} \geq 1 - \frac{M_n(T)}{N(T)(n-1)!}.$$

Thus,

$$\liminf_{T \to \infty} \frac{Z_n(T)}{N(T)} \geq 1 - \frac{c_{n,m}}{(n-1)!},$$

which shows we can use the problem in (4) to obtain a lower bound on the fraction of zeros having multiplicity at most $n-1$.

As an alternative to $M_n(T)$ we could also use the parameters

$$N_k(T) = \sum_{\substack{j \geq 1 \\ \gamma_j \leq T}} m_{\rho_j}^{k-1},$$

which satisfy $N(T) = N_1(T)$ and $N^*(T) = N_2(T)$. We have

$$(5) \qquad N_n(T) = \sum_{k=1}^{n} S(n,k) M_k(T),$$

where $S(n,k)$ are the Stirling numbers of the second kind. Since $S(n,k) \geq 0$ for all n and k, we can use our bounds on $c_{n,m}$, computed in Section 5 and 6, to obtain

$$(6) \qquad \limsup_{T \to \infty} \frac{N_n(T)}{N(T)} \leq \begin{cases} 2.0597 & \text{if } n = 3 \text{ and } m = 1, \\ 5.8984 & \text{if } n = 3 \text{ and } m = 2, \\ 3.8834 & \text{if } n = 4 \text{ and } m = 1, \end{cases}$$

provided the hypothesis of Theorem 1 holds. We also adapted the problem in (4) to bound $N_n(T)$ directly, but we were not able to improve over the results in (6) in this way.

We end this section with a possible formal solution to the problem of computing $c_{n,m}$. Note that the following result is true for H_{n-1} replaced by any compact set with a nonempty interior, with essentially the same proof.

Theorem 2. *For $n, m > 0$ there exists a kernel $K \colon \mathbb{C}^{n-1} \times \mathbb{C}^{n-1} \to \mathbb{C}$ such that*

$$(7) \qquad g(w) = \int_{\mathbb{R}^{n-1}} g(v) \overline{K(w,v)} \, d\nu_n(v)$$

for all $g \in \mathrm{PW}(\frac{1}{m} H_{n-1})$ and $w \in \mathbb{C}^{n-1}$. We have

$$c_{n,m} \leq \frac{1}{K(0,0)},$$

and equality is attained if every nonnegative $g \in L^1(\mathbb{R}^n)$ with $\mathrm{supp}\, \widehat{g} \subseteq \frac{2}{m} H_{n-1}$ is a sum of squares in the sense that there are $g_{j,N} \in \mathrm{PW}(\frac{1}{m} H_{n-1})$ such that

$$(8) \qquad g(x) = \lim_{N \to \infty} \sum_{j=1}^{N} |g_{j,N}(x)|^2,$$

with almost everywhere convergence.

Proof. We have that $0 \leq W_n(x) \leq 1$ for all x, and $W_n(x) = 0$ if and only if $x_i = x_j$ for some $i \neq j$. Using induction it can be shown that for every $\epsilon > 0$ there exists $c(\epsilon) > 0$ such that $W_n(x) \geq c(\epsilon)$ whenever $|x_i - x_j| \geq \epsilon$ for all $i \neq j$. Define

$$S_\epsilon = \{x \in \mathbb{R}^{n-1} : |x_i| > \epsilon \text{ and } |x_i - x_j| > \epsilon \text{ for all distinct } i, j = 1, \ldots, n-1\}.$$

Then $\nu_n(|g|^2) \leq \|g\|_2^2$ and

$$\nu_n(|g|^2) \geq c(\epsilon) \int_{S_\epsilon} |g(x)|^2 \, dx.$$

Observe that the set S_ϵ is relatively dense, that is, there is a cube Q (e.g., $Q = [-3\epsilon, 3\epsilon]^{n-1}$) and $\gamma > 0$ such that

$$\inf_{x \in \mathbb{R}^{b-1}} \mathrm{Vol}(S_\epsilon \cap (Q + x)) \geq \gamma \, \mathrm{Vol}(Q).$$

We could then apply the Logvinenko-Sereda Theorem [21, p. 112], which says there exists $b(\epsilon) > 0$ such that

$$\int_{S_\epsilon} |g(x)|^2 \, dx \geq b(\epsilon) \|g\|_2^2,$$

proving the norms $\nu_n(|g|^2)$ and $\|g\|_2^2$ are equivalent. For completeness, we give a direct proof of the above inequality in our particular case.

We apply the Hardy-Littlewood-Sobolev theorem of fractional integration (see, e.g., [33, Section V.1.2]), which implies that there exists a constant $C > 0$ such that

$$\| h(\cdot) | \cdot |^{-1/4} \|_2 \leq C \| \widehat{h} \|_{4/3}$$

for all $h \in L^2(\mathbb{R})$. If in addition $\overline{\mathrm{supp}}(\widehat{h}) \subseteq [-a, a]$, then using Hölder's inequality we obtain

$$\| h(\cdot) | \cdot |^{-1/4} \|_2 \leq C \| \widehat{h} \|_{4/3} \leq (2a)^{1/4} C \| \widehat{h} \|_2 = (2a)^{1/4} C \| h \|_2.$$

Then, with $h(x_i) = \widetilde{g}(x + x_j e_i)$ and $a = 1/2$, we get

$$\int_{\{x : |x_i - x_j| < \epsilon\}} |g(x)|^2 \, dx \leq \epsilon^{1/2} \int_{\{x : |x_i - x_j| < \epsilon\}} \left| \frac{g(x)}{|x_i - x_j|^{1/4}} \right|^2 dx \leq C \epsilon^{1/2} \|g\|_2^2.$$

A similar procedure shows that $\int_{\{x:|x_i|<\epsilon\}} |g(x)|^2\, dx \leq C\epsilon^{1/2}\|g\|_2^2$. Hence,

$$\int_{S_\epsilon} |g(x)|^2\, dx \geq \|g\|_2^2 - \sum_{i=1}^{n-1} \int_{\{x:|x_i|<\epsilon\}} |g(x)|^2\, dx - \sum_{1\leq i<j\leq n} \int_{\{x:|x_i-x_j|<\epsilon\}} |g(x)|^2\, dx$$

$$= \left(1 - \binom{n}{2}C\epsilon^{1/2}\right)\|g\|_2^2.$$

By choosing $\epsilon > 0$ small enough the constant $1 - \binom{n}{2}C\epsilon^{1/2}$ is positive, which shows ν_n defines a norm equivalent to the L^2 norm. Hence, $\mathrm{PW}(\frac{1}{m}H_{n-1})$ is a Hilbert space with the inner product given by ν_n.

Using Fourier inversion, Cauchy's inequality, and Plancherel's theorem it can be shown that the evaluation functions $f \mapsto f(x)$ on $\mathrm{PW}(\frac{1}{m}H_{n-1})$ are continuous in the L^2 topology, so by the Riesz representation theorem there exists a kernel $K\colon \mathbb{C}^{n-1} \times \mathbb{C}^{n-1} \to \mathbb{C}$ with $K(x,\cdot) \in L^2(\mathbb{C}^{n-1})$ satisfying (7).

To finish, observe that if g satisfies conditions (i), (ii), and (iii) and condition (8), then by the monotone convergence theorem, limit (8) holds also in the $L^1(\mathbb{R}^{n-1})$-sense, and since $\mathrm{PW}(\frac{1}{m}H_{n-1}) \cap L^1(\mathbb{R}^{n-1})$ is a reproducing kernel space, it is simple to show that we actually have uniform convergence in compact sets. Then,

$$1 = g(0) = \lim_{N\to\infty} \sum_{j=1}^{N} |g_{j,N}(0)|^2 = \lim_{N\to\infty} \sum_{j=1}^{N} |\nu_n(g_{j,N}(\cdot)K(0,\cdot))|^2$$

$$\leq \lim_{N\to\infty} \sum_{j=1}^{N} \nu_n(|g_{j,N}|^2)K(0,0) = \nu_n(g)K(0,0).$$

This shows $c_{n,m} \geq 1/K(0,0)$. Since $g(x) = K(0,x)^2/K(0,0)^2$ satisfies conditions (i), (ii), and (iii) and $\nu_n(g) = 1/K(0,0)$, we have $c_{n,m} \leq 1/K(0,0)$, which completes the proof. $\qquad\square$

It is worth mentioning that condition (8) holds true, and so equality $c_{n,m} = K(0,0)^{-1}$ is true, in the one-dimensional case (Hadamard factorization), which implies this condition is true in higher dimensions if H_{n-1} is replaced by a cube. Condition (8) also holds true for a ball (see [16]) and radial g, which is enough to show $c_{n,m} = K(0,0)^{-1}$. It is an open problem to prove condition (8) when H_{n-1} is replaced by a generic convex body. J. Vaaler, via personal communication, proposed an interesting way of obtaining (8). He conjectures the following: For any centrally symmetric convex body K there is a constant $c(K) \in (0,1)$ such that for any nonnegative $g \in \mathrm{PW}(K) \cap L^1$ there is $h \in \mathrm{PW}(K)$ such that

$$g \geq |h|^2 \quad \text{and} \quad \|h\|_2^2 \geq c(K)\|g\|_1.$$

If this conjecture is true, iterating this procedure one finds functions $h_1, h_2, \ldots$ such that $g \geq |h_1|^2 + \ldots + |h_N|^2$ and

$$\|h_N\|_2^2 \geq c(K)(\|g\|_1 - \|h_1\|_2^2 - \ldots - \|h_{N-1}\|_2^2).$$

Then it is easy to see that we must have $g = \sum_{n\geq 1} |h_n|^2$ pointwise.

3. Analytic solution for $n = 2$

In this section, we compute the kernel K of Theorem 2 for $n = 2$ and all $m \geq 1$. We note that this kernel was already computed in [6] but only for $m = 1$, and it relied heavily on the theory of de Branges spaces and Fourier transform techniques.

In what follows, we present a direct and simple approach that avoids any such things. Moreover, if one wants to compute only $K(0,0)$, then the argument is really short.

We want to compute the reproducing kernel $K(w, z)$ such that

$$f(w) = \int_{\mathbb{R}} f(x)\overline{K(w,x)}(1 - s(x)^2)\, dx$$

for every $w \in \mathbb{C}$ and $f \in \mathrm{PW}([-\frac{1}{2m}, \frac{1}{2m}])$, where $s(x) = \frac{\sin(\pi x)}{\pi x}$. Letting $k(w, z) = mK(mw, mz)$ we obtain

$$f(w) = \int_{\mathbb{R}} f(x)\overline{k(w,x)}(1 - s(mx)^2)\, dx =: \langle f | k(w, \cdot) \rangle$$

for every $w \in \mathbb{C}$ and $f \in \mathrm{PW}([-\frac{1}{2}, \frac{1}{2}])$. In what follows we use the trigonometric identity $2\sin^2(\theta) = 1 - \cos(2\theta)$. Observe that if $g \in \mathrm{PW}([-1, 1])$ is even then

$$\int_{\mathbb{R}} g(x)s(mx)^2 dx = \int_{\mathbb{R}} \frac{g(x) - g(0)}{2(\pi mx)^2}(1 - \cos(2\pi mx))dx + \frac{1}{m}g(0)$$

$$= \int_{\mathbb{R}} \frac{g(x) - g(0)}{2(\pi mx)^2}dx + \frac{1}{m}g(0).$$

Since $1 - s(x)^2$ is even, a simple computation shows $k(-w, z) = k(w, -z)$, and so $k(0, x)$ is even. Note also that any reproducing kernel satisfies $k(w, z) = \overline{k(z, w)} = k(\overline{z}, \overline{w})$. For simplicity we let

$$k_{\pm}(w, z) = \frac{1}{2}(k(w, z) \pm k(-w, z)) \quad \text{and} \quad s_{\pm}(w, z) = \frac{1}{2}(s(w - z) \pm s(w + z)).$$

For $x, y \in \mathbb{R}$ we obtain

$$s_+(x, y) = \langle s_+(x, \cdot) | k_+(y, \cdot) \rangle$$

$$= k_+(x, y) - \frac{1}{m}s(x)k(0, y) - \int_{\mathbb{R}} \frac{s_+(x, t)k_+(t, y) - s(x)k(0, y)}{2(\pi mt)^2}dt$$

$$= k_+(x, y) - \frac{1}{m}s_+(x, 0)k(0, y) - \int_{\mathbb{R}} s_+(x, t)\frac{k_+(t, y) - k(0, y)}{2(\pi mt)^2}dt$$

$$\quad - k(0, y)\int_{\mathbb{R}} \frac{s_+(x, t) - s(x)}{2(\pi mt)^2}dt$$

$$= k_+(x, y) - \frac{1}{m}s(x)k(0, y) - \frac{k_+(x, y) - k(0, y)}{2(\pi mx)^2}$$

$$\quad - k(0, y)\frac{1 - \pi x\sin(\pi x) - \cos(\pi x)}{2(\pi mx)^2}$$

$$= k_+(x, y)\left(1 - \frac{1}{2(\pi mx)^2}\right) + k(0, y)\left(-\frac{1}{m}s(x) + \frac{\pi x\sin(\pi x) + \cos(\pi x)}{2(\pi mx)^2}\right),$$

where we used the identity

$$\int_{\mathbb{R}} \frac{s_+(x, t) - s(x)}{2(\pi mt)^2}dt = \frac{1 - \pi x\sin(\pi x) - \cos(\pi x)}{2(\pi mx)^2}$$

which can be proven via the residue theorem. We now evaluate at $x = u_m$ with $u_m = (\pi m\sqrt{2})^{-1}$ to get

$$k(0, y) = \frac{s_+(u_m, y)}{-\sqrt{2}\sin(\pi u_m) + \pi u_m\sin(\pi u_m) + \cos(\pi u_m)}$$

which gives

$$K(0,0) = \frac{k(0,0)}{m} = \frac{1}{\frac{1}{\sqrt{2}}\cot(\frac{1}{\sqrt{2}m}) - \frac{2m-1}{2m}}.$$

We note that from this point on one can easily extract $k_+(x,y)$ by back substitution, if we let $a(x) = -s(x)/m + \frac{\pi x \sin(\pi x) + \cos(\pi x)}{2(\pi m x)^2}$ then

$$k_+(x,y) = \frac{s_+(x,y) - s_+(u_m,y)a(x)/a(u_m)}{1 - \frac{1}{2(\pi m x)^2}}.$$

For $k_-(x,y)$, one can do a similar trick to extract $\partial_t k(y,t)|_{t=0}$. We have

$$\begin{aligned}
s_-(x,y) &= k_-(x,y) - \int_{\mathbb{R}} \frac{s_-(x,t)k_-(y,t)}{2(\pi m t)^2}dt \\
&= k_-(x,y) - \frac{1}{x}\int_{\mathbb{R}} \frac{(s_+(x,t) - \cos(\pi x)s(t))k_-(y,t)/t}{2(\pi m)^2}dt \\
&= k_-(x,y)\left(1 - \frac{1}{2(\pi m x)^2}\right) + \frac{\cos(\pi x)}{2(\pi m)^2 x}\partial_t k(y,t)|_{t=0},
\end{aligned}$$

where we used that $s_-(x,t)/t = s_+(x,t) - \cos(\pi x)s(t)$, hence evaluation at $x = u_m$ gives

$$\partial_t k(y,t)|_{t=0} = \frac{s_-(u_m,y)}{u_m \cos(\pi u_m)}.$$

Letting $b(x) = \frac{\cos(\pi x)}{2(\pi m)^2 x}$ we get

$$k_-(x,y) = \frac{s_-(x,y) - s_-(u_m,y)b(x)/b(u_m)}{1 - \frac{1}{2(\pi m x)^2}}$$

and

$$K(x,y) = \frac{1}{m}(k_+(x/m,y/m) + k_-(x/m,y/m)).$$

4. SYMMETRY AND RANK-1 STRUCTURE

In this section, we show how we can use symmetry and a rank-1 structure to solve the problem in (4) efficiently.

Let G_n be the symmetry group of H_{n-1}; that is, let G_n be the group containing the matrices $A \in \mathbb{R}^{(n-1)\times(n-1)}$ with $AH_{n-1} = H_{n-1}$. Let

$$\Gamma_n = \{A^\mathsf{T} : A \in G_n\}.$$

If g is a function satisfying conditions (i), (ii), and (iii), then, for $\gamma \in \Gamma_n$, the function $L(\gamma)g$ defined by $L(\gamma)g(x) = g(\gamma^{-1}x)$ also satisfies these constraints and $\nu_n(g) = \nu_n(L(\gamma)g)$. It follows that the function $\overline{g}$ defined by

$$\overline{g}(x) = \frac{1}{|\Gamma_n|}\sum_{\gamma \in \Gamma_n} L(\gamma)g(x)$$

also satisfies these constraints and $\nu_n(\overline{g}) = \nu_n(g)$. Since $\overline{g}$ is Γ_n-invariant, this shows we may restrict to Γ_n-invariant functions.

Now assume F is some Γ_n-invariant space of functions $\mathbb{R}^{n-1} \to \mathbb{R}$. Consider a complete set $\widehat{\Gamma}_n$ of irreducible, unitary representations of Γ_n. Let $\{g_{\pi,i,j}\}$ be a symmetry adapted system of the space F. By this we mean that $\{g_{\pi,i,j}\}$ is a basis of F such that $H_{\pi,i} := \mathrm{span}\{g_{\pi,i,j} : j = 1,\ldots,d_\pi\}$ is a Γ_n-irreducible representation with $H_{\pi,i}$ equivalent to $H_{\pi',i'}$ if and only if $\pi = \pi'$, and for each π, i and i' there

exists a Γ_n-equivariant isomorphism $T_{\pi,i,i'} \colon H_{\pi,i} \to H_{\pi,i'}$ such that $g_{\pi,i',j} = Tg_{\pi,i,j}$ for all j. In other words, a symmetry adapted system is a basis of F according to a decomposition of F into Γ_n-irreducible subspaces, where the bases of equivalent irreducibles transform in the same way under the action of Γ_n.

Then, assuming the representations of Γ_n are of real type, we have the following block-diagonalization result: any function g that is a sum of squares of functions from F can be written as

$$g(x) = \sum_{\pi} \sum_{i,i'} X_{i,i'}^{(\pi)} \sum_{j} g_{\pi,i,j}(x) g_{\pi,i',j}(x),$$

for positive semidefinite matrices $X^{(\pi)}$. This follows from Schur's lemma as explained in [18] (see [15, Proposition 4.1] for a detailed proof).

To generate a concrete symmetry-adapted system $\{g_{\pi,i,j}\}$ for F we use an implementation of the projection algorithm as described in [31]. For this, first define the operators

$$(9) \qquad p_{j,j'}^{(\pi)} = \frac{d_\pi}{|\Gamma|} \sum_{\gamma \in \Gamma} \pi(\gamma^{-1})_{j,j'} L(\gamma),$$

where d_π is the dimension of π and $L(\gamma)$ is the operator $L(\gamma)g(x) = g(\gamma^{-1}x)$. Then choose bases $\{g_{\pi,i,1}\}_i$ of $\mathrm{Im}(p_{1,1}^{(\pi)})$ and set $g_{\pi,i,j} = p_{j,1}^{(\pi)} g_{\pi,i,1}$.

Lemma 3. *If π is not the trivial representation, then $g_{\pi,i,j}(0) = 0$.*

Proof. Let $p_{j,j'}^{(\pi)}$ be the operator as defined in (9) and $g \in F$. Then,

$$(p_{j,1}^{(\pi)} p_{1,1}^{(\pi)} g)(x) = \frac{d_\pi^2}{|\Gamma|^2} \sum_{\beta,\gamma \in \Gamma} \pi(\beta^{-1})_{j,1} \pi(\gamma^{-1})_{1,1} g(\beta^{-1}\gamma^{-1}x),$$

and thus

$$(p_{j,1}^{(\pi)} p_{1,1}^{(\pi)} g)(0) = \frac{d_\pi^2}{|\Gamma|^2} \left(\sum_{\beta \in \Gamma} \pi(\beta^{-1})_{j,1} \right) \left(\sum_{\gamma \in \Gamma} \pi(\gamma^{-1})_{1,1} \right) g(0).$$

If π is not the trivial representation, then $\sum_{\gamma \in \Gamma} \pi(\gamma^{-1})_{j,j'} = 0$ by orthogonality of matrix coefficients. By linearity, the result then follows. $\square$

This shows optimizing over functions of the form (3) is the same as optimizing over functions of the form

$$g(x) = \sum_{i,i'} X_{i,i'} g_{1,i,1}(x) g_{1,i',1}(x),$$

where X is positive semidefinite and where we denote the trivial representation by 1. That is, instead of using a Γ-invariant space of functions, we can use the much smaller space of Γ-invariant functions $g_i(x) = g_{1,i,1}(x)$. In other words, the problem in (4) reduces to the simpler semidefinite program

$$
\begin{aligned}
& \text{minimize} && \langle A, X \rangle \\
(10) \qquad & \text{subject to} && \langle bb^\mathsf{T}, X \rangle = 1, \\
& && X \succeq 0,
\end{aligned}
$$

where $A_{i,i'} = \nu_n(g_i g_{i'})$ and $b_i = g_i(0)$. Here we use the notation $\langle A, B \rangle = \mathrm{tr}(A^\mathsf{T} B)$.

A semidefinite program with m equality constraints has an optimal solution of rank r with $r(r+1)/2 \leq m$ [28]. Since the above semidefinite program has only one equality constraint, we know that there exists an optimal solution of rank 1. In fact, Lemma 4 shows we can find this rank 1 solution by solving a linear system. We can view this lemma as a finite-dimensional version of Theorem 2.

Lemma 4. *Let A be a positive semidefinite matrix and let x be a solution to the system $Ax = b$. Then $xx^{\mathsf{T}}/(x^{\mathsf{T}}b)^2$ is an optimal solution to the semidefinite program*

$$\text{minimize} \quad \langle A, X \rangle$$

$$\text{subject to} \quad \langle bb^{\mathsf{T}}, X \rangle = 1,$$
$$X \succeq 0.$$

Proof. Let X be feasible to the semidefinite program and consider the spectral decomposition $X = \sum_i v_i v_i^{\mathsf{T}}$. Using Cauchy-Schwarz we have

$$1 = b^{\mathsf{T}} X b = \sum_i (b^{\mathsf{T}} v_i)^2 = \sum_i (x^{\mathsf{T}} A v_i)^2 \leq \sum_i (x^{\mathsf{T}} A x)(v_i^{\mathsf{T}} A v_i) = x^{\mathsf{T}} b \langle A, X \rangle,$$

so

$$\langle A, X \rangle \geq \frac{1}{x^{\mathsf{T}} b} = \left\langle A, \frac{xx^{\mathsf{T}}}{(x^{\mathsf{T}} b)^2} \right\rangle. \qquad \square$$

5. Parametrization using polynomials

Here we consider the case $(n, m) = (3, 1)$. Let $\mathcal{X}_{H_2}(x)$ be the indicator function of the region H_2 and define the functions $g_\alpha(x)$ for $\alpha = (\alpha_1, \alpha_2) \in \mathbb{N}_0^2$ by

$$\widehat{g}_\alpha(x) = x_1^{\alpha_1} x_2^{\alpha_2} \mathcal{X}_{H_2}(x).$$

Fix a degree d and let $F = \text{span}\{g_\alpha : \alpha_1 + \alpha_2 \leq d\}$. As before, we let $\{g_i\}$ be a basis for the Γ_n-invariant functions in F, and we use the parametrization

$$g(x) = \sum_{i,i'} X_{i,i'} g_i(x) g_{i'}(x).$$

Since each function g_i is a linear combination of the functions in F we have that $\widehat{g}_i(x) = p_i(x) \mathcal{X}_{H_2}(x)$ for some polynomial p_i of degree at most d; and as explained in Section 4 these polynomials p_i can be computed explicitly.

To set up the linear system for solving (10) we need to compute explicitly how the linear functionals $g(0)$ and $\nu_3(g)$ depend on the entries of the matrix X.
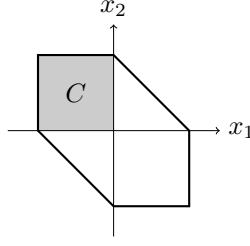
The region H_2 is the open hexagon with vertices $(1/2, 0)$, $(1/2, -1/2)$, $(0, -1/2)$, $(-1/2, 0)$, $(-1/2, 1/2)$, $(0, 1/2)$. Its symmetry group G_3 is the dihedral group of order 12 with generators

$$r = \begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix} \quad \text{and} \quad s = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

With $C = [-1/2, 0] \times [0, 1/2]$ we have $H_2 = C \cup r^2 C \cup r^4 C$; see Figure 1.

Since g_i is Γ_3-invariant, the polynomial $p_i(x)$ is G_3-invariant, so

$$g_i(0) = \int_{H_2} p_i(x) \, dx = \int_C \big(p_i(x) + p_i(r^2 x) + p_i(r^4 x) \big) \, dx = 3 \int_C p_i(x) \, dx$$

$$= 3 \int_0^{1/2} \int_{-1/2}^0 p_i(x_1, x_2) \, dx_1 dx_2,$$

FIGURE 1. The hexagon H_2 and the square C (shaded)

which can be computed explicitly. This shows how we can write

$$g(0) = \sum_{i,i'} X_{i,i'} g_i(0) g_{i'}(0)$$

explicitly as a linear combination of the entries of the matrix X.

As computed in Hejhal [22], we have

$$\nu_3(g) = \int_{\mathbb{R}^2} g(x_1, x_2) W_3(x_1, x_2, 0)\, dx_1 dx_2$$

$$= 2 + \widehat{g}(0) + 6 \int_0^1 \widehat{g}(x, 0)(x - 1)\, dx - 12 \int_0^1 \int_{-x_2}^0 \widehat{g}(x_1, x_2) x_2 \, dx_1 dx_2.$$

To compute this explicitly, note that

$$\widehat{g}(x) = \sum_{i,i'} X_{i,i'} (\widehat{g}_i * \widehat{g}_{i'})(x).$$

The term $\widehat{g}(0)$ can be computed similarly to how $g_i(0)$ is computed above, since

$$\widehat{g}(0) = \sum_{i,i'} X_{i,i'} \int_{H_2} p_i(x) p_{i'}(x)\, dx,$$

where we used that $p_{i'}(-x) = p_{i'}(x)$.

Since $\widehat{g}_i$ and $\widehat{g}_{i'}$ have bounded support, the convolution $(\widehat{g}_i * \widehat{g}_{i'})(x)$ is an integral over a bounded region whose shape depends on x. For the third term, symmetry gives

$$\int_0^1 \widehat{g}(x, 0)(x - 1)\, dx = \int_0^1 \widehat{g}(x, -x)(x - 1)\, dx.$$

Figure 2 shows the shape of the integration region used to compute $\widehat{g}(x, -x)$ for different values of x. This gives

$$\int_0^1 \widehat{g}(x, -x)(x-1)\, dx = \sum_{i,i} X_{i,i'} \int_0^1 \mathcal{J}_x\, p_i(u_1, u_2) p_{i'}(u_1+x, u_2-x)(x-1)\, du_1 du_2 dx,$$

where

$$\mathcal{J}_x = \begin{cases} \int_{-\frac{1}{2}+x}^0 \int_{-\frac{1}{2}-u_2}^{\frac{1}{2}-x} + \int_0^x \int_{-\frac{1}{2}}^{\frac{1}{2}-x} + \int_x^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}-u_2} & 0 \leq x \leq \frac{1}{2}, \\ \int_{x-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}-x} & \frac{1}{2} \leq x \leq 1. \end{cases}$$

Similarly, we split the convolution integral for the fourth term into the 4 regions $R_1 = \{-1 \leq -x_2 \leq x_1 \leq -\frac{1}{2}\}$, $R_2 = \{-\frac{1}{2} \leq \frac{1}{2} - x_2 \leq x_1 \leq 0\}$, $R_3 = \{0 \leq -2x_1 \leq$
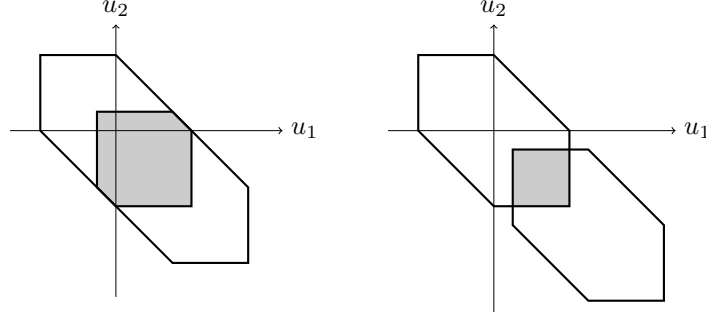
FIGURE 2. The possible shapes of the intersection of the supports of $g_i(u_1, u_2)$ and $g_{i'}(u_1 + x, u_2 - x)$ for $0 \leq x \leq 1/2$ (left) and $1/2 \leq x \leq 1$ (right)

TABLE 1. Upper bounds on the best possible value for $c_{3,1}$ obtained using a parametrization using polynomials of degree d

d	$c_{3,1}$
10	0.077516654
20	0.077222625
30	0.077206761
40	0.077200000
50	0.077198398
60	0.077197284

$x_2 \leq \frac{1}{2} - x_1 \leq 1\}$ and $R_4 = \{0 \leq -x_1 \leq x_2 \leq -2x_1 \leq 1\}$. Then the fourth term can be computed as

$$\int_0^1 \int_{-x_2}^0 \widehat{g}(x_1, x_2) x_2 \, dx_1 dx_2 = \sum_{i,i'} X_{i,i'} \int_0^1 \int_{-x_2}^0 \mathcal{I}_x \, p_i(u) p_{i'}(u - x) x_2 \, du_1 du_2 dx_1 dx_2,$$

where

$$\mathcal{I}_x = \begin{cases} \int_{x_2 - \frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{x_1 + \frac{1}{2}} & (x_1, x_2) \in R_1, \\ \int_{x_2 - \frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2} - u_2 + x_1 + x_2}^{\frac{1}{2} - u_2} & (x_1, x_2) \in R_2, \\ \int_{x_1 + x_2}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2} - u_2} + \int_{-x_1}^{x_1 + x_2} \int_{x_1 + x_2 - u_2 - \frac{1}{2}}^{\frac{1}{2} - u_2} + \int_{x_2 - \frac{1}{2}}^{-x_1} \int_{x_1 + x_2 - u_2 - \frac{1}{2}}^{x_1 + \frac{1}{2}} & (x_1, x_2) \in R_3, \\ \int_{-x_1}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2} - u_2} + \int_{x_1 + x_2}^{-x_1} \int_{-\frac{1}{2}}^{x_1 + \frac{1}{2}} + \int_{x_2 - \frac{1}{2}}^{x_1 + x_2} \int_{x_1 + x_2 - u_2 - \frac{1}{2}}^{x_1 + \frac{1}{2}} & (x_1, x_2) \in R_4. \end{cases}$$

In Table 1 we show the bounds on $c_{3,1}$ obtained with this parametrization for degree d. This proves the $(n, m) = (3, 1)$ case of Theorem 1. As ancillary files to the arXiv version of this paper we give the GAP source code to compute the polynomials p_i in exact arithmetic and a Julia file to compute the above bound rigorously by solving the linear system from Section 4 in ball arithmetic.

6. Parametrization using shifts

Now we consider the functions g_λ obtained by shifting the Fourier transform of the indicator function of $\frac{1}{m}H_{n-1}$ by $\lambda \in m\mathbb{Z}^{n-1}$:

$$g_\lambda(x) = \widehat{\chi_{\frac{1}{m}H_{n-1}}}(x - \lambda) = \frac{1}{m^{n-1}}\widehat{\chi_{H_{n-1}}}\left(\frac{1}{m}(x - \lambda)\right).$$

Then $g_\lambda(x)$ is the Fourier transform of $\chi_{\frac{1}{m}H_{n-1}}(\cdot)e^{-2\pi i\langle\lambda,\cdot\rangle}$, so $g_\lambda(\gamma x) = g_{\gamma^{-1}\lambda}(x)$ for all γ in the group Γ_n as defined in Section 4.

We observe that for $n = 2$, the functions g_λ for $\lambda \in \Lambda = m\mathbb{Z}^{n-1}$ form an orthogonal basis of $\mathrm{PW}(\frac{1}{m}H_{n-1})$ with respect to the Lebesgue L^2-norm. This, however, is not true for $n \geq 3$. For $n = 3$, a classical result of Venkov [34] shows that it is an orthogonal basis if we take Λ as the dual lattice of

$$\{(u/2 + v, u/2 - v/2) : u, v \in \frac{1}{m}\mathbb{Z}\}.$$

For $n \geq 4$, a recent result [20, 24] implies that no set of translations Λ exists for which $\{g_\lambda\}_{\lambda\in\Lambda}$ is an orthogonal basis of $\mathrm{PW}(\frac{1}{m}H_{n-1})$, otherwise H_{n-1} would need to be centrally symmetric, have only centrally symmetric faces and tile the space by translations, but none of these properties hold. In any case, in practice, using $\Lambda = m\mathbb{Z}^{n-1}$ works reasonably well since $\{g_\lambda\}_{\lambda\in\Lambda}$ is an orthogonal basis of $\mathrm{PW}(\frac{1}{m}[-1/2, 1/2]^{n-1})$ which contains $\mathrm{PW}(\frac{1}{m}H_{n-1})$.

Let F be a finite-dimensional, Γ_n-invariant subspace of $\mathrm{span}\{g_\lambda : \lambda \in m\mathbb{Z}^{n-1}\}$, and again use the parametrization

$$g(x) = \sum_{i,i'} X_{i,i'}g_i(x)g_{i'}(x),$$

where $\{g_i\}$ is a basis for the Γ_n-invariant functions in F.

To set up the linear system from Section 4 we need to compute the matrix $A_{i,i'} = \nu_n(g_ig_{i'})$ and the vector $b_i = g_i(0)$. By Lemma 4 the optimal function then is given by

$$g(x) = \frac{(\sum_i c_ig_i(x))^2}{(c^\mathsf{T}b)^2}$$

with c a solution to $Ac = b$.

In Appendix A we calculate the Fourier transform of $\chi_{H_{n-1}}(x)$ for general n. This function has removable singularities whenever $x_i = 0$ for some i or $x_i = x_j$ for some $i \neq j$. The function g_i is a linear combination of shifts of the Fourier transform, and thus can also have removable singularities. To compute $g_i(0)$ we consider each term individually, check whether the denominator evaluates to zero and if it does, we use repeated applications of L'Hôpital's rule.

To compute the entries $A_{i,i'} = \nu_n(g_ig_{i'})$, we need to compute integrals of the form $\int_{\mathbb{R}^{n-1}} f(x)\,dx$, where $f(x) = g_i(x)g_{i'}(x)W_n(x, 0)$. To simplify the computations we change variables to $m^{-1}x$. Since the Fourier transform of $g_i(mx)$ is supported in $[-1/2, 1/2]^{n-1}$ and the Fourier transform of $W_n(mx, 0)$ is supported in $[-m, m]^{n-1}$, the Fourier transform of f is supported in $[-(m + 1), (m + 1)]^{n-1}$. By Poisson summation, we then have

$$\int_{\mathbb{R}^{n-1}} f(x)\,dx = \widehat{f}(0) = \sum_{k\in(m+1)\mathbb{Z}^{n-1}}\widehat{f}(k) = \frac{1}{(m+1)^{n-1}}\sum_{k\in\frac{1}{m+1}\mathbb{Z}^{n-1}}f(k).$$

By again using Poisson summation, we have

$$\sum_{k \in \frac{1}{m+1}\mathbb{Z}^{n-1}} f(k) = (m+1)^{n-1}\widehat{f}(0)$$

$$= (m+1)^{n-1} \sum_{k \in (m+1)\mathbb{Z}^{n-1}} \widehat{f}(k) e^{2\pi i \langle k, s \rangle}$$

$$= \sum_{k \in \frac{1}{(m+1)}\mathbb{Z}^{n-1}} f(k+s)$$

for any $s \in \mathbb{R}^{n-1}$. To avoid evaluation of f on a removable singularity, we set

$$s = \left(\frac{1}{m(m+1)n}, \frac{2}{m(m+1)n}, \dots, \frac{n-1}{m(m+1)n} \right),$$

and compute the integral as

$$\int_{\mathbb{R}^{n-1}} f(x)\, dx = \frac{1}{(m+1)^{n-1}} \sum_{k \in \frac{1}{(m+1)}\mathbb{Z}^{n-1}} f(k+s).$$

Because of the sines and cosines in the formula of $\widehat{\chi}_{H_{n-1}}$ (see Appendix A), each series $\sum_k f(k+s)$ can be split into $(2(m+1))^{n-1}$ series of rational functions over the lattice $\mathbb{Z}^{n-1}$, one for each value appearing for the sines and cosines.

Computing these series exactly is the computational bottleneck in our approach. Maple is the only system among the computer algebra systems we tried in which we could successfully compute the sums of all the series, and for this we needed several ad hoc tricks. For instance, for series over $\mathbb{Z}^3$, we first compute the outer series over $\mathbb{Z}$, and then use partial fraction decomposition to simplify the terms before summing over $\mathbb{Z}^2$. Here a complicating factor was that after partial fraction decomposition the series of some terms no longer converge, which meant we needed to recombine certain terms in ad hoc ways before summing over $\mathbb{Z}^2$.

Unfortunately, Maple 2022.2 contains a bug where it acts nondeterministically and sometimes gives a completely wrong answer. We, therefore, check that the sum computed with Maple deviates at most 0.1% from the sum we obtain by truncating the series to the box $[-C/(m+1), C/(m+1)]^{n-1}$, where for $n = 3$ we use $C = 400$ (or $C = 1300$ for the cases where this is not sufficient) and for $n = 4$ we use $C = 25$. We give text files containing the series in Maple syntax and for each series an interval containing the correct sum given by decimal expressions of a midpoint and a radius. We also give a Julia file with the code to obtain the rigorous bounds using the data in these text files.

For $(n, m) = (3, 1)$ and $(n, m) = (3, 2)$, Table 2 gives the results for the subspaces $F = \text{span}\{g_\lambda : \lambda \in S_d\}$, where

$$S_d = \Gamma_n\{m\lambda \in \mathbb{Z}^{n-1} : \|\lambda\|_1 \le d\}.$$

This proves the case $(3, 2)$ of Theorem 1 (the case $(3, 1)$ was already done in Section 5). For $(n, m) = (4, 1)$, we only compute the series exactly for $\lambda = 0$ (partly because of the aforementioned Maple bug), which gives $c_{4,1} \le 447/3500 \approx 0.1277$ as used in Theorem 1. Numerically we estimate that by using more values of λ this can be improved to $c_{4,1} \le 0.026$. This would improve the lower bound in Theorem 1 from 0.9787 to 0.9956.

TABLE 2. Upper bounds on the best possible value for $c_{n,m}$ obtained through a parametrization using shifts S_d^2

d	$c_{3,1}$	$c_{3,2}$
0	0.144444445	1.488888889
1	0.077710979	1.401604735
2	0.077580416	1.401343568
3	0.077261926	1.400616000
4	0.077247720	1.400581457
5	0.077213324	1.400506625

APPENDIX A. THE FOURIER TRANSFORM OF $\chi_{H_{n-1}}$

To compute the Fourier transform of the indicator function of H_{n-1} we use the Fourier transform of the indicator function of the simplex $S_n = \{x \in \mathbb{R}^n : x_j \geq 0, x_1 + \ldots + x_n \leq 1\}$ as computed in [4, Eq. 18]:

$$\widehat{\chi}_{S_n}(y) = \frac{(-1)^{n+1}}{(2\pi i)^n} \sum_{j=1}^{n} \frac{1 - e^{-2\pi i y_j}}{y_j \prod_{i \neq j}(y_j - y_i)}.$$

The Fourier transform of the indicator function of the cross-polytope $C_n = \{x \in \mathbb{R}^n : |x_1| + \ldots + |x_n| \leq 1\}$ is given by

$$\widehat{\chi}_{C_n}(y) = \sum_{\sigma \in \{\pm 1\}^n} \widehat{\chi}_{S_n}(\sigma_1 y_1, \ldots, \sigma_n y_n).$$

If we consider each term in $\widehat{\chi}_{S_n}(y)$ individually, then it is simple to deduce that

$$\sum_{\sigma \in \{\pm 1\}^n} \frac{1 - e^{-2\pi i \sigma_j y_j}}{\sigma_j y_j \prod_{i \neq j}(\sigma_j y_j - \sigma_i y_i)} = \sum_{\sigma \in \{\pm 1\}} (2\sigma y_j)^{n-1} \frac{1 - e^{-2\pi i \sigma y_j}}{\sigma y_j \prod_{i \neq j}(y_j^2 - y_i^2)},$$

while the latter depends on the parity of n. This implies that

$$\widehat{\chi}_{C_n}(y) = \begin{cases} \pi^{-n}(-1)^{(n-1)/2} \sum_{j=1}^{n} \frac{y_j^{n-2} \sin(2\pi y_j)}{\prod_{i \neq j}(y_j^2 - y_i^2)} & \text{if } n \text{ is odd, and} \\ \pi^{-n}(-1)^{n/2-1} \sum_{j=1}^{n} \frac{2y_j^{n-2} \sin(\pi y_j)^2}{\prod_{i \neq j}(y_j^2 - y_i^2)} & \text{if } n \text{ is even.} \end{cases}$$

Finally, notice that H_{n-1} can be identified with $C_n \cap \{x : x_1 + \ldots + x_n = 0\}$ and thus one can rigorously justify that

$$\widehat{\chi}_{H_{n-1}}(y_1, \ldots, y_{n-1}) = \lim_{T \to \infty} \int_{-T}^{T} \widehat{\chi}_{C_n}(y_1 + t, \ldots, y_{n-1} + t, t) \, dt.$$

The function under the integral sign above only has simple poles at $t = -\frac{y_j + y_k}{2}$ for $k \neq j$ and $t = -y_j/2$ (for generic $y \in \mathbb{R}^{n-1}$). A routine application of the residue theorem and a grouping of terms shows that $\widehat{\chi}_{H_{n-1}}(y)$ is equal to

$$\frac{(-1)^{(n-1)/2}}{2^{n-2}\pi^{n-1}} \left[- \sum_{1 \leq j < k \leq n-1} \frac{(y_j - y_k)^{n-3} \cos(\pi(y_j - y_k))}{y_j y_k \prod_{i \neq j,k}(y_j - y_i)(y_k - y_i)} + \sum_{j=1}^{n-1} \frac{y_j^{n-3} \cos(\pi y_j)}{\prod_{i \neq j}(y_j - y_i) y_i} \right]$$

if n is odd, and equal to

$$\frac{(-1)^{n/2-1}}{2^{n-2}\pi^{n-1}}\left[\sum_{1\le j<k\le n-1}\frac{(y_j-y_k)^{n-3}\sin(\pi(y_j-y_k))}{y_jy_k\prod_{i\ne j,k}(y_j-y_i)(y_k-y_i)}+\sum_{j=1}^{n-1}\frac{y_j^{n-3}\sin(\pi y_j)}{\prod_{i\ne j}(y_j-y_i)y_i}\right]$$

if n is even.

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