A new upper bound for finite additive bases

by

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1. An extremal problem for finite bases. Let $\mathbb{N}_0$ and $\mathbb{Z}$ denote the nonnegative integers and integers, respectively, and let $|A|$ denote the cardinality of the set A.

Let A be a set of integers, and consider the *sumset*

$$2A = \{a + a' : a, a' \in A\}.$$

Let S be a set of integers. The set A is a *basis of order* 2 *for S* if $S \subseteq 2A$. The set A is called a *basis of order* 2 *for n* if the sumset $2A$ contains the first n nonnegative integers, that is, if A is a basis of order 2 for the interval of integers $[0, n-1] := \{0, 1, \ldots, n-1\}$. We define $n(2, A)$ as the largest integer n such that A is a basis of order 2 for n, that is,

$$n(2, A) = \max\{n : [0, n-1] \subseteq 2A\}.$$

Rohrbach [6] introduced the extremal problem of determining the largest integer n for which there exists a set A consisting of at most k nonnegative integers such that A is a basis of order 2 for n. Let

$$n(2, k) = \max\{n(2, A) : A \subseteq \mathbb{N}_0 \text{ and } |A| = k\}.$$

Rohrbach's problem is to compute or estimate the extremal function $n(2, k)$. The set A is called an *extremal k-basis of order* 2 if $|A| \leq k$ and $n(2, A) = n(2, k)$.

For example, $n(2, 1) = 1$ and $n(2, 2) = 3$. The unique extremal 1-basis of order 2 is $\{0\}$, and the unique extremal 2-basis of order 2 is $\{0, 1\}$. For $k = 3$ we have $n(2, 3) = 5$, and the extremal 3-bases of order 2 are $\{0, 1, 2\}$ and $\{0, 1, 3\}$. If $k \geq 2$ and A is an extremal k-basis of order 2, then $0, 1 \in A$.

If A is a finite set of k nonnegative integers and $n(2, A) = n$, then $n \notin A$. If $a \in A$ and $a > n$, then the set $A' = (A \setminus \{a\}) \cup \{n\}$ has cardinality k, and $n(2, A') \geq n + 1 > n(2, A)$. Therefore, if A is an extremal k-basis of order 2 and $n(2, k) = n$, then

$$\{0, 1\} \subseteq A \subseteq \{0, 1, \ldots, n - 1\} \subseteq 2A.$$

If A is an extremal k-basis for n, then $|A| = k$ and $A \subseteq \{0, 1, \ldots, n - 1\}$.

Rohrbach determined order of magnitude of $n(2, k)$. He observed that if A is a set of cardinality k, then there are exactly $\binom{k+1}{2}$ ordered pairs of the form (a, a') with $a, a' \in A$ and $a \leq a'$. This gives the upper bound

$$n(2, k) \leq \binom{k + 1}{2} = \frac{k^2}{2} + O(k).$$

To derive a lower bound, he set $r = [k/2]$ and constructed the set

$$A = \{0, 1, \ldots, r - 1, r, 2r, \ldots, (r - 1)r\}.$$

We have

$$|A| = 2r - 1 \leq k$$

and $\{0, 1, \ldots, r^2\} \subseteq 2A$. Then

$$n(2, A) \geq r^2 + 1 \geq (k - 1)^2/4 + 1 = k^2/4 + O(k)$$

and so

$$n(2, k) \geq k^2/4 + O(k).$$

Thus,

$$\liminf_{n \to \infty} \frac{n(2, k)}{k^2} \geq \frac{1}{4} = 0.25, \quad \limsup_{n \to \infty} \frac{n(2, k)}{k^2} \leq \frac{1}{2} = 0.5.$$

It is an open problem to compute these upper and lower limits. Mrose [5] (see also [1]) proved that

$$\liminf_{n \to \infty} \frac{n(2, k)}{k^2} \geq \frac{2}{7} = 0.2857 \ldots,$$

and this is still the best lower bound. Rohrbach used a combinatorial argument to get the nontrivial upper bound

$$\limsup_{n \to \infty} \frac{n(2, k)}{k^2} \leq 0.4992.$$

Moser [3] introduced a Fourier series argument to obtain

$$\limsup_{n \to \infty} \frac{n(2, k)}{k^2} \leq 0.4903,$$

and subsequent improvements by Moser, Pounder, and Riddell [4] produced

$$\limsup_{n \to \infty} \frac{n(2, k)}{k^2} \leq 0.4847.$$

Combining Moser's analytic method and Rohrbach's combinatorial technique, Klotz [2] proved that

$$\limsup_{n\to\infty} \frac{n(2,k)}{k^2} \leq 0.4802.$$

In this paper, we use Fourier series for functions of two variables to obtain

$$\limsup_{n\to\infty} \frac{n(2,k)}{k^2} \leq 0.4789.$$

We note that Rohrbach used a slightly different function $n(2,k)$: He defined $n(2,k)$ as the largest integer n for which there exists a set A consisting of $k+1$ nonnegative integers such that the sumset $2A$ contains the first $n+1$ nonnegative integers. Of course, Rohrbach's function and our function have the same asymptotics.

2. Moser's application of Fourier series. In this section we describe Moser's use of harmonic analysis to obtain an upper bound for $n(2,k)$. Let A be an extremal k-basis of order 2. Let $r_{2,A}(j)$ denote the number of representations of j as a sum of two elements of A, that is,

$$r_{2,A}(j) = \text{card}(\{(a_1,a_2) \in A \times A : a_1 + a_2 = j \text{ and } a_1 \leq a_2\}).$$

We introduce the generating function

$$f_A(q) = \sum_{a\in A} q^a.$$

Then

$$k = f_A(1) = |A| \quad \text{and} \quad \frac{f_A(q)^2 + f_A(q^2)}{2} = \sum_{j\in 2A} r_{2,A}(j)q^j.$$

If $[0,n-1] \subseteq 2A$, then $r_{2,A}(j) \geq 1$ for all $0 \leq j \leq n-1$. Hence there exist integers $\delta(j) \geq 0$ such that

$$\frac{f_A(q)^2 + f_A(q^2)}{2} = 1 + q + q^2 + \cdots + q^{n-1} + \sum_{j\in 2A} \delta(j)q^j,$$

where

$$\delta(j) = \begin{cases} r_{2,A}(j) - 1 & \text{if } j \in \{0,1,\ldots,n-1\}, \\ r_{2,A}(j) & \text{otherwise.} \end{cases}$$

Let

$$\Delta(q) = \sum_{j\in 2A} \delta(j)q^j.$$

Then $\Delta(q) \geq 0$ for $q \geq 0$, and

$$(1) \qquad \frac{f_A(q)^2 + f_A(q^2)}{2} = 1 + q + q^2 + \cdots + q^{n-1} + \Delta(q).$$

Evaluating the generating function identity (1) at $q = 1$, we obtain

(2) $$(k^2 + k)/2 = n + \Delta(1).$$

Since $\Delta(1) \geq 0$, we have

$$n \leq k^2/2 + O(k).$$

The strategy is to find a lower bound for $\Delta(1)$ of the form

$$\Delta(1) \geq ck^2 + O(k)$$

for some $c > 0$, and deduce

$$n \leq \left(\frac{1}{2} - c\right)k^2 + O(k).$$

One obtains a simple combinatorial lower bound for $\Delta(1)$ by noting that if $a_1, a_2 \in A$ and $n/2 \leq a_1 \leq a_2$, then $a_1 + a_2 \geq n$. Let ℓ denote the number of elements $a \in A$ such that $a \geq n/2$. Then

(3) $$\Delta(1) \geq \sum_{j \geq n} \delta(j) = \sum_{j \geq n} r_{2,A}(j) \geq \frac{\ell(\ell+1)}{2} \geq \frac{\ell^2}{2}.$$

Let $\omega = e^{2\pi i/n}$ be a primitive nth root of unity. Let r be an integer not divisible by n. Then

$$1 + \omega^r + \omega^{2r} + \cdots + \omega^{(n-1)r} = 0$$

and so

$$\frac{f_A(\omega^r)^2 + f_A(\omega^{2r})}{2} = 1 + \omega^r + \omega^{2r} + \cdots + \omega^{(n-1)r} + \sum_j \delta(j)\omega^{jr} = \Delta(\omega^r).$$

Applying the triangle inequality, we obtain

$$\Delta(1) \geq |\Delta(\omega^r)| = \frac{|f_A(\omega^r)^2 + f_A(\omega^{2r})|}{2} \geq \frac{|f_A(\omega^r)|^2 - k}{2}.$$

Let

$$M = \max\{|f_A(\omega^r)| : r \not\equiv 0 \ (\mathrm{mod}\, n)\}.$$

Then

(4) $$0 \leq M \leq k$$

and

(5) $$\Delta(1) \geq (M^2 - k)/2.$$

It is also possible to obtain an analytic lower bound for $\Delta(1)$. For all integers r not divisible by n, we have

$$M \geq |f_A(\omega^r)| = \left|\sum_{a \in A} e^{2\pi i ra/n}\right| = \left|\sum_{a \in A} \cos(2\pi ra/n) + i\sin(2\pi ra/n)\right|,$$

and so

$$\left| \sum_{a \in A} \cos(2\pi ra/n) \right| \le M, \quad \left| \sum_{a \in A} \sin(2\pi ra/n) \right| \le M.$$

Let $\varphi(t)$ be a real-valued function with period 1 and with a Fourier series

$$\varphi(t) = \sum_{r=0}^{\infty} a_r \cos(2\pi rt) + \sum_{r=1}^{\infty} b_r \sin(2\pi rt)$$

whose Fourier coefficients are absolutely summable, that is,

$$\sum_{r=0}^{\infty} |a_r| + \sum_{r=1}^{\infty} |b_r| < \infty.$$

Define $C = C(n)$ by

$$C = \sum_{\substack{r=0 \\ n|r}}^{\infty} |a_r|.$$

For any integer a we have

$$
\begin{aligned}
\sum_{a \in A} \varphi\left(\frac{a}{n}\right) &= \sum_{a \in A} \sum_{r=0}^{\infty} a_r \cos(2\pi ra/n) + \sum_{a \in A} \sum_{r=1}^{\infty} b_r \sin(2\pi ra/n) \\
&= \sum_{r=0}^{\infty} a_r \sum_{a \in A} \cos(2\pi ra/n) + \sum_{r=1}^{\infty} b_r \sum_{a \in A} \sin(2\pi ra/n) \\
&= \sum_{\substack{r=0 \\ n \nmid r}}^{\infty} a_r \sum_{a \in A} \cos(2\pi ra/n) + \sum_{\substack{r=1 \\ n \nmid r}}^{\infty} b_r \sum_{a \in A} \sin(2\pi ra/n) + k \sum_{\substack{r=0 \\ n|r}}^{\infty} a_r,
\end{aligned}
$$

and so

$$\left| \sum_{a \in A} \varphi\left(\frac{a}{n}\right) \right| \le M \sum_{\substack{r=1 \\ n \nmid r}}^{\infty} (|a_r| + |b_r|) + kC.$$

Let α_1 and α_2 be real numbers such that

$$\varphi(t) \ge \begin{cases} \alpha_1 & \text{for } 0 \le t < 1/2, \\ \alpha_2 & \text{for } 1/2 \le t < 1. \end{cases}$$

Recall that ℓ denotes the number of elements $a \in A$ such that $n/2 \le a \le n-1$. Then

$$\sum_{a \in A} \varphi\left(\frac{a}{n}\right) \ge (k - \ell)\alpha_1 + \ell\alpha_2 = k\alpha_1 - (\alpha_1 - \alpha_2)\ell.$$

We obtain the inequality

$$(6) \qquad k\alpha_1 - (\alpha_1 - \alpha_2)\ell \leq M \sum_{\substack{r=1 \\ n \nmid r}}^{\infty} (|a_r| + |b_r|) + kC.$$

In this way, the function $\varphi(t)$ produces a lower bound for M, which, by (5), gives a lower bound for $\Delta(1)$.

Moser applied inequality (6) to the function

$$\varphi(t) = \frac{1}{2}\cos(4\pi t) + \sin(2\pi t),$$

whose nonzero Fourier coefficients are $a_2 = 1/2$ and $b_1 = 1$. Then $C = 0$ for $n \geq 3$, and

$$\left| \sum_{a \in A} \varphi\left(\frac{a}{n}\right) \right| \leq \frac{3M}{2}.$$

The function $\varphi(t)$ satisfies the inequality

$$\varphi(t) \geq \begin{cases} 1/2 & \text{for } 0 \leq t < 1/2, \\ -3/2 & \text{for } 1/2 \leq t < 1, \end{cases}$$

and so

$$\sum_{a \in A} \varphi\left(\frac{a}{n}\right) \geq \frac{k-\ell}{2} - \frac{3\ell}{2} = \frac{k-4\ell}{2}.$$

This implies that

$$M \geq \frac{2}{3}\left| \sum_{a \in A} \varphi\left(\frac{a}{n}\right) \right| \geq \frac{k-4\ell}{3}.$$

Defining $\lambda = \ell/k$ and $\mu = M/k$, which both lie in $[0,1]$, we obtain the constraint

$$\frac{4}{3}\lambda + \mu \geq \frac{1}{3}.$$

Recalling the combinatorial lower bound (3) and the analytical bound (5), we next obtain

$$\frac{2\Delta(1)}{k^2} \geq \max\left(\lambda^2, \mu^2 - \frac{1}{k}\right) \geq \max(\lambda, \mu)^2 - \frac{1}{k}.$$

It is now easy to see that

$$\max(\lambda, \mu) \geq \frac{\frac{4}{3}\lambda + \mu}{\frac{4}{3} + 1} \geq \frac{1}{7},$$

hence we obtain

$$\Delta(1) \geq \frac{k^2}{98} - \frac{k}{2}.$$

Inserting this into inequality (2), we obtain

$$\frac{k^2 + k}{2} = n + \Delta(1) \geq n + \frac{k^2}{98} - \frac{k}{2},$$

and so

$$n \leq \left(\frac{1}{2} - \frac{1}{98}\right) k^2 + k \leq 0.4898 k^2 + k,$$

which, in fact, has a slightly better constant than derived by Moser originally. The constant in this estimate can be further improved by optimizing the function φ.

In the next section we shall employ a more general method using Fourier series in two variables that ultimately yields an even better lower bound for $\Delta(1)$.

3. Fourier series in two variables. We use the same notation as in the previous section. In particular, ℓ denotes the number of integers $a \in A$ such that $a \geq n/2$. Let L denote the number of pairs $(a_1, a_2) \in A \times A$ such that $a_1 + a_2 \geq n$. Then $L \geq \ell^2$, and $k^2 - L$ is the number of pairs $(a_1, a_2) \in A \times A$ such that $a_1 + a_2 \leq n - 1$. We have the combinatorial lower bound

$$(7) \qquad \Delta(1) \geq \sum_{j \geq n} r_{2,A}(j) = (L + \ell)/2 \geq L/2.$$

Let $\varphi(t_1, t_2)$ be a real-valued function with period 1 in each variable and with a Fourier series

$$\varphi(t_1, t_2) = \sum_{r_1 \in \mathbb{Z}} \sum_{r_2 \in \mathbb{Z}} \widehat{\varphi}(r_1, r_2) e^{2\pi i r_1 t_1} e^{2\pi i r_2 t_2}$$

which converges absolutely, that is,

$$\sum_{r_1 \in \mathbb{Z}} \sum_{r_2 \in \mathbb{Z}} |\widehat{\varphi}(r_1, r_2)| < \infty.$$

We choose $\varphi(t_1, t_2)$ with zero mean, that is,

$$\widehat{\varphi}(0,0) = \int_0^1 \int_0^1 \varphi(t_1, t_2) \, dt_1 \, dt_2 = 0.$$

Let

$$R_1 = \{(t_1, t_2) \in [0,1) \times [0,1) : t_1 + t_2 < 1\},$$
$$R_2 = \{(t_1, t_2) \in [0,1) \times [0,1) : t_1 + t_2 \geq 1\}.$$

If $a_1, a_2 \in A$ and $a_1 + a_2 \leq n - 1$, then $(a_1/n, a_2/n) \in R_1$. If $a_1 + a_2 \geq n$, then $(a_1/n, a_2/n) \in R_2$.

Let α_1 and α_2 be real numbers such that

$$\varphi(t_1, t_2) \geq \begin{cases} \alpha_1 & \text{for } (t_1, t_2) \in R_1, \\ \alpha_2 & \text{for } (t_1, t_2) \in R_2. \end{cases}$$

We choose the function $\varphi(t_1, t_2)$ such that $\alpha_1 > \alpha_2$. Then

$$(8) \qquad \sum_{a_1 \in A} \sum_{a_2 \in A} \varphi\left(\frac{a_1}{n}, \frac{a_2}{n}\right) \geq (k^2 - L)\alpha_1 + L\alpha_2 = \alpha_1 k^2 - (\alpha_1 - \alpha_2)L.$$

We can rewrite this sum as follows:

$$\sum_{a_1 \in A} \sum_{a_2 \in A} \varphi\left(\frac{a_1}{n}, \frac{a_2}{n}\right) = \sum_{a_1 \in A} \sum_{a_2 \in A} \sum_{r_1 \in \mathbb{Z}} \sum_{r_2 \in \mathbb{Z}} \widehat{\varphi}(r_1, r_2) e^{2\pi i r_1 a_1/n} e^{2\pi i r_2 a_2/n}$$

$$= \sum_{r_1 \in \mathbb{Z}} \sum_{r_2 \in \mathbb{Z}} \widehat{\varphi}(r_1, r_2) \sum_{a_1 \in A} e^{2\pi i r_1 a_1/n} \sum_{a_2 \in A} e^{2\pi i r_2 a_2/n}$$

$$= \sum_{r_1 \in \mathbb{Z}} \sum_{r_2 \in \mathbb{Z}} \widehat{\varphi}(r_1, r_2) f_A(\omega^{r_1}) f_A(\omega^{r_2}).$$

Consider the partition of the integer lattice $\mathbb{Z}^2 = S_0 \cup S_1 \cup S_2$, where

$$S_0 = \{(r_1, r_2) \in \mathbb{Z}^2 : r_1 \equiv r_2 \equiv 0 \ (\text{mod } n)\},$$
$$S_1 = \{(r_1, r_2) \in \mathbb{Z}^2 : r_1 \equiv 0 \ (\text{mod } n), r_2 \not\equiv 0 \ (\text{mod } n)\}$$
$$\cup \{(r_1, r_2) \in \mathbb{Z}^2 : r_1 \not\equiv 0 \ (\text{mod } n), r_2 \equiv 0 \ (\text{mod } n)\},$$
$$S_2 = \{(r_1, r_2) \in \mathbb{Z}^2 : r_1 \not\equiv 0 \ (\text{mod } n), r_2 \not\equiv 0 \ (\text{mod } n)\}.$$

We define $C_i = C_i(n)$ for $i = 0, 1, 2$ by

$$C_i = \sum_{(r_1, r_2) \in S_i} |\widehat{\varphi}(r_1, r_2)|.$$

Recall that $|f_A(\omega^r)| \leq M$ if r is not divisible by n and $|f_A(\omega^r)| = k$ if r is divisible by n. Then

$$(9) \qquad \left| \sum_{a_1 \in A} \sum_{a_2 \in A} \varphi\left(\frac{a_1}{n}, \frac{a_2}{n}\right) \right| \leq C_0 k^2 + C_1 k M + C_2 M^2.$$

Combining (8) and (9), we obtain

$$\alpha_1 k^2 - (\alpha_1 - \alpha_2)L \leq C_0 k^2 + C_1 k M + C_2 M^2.$$

Since $\alpha_1 > \alpha_2$, we have

$$L \geq \frac{(\alpha_1 - C_0)k^2 - C_1 k M - C_2 M^2}{\alpha_1 - \alpha_2}.$$

We again define $\mu = M/k$. Since $0 \leq M \leq k$, we have $0 \leq \mu \leq 1$. By (7), we have $2\Delta(1) \geq L$, and so

$$\frac{2\Delta(1)}{k^2} \geq \frac{L}{k^2} \geq \frac{(\alpha_1 - C_0) - C_1 \mu - C_2 \mu^2}{\alpha_1 - \alpha_2}.$$

By (5), we also have $2\Delta(1) \geq M^2 - k$, and so

(10)
$$\frac{2\Delta(1)}{k^2} \geq \max\left(\mu^2, \frac{(\alpha_1 - C_0) - C_1\mu - C_2\mu^2}{\alpha_1 - \alpha_2}\right) - \frac{1}{k}.$$

Since the Fourier series of $\varphi(t_1, t_2)$ converges absolutely and since $\widehat{\varphi}(0, 0) = 0$, we can arrange the Fourier series in the form of a sum over concentric squares

$$\sum_{R=1}^{\infty} \sum_{\max(|r_1|, |r_2|)=R} \widehat{\varphi}(r_1, r_2) e^{2\pi i r_1 t_1} e^{2\pi i r_2 t_2}.$$

For any $\varepsilon > 0$ there exists an integer $N = N(\varepsilon)$ such that

$$\sum_{n=N}^{\infty} \sum_{\max(|r_1|, |r_2|)=n} |\widehat{\varphi}(r_1, r_2)| < \varepsilon(\alpha_1 - \alpha_2).$$

For all $n \geq N$, we shall approximate the sums C_0, C_1, and C_2 by 0, C_{axial}, and C_{main}, respectively, where

$$C_{\text{axial}} = \sum_{\substack{r \in \mathbb{Z} \\ r \neq 0}} (|\widehat{\varphi}(0, r)| + |\widehat{\varphi}(r, 0)|), \quad C_{\text{main}} = \sum_{\substack{r_1 \in \mathbb{Z} \\ r_1 \neq 0}} \sum_{\substack{r_2 \in \mathbb{Z} \\ r_2 \neq 0}} |\widehat{\varphi}(r_1, r_2)|.$$

Then

$$\begin{aligned}
|(\alpha_1 - C_0) - C_1\mu - C_2\mu^2 - (\alpha_1 - C_{\text{axial}}\mu - C_{\text{main}}\mu^2)| \\
= |C_0 + (C_1 - C_{\text{axial}})\mu + (C_2 - C_{\text{main}})\mu^2| \\
\leq |C_0| + |C_1 - C_{\text{axial}}| + |C_2 - C_{\text{main}}| \\
\leq \sum_{\max(|r_1|, |r_2|) \geq N} |\widehat{\varphi}(r_1, r_2)| < \varepsilon(\alpha_1 - \alpha_2),
\end{aligned}$$

and so

$$\left| \frac{(\alpha_1 - C_0) - C_1\mu - C_2\mu^2}{\alpha_1 - \alpha_2} - \frac{\alpha_1 - C_{\text{axial}}\mu - C_{\text{main}}\mu^2}{\alpha_1 - \alpha_2} \right| < \varepsilon.$$

It follows from inequality (10) that

$$\frac{2\Delta(1)}{k^2} \geq \max\left(\mu^2, \frac{\alpha_1 - C_{\text{axial}}\mu - C_{\text{main}}\mu^2}{\alpha_1 - \alpha_2}\right) - \varepsilon - \frac{1}{k}.$$

Let

(11)
$$\varrho = \inf_{0 \leq \mu \leq 1} \max\left(\mu^2, \frac{\alpha_1 - C_{\text{axial}}\mu - C_{\text{main}}\mu^2}{\alpha_1 - \alpha_2}\right).$$

From (10) and the definition of ϱ in (11), we now have

$$2\Delta(1)/k^2 \geq \varrho - \varepsilon - 1/k.$$

Applying (2), we obtain

$$\frac{k^2 + k}{2} = n + \Delta(1) \geq n + \frac{(\varrho - \varepsilon)k^2 - k}{2}.$$

Therefore, we obtain the desired estimate

(12) $$n \leq \frac{1 - \varrho + \varepsilon}{2} k^2 + k$$

for all sufficiently large n, where the number ϱ depends only on the function $\varphi(t_1, t_2)$ and $\varepsilon > 0$ can be arbitrarily small.

It is clear that we always have $\varrho \geq 0$, and that $\varrho > 0$ if and only if $\alpha_1 > 0$. It is also clear that when $\alpha_1 \geq 0$, we have $\varrho = \xi^2$, where ξ is the unique solution in $[0, 1]$ to the quadratic equation

$$\xi^2 = \frac{\alpha_1 - C_{\text{axial}}\xi - C_{\text{main}}\xi^2}{\alpha_1 - \alpha_2},$$

i.e.,

$$(\alpha_1 - \alpha_2 + C_{\text{main}})\xi^2 + C_{\text{axial}}\xi - \alpha_1 = 0,$$

which yields the formula

(13) $$\varrho = \left(\frac{-C_{\text{axial}} + \sqrt{C_{\text{axial}}^2 + 4\alpha_1(\alpha_1 - \alpha_2 + C_{\text{main}})}}{2(\alpha_1 - \alpha_2 + C_{\text{main}})}\right)^2.$$

Hence we have an optimization problem in which we maximize ϱ over all real-valued functions φ defined on the unit square $[0, 1)^2$ such that φ has zero mean and $\varphi > 0$ on R_1. We do not know the optimal function for this problem, but we have found a simple piecewise polynomial function that improves Klotz's upper bound for $n(2, k)$. Before we proceed to the main result of this paper, which also includes the definition of this function, let us present some of the heuristics which have lead us to our "educated guess."

First, without loss of generality, we may assume that $\alpha_1 = 1$. We then necessarily have

$$0 = \iint\limits_{R_1} \varphi(t_1, t_2) \, dt_1 \, dt_2 + \iint\limits_{R_2} \varphi(t_1, t_2) \, dt_1 \, dt_2 \geq \frac{1}{2} + \frac{1}{2}\alpha_2,$$

hence $\alpha_2 \leq -1$. We also have

$$C_{\text{axial}} \geq \left|\sum_r (\widehat{\varphi}(r, 0) + \widehat{\varphi}(0, r))\right| = \left|\int_0^1 (\varphi(0, t) + \varphi(t, 0)) \, dt\right| \geq 2$$

and

$$C_{\text{main}} \geq \left|\sum_r \widehat{\varphi}(r, r)\right| = \left|\int_0^1 \varphi(t, 1 - t) \, dt\right| \geq 1.$$

In any case we are interested in the positive root $\xi_{\kappa,\tau}$ of the equation

$$\kappa\xi^2 + \tau\xi - 1 = 0$$

where $\kappa = 1 - \alpha_2 + C_{\text{main}} \geq 3$ and $\tau = C_{\text{axial}} \geq 2$. Clearly, the smaller κ and τ are, the larger this root will be. The bounds $\kappa \geq 3$ and $\tau \geq 2$ already imply that $\xi_{\kappa,\tau} \leq 1/3$, hence $\varrho = \xi_{\kappa,\tau}^2 \leq 1/9$. In reality, $\alpha_2 < -1$ because equality can happen only if φ is constant on both R_1 and R_2, in which case $\widehat{\varphi}$ is not absolutely summable. This results in the heuristic that if we try to push α_2 close to -1, then C_{axial} and C_{main} will become large, and conversely if we try to push C_{axial} and C_{main} close to their respective minimum values, then φ may not be bounded from below on R_2 by a small value. The right trade-off between these two competing quantities will result in the solution of this optimization problem.

It is interesting to note that the value of ϱ is fairly robust with respect to variations in κ and τ, which we will only be able to estimate numerically and not compute exactly. The following lemma gives an explicit estimate for this purpose:

LEMMA 1. *Let $\xi_{\kappa,\tau}$ and ξ_{κ_0,τ_0} be the respective positive roots of the equations $\kappa\xi^2 + \tau\xi - 1 = 0$ and $\kappa_0\xi^2 + \tau_0\xi - 1 = 0$. Let $\varrho = \xi_{\kappa,\tau}^2$ and $\varrho_0 = \xi_{\kappa_0,\tau_0}^2$. If $\min(\kappa,\kappa_0) \geq 3$ and $\min(\tau,\tau_0) \geq 2$, then*

$$(14) \qquad |\varrho - \varrho_0| \leq \frac{1}{54}|\kappa - \kappa_0| + \frac{1}{18}|\tau - \tau_0|.$$

The proof of this lemma is given in the Appendix. Now we can state and prove the main theorem of this paper.

THEOREM 1. *We have*

$$\limsup_{n\to\infty} \frac{n(2,k)}{k^2} \leq 0.4789.$$

Proof. We define the function $\varphi(t_1,t_2)$ on the unit square $[0,1)^2$ by

$$(15) \qquad \varphi(t_1,t_2)$$
$$= \begin{cases} 1, & (t_1,t_2) \in R_1, \\ 1 - 40(1-t_1)(1-t_2)(1 - (2 - t_1 - t_2)^6), & (t_1,t_2) \in R_2. \end{cases}$$

The graph of this function is plotted in Figure 1.

Clearly we have $\alpha_1 = 1$. Computation of the three other parameters used in formula (11) for ϱ yields

$$\alpha_2 = 1 - \frac{15}{2^{5/3}} = -3.72470\ldots,$$

$$2.90278 \leq C_{\text{axial}} \leq 2.90289, \qquad 4.75145 \leq C_{\text{main}} \leq 4.76146.$$

Taking $\kappa_0 = 1 + 3.72471 + 4.76146 = 9.48617$ and $\tau_0 = 2.90289$, we obtain $\varrho_0 > 0.04240$, $|\kappa - \kappa_0| < 0.01002$ and $|\tau - \tau_0| < 0.00011$, so it follows that
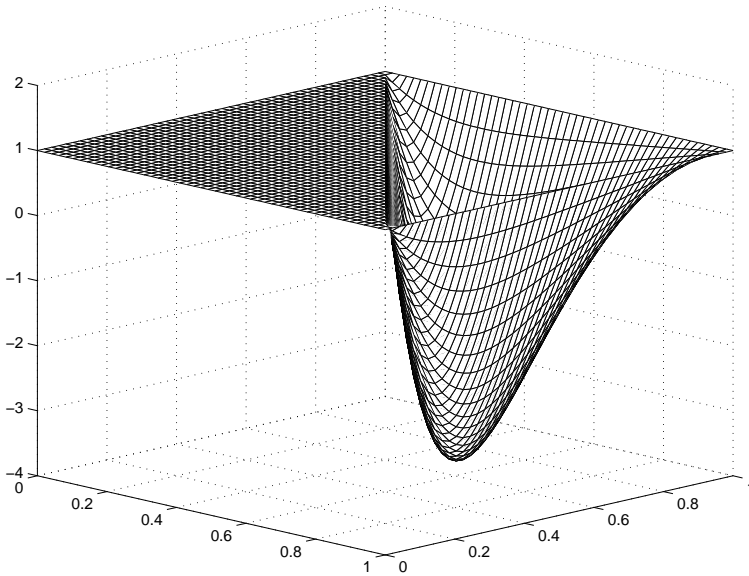
Fig. 1. Graph of the function φ defined in (15)

$|\varrho - \varrho_0| < 0.0002$. Hence

$$\varrho \geq \varrho_0 - |\varrho - \varrho_0| > 0.0422.$$

Consequently, choosing ε sufficiently small and using (12), we obtain

$$n \leq 0.4789 \, k^2 + k.$$

The details of the computations are in the Appendix to this paper. This completes the proof. ∎

4. Open problems. A major open problem concerning the extremal function

$$n(2, k) = \max\{n(2, A) : A \subseteq \mathbb{N}_0 \text{ and } |A| \leq k\}$$

is to compute $\liminf_{n \to \infty} n(2, k)/k^2$ and $\limsup_{n \to \infty} n(2, k)/k^2$, and to determine if the limit $\lim_{n \to \infty} n(2, k)/k^2$ exists. We have no conjecture about the existence of this limit, nor about the values of the lim inf and lim sup.

It is also difficult to compute the exact values of the function $n(2, k)$.

We can generalize the extremal functions $n(2, A)$ and $n(2, k)$ as follows. Let A be a finite set of integers, and let $m(2, A)$ denote the largest integer n such that the sumset $2A$ contains n consecutive integers. Let

$$m(2, k) = \max\{m(2, A) : A \subseteq \mathbb{Z} \text{ and } |A| \leq k\}.$$

Let $\ell(2, A)$ denote the largest integer n such that the sumset $2A$ contains

an arithmetic progression of length n, and let

$$\ell(2, k) = \max\{\ell(2, A) : A \subseteq \mathbb{Z} \text{ and } |A| \leq k\}.$$

We can also define the extremal function

$$n'(2, k) = \max\{n(2, A) : A \subseteq \mathbb{Z} \text{ and } |A| \leq k\}.$$

Then

$$n(2, A) \leq n'(2, A) \leq m(2, A) \leq \ell(2, A),$$

and so

$$n(2, k) \leq n'(2, k) \leq m(2, k) \leq \ell(2, k).$$

For any integer t and set A, we have the translation $A + t = \{a + t : a \in A\}$. The functions ℓ and m are translation invariant, that is, $\ell(2, A+t) = \ell(2, A)$ and $m(2, A + t) = m(2, A)$. We also have the trivial upper bound $\ell(2, k) \leq \binom{k+1}{2}$, but it is an open problem to obtain nontrivial upper bounds for any of the extremal functions $n'(2, k)$, $m(2, k)$, or $\ell(2, k)$.

Appendix. We describe here the computations.

Proof of Lemma 1. We start with the formula

$$\xi_{\kappa,\tau} = \frac{-\tau + \sqrt{\tau^2 + 4\kappa}}{2\kappa} = \frac{2}{\tau + \sqrt{\tau^2 + 4\kappa}}.$$

We next evaluate the partial derivatives of $\xi_{\kappa,\tau}$ with respect to κ and τ:

$$(16) \qquad \frac{\partial \xi_{\kappa,\tau}}{\partial \kappa} = -\frac{4}{\sqrt{\tau^2 + 4\kappa}\,(\tau + \sqrt{\tau^2 + 4\kappa})^2},$$

$$(17) \qquad \frac{\partial \xi_{\kappa,\tau}}{\partial \tau} = -\frac{2}{\sqrt{\tau^2 + 4\kappa}\,(\tau + \sqrt{\tau^2 + 4\kappa})}$$

from which it follows that in the set $\{(\kappa, \tau) : \kappa \geq 3,\ \tau \geq 2\}$, we have

$$\left|\frac{\partial \xi_{\kappa,\tau}}{\partial \kappa}\right| \leq \frac{1}{36} \quad \text{and} \quad \left|\frac{\partial \xi_{\kappa,\tau}}{\partial \tau}\right| \leq \frac{1}{12}.$$

These bounds then imply

$$|\xi_{\kappa,\tau} - \xi_{\kappa_0,\tau_0}| \leq \frac{1}{36}\,|\kappa - \kappa_0| + \frac{1}{12}\,|\tau - \tau_0|.$$

We then note that $\xi_{\kappa,\tau} \leq 1/3$, which yields

$$|\varrho - \varrho_0| = |\xi_{\kappa,\tau} - \xi_{\kappa_0,\tau_0}|\,|\xi_{\kappa,\tau} + \xi_{\kappa_0,\tau_0}| \leq \frac{2}{3}|\xi_{\kappa,\tau} - \xi_{\kappa_0,\tau_0}|,$$

hence the result of the lemma. ∎

Absolute summability of $\widehat{\varphi}$. While the result explained in this subsection is elementary, we will provide a certain amount of detail in its derivation because our main concern is more than absolute summability of $\widehat{\varphi}$. We would like to provide explicit estimates on the rate of the convergence; this will be necessary later in the section when we will analyze the accuracy of the numerical computation of the constants C_{main} and C_{axial}.

LEMMA 2. *Let f be a smooth function on $[0,1]$. Then for all $L \geq 0$ and $n \neq 0$, the following formula holds:*

$$(18) \qquad \widehat{f}(n) = \sum_{k=0}^{L} \frac{f^{(k)}(0) - f^{(k)}(1)}{(2\pi in)^{k+1}} + \frac{\widehat{f^{(L+1)}}(n)}{(2\pi in)^{L+1}}.$$

Proof. The case $L = 0$ follows from integration by parts and the general case follows from iterating this result. ∎

THEOREM 2. *Let F be a smooth function on $\mathbb{R}^2$ which vanishes on the boundary of R_2, i.e.,*

$$F(t, 1-t) = F(1,t) = F(t,1) = 0 \quad \text{for all } t \in [0,1].$$

Define

$$\Psi_F(t_1, t_2) = \begin{cases} 0 & \text{if } (t_1, t_2) \in R_1, \\ F(t_1, t_2) & \text{if } (t_1, t_2) \in R_2. \end{cases}$$

Then the Fourier series expansion of Ψ_F is absolutely convergent.

Note. Later we will simply set $\varphi = \Psi_F + 1$.

Proof. We will prove this result by deriving a suitable decay estimate on $|\widehat{\Psi}_F(r_1, r_2)|$, where

$$\widehat{\Psi}_F(r_1, r_2) = \int_0^1 e^{-2\pi i r_1 t_1} \left\{ \int_{1-t_1}^1 F(t_1, t_2) e^{-2\pi i r_2 t_2} \, dt_2 \right\} dt_1.$$

The case $r_1 = 0$ or $r_2 = 0$. Due to the symmetry on the assumptions on F, it suffices to consider only one of these cases. Let us assume that $r_2 = 0$. Define

$$J_1(t_1) = \int_{1-t_1}^1 F(t_1, t_2) \, dt_2,$$

so that

$$(19) \qquad \widehat{\Psi}_F(r_1, 0) = \widehat{J}_1(r_1).$$

Clearly we have $J_1(0) = J_1(1) = 0$. Setting $L = 1$ and $f = J_1$ in Lemma 2, we see that for $r_1 \neq 0$,

$$(20) \qquad |\widehat{\Psi}_F(r_1, 0)| \leq \frac{1}{|2\pi r_1|^2} \left(|J_1'(0) - J_1'(1)| + \int_0^1 |J_1''| \right) = O\left(\frac{1}{r_1^2} \right).$$

With a similar estimate for $|\widehat{\Psi}_F(0, r_2)|$, we have

$$\sum_{r \neq 0} (|\widehat{\Psi}_F(r, 0)| + |\widehat{\Psi}_F(0, r)|) < \infty.$$

The case $r_1 \neq 0$ and $r_2 \neq 0$. We will derive a general formula for $\widehat{\Psi}_F(r_1, r_2)$. To do this, we momentarily forget that F vanishes on the boundary of R_2, and for $t \in [0, 1]$, define the following functions:

$$
\begin{aligned}
g_0(t) &= F(t, 1-t), & h_0(t) &= F(t, 1), \\
g_1(t) &= (\partial_2 F)(t, 1-t), & h_1(t) &= (\partial_2 F)(1, t), \\
g_2(t) &= (\partial_1 \partial_2 F)(t, 1-t), & h_2(t) &= (\partial_1 \partial_2 F)(t, 1), \\
g_3(t) &= (\partial_1 \partial_2^2 F)(t, 1-t), & h_3(t) &= (\partial_1 \partial_2^2 F)(1, t).
\end{aligned}
$$

We start with the formula for $\widehat{\Psi}_F(r_1, r_2)$ above. Integrating by parts in the second variable, we obtain

$$
\widehat{\Psi}_F(r_1, r_2) = \int_0^1 dt_1\, e^{-2\pi i r_1 t_1} \left\{ \left[\frac{e^{2\pi i r_2 t_2}}{-2\pi i r_2} F(t_1, t_2) \right]_{t_2 = 1-t_1}^{t_2 = 1} \right.
$$
$$
\left. - \int_{1-t_1}^1 dt_2\, \frac{e^{-2\pi i r_2 t_2}}{-2\pi i r_2} (\partial_2 F)(t_1, t_2) \right\}
$$
$$
= \frac{1}{(2\pi i) r_2} \left(\widehat{g}_0(r_1 - r_2) - \widehat{h}_0(r_1) + \widehat{\Psi}_{\partial_2 F}(r_1, r_2) \right).
$$

We apply the same method to $\widehat{\Psi}_{\partial_2 F}(r_1, r_2)$, but integrate by parts in the first variable. This results in

$$
\widehat{\Psi}_F(r_1, r_2) = \frac{1}{(2\pi i) r_2} \left(\widehat{g}_0(r_1 - r_2) - \widehat{h}_0(r_1) \right)
$$
$$
+ \frac{1}{(2\pi i)^2 r_1 r_2} \left(\widehat{g}_1(r_1 - r_2) - \widehat{h}_1(r_2) + \widehat{\Psi}_{\partial_1 \partial_2 F}(r_1, r_2) \right).
$$

We repeat the first two steps in the same order, which gives us

$$
(21) \quad \widehat{\Psi}_F(r_1, r_2) = \frac{1}{(2\pi i) r_2} \left(\widehat{g}_0(r_1 - r_2) - \widehat{h}_0(r_1) \right)
$$
$$
+ \frac{1}{(2\pi i)^2 r_1 r_2} \left(\widehat{g}_1(r_1 - r_2) - \widehat{h}_1(r_2) \right)
$$
$$
+ \frac{1}{(2\pi i)^3 r_1 r_2^2} \left(\widehat{g}_2(r_1 - r_2) - \widehat{h}_2(r_1) \right)
$$
$$
+ \frac{1}{(2\pi i)^4 r_1^2 r_2^2} \left(\widehat{g}_3(r_1 - r_2) - \widehat{h}_3(r_2) + \widehat{\Psi}_{\partial_1^2 \partial_2^2 F}(r_1, r_2) \right).
$$

Note that from our assumptions on F, we have $g_0 = h_0 = h_1 = 0$. We will have two subcases:

(1) $r_1 = r_2 = r$. In this case, we easily see from the second formula above that

$$(22) \qquad |\widehat{\Psi}_F(r, r)| \leq \frac{|\widehat{g}_1(0)| + \|\Psi_{\partial_1 \partial_2 F}\|_1}{4\pi^2 r^2}.$$

(2) $r_1 \neq r_2$. This case is slightly more subtle. We first note that $g_1(1) = h_1(0) = 0$. It is also true that $g_1(0) = (\partial_2 F)(0, 1)$. To see this, note that $(\partial_1 F)(0, 1) = 0$ and $\nabla F(0, 1) \cdot (1, -1) = 0$, both of which follow from the fact that F vanishes on the boundary of R_2. The function g_1 being smooth otherwise, we conclude that

$$|\widehat{g}_1(r_1 - r_2)| \leq \frac{|g_1'(1) - g_1'(0)| + \|g_1''\|_1}{4\pi^2 |r_1 - r_2|^2}.$$

The estimates for g_2 and h_2 are simpler in nature. We use the bounds

$$|\widehat{g}_2(r_1 - r_2)| \leq \frac{|g_2(1) - g_2(0)| + \|g_2'\|_1}{2\pi |r_1 - r_2|},$$

$$|\widehat{h}_2(r_1)| \leq \frac{|h_2(1) - h_2(0)| + \|h_2'\|_1}{2\pi |r_1|},$$

as well as

$$|\widehat{g}_3(r_1 - r_2)| \leq \|g_3\|_1, \quad |\widehat{h}_3(r_1)| \leq \|h_3\|_1, \quad |\widehat{\Psi}_{\partial_1^2 \partial_2^2 F}(r_1, r_2)| \leq \|\Psi_{\partial_1^2 \partial_2^2 F}\|_1.$$

Putting all these together, we see that

$$|\widehat{\Psi}_F(r_1, r_2)| = O\left(\frac{1}{|r_1 r_2|(r_1 - r_2)^2} + \frac{1}{|r_1(r_1 - r_2)|r_2^2} + \frac{1}{r_1^2 r_2^2} \right),$$

which is easily verified to be summable over all admissible values of r_1 and r_2. We will return to this shortly for a more explicit estimate. ∎

Explicit numerical estimates. In this subsection we will work with the specific function φ in (15) for which

$$F(t_1, t_2) = -40(1 - t_1)(1 - t_2)(1 - (2 - t_1 - t_2)^6).$$

We will numerically estimate C_{axial} and C_{main} using appropriate tail bounds on their defining infinite series. This procedure is illustrated in Figure 2.

Estimating the value of C_{axial}. Since F is symmetric, we have $\widehat{\varphi}(r, 0) = \widehat{\varphi}(0, r)$. We use the formula (19) to evaluate $\widehat{\varphi}(r_1, 0)$. It is a simple calculation to show that

$$J_1(t_1) = -15(1 - t_1) + \frac{240}{7}(1 - t_1)^2 - 20(1 - t_1)^3 + \frac{5}{7}(1 - t_1)^9.$$

Using this expression, we find that $|J_1'(0) - J_1'(1)| = 15$ and

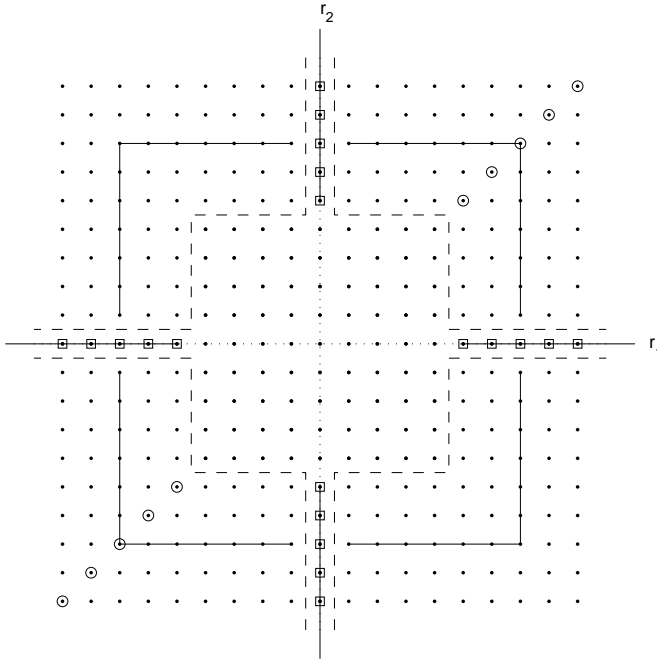$$\int_0^1 |J_1''| \leq \left(\int_0^1 (J_1'')^2 \right)^{1/2} = 8\sqrt{15}.$$

Fig. 2. Estimating the values of C_{axial} and C_{main}. Circled dots correspond to the Fourier coefficients along the diagonal for which a separate decay estimate holds.

Hence by (20), we obtain the estimate

$$|\widehat{\varphi}(r,0)| = |\widehat{\varphi}(0,r)| \leq \frac{15 + 8\sqrt{15}}{4\pi^2} \frac{1}{r^2}.$$

If we define

$$(23) \qquad C_{\text{axial}}(N) = \sum_{|r| \leq N} (|\widehat{\varphi}(r,0)| + |\widehat{\varphi}(0,r)|),$$

then it follows that

$$0 \leq C_{\text{axial}} - C_{\text{axial}}(N) \leq \frac{15 + 8\sqrt{15}}{\pi^2} \frac{1}{N} < \frac{5}{N}.$$

To estimate $C_{\text{axial}}(N)$, we still need the actual expression for $\widehat{\varphi}(r,0)$, which is given in (30). Taking $N = 50000$, numerical computation shows that $C_{\text{axial}}(N) = 2.90278\ldots$; hence it follows that

$$2.90278 \leq C_{\text{axial}} \leq 2.90289.$$

Estimating the value of C_{main}. We shall estimate the diagonal terms first. We have

$$g_1(t) = -240t(1-t)$$

from which we obtain

$$|\widehat{g}_1(0)| = 40,$$

and

$$|\partial_1\partial_2 F(t_1, t_2)| = |1200(1 - t_1)(1 - t_2)(2 - t_1 - t_2)^4 + 280(2 - t_1 - t_2)^6 - 40|$$
$$\leq 1200(1 - t_1)(1 - t_2)(2 - t_1 - t_2)^4 + 280(2 - t_1 - t_2)^6 + 40$$

from which we obtain

$$\|\Psi_{\partial_1\partial_2 F}\|_{L^1([0,1)^2)} \leq 80.$$

Hence by (22), we obtain the estimate

$$|\widehat{\varphi}(r, r)| \leq \frac{30}{\pi^2} \frac{1}{r^2}$$

from which it follows that

$$\sum_{|r|=N+1}^{\infty} |\widehat{\varphi}(r, r)| \leq \frac{60}{\pi^2} \frac{1}{N}.$$

We next estimate $\widehat{\varphi}(r_1, r_2)$ in the case when $r_1 \neq r_2$. We begin by noting that

$$\widehat{g}_1(r_1 - r_2) = \frac{120}{\pi^2(r_1 - r_2)^2}, \qquad r_1 \neq r_2.$$

We have

$$g_2(t) = 240(1 + 5t(1 - t)), \qquad g_3(t) = 240(-12 - 15t + 20t^2),$$
$$h_2(t) = -40 + 280(1 - t)^6, \qquad h_3(t) = -1680(1 - t)^5,$$
$$\partial_1^2\partial_2^2 F(t_1, t_2) = 14400(2 - t_1 - t_2)^2(5 + t_1^2 + t_2^2 - 5t_1 - 5t_2 + 3t_1 t_2),$$

from which we obtain

$$\widehat{g}_2(r_1 - r_2) = -\frac{600}{\pi^2(r_1 - r_2)^2}, \qquad r_1 \neq r_2,$$

$$|\widehat{h}_2(r_1)| \leq \frac{280}{\pi|r_1|}, \qquad r_1 \neq 0,$$

$$|\widehat{g}_3(r_1 - r_2)| \leq 3080, \qquad |\widehat{h}_3(r_1)| \leq 280, \qquad \|\Psi_{\partial_1^2\partial_2^2 F}\|_1 = 2800.$$

Putting these together, we finally obtain the estimate

$$(24) \qquad |\widehat{\varphi}(r_1, r_2)| \leq \frac{105}{\pi^4} \frac{1}{|r_1 r_2|(r_1 - r_2)^2} + \frac{420}{\pi^4} \frac{1}{r_1^2 r_2^2}.$$

The following is a simple lemma:

LEMMA 3. *For any $N \geq 1$, one has*

$$(25) \qquad \sum_{R=N+1}^{\infty} \sum_{\substack{\max(|r_1|,|r_2|)=R \\ \min(|r_1|,|r_2|)\neq 0}} \frac{1}{r_1^2 r_2^2} < \frac{4\pi^2}{3} \frac{1}{N}$$

and

$$(26) \qquad \sum_{R=N+1}^{\infty} \sum_{\substack{\max(|r_1|,|r_2|)=R \\ \min(|r_1|,|r_2|)\neq 0 \\ r_1\neq r_2}} \frac{1}{|r_1 r_2|(r_1-r_2)^2} < 4\left(\frac{\pi^2}{3}+1\right)\frac{1}{N}.$$

Proof. The first inequality simply follows from

$$\sum_{\substack{\max(|r_1|,|r_2|)=R \\ \min(|r_1|,|r_2|)\neq 0}} \frac{1}{r_1^2 r_2^2} = \frac{8}{R^2}\sum_{r=1}^{R-1}\frac{1}{r^2} \leq \frac{4\pi^2}{3}\frac{1}{R^2}.$$

For the second inequality, we first use the symmetries to write

$$\sum_{\substack{\max(|r_1|,|r_2|)=R \\ \min(|r_1|,|r_2|)\neq 0 \\ r_1\neq r_2}} \frac{1}{|r_1 r_2|(r_1-r_2)^2} = \frac{4}{R}\sum_{r=1}^{R-1}\frac{1}{r(R-r)^2} + \frac{4}{R}\sum_{r=1}^{R}\frac{1}{r(R+r)^2} - \frac{1}{2R^4}.$$

Using the identity

$$\frac{1}{r(R-r)^2} = \frac{1}{Rr(R-r)} + \frac{1}{R(R-r)^2}$$

and the Cauchy–Schwarz inequality we have

$$\frac{4}{R}\sum_{r=1}^{R-1}\frac{1}{r(R-r)^2} = \frac{4}{R^2}\left(\sum_{r=1}^{R-1}\frac{1}{r(R-r)} + \sum_{r=1}^{R-1}\frac{1}{(R-r)^2}\right) < \frac{4\pi^2}{3}\frac{1}{R^2}.$$

For the remaining terms, we use the trivial estimate

$$\frac{4}{R}\sum_{r=1}^{R}\frac{1}{r(R+r)^2} - \frac{1}{2R^4} < \frac{4}{R^2}.$$

Hence

$$\sum_{\substack{\max(|r_1|,|r_2|)=R \\ \min(|r_1|,|r_2|)\neq 0 \\ r_1\neq r_2}} \frac{1}{|r_1 r_2|(r_1-r_2)^2} < 4\left(\frac{\pi^2}{3}+1\right)\frac{1}{R^2},$$

and the result follows. ∎

If we define

$$(27) \qquad C_{\mathrm{main}}(N) = \sum_{R=1}^{N} \sum_{\substack{\max(|r_1|,|r_2|)=R \\ \min(|r_1|,|r_2|)\neq 0}} |\widehat{\varphi}(r_1,r_2)|,$$

then we have

$$(28) \qquad 0 \leq C_{\mathrm{main}} - C_{\mathrm{main}}(N) < \left(\frac{340}{\pi^2} + \frac{420}{\pi^4}\right)\frac{1}{N} < \frac{40}{N}.$$

For $N = 4000$, numerical computation using the formulas (31) and (32) reveals that $C_{\mathrm{main}}(N) = 4.75145\ldots$; hence with the above error estimate, we have

$$(29) \qquad\qquad 4.75145 \leq C_{\mathrm{main}} \leq 4.76146.$$

Explicit expressions for $\widehat{\varphi}(r_1, r_2)$. The following formulas have been computed using Mathematica, though it is also possible to compute them easily using the iterative procedure based on integration by parts which was outlined in this section earlier.

$$(30) \qquad \widehat{\varphi}(r,0) = \frac{15}{4\pi^2 r^2}\left(1 - \frac{6}{\pi^2 r^2} + \frac{45}{\pi^4 r^4} - \frac{135}{\pi^6 r^6}\right)$$
$$- i\,\frac{60}{7\pi^3 r^3}\left(1 + \frac{63}{8\pi^2 r^2} - \frac{315}{8\pi^4 r^4} + \frac{945}{16\pi^6 r^6}\right),$$

$$(31) \qquad \widehat{\varphi}(r,r) = \frac{10}{\pi^2 r^2}\left(1 - \frac{21}{\pi^2 r^2} + \frac{315}{2\pi^4 r^4} - \frac{945}{2\pi^6 r^6}\right)$$
$$+ i\,\frac{55}{\pi^3 r^3}\left(1 - \frac{126}{11\pi^2 r^2} + \frac{630}{11\pi^4 r^4} - \frac{945}{11\pi^6 r^6}\right),$$

$$(32) \quad \widehat{\varphi}(r,s)$$
$$= -\frac{1575}{4\pi^8 r^6 (r-s)^2} + \frac{525}{4\pi^6 r^4 (r-s)^2} - \frac{35}{2\pi^4 r^2 (r-s)^2} - \frac{1575}{4\pi^8 (r-s)^2 s^6}$$
$$+ \frac{225}{2\pi^8 r (r-s)^2 s^5} + \frac{525}{4\pi^6 (r-s)^2 s^4} + \frac{225}{2\pi^8 r^2 (r-s)^2 s^4} + \frac{225}{2\pi^8 r^3 (r-s)^2 s^3}$$
$$- \frac{75}{2\pi^6 r (r-s)^2 s^3} - \frac{35}{2\pi^4 (r-s)^2 s^2} + \frac{225}{2\pi^8 r^4 (r-s)^2 s^2} - \frac{75}{2\pi^6 r^2 (r-s)^2 s^2}$$
$$+ \frac{225}{2\pi^8 r^5 (r-s)^2 s} - \frac{75}{2\pi^6 r^3 (r-s)^2 s} + \frac{5}{\pi^4 r (r-s)^2 s}$$
$$+ i\left(-\frac{1575}{4\pi^9 r^7 (r-s)^2} + \frac{525}{2\pi^7 r^5 (r-s)^2} - \frac{105}{2\pi^5 r^3 (r-s)^2} - \frac{1575}{4\pi^9 (r-s)^2 s^7} \right.$$
$$+ \frac{225}{2\pi^9 r (r-s)^2 s^6} + \frac{525}{2\pi^7 (r-s)^2 s^5} + \frac{225}{2\pi^9 r^2 (r-s)^2 s^5} + \frac{225}{2\pi^9 r^3 (r-s)^2 s^4}$$
$$- \frac{75}{\pi^7 r (r-s)^2 s^4} - \frac{105}{2\pi^5 (r-s)^2 s^3} + \frac{225}{2\pi^9 r^4 (r-s)^2 s^3} - \frac{75}{\pi^7 r^2 (r-s)^2 s^3}$$
$$+ \frac{225}{2\pi^9 r^5 (r-s)^2 s^2} - \frac{75}{\pi^7 r^3 (r-s)^2 s^2} + \frac{15}{\pi^5 r (r-s)^2 s^2} + \frac{225}{2\pi^9 r^6 (r-s)^2 s}$$
$$\left. - \frac{75}{\pi^7 r^4 (r-s)^2 s} + \frac{15}{\pi^5 r^2 (r-s)^2 s} \right).$$

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