

## Note on the Goldbach Conjecture and Landau-Siegel Zeros

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## NOTE ON THE GOLDBACH CONJECTURE AND LANDAU-SIEGEL ZEROS

D. A. GOLDSTON AND ADE IRMA SURIAJAYA

ABSTRACT. We generalize the work of Fei, Bhowmik and Halupczok, and Jia relating the Goldbach conjecture to real zeros of Dirichlet  $L$ -functions.

## 1. INTRODUCTION

Let

$$(1.1) \quad \psi_2(n) = \sum_{m+m'=n} \Lambda(m)\Lambda(m'),$$

where  $\Lambda$  is the von Mangoldt function, defined by  $\Lambda(n) = \log p$  if  $n = p^m$ ,  $p$  a prime and  $m \geq 1$ , and  $\Lambda(n) = 0$  otherwise. Thus  $\psi_2(n)$  counts the “Goldbach” representations of  $n$  as sums of both primes and prime powers, and these primes are weighted to make them have a “density” of 1 on the integers.

Hardy and Littlewood [HL22] conjectured that, for  $n$  even

$$(1.2) \quad \psi_2(n) \sim \mathfrak{S}(n)n, \quad \text{as } n \rightarrow \infty,$$

where

$$(1.3) \quad \mathfrak{S}(k) = \begin{cases} 2C_2 \prod_{\substack{p|k \\ p>2}} \left( \frac{p-1}{p-2} \right) & \text{if } k \text{ is even, } k \neq 0, \\ 0 & \text{if } k \text{ is odd} \end{cases}$$

and

$$(1.4) \quad C_2 = \prod_{p>2} \left( 1 - \frac{1}{(p-1)^2} \right) = 0.66016\dots$$

When  $n$  is odd then the only possible non-zero terms in the sum in (1.1) are when  $m$  or  $m'$  is a power of 2, and since there are  $\ll \log n$  such terms we have

$$(1.5) \quad \psi_2(n) \ll \log^2 n, \quad \text{for } n \text{ odd.}$$

In this paper we will use the following weaker form of (1.2).

**Weak Hardy-Littlewood Goldbach Conjecture.** *Given a fixed constant  $0 < \delta < 1$ , then for sufficiently large even  $n$ , we have  $|\psi_2(n) - \mathfrak{S}(n)n| \leq (1 - \delta)\mathfrak{S}(n)n$ . Equivalently, we have*

$$(1.6) \quad \text{(A) } \delta\mathfrak{S}(n)n \leq \psi_2(n), \quad \text{and} \quad \text{(B) } \psi_2(n) \leq (2 - \delta)\mathfrak{S}(n)n.$$

We show this conjecture implies that a sequence of Landau-Siegel zeros can only slowly approach 1.

**Theorem 1.** *Assume the Weak Hardy-Littlewood Goldbach Conjecture. Let  $q$  be sufficiently large, and suppose that  $\chi_1$  is the single real character (mod  $q$ ), if it exists, for which  $L(s, \chi_1)$  has a real zero  $\beta_1$  satisfying  $1 - c/\log q < \beta_1$  for a certain positive absolute constant  $c$ . Then we have  $\beta_1 < 1 - C(\delta)/\log^2 q$ , where  $C(\delta)$  is a positive effective constant that depends on  $\delta$ . In particular, if  $\chi(-1) = -1$  then this follows from (A) in (1.6), and if  $\chi(-1) = 1$  then this follows from (B) in (1.6).*

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Fei [Fei16] obtained this result when  $q$  is taken to be a prime  $q \equiv 3 \pmod{4}$ . Bhowmik and Halupczok [BH20] obtained the theorem when  $\chi(-1) = -1$ ; actually they use a slightly different form of (A) in (1.6) which is weaker when  $q$  has many prime factors, and the corresponding result on real zeros is consequently also slightly weaker for these  $q$ . Jia [Jia20] noticed this in the original preprint of [BH20] and then used (A) in (1.6) to prove precisely the result in the theorem above when  $\chi(-1) = -1$ . It should also be pointed out that Bhowmik and Halupczok proved their result when the Weak Goldbach Conjecture is allowed to not hold on a certain exceptional set. In a recent talk Bhowmik mentioned as a goal proving the current theorem when  $\chi(-1) = 1$  using (B) of (1.6).

We follow the method of Fei [Fei16] and Bhowmik and Halupczok [BH20], but make use of power series generating functions instead of exponential generating functions, which makes possible the use of the upper bound (B) in (1.6). By rearranging the earlier proofs we are also able to remove the need for Gaussian sums in our proof.

With minor adjustments to our proof, we can prove a form of Theorem 1 using a prime-pair conjecture in place of the Goldbach conjecture. For  $k \geq 0$  let

$$(1.7) \quad \psi_2(x, k) := \sum_{n \leq x} \Lambda(n) \Lambda(n - k) = \sum_{k < n \leq x} \Lambda(n) \Lambda(n - k).$$

The Hardy-Littlewood conjecture we need here is that, for even  $2 \leq k \leq x$ ,

$$(1.8) \quad \psi_2(x, k) = \mathfrak{S}(k)(x - k) + o(\mathfrak{S}(k)x).$$

Note that this is true in the range  $x - o(x) \leq k \leq x$  by a standard sieve result [HR11, Cor. 5.8.1]. If  $k$  is odd then in the same way we obtained (1.5) we have

$$(1.9) \quad \psi_2(x, k) \ll \log^2 x.$$

The conjecture we need is an upper bound that is slightly smaller than twice the conjectured main term.

**Hardy-Littlewood Prime-Pair Upper Bound Conjecture.** *Given a fixed constant  $0 < \delta < 1$ , then for even  $2 \leq k \leq x$  and sufficiently large  $x$ , we have*

$$(1.10) \quad \psi_2(x, k) \leq (2 - \delta)\mathfrak{S}(k)(x - k) + o(\mathfrak{S}(k)x).$$

**Theorem 2.** *Theorem 1 holds if we replace the Weak Hardy-Littlewood Goldbach Conjecture with the Hardy-Littlewood Prime-Pair Upper Bound Conjecture.*

## 2. EVALUATING $\mathcal{S}(q)$ IN TWO WAYS

Here all sums run over the positive integers unless specified otherwise. We use the power series generating function

$$(2.1) \quad \Psi(z) = \sum_n \Lambda(n) z^n, \quad z = re(\alpha), \quad e(\alpha) = e^{2\pi i \alpha},$$

for  $|z| = r < 1$ . Squaring, we have

$$(2.2) \quad \Psi(z)^2 = \sum_{m, m'} \Lambda(m) \Lambda(m') z^{m+m'} = \sum_n \psi_2(n) z^n.$$

Fei's idea is equivalent in this setting to computing

$$(2.3) \quad \mathcal{S}(q) := \frac{1}{q} \sum_{a=1}^q \Psi(re(a/q))^2$$

in two ways. First, using (2.2) and  $\frac{1}{q} \sum_{a=1}^q e(an/q) = \mathbb{1}_{q|n}$ , we have

$$(2.4) \quad \mathcal{S}(q) = \frac{1}{q} \sum_{a=1}^q \sum_n \psi_2(n) r^n e(an/q) = \sum_{\substack{n \\ q|n}} \psi_2(n) r^n.$$

Summing  $\psi_2(n)$  over multiples of  $q$  is a problem that has already occurred in [Gran07], [Gran08], and [BHMS19].

To obtain the second formula for  $\mathcal{S}(q)$ , as in the circle method we separate the terms in  $\Psi(re(a/q))$  according to the arithmetic progressions they belong to modulo  $q$ . Letting

$$(2.5) \quad \Psi(r; q, b) := \sum_{\substack{n \\ n \equiv b \pmod{q}}} \Lambda(n)r^n,$$

we have

$$\Psi(re(a/q)) = \sum_{b=1}^q \sum_{\substack{n \\ n \equiv b \pmod{q}}} \Lambda(n)r^n e(an/q) = \sum_{b=1}^q e(ab/q)\Psi(r; q, b),$$

and therefore

$$\begin{aligned} \mathcal{S}(q) &= \frac{1}{q} \sum_{a=1}^q \sum_{\substack{1 \leq b, b' \leq q \\ q|b+b'}} e(a(b+b')/q)\Psi(r; q, b)\Psi(r; q, b') \\ &= \sum_{\substack{1 \leq b, b' \leq q \\ q|b+b'}} \Psi(r; q, b)\Psi(r; q, b'). \end{aligned}$$

The conditions on  $b$  and  $b'$  in the last sum imply that  $b' = q - b$  for  $1 \leq b \leq q - 1$  or  $b = b' = q$ , and therefore we conclude, since  $\Psi(r; q, q - b) = \Psi(r; q, -b)$ ,

$$(2.6) \quad \mathcal{S}(q) = \sum_{b=1}^q \Psi(r; q, b)\Psi(r; q, -b).$$

### 3. EVALUATING $\mathcal{S}(q)$ USING THE GOLDBACH CONJECTURE

Letting

$$(3.1) \quad r = e^{-1/N},$$

then on taking  $n = qk$  and using (1.5) we have

$$\mathcal{S}(q) \stackrel{(2.4)}{=} \sum_{\substack{n \\ q|n}} \psi_2(n)r^n = \sum_k \mathbb{1}_{2|qk} \psi_2(qk)e^{-qk/N} + O\left(\sum_n (\log^2 n)e^{-n/N}\right) = \sum_k \mathbb{1}_{2|qk} \psi_2(qk)e^{-qk/N} + O(N \log^2 N).$$

From now on we specify that

$$(3.2) \quad 1 \leq q \leq N.$$

Letting

$$(3.3) \quad V_q(N) := q \sum_k \mathfrak{S}(qk)ke^{-qk/N},$$

we conclude from (1.6) that the Weak Goldbach Conjecture implies

$$(3.4) \quad \delta V_q(N) + O(N \log^2 N) \leq \mathcal{S}(q) \leq (2 - \delta)V_q(N) + O(N \log^2 N).$$

To evaluate  $V_q(N)$ , we need a formula for the singular series average

$$(3.5) \quad G_q(x) := \sum_{k \leq x} \mathfrak{S}(qk).$$

**Lemma 1** (Montgomery). *For  $x \geq 1$  we have*

$$(3.6) \quad G_q(x) = \frac{q}{\phi(q)}x + O\left(\frac{q}{\phi(q)} \log 2x\right)$$

*uniformly for all  $q \geq 1$ .*

This lemma follows from [Mon71, Lemma 17.4]; we will give a complete proof in Section 6. Writing Lemma 1 in the form  $G_q(x) = \frac{q}{\phi(q)}x + R_q(x)$  for  $x \geq 1$ , we obtain by partial summation

$$\begin{aligned} V_q(N) &= q \int_{1^-}^{\infty} ue^{-qu/N} dG_q(u) \\ &= \frac{q^2}{\phi(q)} \int_1^{\infty} ue^{-qu/N} du + q \int_{1^-}^{\infty} ue^{-qu/N} dR_q(u) \\ &:= I_1 + I_2. \end{aligned}$$

Using the condition  $1 \leq q \leq N$ , we have on letting  $v = qu/N$

$$\begin{aligned} I_1 &= \frac{N^2}{\phi(q)} \int_{q/N}^{\infty} ve^{-v} dv \\ &= \frac{N^2}{\phi(q)} \left( \int_0^{\infty} ve^{-v} dv + O\left(\frac{q}{N}\right) \right) \\ &= \frac{N^2}{\phi(q)} + O\left(\frac{qN}{\phi(q)}\right). \end{aligned}$$

Next, integrating by parts and using  $R_q(x) \ll \frac{q}{\phi(q)} \log(2x)$ , we have

$$\begin{aligned} I_2 &= O\left(\frac{q^2}{\phi(q)} e^{-q/N}\right) - q \int_1^{\infty} \left(1 - \frac{q}{N}u\right) e^{-qu/N} R_q(u) du \\ &\ll \frac{q^2}{\phi(q)} + \frac{q^2}{\phi(q)} \int_1^{N/q} e^{-qu/N} \log(2u) du + \frac{q^3}{\phi(q)N} \int_{N/q}^{\infty} ue^{-qu/N} \log(2u) du \\ &\ll \frac{q^2}{\phi(q)} + \frac{q}{\phi(q)} N \log(2N/q) + \frac{qN}{\phi(q)} \int_1^{\infty} ve^{-v} \log(2Nv/q) dv \\ &\ll \frac{q^2}{\phi(q)} + \frac{q}{\phi(q)} N \log(2N/q). \end{aligned}$$

Since

$$(3.7) \quad \frac{q}{\phi(q)} \ll \log \log 3q \stackrel{(3.2)}{\ll} \log \log N$$

holds, we conclude that

$$(3.8) \quad V_q(N) = \frac{N^2}{\phi(q)} + O(N \log N \log \log N).$$

Thus by (3.4)

$$(3.9) \quad \delta \frac{N^2}{\phi(q)} + O(N \log^2 N) \leq \mathcal{S}(q) \leq (2 - \delta) \frac{N^2}{\phi(q)} + O(N \log^2 N).$$

#### 4. EVALUATING $\mathcal{S}(q)$ USING THE PRIME NUMBER THEOREM FOR ARITHMETIC PROGRESSIONS

Let

$$(4.1) \quad \psi(x; q, a) := \sum_{\substack{n \leq x \\ n \equiv a \pmod{q}}} \Lambda(n).$$

We will make use of the prime number theorem for arithmetic progressions for a modulus  $q$  which has a possible exceptional real character  $\chi_1$  as described in our theorem. By [MV07, Cor. 11.17], we have that there is a positive constant  $c_1$  such that for  $(a, q) = 1$

$$(4.2) \quad \psi(x; q, a) = \frac{x}{\phi(q)} - \frac{\chi_1(a)x^{\beta_1}}{\phi(q)\beta_1} + O(xe^{-c_1\sqrt{\log x}}).$$

As explained in [MV07, proof of Corollary 11.17], a bound on  $q$  such as  $q \leq e^{2c_1\sqrt{\log x}}$  which is usually imposed on (4.2) is not needed because  $\psi(x; q, a)$  trivially satisfies a smaller bound than the right-hand side of (4.2) when  $q \geq e^{2c_1\sqrt{\log x}}$ . Thus by partial summation we have using (2.5) and (3.1) that, with  $(b, q) = 1$ ,

$$\begin{aligned}\Psi(r; q, b) &= \sum_{n \equiv b \pmod{q}} \Lambda(n) e^{-n/N} = \int_{2^-}^{\infty} e^{-u/N} d\psi(u; q, b) \\ &= \int_0^{\infty} e^{-u/N} \left( \frac{1}{\phi(q)} - \frac{\chi_1(b) u^{\beta_1-1}}{\phi(q)} \right) du + O\left( \frac{1}{N} \int_2^{\infty} u e^{-u/N} e^{-c_1\sqrt{\log u}} du \right) \\ &= \frac{N}{\phi(q)} \int_0^{\infty} e^{-t} dt + \frac{\chi_1(b) N^{\beta_1}}{\phi(q)} \int_0^{\infty} t^{\beta_1-1} e^{-t} dt + O(N e^{-c_1\sqrt{\log N}}).\end{aligned}$$

Recalling the gamma function

$$(4.3) \quad \Gamma(s) = \int_0^{\infty} t^{s-1} e^{-t} dt, \quad \operatorname{Re}(s) > 0,$$

we conclude, for  $(b, q) = 1$ ,

$$(4.4) \quad \Psi(r; q, b) = \frac{N}{\phi(q)} + \frac{\chi_1(b) \Gamma(\beta_1) N^{\beta_1}}{\phi(q)} + O(N e^{-c_1\sqrt{\log N}}).$$

To apply this result to  $\mathcal{S}(q)$ , we first show that

$$(4.5) \quad \mathcal{S}(q) \stackrel{(2.6)}{=} \sum_{b=1}^q \Psi(r; q, b) \Psi(r; q, -b) = \sum_{\substack{1 \leq b \leq q \\ (b, q)=1}} \Psi(r; q, b) \Psi(r; q, -b) + O(q(\log q \log N)^2),$$

which follows immediately from

$$(4.6) \quad \Psi(r; q, b) \ll \log q \log N, \quad \text{when } (b, q) = d > 1.$$

To prove this estimate, first note that when  $(b, q) = d > 1$ ,

$$\Psi(r; q, b) = \sum_{\substack{n \equiv b \pmod{q} \\ (b, q)=d > 1}} \Lambda(n) r^n = \sum_{d|n} \Lambda(n) r^n = \sum_m \Lambda(dm) r^{dm}.$$

Now  $\Lambda(dm) = \log p$  if and only if  $dm = p^j$ ,  $j \geq 1$  while  $\Lambda(dm) = 0$  otherwise. Therefore

$$\Psi(r; q, b) \leq \log q \sum_j e^{-2^j/N}.$$

The estimate (4.6) now follows from

$$(4.7) \quad \sum_j e^{-2^j/N} \ll \sum_{j < 2 \log N} 1 + \sum_{j \geq 2 \log N} e^{-2^j/N} \ll \log N,$$

since for the second sum on the right-hand side we have  $e^{-2^j/N} < 1/e < 1/2$  and also  $e^{-2^{j+k}/N} = (e^{-2^j/N})^{2^k}$ ; therefore

$$\sum_{j \geq 2 \log N} e^{-2^j/N} < 1/2 + 1/2^2 + 1/2^4 + 1/2^8 + \dots < 1.$$

We now compute  $\mathcal{S}(q)$ . First, by (4.4) when  $(b, q) = 1$  we obtain

$$\begin{aligned}\Psi(r; q, b) \Psi(r; q, -b) &= \frac{N^2}{\phi(q)^2} + \frac{N^{1+\beta_1} \Gamma(\beta_1)}{\phi(q)^2} (\chi_1(b) + \chi_1(-b)) + \frac{\chi_1(b) \chi_1(-b) \Gamma(\beta_1)^2 N^{2\beta_1}}{\phi(q)^2} \\ &\quad + O\left( \frac{N^2 e^{-c_1\sqrt{\log N}}}{\phi(q)} \right) + O\left( N^2 e^{-2c_1\sqrt{\log N}} \right).\end{aligned}$$

Thus

$$\sum_{\substack{1 \leq b \leq q \\ (b, q) = 1}} \Psi(r; q, b) \Psi(r; q, -b) = \frac{N^2}{\phi(q)} + \frac{\chi_1(-1) \Gamma(\beta_1)^2 N^{2\beta_1}}{\phi(q)} + O\left(N^2 e^{-c_1 \sqrt{\log N}}\right) + O\left(\phi(q) N^2 e^{-2c_1 \sqrt{\log N}}\right),$$

where we used the fact that the sum of a Dirichlet character over a reduced residue class vanishes, and that  $\chi_1$  is a real character so that  $\chi_1(b)\chi_1(-b) = \chi_1(-1)$ . Anticipating our choice of  $N$  in the next section, we now take  $q \leq e^{c_1 \sqrt{\log N}}$ . Next we apply (4.5), and since the error term  $O(q(\log q \log N)^2)$  from that equation and the last error term above may both be absorbed into the first error term, we conclude

$$(4.8) \quad \mathcal{S}(q) = \frac{N^2}{\phi(q)} + \frac{\chi_1(-1) \Gamma(\beta_1)^2 N^{2\beta_1}}{\phi(q)} + O(N^2 e^{-c_1 \sqrt{\log N}}).$$

## 5. PROOF OF THEOREM 1

We will now prove the following more precise version of Theorem 1.

**Theorem 3.** *Assume the Weak Goldbach Conjecture with a given fixed  $0 < \delta < 1$ . For  $q$  sufficiently large suppose  $\chi_1$  is a real character modulo  $q$  for which  $L(s, \chi_1)$  has a real zero  $\beta_1$  with  $1 - c/\log q < \beta_1$  for a positive constant  $c$ . Let  $c_1$  be the positive constant in the prime number theorem for arithmetic progressions (4.2). Then for any fixed positive constant  $c' < c_1$  we have*

$$(5.1) \quad \beta_1 < 1 - \frac{\frac{1}{2}(c')^2 \log\left(\frac{1}{1-\delta}\right)}{\log^2 q}.$$

*Proof of Theorem 3.* We substitute (4.8) into (3.9) and obtain

$$\delta \frac{N^2}{\phi(q)} + O(N \log N) \leq \frac{N^2}{\phi(q)} + \frac{\chi_1(-1) \Gamma(\beta_1)^2 N^{2\beta_1}}{\phi(q)} + O(N^2 e^{-c_1 \sqrt{\log N}}) \leq (2 - \delta) \frac{N^2}{\phi(q)} + O(N \log^2 N),$$

and therefore

$$-(1 - \delta) + O(\phi(q) e^{-c_1 \sqrt{\log N}}) \leq \chi_1(-1) \Gamma(\beta_1)^2 N^{2(\beta_1 - 1)} \leq (1 - \delta) + O(\phi(q) e^{-c_1 \sqrt{\log N}}).$$

If  $\chi(-1) = -1$  then from the lower bound above we obtain

$$(5.2) \quad \Gamma(\beta_1)^2 N^{2(\beta_1 - 1)} \leq (1 - \delta) + O(\phi(q) e^{-c_1 \sqrt{\log N}}),$$

while if  $\chi(-1) = 1$  the upper bound above gives (5.2). Thus (5.2) holds in both cases.

Now choose  $c' > 0$  to be any fixed constant with  $c' < c_1$  and a second constant  $c''$  such that  $c' < c'' < c_1$ . Defining  $N$  by

$$\log N := \left( \frac{1}{c''} \log q \right)^2,$$

so that  $N \rightarrow \infty$  as  $q \rightarrow \infty$ . Solving for  $q$  we have  $q = e^{c'' \sqrt{\log N}}$ , which verifies our earlier use of the inequality  $q \leq e^{c_1 \sqrt{\log N}}$ . Further notice that the error term in (5.2) is  $o(1)$  as  $q \rightarrow \infty$  since

$$\phi(q) e^{-c_1 \sqrt{\log N}} \leq e^{-(c_1 - c'') \sqrt{\log N}} = o(1).$$

Rewriting (5.2) we obtain

$$\beta_1 \leq 1 + \frac{\log\left(\frac{1-\delta+o(1)}{\Gamma(\beta_1)^2}\right)}{2 \log N} = 1 - \frac{\frac{1}{2}(c'')^2 \log\left(\frac{\Gamma(\beta_1)^2}{1-\delta+o(1)}\right)}{\log^2 q}.$$

It is easy to verify from the definition of the gamma function  $\Gamma(s)$  given in (4.3) that  $\Gamma'(s)$  is analytic when  $\operatorname{Re}(s) > 0$  and since  $1 - c/\log q \leq \beta_1 < 1$  and  $\Gamma(1) = 1$  we see by the mean value theorem that  $\Gamma(\beta_1) = 1 + O(1/\log q) = 1 + o(1)$  as  $q \rightarrow \infty$ . We conclude

$$\beta_1 \leq 1 - \frac{\frac{1}{2}(c'')^2 \log\left(\frac{1+o(1)}{1-\delta+o(1)}\right)}{\log^2 q} < 1 - \frac{\frac{1}{2}(c')^2 \log\left(\frac{1}{1-\delta}\right)}{\log^2 q}$$

on taking  $q$  sufficiently large, which proves Theorem 3.  $\square$

## 6. PROOF OF LEMMA 1

*Proof.* We define

$$(6.1) \quad H_q(k) := \prod_{\substack{p|k \\ (p,2q)=1}} \left( \frac{p-1}{p-2} \right),$$

and take  $H(k) := H_1(k)$ . Thus we can rewrite (1.3) as

$$(6.2) \quad \mathfrak{S}(k) = \mathbb{1}_{2|k} 2C_2 H(k).$$

Since clearly

$$(6.3) \quad H(qk) = H(q)H_q(k),$$

we have

$$G_q(x) = \sum_{k \leq x} \mathfrak{S}(qk) = 2C_2 H(q) \sum_{k \leq x} \mathbb{1}_{2|qk} H_q(k).$$

Using  $\mathbb{1}_{2|qk} = \mathbb{1}_{2|q} + \mathbb{1}_{2 \nmid q} \mathbb{1}_{2|k}$ , we have

$$G_q(x) = 2C_2 H(q) \left( \mathbb{1}_{2|q} \sum_{k \leq x} H_q(k) + \mathbb{1}_{2 \nmid q} \sum_{\substack{k \leq x \\ 2|k}} H_q(k) \right).$$

Writing

$$(6.4) \quad \tilde{G}_q(x) := \sum_{k \leq x} H_q(k),$$

we conclude, on noting  $H_q(2k) = H_q(k)$ , that

$$(6.5) \quad G_q(x) = 2C_2 H(q) \left( \mathbb{1}_{2|q} \tilde{G}_q(x) + \mathbb{1}_{2 \nmid q} \tilde{G}_q(x/2) \right).$$

We will prove below that

$$(6.6) \quad \tilde{G}_q(x) = \frac{q}{(2,q)\phi(q)C_2 H(q)} x + O(\log 2x),$$

which on substituting into (6.5) gives immediately

$$G_q(x) = \frac{q}{\phi(q)} x + O(H(q) \log 2x).$$

Lemma 1 now follows from the estimate  $H(q) \ll q/\phi(q)$  which can be verified by the calculation

$$(6.7) \quad \frac{\phi(q)}{q} H(q) = \frac{1}{(2,q)} \prod_{\substack{p|q \\ p>2}} \left( 1 - \frac{1}{p} \right) \left( \frac{p-1}{p-2} \right) \leq \prod_{p>2} \left( 1 + \frac{1}{p(p-2)} \right) \ll 1.$$

□

*Proof of (6.6).* We give an expanded version of Montgomery's very nice proof [Mon71, Lemma 17.4]. First,

$$H_q(k) = \prod_{\substack{p|k \\ (p,2q)=1}} \left( 1 + \frac{1}{p-2} \right) = \sum_{d|k} f_q(d),$$

where

$$f_q(d) = \mathbb{1}_{(d,2q)=1} \mu(d)^2 \prod_{p|d} \left( \frac{1}{p-2} \right).$$

Hence

$$\begin{aligned}
\tilde{G}_q(x) &= \sum_{k \leq x} \sum_{d|k} f_q(d) \\
&= \sum_{d \leq x} f_q(d) \sum_{\substack{k \leq x \\ d|k}} 1 \\
(6.8) \quad &= x \sum_{d \leq x} \frac{f_q(d)}{d} + O\left(\sum_{d \leq x} f_q(d)\right) \\
&= x \sum_{d=1}^{\infty} \frac{f_q(d)}{d} + O\left(x \sum_{d > x} \frac{f_1(d)}{d}\right) + O\left(\sum_{d \leq x} f_1(d)\right).
\end{aligned}$$

Since  $f_q(d)$  is multiplicative and  $d$  square-free, recalling the equality (6.7), we have

$$\begin{aligned}
\sum_{d=1}^{\infty} \frac{f_q(d)}{d} &= \prod_p \left(1 + \frac{f_q(p)}{p}\right) \\
&= \prod_{\substack{p \\ (p, 2q)=1}} \left(1 + \frac{1}{p(p-2)}\right) \\
&= \prod_{p > 2} \left(1 + \frac{1}{p(p-2)}\right) \prod_{\substack{p|q \\ p > 2}} \left(1 + \frac{1}{p(p-2)}\right)^{-1} \\
&= \frac{1}{C_2} \prod_{\substack{p|q \\ p > 2}} \left(\frac{p(p-2)}{(p-1)^2}\right) \\
&= \frac{q}{(2, q)\phi(q)C_2H(q)},
\end{aligned}$$

which gives the main term in (6.6). For the two error terms above, we see that  $f_1(d) = \mu(d)^2/\phi_2(d)$ , where  $\phi_2(p) := p - 2$  and this is extended to  $\phi_2(d)$  for squarefree  $d$  with  $(d, 2) = 1$  by multiplicativity. Thus

$$\begin{aligned}
S(x, f_1) &:= \sum_{d \leq x} f_1(d) = \sum_{\substack{d \leq x \\ (d, 2)=1}} \frac{\mu(d)^2}{\phi_2(d)} \\
&\ll \prod_{2 < p \leq x} \left(1 + \frac{1}{p-2}\right) \\
&= \exp\left(\sum_{2 < p \leq x} \log\left(1 + \frac{1}{p-2}\right)\right) \\
&\ll \exp\left(\sum_{p \leq x} \frac{1}{p}\right) \ll \exp(\log \log 2x + O(1)) \ll \log 2x,
\end{aligned}$$

by Mertens formula. Finally by partial summation

$$\sum_{d > x} \frac{f_1(d)}{d} = \int_{x+}^{\infty} \frac{dS(u, f_1)}{u} \ll \frac{\log 2x}{x} + \int_x^{\infty} \frac{\log 2u}{u^2} du \ll \frac{\log 2x}{x}.$$

Using these estimates in (6.8) completes the proof of (6.6).  $\square$

## 7. PROOF OF THEOREM 2

Define

$$(7.1) \quad \Psi_2(r, k) := \sum_n \Lambda(n) \Lambda(n-k) r^{2n-k}.$$

Then in place of (2.2) we have, on letting  $k = n - n'$ ,

$$|\Psi_2(z)|^2 = \sum_{n, n'} \Lambda(n) \Lambda(n') r^{n+n'} e((n-n')\alpha) = \sum_{k=-\infty}^{\infty} \Psi_2(r, k) e(k\alpha).$$

Since  $\Psi_2(r, k) = \Psi_2(r, -k)$ , we have

$$(7.2) \quad |\Psi_2(z)|^2 = \Psi_2(r, 0) + 2\operatorname{Re} \sum_k \Psi_2(r, k) e(k\alpha).$$

Recalling that  $r = e^{-1/N} < 1$  from (3.1), we first show that, for odd  $k \geq 1$ ,

$$(7.3) \quad \Psi_2(r, k) \ll e^{-k/N} \log^2 N + (\log k) e^{-k/N} \log N,$$

which corresponds to (1.9). To prove this, note first that  $\Lambda(n-k) = 0$  for  $k \geq n$ . Next, for  $k \geq 1$  odd,  $\Lambda(n)\Lambda(n-k) = 0$  holds i) if  $n$  is even and  $n \neq 2^j$ , or ii) if  $n$  is odd and  $n-k \neq 2^j$ . Hence

$$\begin{aligned} \Psi_2(r, k) &= (\log 2) \sum_{k < 2^j} \Lambda(2^j - k) r^{2^j + (2^j - k)} + (\log 2) \sum_j \Lambda(2^j + k) r^{2^j + 1 + k} \\ &\ll e^{-k/N} \left( \sum_{k < 2^j} \log(2^j - k) e^{-(2^j - k)/N} + \sum_j \log(2^j + k) e^{-2^j + 1 + k/N} \right). \end{aligned}$$

To estimate these last two sums we use  $\sum_j e^{-2^j/N} \ll \log N$  from (4.7) together with the estimate  $\sum_j j e^{-2^j/N} \ll \log^2 N$  obtained immediately by the argument used to obtain (4.7). For the first sum there is one  $j$  satisfying  $k < 2^j \leq 2k$  and therefore we have

$$\sum_{k < 2^j \leq 2k} \log(2^j - k) e^{-(2^j - k)/N} \ll \log k.$$

For  $2^j > 2k$ , we have  $2^j - k > 2^j - 2^{j-1} = 2^{j-1}$ , and therefore

$$\sum_{2k < 2^j} \log(2^j - k) e^{-(2^j - k)/N} \ll \sum_j j e^{-2^{j-1}/N} \ll \log^2 N.$$

For the second sum, since  $\log(2^j + k) \ll j + \log k$ , we have

$$\sum_j \log(2^j + k) e^{-2^j + 1 + k/N} \ll \sum_j (j + \log k) e^{-2^j/N} \ll \log^2 N + (\log k)(\log N).$$

Substituting we have

$$\Psi_2(r, k) \ll e^{-k/N} (\log^2 N + (\log k)(\log N))$$

which proves (7.3).

Next

$$\Psi_2(r, 0) = \sum_n \Lambda(n)^2 r^{2n} \leq \sum_n \Lambda(n) (\log n) e^{-2n/N}.$$

Letting  $\psi(x) := \sum_{n \leq x} \Lambda(n)$  and using the Chebyshev bound  $\psi(x) \ll x$  we have by partial summation

$$(7.4) \quad \begin{aligned} \Psi_2(r, 0) &\ll \int_2^\infty \psi(u) \frac{d}{du} \left( (\log u) e^{-2u/N} \right) du \\ &\ll \int_2^\infty u e^{-2u/N} \left( \frac{1}{u} + \frac{2}{N} \log u \right) du \\ &\ll \log N \int_2^N e^{-2u/N} du + \frac{1}{N} \int_N^\infty (u \log u) e^{-2u/N} du \\ &\ll N \log N. \end{aligned}$$

For  $k \geq 2$  even, we use partial summation with  $\psi_2(x, k)$  and the upper bound conjecture (1.10) to obtain

$$\begin{aligned}
(7.5) \quad \Psi_2(r, k) &= - \int_k^\infty \psi_2(u, k) \frac{d}{du} e^{-(2u-k)/N} du = \frac{2e^{-k/N}}{N} \int_k^\infty \psi_2(u, k) e^{-2(u-k)/N} du \\
&\leq \frac{2(2-\delta)\mathfrak{S}(k)e^{-k/N}}{N} \int_k^\infty ((u-k) + o(u)) e^{-2(u-k)/N} du \\
&= \frac{2-\delta}{2} \mathfrak{S}(k) N e^{-k/N} \int_0^\infty (v + o(v) + o(k/N)) e^{-v} dv \\
&= \frac{2-\delta}{2} \mathfrak{S}(k) N e^{-k/N} (1 + o(1) + o(k/N)).
\end{aligned}$$

Corresponding to  $\mathcal{S}(q)$  in (2.3), we define

$$(7.6) \quad \mathcal{T}(q) := \frac{1}{q} \sum_{a=1}^q |\Psi_2(re(a/q))|^2$$

and have by (7.2) that

$$\mathcal{T}(q) = \Psi_2(r, 0) + 2 \sum_{\substack{k \\ q|k}} \Psi_2(r, k) = \Psi_2(r, 0) + 2 \sum_j \Psi_2(r, qj).$$

Applying our estimates (7.3), (7.4), and (7.5) for  $\Psi_2(r, k)$ , and recalling  $1 \leq q \leq N$  by (3.2), we have

$$\begin{aligned}
\mathcal{T}(q) &\leq O(N \log N) + (2-\delta)N \sum_j \mathfrak{S}(qj) e^{-qj/N} (1 + o(1) + o(qj/N)) \\
&\quad + O\left( (\log^2 N) \sum_j e^{-qj/N} + (\log N) \sum_j \log(qj) e^{-qj/N} \right) \\
&\leq (2-\delta)N(1 + o(1)) \sum_j \mathfrak{S}(qj) e^{-qj/N} + o(V_q(N)) + O(N \log^2 N),
\end{aligned}$$

where  $V_q(N)$  is defined in (3.3) and by (3.8)  $V_q(N) = \frac{N^2}{\phi(q)} + O(N \log N \log \log N)$ . We show below that

$$(7.7) \quad \sum_j \mathfrak{S}(qj) e^{-qj/N} = \frac{N}{\phi(q)} + O(\log N \log \log N),$$

and thus we conclude

$$(7.8) \quad \mathcal{T}(q) \leq (2-\delta) \frac{N^2}{\phi(q)} (1 + o(1)) + O(N \log^2 N).$$

The calculation for (7.7) is nearly the same as the earlier one for obtaining (3.8). We have

$$\begin{aligned}
\sum_j \mathfrak{S}(qj) e^{-qj/N} &= \int_{1^-}^\infty e^{-qu/N} dG_q(u) \\
&= \frac{q}{\phi(q)} \int_1^\infty e^{-qu/N} du + \int_{1^-}^\infty e^{-qu/N} dR_q(u) \\
&= \frac{N}{\phi(q)} \int_{q/N}^\infty e^{-v} dv + O\left( \frac{q^2}{\phi(q)N} \int_1^\infty e^{-qu/N} \log 2u du \right) \\
&= \frac{N}{\phi(q)} + O\left( \frac{q}{\log q} \right) + O\left( \frac{q}{\phi(q)} \log(2N/q) \right) = \frac{N}{\phi(q)} + O\left( \frac{q}{\phi(q)} \log N \right).
\end{aligned}$$

Combining this with (3.7) gives (7.7).

The evaluation of  $\mathcal{T}(q)$  using the prime number theorem for arithmetic progressions is almost identical to the earlier evaluation of  $\mathcal{S}(q)$ . Using

$$\Psi(re(a/q)) = \sum_{b=1}^q e(ab/q) \Psi(r; q, b)$$

in (7.6), we have

$$\begin{aligned}
\mathcal{T}(q) &= \frac{1}{q} \sum_{a=1}^q \sum_{1 \leq b, b' \leq q} e(a(b-b')/q) \Psi(r; q, b) \Psi(r; q, b') \\
&= \sum_{\substack{1 \leq b, b' \leq q \\ q | b-b'}} \Psi(r; q, b) \Psi(r; q, b') \\
&= \sum_{b=1}^q \Psi(r; q, b)^2 = \sum_{\substack{1 \leq b \leq q \\ (b, q)=1}} \Psi(r; q, b)^2 + O(q(\log q \log N)^2),
\end{aligned}$$

on using (4.6). From (4.4) we obtain

$$\Psi(r; q, b)^2 = \frac{N^2}{\phi(q)^2} + \frac{2\chi_1(b)N^{1+\beta_1}\Gamma(\beta_1)}{\phi(q)^2} + \frac{\Gamma(\beta_1)^2 N^{2\beta_1}}{\phi(q)^2} + O\left(\frac{N^2 e^{-c_1\sqrt{\log N}}}{\phi(q)}\right) + O\left(N^2 e^{-2c_1\sqrt{\log N}}\right),$$

and substituting this into the previous equation and noting the term with  $\chi_1(b)$  vanishes when summed, we obtain as before

$$(7.9) \quad \mathcal{T}(q) = \frac{N^2}{\phi(q)} + \frac{\Gamma(\beta_1)^2 N^{2\beta_1}}{\phi(q)} + O(N^2 e^{-c_1\sqrt{\log N}}),$$

which is the same as the result for  $\mathcal{S}(q)$  when  $\chi(-1) = 1$ . Combining (7.8) and (7.9) we obtain (5.2). The proof of Theorem 3 (and thus of Theorem 1) then follows as before. This concludes the proof of Theorem 2.

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