

THE TAIL OF THE SINGULAR SERIES FOR THE PRIME PAIR AND GOLDBACH PROBLEMS

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Abstract: We obtain an asymptotic formula for a weighted sum of the square of the tail in the singular series for the Goldbach and prime-pair problems.

Keywords: Hardy-Littlewood conjecture; prime numbers; singular series.

1. Introduction and statement of results

Hardy and Littlewood [5] conjectured in 1922 an asymptotic formula for the number of pairs of primes differing by k . The first major step forward on this conjecture only occurred in 2013 when Zhang [15] proved that there exist some k 's for which there are infinitely many such pairs of primes. Let $\Lambda(n)$ be the von Mangoldt function defined by $\Lambda(n) = \log p$ if $n = p^m$, p a prime, $m \geq 1$ an integer, and $\Lambda(n) = 0$ otherwise. Hardy and Littlewood's conjecture is equivalent, for k even, to

$$\psi_2(N, k) := \sum_{\substack{n, n' \leq N \\ n' - n = k}} \Lambda(n)\Lambda(n') \sim \mathfrak{S}(k)(N - |k|) \quad \text{as } N \rightarrow \infty, \quad (1.1)$$

where

$$\mathfrak{S}(k) = \begin{cases} 2C_2 \prod_{\substack{p|k \\ p > 2}} \left(\frac{p-1}{p-2} \right) & \text{if } k \text{ is even, } k \neq 0, \\ 0 & \text{if } k \text{ is odd} \end{cases} \quad (1.2)$$

and

$$C_2 = \prod_{p > 2} \left(1 - \frac{1}{(p-1)^2} \right) = 0.66016 \dots \quad (1.3)$$

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For odd k the sum in (1.1) has non-zero terms only when n or n' is a power of 2, so $\psi_2(N, k) = O((\log N)^2)$. For the Goldbach problem Hardy and Littlewood conjectured an analogous formula for the number of ways an even number k can be expressed as the sum of two primes, which also includes the arithmetic function $\mathfrak{S}(k)$.

The function $\mathfrak{S}(k)$ is called the singular series, a name given it by Hardy and Littlewood because it first occurred as the series

$$\mathfrak{S}(k) = \sum_{q=1}^{\infty} \frac{\mu(q)^2}{\phi(q)^2} c_q(-k), \tag{1.4}$$

where the Ramanujan sum $c_q(n)$ is defined by

$$c_q(n) = \sum_{\substack{1 \leq a \leq q \\ (a,q)=1}} e\left(\frac{an}{q}\right), \quad e(\alpha) = e^{2\pi i \alpha}. \tag{1.5}$$

Some well-known properties of $c_q(n)$ (see, e.g., [10]) are that $c_q(-n) = c_q(n)$, $c_q(n)$ is a multiplicative function of q , and

$$c_q(n) = \sum_{\substack{d|n \\ d|q}} d\mu\left(\frac{q}{d}\right) = \frac{\mu\left(\frac{q}{(n,q)}\right)\phi(q)}{\phi\left(\frac{q}{(n,q)}\right)}. \tag{1.6}$$

Since the singular series is a sum of multiplicative functions in q , it is easy to verify that (1.4) is equivalent to the product in (1.2). The series in (1.4) is a Ramanujan series; many arithmetic functions can be expanded into these series which have the property that the first term $q = 1$ is the average or expected value of the arithmetic function. Thus we see that the $q = 1$ term in (1.4) says that $\mathfrak{S}(k)$ has average value 1. If we consider the first two terms we have

$$\mathfrak{S}(k) = 1 + e\left(-\frac{k}{2}\right) + \sum_{q=3}^{\infty} \frac{\mu(q)^2}{\phi(q)^2} c_q(-k),$$

and therefore we obtain the refinement that on average $\mathfrak{S}(k)$ is 0 if k is odd and is 2 if k is even.

In applications it is often useful to truncate the singular series; we write

$$\mathfrak{S}(k) = \mathfrak{S}_y(k) + \tilde{\mathfrak{S}}_y(k), \tag{1.7}$$

where

$$\mathfrak{S}_y(k) = \sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^2} c_q(-k), \quad \tilde{\mathfrak{S}}_y(k) = \sum_{q > y} \frac{\mu(q)^2}{\phi(q)^2} c_q(-k). \tag{1.8}$$

We refer to $\tilde{\mathfrak{S}}_y(k)$ as the tail of the singular series. Montgomery and Vaughan [9], by a simple argument using (1.5), proved for $y \geq 1$ the bound

$$\tilde{\mathfrak{S}}_y(k) \ll d(k) \frac{(\log \log 3y)^2}{y}. \tag{1.9}$$

Using a result of Ramanujan (for a proof see [14])

$$\sum_{k \leq N} d(k)^2 \sim \frac{1}{\pi^2} N(\log N)^3,$$

this bound immediately gives the mean square estimate

$$\sum_{k \leq N} \tilde{\mathfrak{S}}_y(k)^2 \ll \frac{N(\log N)^3(\log \log 3y)^4}{y^2}.$$

In [4]¹ the first-named author improved this last bound by showing

$$\sum_{k \leq N} \tilde{\mathfrak{S}}_y(k)^2 \ll \frac{N \log N}{y^2}. \tag{1.10}$$

Bounds of this type are useful in applications related to both the Goldbach and prime pair conjectures. For a recent application, see [1]. The proof of (1.10) is rather complicated and left open the question of whether the result can be improved further or is best possible. Our first result answers this question in the range $1 \leq y \leq \sqrt{N}$.

Theorem 1. *We have, for $1 \leq y \leq \sqrt{N}$ and any fixed δ , $0 < \delta < 1$,*

$$\sum_{k \leq N} (N - k)^2 \tilde{\mathfrak{S}}_y(k)^2 = \mathcal{T}(y) \frac{N^3}{3} \left(1 + O_\delta \left(\left(\frac{y^2}{N} \right)^\delta \right) \right), \tag{1.11}$$

where

$$\mathcal{T}(y) := \sum_{q > y} \frac{\mu(q)^2}{\phi(q)^3}. \tag{1.12}$$

From (2.8) below we have

$$\mathcal{T}(y) = \frac{\mathcal{A}}{y^2} (1 + o(1)), \quad \text{where } \mathcal{A} = \prod_p \left(1 + \frac{2 - 1/p}{(p - 1)^2} \right). \tag{1.13}$$

A simple argument then gives the following result. Here $f \asymp g$ means $f \ll g$ and $g \ll f$.

Corollary 1. *We have, for some sufficiently small constant c ,*

$$\sum_{k \leq N} \tilde{\mathfrak{S}}_y(k)^2 \asymp \frac{N}{y^2}, \quad \text{for } 1 \leq y \leq c\sqrt{N}. \tag{1.14}$$

and for $1 \leq y \leq \sqrt{N}$ and any fixed δ , $0 < \delta < 1$,

$$\sum_{k \leq N} \tilde{\mathfrak{S}}_y(k)^2 = \mathcal{T}(y) N \left(1 + O_\delta \left(\left(\frac{y^2}{N} \right)^{\delta/4} \right) \right). \tag{1.15}$$

¹Beware that in [4] $\mathfrak{S}_y(k)$ and $\tilde{\mathfrak{S}}_y(k)$ are defined differently than they are in this paper.

Our main result is a refinement of Theorem 1.

Theorem 2. *We have, for $1 \leq y \leq \sqrt{N}$,*

$$\sum_{k \leq N} (N - k)^2 \tilde{\mathfrak{S}}_y(k)^2 = \mathcal{T}(y) \frac{N^3}{3} - \frac{1}{4} N^2 \left(\log \frac{N}{y^2} \right)^2 + c N^2 \log \frac{N}{y^2} + O(N^2) + O\left(\frac{N^2}{\sqrt{y}} \log(2N) \right), \tag{1.16}$$

where

$$c = \frac{3}{4} - \frac{1}{2} \log 2\pi + \frac{1}{2} \sum_p \frac{(p - 2) \log p}{p(p - 1)^2}.$$

The proof of Theorem 2 requires a less direct approach than Theorem 1. To proceed from the proof of Theorem 1 we want to take the parameter $\delta \geq 1$, but then the sums that result from the tail of the singular series diverge. Therefore we are forced to consider $\tilde{\mathfrak{S}}_y(k)^2 = (\mathfrak{S}(k) - \mathfrak{S}_y(k))^2$, multiply this out, and evaluate each of the three terms separately.

With a little additional work, by not dropping lower-order terms in (6.15), (7.15), (7.16) and (7.21) we can replace the $O(N^2)$ in Theorem 2 by $CN^2 + O_\epsilon(N^2 y^{-\frac{1}{2} + \epsilon})$ for a complicated constant C .

The weight $(N - k)^2$ in our sum was chosen because it occurs naturally in the prime-pair problem. Obviously other weights or families of weights can be used.

We have not been able to extend these results to the range $\sqrt{N} \leq y \leq N$ so in this range (1.10) remains the best result known. For $y \geq N$, the method of [4] yields $\sum_{k \leq N} \tilde{\mathfrak{S}}_y(k)^2 \ll_A \frac{N \log N}{y^2 \log(2y/N)^A}$.

Notation. We follow some common conventions. A sum will normally be over integers; any sum without a lower bound on the summation variable will start at 1. Empty sums will equal 0 and empty products will equal 1. The letter p will always denote a prime. The letter ϵ will denote a small positive real number which may change from equation to equation.

2. Lemmas

We gather here some of the results we need later.

Lemma 1. *Let $s(x) = x - [x] - \frac{1}{2}$. Then for $x \geq 0$ we have*

$$\sum_{1 \leq k \leq x} (x - k) = \frac{1}{2} \left(\left(x - \frac{1}{2} \right)^2 - s(x)^2 \right) \tag{2.1}$$

and

$$\sum_{1 \leq k \leq x} (x - k)^2 = \frac{1}{3} \left(x - \frac{1}{2} \right)^3 - \int_{\frac{1}{2}}^x s(u)^2 du. \tag{2.2}$$

Since $|s(x)| \leq \frac{1}{2}$, we have

$$\sum_{1 \leq k \leq x} (x - k) = \frac{1}{2}x^2 - \frac{1}{2}x + O(1). \tag{2.3}$$

Since $s(x)$ is periodic with period 1 and $\int_0^1 s(u)^2 du = \frac{1}{12}$, we have

$$\sum_{1 \leq k \leq x} (x - k)^2 = \frac{1}{3}x^3 - \frac{1}{2}x^2 + \frac{1}{6}x + O(1). \tag{2.4}$$

Proof. For the first identity, we use $\lfloor x \rfloor = x - \frac{1}{2} - s(x)$ to write

$$\begin{aligned} S_1(x) &:= \sum_{1 \leq k \leq x} (x - k) = \sum_{1 \leq k \leq \lfloor x \rfloor} (x - k) \\ &= x \lfloor x \rfloor - \frac{\lfloor x \rfloor (\lfloor x \rfloor + 1)}{2} \\ &= \frac{1}{2} \lfloor x \rfloor \left(x - \frac{1}{2} + s(x) \right) \\ &= \frac{1}{2} \left(x - \frac{1}{2} - s(x) \right) \left(x - \frac{1}{2} + s(x) \right) \\ &= \frac{1}{2} \left(\left(x - \frac{1}{2} \right)^2 - s(x)^2 \right). \end{aligned}$$

For the second identity, we use the first in

$$\sum_{1 \leq k \leq x} (x - k)^2 = 2 \int_{\frac{1}{2}}^x S_1(u) du. \quad \blacksquare$$

Lemma 2. For fixed real numbers a and b , let

$$G(x; a, b) := \sum_{r \leq x} \frac{\mu(r)^2 r^a}{\phi(r)^b}, \tag{2.5}$$

and

$$g(s; a, b) := \prod_p \left(1 - \frac{1 - p^{s-a+b} (1 - (1 - \frac{1}{p})^b)}{(p-1)^b p^{2(s-a)+b}} \right). \tag{2.6}$$

Then we have

$$G(x; a, b) = \begin{cases} \frac{g(a-b+1; a, b)}{a-b+1} x^{a-b+1} + o_{a,b}(x^{a-b+1}) & \text{if } a - b > -1, \\ g(0; b - 1, b) \log x + O_{a,b}(1) & \text{if } a = b - 1, \\ \zeta(b - a) g(0; a, b) + \frac{g(a-b+1; a, b)}{a-b+1} x^{a-b+1} \\ \quad + o_{a,b}(x^{a-b+1}) & \text{if } a - b < -1, \end{cases} \tag{2.7}$$

where $\zeta(s)$ is the Riemann zeta function (3.3).

This is Lemma 2 of [3]. In this paper we frequently apply this lemma to obtain only an upper bound for $G(x; a, b)$, but it is useful to know that the estimates obtained are essentially sharp. We note that when $a - b < -1$

$$\begin{aligned} \sum_{r>x} \frac{\mu(r)^2 r^a}{\phi(r)^b} &= \lim_{y \rightarrow \infty} (G(y; a, b) - G(x; a, b)) \\ &= \frac{g(a - b + 1; a, b)}{b - a - 1} x^{a-b+1} + o_{a,b}(x^{a-b+1}). \end{aligned} \tag{2.8}$$

Lemma 3 (Hildebrand). *For $x \geq 1, d \geq 1$, we have*

$$\begin{aligned} \sum_{\substack{q \leq x \\ (q,d)=1}} \frac{\mu^2(q)}{\phi(q)} &= \frac{\phi(d)}{d} \left(\log x + \gamma + \sum_p \frac{\log p}{p(p-1)} + \sum_{p|d} \frac{\log p}{p} \right) \\ &\quad + O\left(x^{-\frac{1}{2}} \prod_{p|d} (1 + p^{-\frac{1}{2}})\right). \end{aligned} \tag{2.9}$$

This is Hilfssatz 2 of [6].

Lemma 4. *For $x \geq 1$,*

$$\sum_{k \leq x} (x - k) \mathfrak{S}(k) = \frac{1}{2} x^2 - \frac{1}{2} x \log x + \frac{1}{2} (1 - \gamma - \log 2\pi) x + O_\epsilon(x^{\frac{1}{2}+\epsilon}). \tag{2.10}$$

This was first stated in [3], and also appeared in [2], but the first published proof is in [8].

Our next lemma is a generalization and strengthening of Lemma 4 due to Vaughan. We let

$$\mathfrak{S}_d(k) = 2C(d) \prod_{\substack{p|k \\ (p,2d)=1}} \left(\frac{p-1}{p-2} \right), \tag{2.11}$$

where

$$C(d) = \prod_{(p,2d)=1} \left(1 - \frac{1}{(p-1)^2} \right). \tag{2.12}$$

Note that unlike for $\mathfrak{S}(k)$ we do not require that $\mathfrak{S}_d(k)$ be zero if k is odd; instead $\mathfrak{S}_d(k) = \mathfrak{S}_d(2k)$.

Lemma 5 (Vaughan). *For $x \geq 1$, we have*

$$\sum_{k \leq x} (x - k) \mathfrak{S}_d(k) = x^2 - \frac{1}{2} \frac{(d, 2)\phi(d)}{d} x \left(\log x + \gamma - 1 + \log 2\pi + \sum_{p|2d} \frac{\log p}{p-1} \right) + E(x, d) \tag{2.13}$$

where

$$E(x, d) \ll x^{\frac{1}{2}} \exp\left(-c \frac{(\log 2x)^{\frac{3}{5}}}{(\log \log 3x)^{\frac{1}{5}}}\right) \prod_{p|d} (1 - p^{-\frac{1}{4}})^{-1} \tag{2.14}$$

for some positive constant c . If we assume the Riemann Hypothesis then $x^{\frac{1}{2}}$ in (2.14) can be replaced by $x^{\frac{5}{12} + \epsilon}$.

This is Theorem 3 of [13]. (The Riemann Hypothesis estimate is on page 552 of that paper.) We can recover Lemma 4 from Lemma 5 with a stronger error term by using

$$\sum_{k \leq x} (x - k) \mathfrak{S}(k) = 2 \sum_{k \leq \frac{x}{2}} \left(\frac{x}{2} - k\right) \mathfrak{S}_1(k).$$

3. Proof of Theorem 1.

We have

$$S := \sum_{k \leq N} (N - k)^2 \tilde{\mathfrak{S}}_y(k)^2 = \sum_{q > y} \sum_{q' > y} \frac{\mu(q)^2 \mu(q')^2}{\phi(q)^2 \phi(q')^2} \underbrace{\sum_{1 \leq k \leq N} (N - k)^2 c_q(-k) c_{q'}(-k)}_{S'} \tag{3.1}$$

and by the formula $c_q(-k) = \sum_{\substack{d|q \\ d|k}} d \mu\left(\frac{q}{d}\right)$, we have

$$S' = \sum_{d|q} \sum_{d'|q'} d \mu\left(\frac{q}{d}\right) d' \mu\left(\frac{q'}{d'}\right) \sum_{\substack{1 \leq k \leq N \\ [d, d'] | k}} (N - k)^2. \tag{3.2}$$

We now need to evaluate the inner sum over k . In proving Theorem 2 we do this with the elementary Lemma 1, but here we need to use the formula in Theorem B of Ingham [7]: if m is a positive integer, $c > 0$, and $x > 0$, then

$$\frac{m!}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{x^{s+m}}{s(s+1)(s+2)\cdots(s+m)} ds = \begin{cases} 0 & \text{if } 0 < x \leq 1, \\ (x-1)^m & \text{if } x \geq 1. \end{cases}$$

The Riemann zeta function is, for $s = \sigma + it$, $\sigma > 1$,

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \prod_p \left(1 - \frac{1}{p^s}\right)^{-1}. \tag{3.3}$$

The series and product converge absolutely and converge uniformly for $\sigma \geq 1 + \epsilon$. Hence for $x \geq 1$ and $c > 1$ we have

$$\sum_{1 \leq n \leq x} (x - n)^k = \frac{k!}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{\zeta(s) x^{s+k}}{s(s+1)(s+2)\cdots(s+k)} ds. \tag{3.4}$$

Now

$$\sum_{\substack{1 \leq k \leq N \\ [d, d'] | k}} (N - k)^2 = [d, d']^2 \sum_{1 \leq k \leq \frac{N}{[d, d']}} \left(\frac{N}{[d, d']} - k \right)^2,$$

and therefore

$$\sum_{\substack{1 \leq k \leq N \\ [d, d'] | k}} (N - k)^2 = \frac{2!}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{\zeta(s) N^{s+2}}{s(s+1)(s+2)[d, d']^s} ds,$$

making use of the assumption that $y \leq \sqrt{N}$ to ensure that

$$\frac{N}{[d, d']} \geq \frac{N}{dd'} \geq \frac{N}{qq'} \geq \frac{N}{y^2} \geq 1.$$

Hence

$$S = \frac{2!}{2\pi i} \int_{c-i\infty}^{c+i\infty} \zeta(s) B_s(y) \frac{N^{s+2}}{s(s+1)(s+2)} ds, \tag{3.5}$$

where

$$B_s(y) = \sum_{q>y} \sum_{q'>y} \frac{\mu(q)^2}{\phi(q)^2} \frac{\mu(q')^2}{\phi(q')^2} \sum_{d|q} \sum_{d'|q'} \frac{dd' \mu\left(\frac{q}{d}\right) \mu\left(\frac{q'}{d'}\right)}{[d, d']^s}. \tag{3.6}$$

Following the method Selberg introduced for the Selberg sieve [11], we now diagonalize $B_s(y)$. Define $\phi_s(n)$ by the equation $n^s = \sum_{d|n} \phi_s(d)$, so that $\phi_s(n)$ is multiplicative and $\phi_s(p) = p^s - 1$. Letting $n = (d, d')$ we have

$$(d, d')^s = \sum_{\substack{r|d \\ r|d'}} \phi_s(r),$$

and thus

$$\frac{dd'}{[d, d']^s} = (dd')^{1-s} \sum_{\substack{r|d \\ r|d'}} \phi_s(r).$$

Hence

$$B_s(y) = \sum_{r=1}^{\infty} \phi_s(r) \left(\sum_{\substack{q>y \\ r|q}} \frac{\mu(q)^2}{\phi(q)^2} \sum_{\substack{d|q \\ r|d}} d^{1-s} \mu\left(\frac{q}{d}\right) \right)^2. \tag{3.7}$$

The simplest bound on $\zeta(s)$ in the critical strip is that if $0 < \alpha < 1$, $|t| \geq 1$, then

$$|\zeta(s)| < C(\alpha) |t|^{1-\alpha} \quad \text{for } \sigma \geq \alpha \tag{3.8}$$

for some constant $C(\alpha)$, see Theorem 9 of Ingham[7]. We also need the bound, for $0 < \alpha < 1$,

$$B_s(y) \ll \frac{1}{y^{2\alpha}} \quad \text{for } \sigma \geq \alpha, \tag{3.9}$$

which we will prove later in this section. In our formula for S we move the contour to the left past the simple pole with residue 1 at $s = 1$ of $\zeta(s)$ to the line $s = \alpha + it$ with $0 < \alpha < 1$. Since by (3.8) and (3.9) the integrand is $O_\alpha(N^{2+\alpha}y^{-2\alpha}/|t|^{2+\alpha})$ for $|t| \geq 1$, the integrals converge absolutely and we obtain

$$\begin{aligned} S &= B_1(y) \frac{N^3}{3} + \frac{2!}{2\pi i} \int_{\alpha-i\infty}^{\alpha+i\infty} \zeta(s) B_s(y) \frac{N^{s+2}}{s(s+1)(s+2)} ds \\ &= B_1(y) \frac{N^3}{3} + O_\alpha\left(\frac{N^{2+\alpha}}{y^{2\alpha}}\right). \end{aligned} \tag{3.10}$$

We have $\sum_{\substack{d|q \\ r|d}} \mu\left(\frac{q}{d}\right) = \sum_{s|\frac{q}{r}} \mu\left(\frac{q/r}{s}\right) = \begin{cases} 1 & \text{if } q = r, \\ 0 & \text{if } q \neq r, \end{cases}$ and thus

$$\begin{aligned} B_1(y) &= \sum_{r=1}^{\infty} \phi(r) \left(\sum_{\substack{q>y \\ r|q}} \frac{\mu(q)^2}{\phi(q)^2} \sum_{\substack{d|q \\ r|d}} \mu\left(\frac{q}{d}\right) \right)^2 \\ &= \sum_{r=1}^{\infty} \phi(r) \left(\sum_{\substack{q>y \\ q=r}} \frac{\mu(q)^2}{\phi(q)^2} \right)^2 = \sum_{r>y} \frac{\mu(r)^2}{\phi(r)^3} = \mathcal{T}(y). \end{aligned} \tag{3.11}$$

We conclude that

$$S = \mathcal{T}(y) \frac{N^3}{3} + O_\alpha\left(\frac{N^3}{y^2} \left(\frac{y^2}{N}\right)^{1-\alpha}\right),$$

which proves Theorem 1 on taking $\alpha = 1 - \delta$.

It remains to prove (3.9). For the sums over q and d inside the square in (3.7), writing $q = du$, $d = rv$, we have $q = ruv$ and

$$\sum_{\substack{q>y \\ r|q}} \frac{\mu(q)^2}{\phi(q)^2} \sum_{\substack{d|q \\ r|d}} d^{1-s} \mu\left(\frac{q}{d}\right) = \sum_{ruv>y} \frac{\mu(ruv)^2}{\phi(ruv)^2} (rv)^{1-s} \mu(u).$$

Hence

$$B_s(y) = \sum_{r=1}^{\infty} \frac{\mu(r)^2 \phi_s(r) r^{2-2s}}{\phi(r)^4} \left(\sum_{\substack{u=1 \\ (u,r)=1}}^{\infty} \frac{\mu(u)}{\phi(u)^2} \left(\sum_{\substack{v>y/ur \\ (v,ur)=1}} \frac{\mu(v)^2 v^{1-s}}{\phi(v)^2} \right) \right)^2.$$

We note that for squarefree r

$$|\phi_{\alpha+it}(r)| \leq \prod_{p|r} (p^\alpha + 1) = r^\alpha \prod_{p|r} \left(1 + \frac{1}{p^\alpha}\right) = r^\alpha \sigma_{-\alpha}(r),$$

where $\sigma_z(r) = \sum_{d|r} d^z$. We conclude

$$|B_{a+it}(y)| \leq \sum_{r=1}^{\infty} \frac{\mu(r)^2 r^{2-a}}{\phi(r)^4} \sigma_{-a}(r) \left(\sum_{u=1}^{\infty} \frac{\mu(u)^2}{\phi(u)^2} \left(\sum_{v>y/ur} \frac{\mu(v)^2 v^{1-a}}{\phi(v)^2} \right) \right)^2.$$

Clearly the right-hand side is a decreasing function of a , and therefore to prove (3.9) we only need to prove that the right-hand side above satisfies the bound in (3.9) for $a = \alpha$. Since by Lemma 2

$$\sum_{v>y/ur} \frac{\mu(v)^2 v^{1-\alpha}}{\phi(v)^2} \ll_{\alpha} \left(\frac{ur}{y} \right)^{\alpha},$$

we have

$$B_{\alpha+it}(y) \ll_{\alpha} \sum_{r=1}^{\infty} \frac{\mu(r)^2 r^{2-\alpha}}{\phi(r)^4} \sigma_{-\alpha}(r) \left(\sum_{u=1}^{\infty} \frac{\mu(u)^2}{\phi(u)^2} \left(\frac{ur}{y} \right)^{\alpha} \right)^2.$$

Applying Lemma 2 again, the sum over u is

$$\frac{r^{\alpha}}{y^{\alpha}} \sum_{u=1}^{\infty} \frac{\mu(u)^2 u^{\alpha}}{\phi(u)^2} \ll_{\alpha} \frac{r^{\alpha}}{y^{\alpha}},$$

so

$$B_s(y) \ll_{\alpha} \sum_{r=1}^{\infty} \frac{\mu(r)^2 r^{2-\alpha} \sigma_{-\alpha}(r)}{\phi(r)^4} \frac{r^{2\alpha}}{y^{2\alpha}} = \frac{1}{y^{2\alpha}} \sum_{r=1}^{\infty} \frac{\mu(r)^2 r^{2+\alpha} \sigma_{-\alpha}(r)}{\phi(r)^4}.$$

Since $\phi(dm) = \phi(d)\phi(m)$ when $\mu(dm) \neq 0$,

$$\begin{aligned} \sum_{r=1}^{\infty} \frac{\mu(r)^2 r^{2+\alpha}}{\phi(r)^4} \sum_{d|r} \frac{1}{d^{\alpha}} &= \sum_{d,m} \frac{\mu(dm)^2 d^2 m^{2+\alpha}}{\phi(dm)^4} \\ &\leq \left(\sum_{m=1}^{\infty} \frac{\mu(m)^2 m^{2+\alpha}}{\phi(m)^4} \right) \left(\sum_{d=1}^{\infty} \frac{\mu(d)^2 d^2}{\phi(d)^4} \right) \ll_{\alpha} 1 \end{aligned}$$

and $B_s(y) \ll_{\alpha} \frac{1}{y^{2\alpha}}$, which proves (3.9).

To prove Corollary 1, let

$$T_0(N) = \sum_{k \leq N} \tilde{\mathfrak{S}}_y(k)^2, \quad T_m(N) = \sum_{k \leq N} (N-k)^m \tilde{\mathfrak{S}}_y(k)^2 \quad \text{for } m \geq 1.$$

Then by Theorem 1 and (1.13) for $1 \leq y \leq cN^{1/2}$ with c sufficiently small

$$T_2(N) \asymp \frac{N^3}{y^2}$$

and (1.14) follows from

$$\frac{1}{N^2}T_2(N) \leq T_0(N) \leq \frac{1}{N^2}T_2(2N).$$

To prove (1.15) we note for $m \geq 0$ that

$$T_{m+1}(N) = (m+1) \int_1^N T_m(u) du.$$

Since $T_m(N)$ is a nondecreasing function of N , we have, for $1 \leq h \leq N$,

$$T_1(N) \leq \frac{1}{h} \int_N^{N+h} T_1(u) du = \frac{T_2(N+h) - T_2(N)}{2h}$$

and similarly

$$T_1(N) \geq \frac{T_2(N) - T_2(N-h)}{2h}.$$

Now by (1.11) and (1.13)

$$T_2(N) = \mathcal{T}(y) \frac{N^3}{3} + O_\delta \left(\frac{N^3}{y^2} \left(\frac{y^2}{N} \right)^\delta \right),$$

and hence

$$\begin{aligned} \frac{T_2(N \pm h) - T_2(N)}{\pm 2h} &= \frac{1}{2} \mathcal{T}(y) \left(N^2 \pm Nh + \frac{h^2}{3} \right) + O_\delta \left(\frac{N^3}{hy^2} \left(\frac{y^2}{N} \right)^\delta \right) \\ &= \mathcal{T}(y) \frac{N^2}{2} + O \left(\frac{Nh}{y^2} \right) + O_\delta \left(\frac{N^3}{hy^2} \left(\frac{y^2}{N} \right)^\delta \right). \end{aligned}$$

Balancing the two error terms by choosing $h = N \left(\frac{y^2}{N} \right)^{\frac{\delta}{2}}$, we conclude

$$\frac{T_2(N \pm h) - T_2(N)}{\pm 2h} = \mathcal{T}(y) \frac{N^2}{2} + O_\delta \left(\frac{N^2}{y^2} \left(\frac{y^2}{N} \right)^{\frac{\delta}{2}} \right),$$

and hence

$$T_1(N) = \mathcal{T}(y) \frac{N^2}{2} + O_\delta \left(\frac{N^2}{y^2} \left(\frac{y^2}{N} \right)^{\frac{\delta}{2}} \right).$$

By the same argument $T_0(N)$ is bounded between the expressions

$$\frac{T_1(N \pm h) - T_1(N)}{\pm h} = \mathcal{T}(y)N + O \left(\frac{h}{y^2} \right) + O_\delta \left(\frac{N^2}{hy^2} \left(\frac{y^2}{N} \right)^{\frac{\delta}{2}} \right)$$

and the choice $h = N \left(\frac{y^2}{N}\right)^{\frac{\delta}{4}}$ gives

$$T_0(N) = \mathcal{T}(y)N + O_\delta \left(\frac{N}{y^2} \left(\frac{y^2}{N}\right)^{\frac{\delta}{4}} \right),$$

which proves (1.15).

4. The average of the singular series tail

In this section for completeness we give a proof of the average size of the tail of the singular series. This proof illustrates the method we use to prove Theorem 2 without all the complications.

Theorem 3. *We have, for $1 \leq y \leq N$,*

$$\begin{aligned} \sum_{k \leq N} (N - k) \tilde{\mathfrak{S}}_y(k) &= -\frac{1}{2} N \log \frac{N}{y} + \frac{1}{2} \left(1 - \log 2\pi + \sum_p \frac{\log p}{p(p-1)} \right) N \\ &\quad + O(Ny^{-\frac{1}{2}}) + O(y). \end{aligned} \tag{4.1}$$

The reason the average does not have a main term of size $\frac{N^2}{y}$ as one might expect is that the term 1 from $q = 1$ in (1.4) cancels out this term independent of the truncation level y .

Proof. We have

$$\sum_{k \leq N} (N - k) \tilde{\mathfrak{S}}_y(k) = \sum_{k \leq N} (N - k) \mathfrak{S}(k) - \sum_{k \leq N} (N - k) \mathfrak{S}_y(k). \tag{4.2}$$

The first sum is evaluated in Lemma 4. For the second sum, we use (1.8) and (1.6) to obtain

$$\begin{aligned} \sum_{k \leq N} (N - k) \mathfrak{S}_y(k) &= \sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^2} \sum_{k \leq N} (N - k) c_q(-k) \\ &= \sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^2} \sum_{d|q} d \mu\left(\frac{q}{d}\right) \left(\sum_{\substack{1 \leq k \leq N \\ d|k}} (N - k) \right), \end{aligned}$$

and we see on letting $k = dm$ that by Lemma 1

$$\begin{aligned} \sum_{\substack{1 \leq k \leq N \\ d|k}} (N - k) &= d \sum_{1 \leq m \leq \frac{N}{d}} \left(\frac{N}{d} - m \right) \\ &= \frac{1}{2} \frac{N^2}{d} - \frac{1}{2} N + O(d), \end{aligned}$$

and hence

$$\begin{aligned} \sum_{k \leq N} (N - k) \mathfrak{S}_y(k) &= \frac{1}{2} N^2 \sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^2} \sum_{d|q} \mu\left(\frac{q}{d}\right) - \frac{1}{2} N \sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^2} \sum_{d|q} d \mu\left(\frac{q}{d}\right) \\ &\quad + O\left(\sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^2} \sum_{d|q} d^2\right). \end{aligned}$$

By Lemma 2,

$$\sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^2} \sum_{d|q} d^2 = \sum_{dm \leq y} \frac{\mu(dm)^2 d^2}{\phi(dm)^2} \ll \left(\sum_{m \leq y} \frac{\mu(m)^2}{\phi(m)^2}\right) \left(\sum_{d \leq y} \frac{\mu(d)^2 d^2}{\phi(d)^2}\right) \ll y.$$

Hence we see

$$\sum_{k \leq N} (N - k) \mathfrak{S}_y(k) = \frac{1}{2} N^2 - \frac{1}{2} N \sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)} + O(y). \tag{4.3}$$

The theorem now follows from (4.2), (4.3), Lemma 3 with $d = 1$, Lemma 4, and the fact that $N^{\frac{1}{2} + \epsilon} \ll \max(Ny^{-\frac{1}{2}}, y)$ for $\epsilon \leq \frac{1}{6}$.

5. Starting the proof of Theorem 2

To prove Theorem 2 we need to asymptotically evaluate

$$\begin{aligned} \sum_{k \leq N} (N - k)^2 \tilde{\mathfrak{S}}_y(k)^2 &= \sum_{k \leq N} (N - k)^2 (\mathfrak{S}(k) - \mathfrak{S}_y(k))^2 \\ &= \sum_{k \leq N} (N - k)^2 \mathfrak{S}(k)^2 - 2 \sum_{k \leq N} (N - k)^2 \mathfrak{S}(k) \mathfrak{S}_y(k) \\ &\quad + \sum_{k \leq N} (N - k)^2 \mathfrak{S}_y(k)^2 \\ &=: S_1 - 2S_2 + S_3. \end{aligned} \tag{5.1}$$

We evaluate each of these terms in the following sections.

6. The sum S_1

In this section we evaluate

$$S_1 = \sum_{k \leq N} (N - k)^2 \mathfrak{S}(k)^2. \tag{6.1}$$

The proof is along the same lines as the proof in [8] of Lemma 4.

Theorem 4. *We have*

$$\sum_{k \leq N} (N - k)^2 \mathfrak{S}(k)^2 = \prod_p \left(1 + \frac{1}{(p-1)^3} \right) \frac{N^3}{3} - \frac{1}{4} N^2 (\log N)^2 \tag{6.2}$$

$$+ \left(\frac{3}{4} - \gamma - \frac{1}{2} \log 2\pi - \frac{1}{2} \sum_p \frac{\log p}{(p-1)^2} \right) N^2 \log N + O(N^2).$$

Proof. Let $g(k) = \prod_{\substack{p|k \\ p>2}} \left(\frac{p-1}{p-2} \right)^2$, so that $\mathfrak{S}(k)^2 = \begin{cases} 4C_2^2 g(k) & \text{if } 2 \mid k, \text{ and} \\ 0 & \text{if } 2 \nmid k \end{cases}$

$$S_1 = 4C_2^2 \sum_{\substack{1 \leq k \leq N \\ 2|k}} (N - k)^2 g(k) = 16C_2^2 \sum_{1 \leq k \leq \frac{N}{2}} \left(\frac{N}{2} - k \right)^2 g(k) = 16C_2^2 S_{11} \left(\frac{N}{2} \right) \tag{6.3}$$

where $S_{11}(N) = \sum_{1 \leq k \leq N} (N - k)^2 g(k)$. Let

$$G(s) = \sum_{n=1}^{\infty} \frac{g(n)}{n^s} = \prod_p \left(1 + \sum_{m=1}^{\infty} \frac{g(p^m)}{p^{ms}} \right) \tag{6.4}$$

$$= \left(1 - \frac{1}{2^s} \right)^{-1} \prod_{p>2} \left(1 + \left(\frac{p-1}{p-2} \right)^2 \frac{1}{p^s - 1} \right),$$

for $\text{Re } s > 1$. To analytically continue $G(s)$ to the left, we see the dominant factor is

$$\zeta(s) = \prod_p \left(1 - \frac{1}{p^s} \right)^{-1},$$

and therefore we have

$$G(s) = \zeta(s) \prod_{p>2} \left(1 + \left(\frac{p-1}{p-2} \right)^2 \frac{1}{p^s - 1} \right) \left(1 - \frac{1}{p^s} \right) \tag{6.5}$$

$$= \zeta(s) \prod_{p>2} \left(1 + \frac{2p-3}{(p-2)^2 p^s} \right) =: \zeta(s) H(s)$$

with $H(s)$ analytic for $\text{Re } s > 0$. Next we write $H(s) = \zeta(s+1)^2 \left(1 - \frac{1}{2^{s+1}} \right)^2 J(s)$,

$$J(s) = \prod_{p>2} \left(1 + \frac{2p-3}{(p-2)^2 p^s} \right) \left(1 - \frac{1}{p^{s+1}} \right)^2. \tag{6.6}$$

We then have (by Mathematica) that

$$J(s) = \prod_{p>2} \left(1 + \frac{1}{(p-2)^2 p^s} \left(5 - \frac{8}{p} + \frac{1}{p^s} \left(-3 + \frac{2}{p} + \frac{4}{p^2} \right) + \frac{1}{p^{2s}} \left(\frac{2}{p} - \frac{3}{p^2} \right) \right) \right), \tag{6.7}$$

and for $-1 < \operatorname{Re} s < 0$ this is

$$\prod_{p>2} \left(1 + \frac{1}{(p-2)^2 p^s} \left(-\frac{3}{p^s} + O(1) + O\left(\frac{1}{p^{2s+1}}\right) \right) \right),$$

which is analytic for $\operatorname{Re} s > -\frac{1}{2}$.

Now, in the same way we obtained (3.4), we have for $a > 1$

$$S_{11}(N) = \sum_{k=1}^N (N-k)^2 g(k) = \frac{2!}{2\pi i} \int_{a-i\infty}^{a+i\infty} G(s) \frac{N^{s+2}}{s(s+1)(s+2)} ds. \tag{6.8}$$

We move the contour to $\operatorname{Re} s = b$, $-\frac{1}{2} < b < 0$. To ensure convergence and justify moving the contour we need to use a standard bound for $\zeta(s)$ which improves on (3.8). By [12], Chapter 5, for $|t| \geq 1$,

$$\zeta(\sigma + it) \ll (|t| + 3)^{\lambda(\sigma) + \epsilon}, \tag{6.9}$$

where

$$\lambda(\sigma) = \begin{cases} 0 & \text{if } \sigma > 1, \\ \frac{1}{2} - \frac{1}{2}\sigma & \text{if } 0 < \sigma \leq 1, \\ \frac{1}{2} - \sigma & \text{if } \sigma \leq 0. \end{cases} \tag{6.10}$$

This, along with the fact that $J = O_b(1)$ for $\operatorname{Re} s \geq b$, shows that the integrand is $O_b(N^{\sigma+2}/|t|^{2b+\frac{5}{2}})$ for $|t| \geq 1$.

We encounter a simple pole at $s = 1$ and a triple pole at $s = 0$. Since $H(s)$ is analytic at $s = 1$ and $\zeta(s) = \frac{1}{s-1} + O(1)$, the pole at 1 contributes $\frac{1}{3}H(1)N^3$ to $S_{11}(N)$. Expanding around $s = 0$ we have

$$\begin{aligned} G(s) \frac{N^{s+2}}{s(s+1)(s+2)} &= \zeta(s)\zeta(s+1)^2 \left(1 - \frac{1}{2^{s+1}} \right)^2 J(s) \frac{N^{s+2}}{s(s+1)(s+2)} \\ &= \frac{N^2}{4} \cdot \frac{1}{s^3} K(s) N^s \\ &= \frac{N^2}{4} \cdot \frac{1}{s^3} \left(1 + (\log N)s + \frac{(\log N)^2}{2}s^2 + O(s^3) \right) \\ &\quad \times \left(K(0) + K'(0)s + \frac{K''(0)}{2}s^2 + O(s^3) \right), \end{aligned} \tag{6.11}$$

where

$$K(s) = \zeta(s)(s\zeta(s+1))^2(2-2^{-s})^2 \frac{1}{(1+s)(2+s)} J(s).$$

The pole at 0 therefore contributes $\frac{N^2}{2} (\frac{1}{2}K(0)(\log N)^2 + K'(0)\log N + \frac{1}{2}K''(0))$. From the expansion $s\zeta(s+1) = 1 + \gamma s + O(s^2)$, we find that $K(0) = \frac{1}{2}\zeta(0)J(0) = -\frac{1}{4}J(0)$ and, using that if f_1 and f_2 are differentiable then $\frac{(f_1 f_2)'}{f_1 f_2} = \frac{f_1'}{f_1} + \frac{f_2'}{f_2}$, that $\frac{K'(0)}{K(0)} = \frac{\zeta'(0)}{\zeta(0)} + 2\gamma + 2\log 2 - 1 - \frac{1}{2} + \frac{J'(0)}{J(0)}$. We have

$$\begin{aligned} J(0) &= \prod_{p>2} \left(1 + \frac{2p-3}{(p-2)^2}\right) \left(1 - \frac{1}{p}\right)^2 \\ &= \prod_{p>2} \frac{((p-2)^2 + 2p-3)(p-1)^2}{p^2(p-2)^2} \end{aligned} \quad (6.12)$$

$$= \prod_{p>2} \frac{(p-1)^4}{p^2(p-2)^2} = \prod_{p>2} \left(\frac{1}{1 - \frac{1}{(p-1)^2}}\right)^2 = \frac{1}{C_2^2},$$

$$\frac{\zeta'(0)}{\zeta(0)} = \log 2\pi,$$

$$\begin{aligned} \frac{J'(0)}{J(0)} &= \sum_{p>2} \left(2 \frac{(\log p)p^{-s}}{p-p^{-s}} - \frac{(2p-3)(\log p)p^{-s}}{(p-2)^2 + (2p-3)p^{-s}}\right) \Big|_{s=0} \\ &= \sum_{p>2} \frac{\log p}{(p-1)^2}, \end{aligned} \quad (6.13)$$

and

$$\begin{aligned} H(1) &= \prod_{p>2} \left(1 + \frac{2p-3}{(p-2)^2 p}\right) \\ &= \prod_{p>2} \frac{p^3 - 4p^2 + 6p - 3}{(p-2)^2 p} \\ &= \prod_{p>2} \frac{(p-1)^4 + p-1}{p^2(p-2)^2} \\ &= \prod_{p>2} \frac{(p-1)^4}{p^2(p-2)^2} \left(1 + \frac{1}{(p-1)^3}\right) \\ &= \frac{1}{2C_2^2} \prod_p \left(1 + \frac{1}{(p-1)^3}\right). \end{aligned} \quad (6.14)$$

Combining these, we obtain

$$\begin{aligned}
 S_1(N) &= 16C_2^2 S_{11}\left(\frac{N}{2}\right) \\
 &= 16C_2^2 \left(\frac{1}{24} H(1) N^3 + \frac{N^2}{16} (K(0)(\log(N/2))^2 + 2K'(0)\log(N/2) + K''(0)) \right) \\
 &\quad + \frac{2!}{2\pi i} \int_{b-i\infty}^{b+i\infty} G(s) \frac{N^{s+2}}{s(s+1)(s+2)} ds \\
 &= \frac{1}{3} \prod_p \left(1 + \frac{1}{(p-1)^3} \right) N^3 \\
 &\quad - \frac{1}{4} C_2^2 J(0) N^2 ((\log N)^2 - 2(\log 2)\log N + (\log 2)^2) \\
 &\quad - \frac{1}{2} C_2^2 J(0) \left(\log 2\pi + 2\gamma + 2\log 2 - 1 - \frac{1}{2} + \sum_{p>2} \frac{\log p}{(p-1)^2} \right) \\
 &\quad \times N^2 (\log N - \log 2) + O(N^2) \\
 &= \prod_p \left(1 + \frac{1}{(p-1)^3} \right) \frac{N^3}{3} - \frac{1}{4} N^2 (\log N)^2 \\
 &\quad + \left(\frac{3}{4} - \gamma - \frac{1}{2} \log 2\pi - \frac{1}{2} \sum_p \frac{\log p}{(p-1)^2} \right) N^2 \log N + O(N^2),
 \end{aligned} \tag{6.15}$$

as desired.

7. The sum S_2

In this section we evaluate

$$S_2 = \sum_{k \leq N} (N-k)^2 \mathfrak{S}(k) \mathfrak{S}_y(k). \tag{7.1}$$

Theorem 5. *We have*

$$\begin{aligned}
 S_2 &= \left(\sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^3} \right) \frac{N^3}{3} - \frac{N^2}{2} \log N \log y + \frac{N^2}{4} (\log y)^2 \\
 &\quad - \left(\gamma + \sum_p \frac{\log p}{p(p-1)} \right) \frac{N^2}{2} \log N \\
 &\quad - \left(\gamma - \frac{3}{2} + \log 2\pi + \sum_p \frac{\log p}{p(p-1)^2} \right) \frac{N^2}{2} \log y + O(N^2) \\
 &\quad + O_\epsilon(N^{\frac{3}{2}} y^{\frac{1}{2} + \epsilon}) + O(N^2 \log(2N) y^{-\frac{1}{2}}).
 \end{aligned} \tag{7.2}$$

Proof. The definition of \mathfrak{S}_y and the formula $c_q(-k) = \sum_{\substack{d|q \\ d|k}} d\mu\left(\frac{q}{d}\right)$ give

$$S_2 = \sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^2} \sum_{d|q} d\mu\left(\frac{q}{d}\right) \sum_{\substack{1 \leq k \leq N \\ d|k}} (N-k)^2 \mathfrak{S}(k). \tag{7.3}$$

Letting $k = dm$, the inner sum is

$$S_{21}(d) = d^2 \sum_{1 \leq m \leq N/d} (N/d - m)^2 \mathfrak{S}(dm) = d^2 S_{22}(N/d), \tag{7.4}$$

where

$$\begin{aligned} S_{22}(x) &= \sum_{1 \leq m \leq x} (x - m)^2 \mathfrak{S}(dm) \\ &= 2 \int_1^x \sum_{1 \leq m \leq u} (u - m) \mathfrak{S}(dm) du =: 2 \int_1^x S_{23}(u) du. \end{aligned} \tag{7.5}$$

To evaluate this using Lemma 5, we write it in terms of \mathfrak{S}_d :

$$\begin{aligned} S_{23}(x) &= \sum_{1 \leq n \leq x} (x - n) \mathfrak{S}(dn) = \sum_{\substack{1 \leq n \leq x \\ 2|dn}} (x - n) \frac{d}{(d, 2)\phi(d)} \mathfrak{S}_d(n) \\ &= \begin{cases} \frac{d}{2\phi(d)} \sum_{1 \leq n \leq x} (x - n) \mathfrak{S}_d(n) & \text{if } d \text{ is even,} \\ \frac{2d}{\phi(d)} \sum_{1 \leq n \leq \frac{x}{2}} \left(\frac{x}{2} - n\right) \mathfrak{S}_d(n) & \text{if } d \text{ is odd.} \end{cases} \end{aligned} \tag{7.6}$$

The contribution to $S_{23}(x)$ from the main term of Lemma 5 is $\frac{d}{2\phi(d)}x^2$ regardless of the parity of d , and because $\sum_{p|2d} \frac{\log p}{p-1} = \sum_{p|d} \frac{\log p}{p-1}$ if d is even while

$$\log(x/2) + \sum_{p|2d} \frac{\log p}{p-1} = \log x + \sum_{p|d} \frac{\log p}{p-1}$$

if d is odd, the second term contributes

$$-\frac{x}{2} \left(\log x + \gamma - 1 + \log 2\pi + \sum_{p|d} \frac{\log p}{p-1} \right),$$

again regardless of d 's parity. The error term in Lemma 5 is $\ll_\epsilon x^{\frac{1}{2}}d^\epsilon$ and $\frac{d}{\phi(d)} \ll_\epsilon d^\epsilon$. Thus

$$S_{23}(x) = \frac{d}{\phi(d)} \frac{x^2}{2} - \frac{x}{2} \left(\log x + \gamma - 1 + \log 2\pi + \sum_{p|d} \frac{\log p}{p-1} \right) + O_\epsilon(x^{\frac{1}{2}}d^\epsilon). \tag{7.7}$$

Integrating, and denoting $\gamma - \frac{3}{2} + \log 2\pi$ by c_1 ,

$$S_{22}(x) = 2 \int_1^x S_{23}(u) du = \frac{d}{\phi(d)} \frac{x^3}{3} - \frac{x^2}{2} \left(\log x + c_1 + \sum_{p|d} \frac{\log p}{p-1} \right) - \frac{d}{3\phi(d)} + \frac{1}{2} \sum_{p|d} \frac{\log p}{p-1} + O_\epsilon(x^{\frac{3}{2}} d^\epsilon). \tag{7.8}$$

Thus, because $\frac{d}{\phi(d)}$ and $\sum_{p|d} \frac{\log p}{p-1}$ are both $O_\epsilon(d^\epsilon)$,

$$S_{21}(d) = \frac{N^3}{3\phi(d)} - \frac{N^2}{2} \left(\log N - \log d + c_1 + \sum_{p|d} \frac{\log p}{p-1} \right) + O_\epsilon(N^{\frac{3}{2}} d^{\frac{1}{2}+\epsilon}). \tag{7.9}$$

For square-free q ,

$$\sum_{d|q} \frac{d\mu\left(\frac{q}{d}\right)}{\phi(d)} = \mu(q) \prod_{p|q} \left(1 - \frac{p}{p-1} \right) = \prod_{p|q} \frac{1}{p-1} = \frac{1}{\phi(q)},$$

so the term $\frac{N^3}{3\phi(d)}$ contributes

$$\sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^2} \sum_{d|q} \frac{d\mu\left(\frac{q}{d}\right) N^3}{3\phi(d)} = \frac{N^3}{3} \sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^3} \tag{7.10}$$

to S_2 . Next, the terms $-\frac{N^2}{2}(\log N + c_1)$ are easily dealt with, and contribute

$$\begin{aligned} & -\frac{N^2}{2}(\log N + c_1) \sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^2} \sum_{d|q} d\mu\left(\frac{q}{d}\right) \\ &= -\frac{N^2}{2}(\log N + c_1) \sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)} \\ &= -\frac{N^2}{2}(\log N + c_1) \left(\log y + \gamma + \sum_p \frac{\log p}{p(p-1)} \right) + O(N^2 \log(2N)y^{-\frac{1}{2}}) \end{aligned} \tag{7.11}$$

by Lemma 3. The error $O_\epsilon(N^{\frac{3}{2}} d^{\frac{1}{2}+\epsilon})$ contributes

$$\sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^2} \sum_{d|q} O_\epsilon(N^{\frac{3}{2}} d^{\frac{3}{2}+\epsilon}) = O_\epsilon \left(N^{\frac{3}{2}} \sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^2} q^{\frac{3}{2}+\epsilon} \right) = O_\epsilon(N^{\frac{3}{2}} y^{\frac{1}{2}+\epsilon}). \tag{7.12}$$

For the remaining terms, we first evaluate the inner sum:

$$\begin{aligned}
 \sum_{d|q} d\mu\left(\frac{q}{d}\right) \frac{N^2}{2} \left(\log d - \sum_{p|d} \frac{\log p}{p-1} \right) &= \frac{N^2}{2} \sum_{d|q} d\mu\left(\frac{q}{d}\right) \sum_{p|d} \left(1 - \frac{1}{p-1} \right) \log p \\
 &= \frac{N^2}{2} \sum_{p|q} \left(\frac{p-2}{p-1} \log p \sum_{\substack{d|q \\ p|d}} d\mu\left(\frac{q}{d}\right) \right) \\
 &= \frac{N^2}{2} \sum_{p|q} \frac{p-2}{p-1} p \phi\left(\frac{q}{p}\right) \log p \\
 &= \frac{N^2}{2} \phi(q) \sum_{p|q} \frac{p(p-2)}{(p-1)^2} \log p \\
 &= \frac{N^2}{2} \phi(q) \left(\log q - \sum_{p|q} \frac{\log p}{(p-1)^2} \right)
 \end{aligned} \tag{7.13}$$

Thus the contribution of the terms $\frac{N^2}{2} \left(\log d - \sum_{p|d} \frac{\log p}{p-1} \right)$ is $\frac{N^2}{2}$ times

$$\begin{aligned}
 \sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)} \left(\log q - \sum_{p|q} \frac{\log p}{(p-1)^2} \right) &= \log y \sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)} - \sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)} \log(y/q) \\
 &\quad - \sum_{\substack{p \leq y \\ p|q}} \frac{\log p}{(p-1)^2} \sum_{\substack{q \leq y \\ p|q}} \frac{\mu(q)^2}{\phi(q)}
 \end{aligned} \tag{7.14}$$

The first sum is evaluated in Lemma 3, and contributes

$$(\log y)^2 + \left(\gamma + \sum_p \frac{\log p}{p(p-1)} \right) \log y + O(1). \tag{7.15}$$

Writing $q = pr$, the last sum is

$$\begin{aligned}
 \sum_{p \leq y} \frac{\log p}{(p-1)^3} \sum_{\substack{r \leq y/p \\ (r,p)=1}} \frac{\mu(r)^2}{\phi(r)} &= \sum_{p \leq y} \frac{\log p}{p(p-1)^2} (\log(y/p) + O(1)) \\
 &= \left(\sum_p \frac{\log p}{p(p-1)^2} \right) \log y + O(1).
 \end{aligned} \tag{7.16}$$

We do the middle sum via contour integration:

$$\sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)} \log(y/q) = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} G(s) \frac{y^s}{s^2} ds, \tag{7.17}$$

where $G(s) = \sum_{n=1}^{\infty} \frac{\mu(n)^2}{\phi(n)} n^{-s}$ and $a > 0$.

We have

$$\begin{aligned} G(s) &= \prod_p \left(1 + \frac{1}{(p-1)p^s} \right) \\ &= \zeta(s+1) \prod_p \left(1 + \frac{1}{p(p-1)p^s} - \frac{1}{p(p-1)p^{2s}} \right) \\ &=: \zeta(s+1)H(s), \end{aligned} \tag{7.18}$$

where $H(s)$ is analytic for $\operatorname{Re} s > -1/2$ and $H(0) = 1$. Near $s = 0$,

$$\begin{aligned} G(s) \frac{y^s}{s^2} &= \frac{1}{s^2} \zeta(s+1)H(s)y^s \\ &= \frac{1}{s^2} \left(\frac{1}{s} + \gamma - \gamma_1 s + O(s^2) \right) \left(1 + H'(0)s + \frac{H''(0)s^2}{2} + O(s^3) \right) \\ &\quad \times \left(1 + (\log y)s + \frac{(\log y)^2 s^2}{2} + O(s^3) \right). \end{aligned} \tag{7.19}$$

The residue at 0 is then

$$\frac{(\log y)^2}{2} + (\gamma + H'(0)) \log y - \gamma_1 + \gamma H'(0) + \frac{H''(0)}{2}, \tag{7.20}$$

so by moving the contour to $\operatorname{Re} s = b$, $-1/2 < b < 0$ (convergence follows from (6.9)), we get

$$\sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)} \log(y/q) = \frac{(\log y)^2}{2} + (\gamma + H'(0)) \log y + O(1). \tag{7.21}$$

We have

$$\frac{H'(s)}{H(s)} = \sum_p \frac{(2p^{-2s} - p^{-s}) \log p}{p(p-1) + p^{-s} - p^{-2s}},$$

so $H'(0) = \sum_p \frac{\log p}{p(p-1)}$. Then combining (7.21) with (7.15) and (7.16),

$$\sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)} \left(\log q - \sum_{p|q} \frac{\log p}{(p-1)^2} \right) = \frac{1}{2} (\log y)^2 - \left(\sum_p \frac{\log p}{p(p-1)^2} \right) \log y + O(1). \tag{7.22}$$

Combining with the other terms (7.10), (7.11) and (7.12),

$$\begin{aligned}
 S_2 &= \sum_{k \leq N} (N - k)^2 \mathfrak{S}(k) \mathfrak{S}_y(k) \\
 &= \left(\sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^3} \right) \frac{N^3}{3} - \frac{N^2}{2} (\log N + c_1) \left(\log y + \gamma + \sum_p \frac{\log p}{p(p-1)} \right) \\
 &\quad + O(N^2 \log(2N)y^{-\frac{1}{2}}) \\
 &\quad + \frac{N^2}{2} \left(\frac{1}{2} (\log y)^2 - \left(\sum_p \frac{\log p}{p(p-1)^2} \right) \log y + O(1) \right) + O_\epsilon(N^{\frac{3}{2}}y^{\frac{1}{2}+\epsilon}) \quad (7.23) \\
 &= \left(\sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^3} \right) \frac{N^3}{3} - \frac{N^2}{2} \log N \log y + \frac{N^2}{4} (\log y)^2 \\
 &\quad - \left(\gamma + \sum_p \frac{\log p}{p(p-1)} \right) \frac{N^2}{2} \log N - \left(c_1 + \sum_p \frac{\log p}{p(p-1)^2} \right) \frac{N^2}{2} \log y \\
 &\quad + O(N^2) + O_\epsilon(N^{\frac{3}{2}}y^{\frac{1}{2}+\epsilon}) + O(N^2 \log(2N)y^{-\frac{1}{2}}),
 \end{aligned}$$

as claimed. ■

8. The sum S_3

In this section we prove the following result on S_3 .

Theorem 6. *We have, for $1 \leq y \leq \sqrt{N}$,*

$$\begin{aligned}
 S_3 &:= \sum_{k \leq N} (N - k)^2 \mathfrak{S}_y(k)^2 = \left(\sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^3} \right) \frac{N^3}{3} \\
 &\quad - \left(\log y + \gamma + \sum_p \frac{\log p}{p(p-1)} \right)^2 \frac{N^2}{2} + O(N^2 y^{-\frac{1}{2}} \log y) + O(Ny^2). \quad (8.1)
 \end{aligned}$$

Proof. The definition of $\mathfrak{S}_y(k)$ and the formula $c_q(-k) = \sum_{d|q} d \mu\left(\frac{q}{d}\right)$ give

$$S_3 = \sum_{q \leq y} \sum_{q' \leq y} \frac{\mu(q)^2}{\phi(q)^2} \frac{\mu(q')^2}{\phi(q')^2} \underbrace{\sum_{1 \leq k \leq N} (N - k)^2 c_q(-k) c_{q'}(-k)}_{S_{31}}, \quad (8.2)$$

and

$$S_{31} = \sum_{d|q} \sum_{d'|q'} d \mu\left(\frac{q}{d}\right) d' \mu\left(\frac{q'}{d'}\right) \sum_{\substack{1 \leq k \leq N \\ [d, d']|k}} (N - k)^2. \quad (8.3)$$

Using Lemma 1 on

$$\sum_{\substack{1 \leq k \leq N \\ [d, d']|k}} (N - k)^2 = [d, d']^2 \sum_{1 \leq k \leq \frac{N}{[d, d']}} \left(\frac{N}{[d, d']} - k \right)^2,$$

we obtain

$$\begin{aligned}
 S_{31} &= \sum_{d|q} \sum_{d'|q'} [d, d']^2 dd' \mu\left(\frac{q}{d}\right) \mu\left(\frac{q'}{d'}\right) \left(\frac{N^3}{3[d, d']^3} - \frac{N^2}{2[d, d']^2} + O\left(\frac{N}{[d, d']}\right) \right) \\
 &= \frac{N^3}{3} \sum_{d|q} \sum_{d'|q'} (d, d') \mu\left(\frac{q}{d}\right) \mu\left(\frac{q'}{d'}\right) - \frac{N^2}{2} \sum_{d|q} \sum_{d'|q'} dd' \mu\left(\frac{q}{d}\right) \mu\left(\frac{q'}{d'}\right) \\
 &\quad + O\left(N \sum_{d|q} \sum_{d'|q'} d^2 d'^2\right),
 \end{aligned}$$

where we use that $\frac{N}{6[d, d']} + O(1) = O\left(\frac{N}{[d, d']}\right)$ because $[d, d'] \leq dd' \leq qq' \leq y^2 \leq N$. Thus

$$S_3 = A_1(y) \frac{N^3}{3} - A_2(y) \frac{N^2}{2} + O(A_3(y)N), \tag{8.4}$$

where

$$A_1(y) = \sum_{q \leq y} \sum_{q' \leq y} \frac{\mu(q)^2}{\phi(q)^2} \frac{\mu(q')^2}{\phi(q')^2} \sum_{d|q} \sum_{d'|q'} (d, d') \mu\left(\frac{q}{d}\right) \mu\left(\frac{q'}{d'}\right), \tag{8.5}$$

$$\begin{aligned}
 A_2(y) &= \sum_{q \leq y} \sum_{q' \leq y} \frac{\mu(q)^2}{\phi(q)^2} \frac{\mu(q')^2}{\phi(q')^2} \left(\sum_{d|q} d \mu\left(\frac{q}{d}\right) \right) \left(\sum_{d'|q'} d' \mu\left(\frac{q'}{d'}\right) \right) \\
 &= \left(\sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^2} \cdot \phi(q) \right)^2,
 \end{aligned} \tag{8.6}$$

and

$$\begin{aligned}
 A_3(y) &= \sum_{q \leq y} \sum_{q' \leq y} \frac{\mu(q)^2}{\phi(q)^2} \frac{\mu(q')^2}{\phi(q')^2} \left(\sum_{d|q} d^2 \right) \left(\sum_{d'|q'} d'^2 \right) \\
 &= \left(\sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^2} \sum_{d|q} d^2 \right)^2 = \left(\sum_{dr \leq y} \frac{\mu(dr)^2}{\phi(dr)^2} d^2 \right)^2 \\
 &= \left(\sum_{r \leq y} \frac{\mu(r)^2}{\phi(r)^2} \sum_{\substack{d \leq y/r \\ (d,r)=1}} \frac{\mu(d)^2 d^2}{\phi(d)^2} \right)^2 \ll \left(\sum_{r \leq y} \frac{\mu(r)^2}{\phi(r)^2} \cdot \frac{y}{r} \right)^2 \ll y^2,
 \end{aligned} \tag{8.7}$$

using Lemma 2 for the last two steps. We compute $A_1(y)$ the same way we did $B_1(y)$ in §3, using

$$(d, d') = \sum_{\substack{r|d \\ r|d'}} \phi(r)$$

to get

$$A_1(y) = \sum_{r \leq y} \phi(r) \left(\sum_{\substack{q \leq y \\ r|q}} \frac{\mu(q)^2}{\phi(q)^2} \sum_{\substack{d|q \\ r|d}} \mu\left(\frac{q}{d}\right) \right)^2 = \sum_{r \leq y} \frac{\mu(r)^2}{\phi(r)^3}. \quad (8.8)$$

We conclude

$$S_3 = \left(\sum_{r \leq y} \frac{\mu(r)^2}{\phi(r)^3} \right) \frac{N^3}{3} - \left(\sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)} \right)^2 \frac{N^2}{2} + O(Ny^2). \quad (8.9)$$

Theorem 6 now follows from Lemma 3. ■

9. Completion of the proof of Theorem 2

By (5.1) and Theorems 4, 5, and 6, for $1 \leq y \leq \sqrt{N}$ we have

$$\begin{aligned} \sum_{k \leq N} (N-k)^2 \tilde{\mathfrak{S}}_y(k)^2 &= S_1 - 2S_2 + S_3 \\ &= \left(\prod_p \left(1 + \frac{1}{(p-1)^3} \right) - 2 \sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^3} + \sum_{q \leq y} \frac{\mu(q)^2}{\phi(q)^3} \right) \frac{N^3}{3} \\ &\quad - \frac{1}{4} N^2 (\log N)^2 + 2 \left(\frac{1}{2} N^2 \log N \log y - \frac{1}{4} N^2 (\log y)^2 \right) - \frac{1}{2} N^2 (\log y)^2 \\ &\quad + \left(\frac{3}{4} - \gamma - \frac{1}{2} \log 2\pi - \frac{1}{2} \sum_p \frac{\log p}{(p-1)^2} \right) N^2 \log N \\ &\quad + 2 \left(\left(\gamma + \sum_p \frac{\log p}{p(p-1)} \right) \frac{N^2}{2} \log N \right. \\ &\quad \left. + \left(\gamma - \frac{3}{2} + \log 2\pi + \sum_p \frac{\log p}{p(p-1)^2} \right) \frac{N^2}{2} \log y \right) - 2 \left(\gamma + \sum_p \frac{\log p}{p(p-1)} \right) \frac{N^2}{2} \log y \\ &\quad + O(N^2) + O(N^2 \log(2N)y^{-\frac{1}{2}}) + O_\epsilon(N^{3/2}y^{1/2+\epsilon}) + O(N^2y^{-\frac{1}{2}} \log y) + O(Ny^2) \\ &= \left(\sum_{q > y} \frac{\mu(q)^2}{\phi(q)^3} \right) \frac{N^3}{3} + N^2 \left(-\frac{1}{4} (\log N)^2 + \log N \log y - (\log y)^2 \right) \\ &\quad + \left(\frac{3}{4} - \frac{1}{2} \log 2\pi + \sum_p \frac{(p-2) \log p}{2p(p-1)^2} \right) N^2 \log N \\ &\quad + \left(-\frac{3}{2} + \log 2\pi + \sum_p \frac{(2-p) \log p}{p(p-1)^2} \right) N^2 \log y + O(N^2) + O(N^2 \log(2N)y^{-\frac{1}{2}}) \\ &= \left(\sum_{q > y} \frac{\mu(q)^2}{\phi(q)^3} \right) \frac{N^3}{3} - \frac{1}{4} N^2 \left(\log \frac{N}{y^2} \right)^2 + cN^2 \log \frac{N}{y^2} + O(N^2) + O(N^2 \log(2N)y^{-\frac{1}{2}}). \end{aligned}$$

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