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UNEXPECTED AVERAGE VALUES OF GENERALIZED VON MANGOLDT FUNCTIONS IN RESIDUE CLASSES

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Abstract

In order to study integers with few prime factors, the average of $\Lambda_k = \mu * \log^k$ has been a central object of research. One of the more important cases, $k = 2$, was considered by Selberg ['An elementary proof of the prime-number theorem', *Ann. of Math. (2)* **50** (1949), 305–313]. For $k \geq 2$, it was studied by Bombieri ['The asymptotic sieve', *Rend. Accad. Naz. XL (5)* **1**(2) (1975/76), 243–269; (1977)] and later by Friedlander and Iwaniec ['On Bombieri's asymptotic sieve', *Ann. Sc. Norm. Super. Pisa Cl. Sci. (4)* **5**(4) (1978), 719–756], as an application of the asymptotic sieve.

Let $\Lambda_{j,k} := \mu_j * \log^k$, where μ_j denotes the Liouville function for $(j+1)$-free integers, and 0 otherwise. In this paper we evaluate the average value of $\Lambda_{j,k}$ in a residue class $n \equiv a \bmod q$, $(a, q) = 1$, uniformly on q. When $j \geq 2$, we find that the average value in a residue class differs by a constant factor from the expected value. Moreover, an explicit formula of Weil type for $\Lambda_k(n)$ involving the zeros of the Riemann zeta function is derived for an arbitrary compactly supported C^2 function.

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1. Introduction

The generalized von Mangoldt function is defined by

$$\Lambda_k(n) := \sum_{d|n} \mu(d) \log^k \frac{n}{d}. \tag{1-1}$$

This function is supported on integers with at most k distinct prime factors. Also we observe that the sum runs over the square-free divisors of n. In order to obtain a variant of Selberg's inequality [18], Levinson [13] showed that

$$\sum_{n \leq x} \Lambda_k(n) = kxP_{k-1}(\log x) + O(x), \tag{1-2}$$

where P_n is a monic polynomial of degree n. (It should be noted that there is a typo in Levinson's paper and the right-hand side is misprinted as $(k+1)xP_{k-1}(\log x) + O(x)$.) Ivić [11] improved the error term in the asymptotic formula (1-2) and showed that

$$\sum_{n\le x}\Lambda_k(n) = kxP_{k-1}(\log x) + O(x\exp\{-c_k\delta(x)\}),$$

where $c_k > 0$ and $\delta(x) = (\log x)^{3/5}(\log\log x)^{-1/5}$.

For any relatively prime positive integers a and q, let us define

$$a(n) = \begin{cases} 1 & \text{if } n \equiv a \pmod q, \\ 0 & \text{otherwise.} \end{cases}$$

To give an elementary proof of the prime number theorem in arithmetic progressions, Selberg [19] and Shapiro [20] showed that

$$\sum_{n\le x} a(n)\Lambda_2(n) \sim \frac{2x}{\phi(q)}\log x, \tag{1-3}$$

where $\phi(n)$ denotes the Euler totient function, which counts the positive integers up to n which are coprime to n. It seems that the uniformity of q is missing in their results.

In [21, 23], Siegel and Walfisz separately obtained the following result. The asymptotic formula

$$\sum_{n\le x} a(n)\Lambda(n) \sim \frac{x}{\phi(q)} \tag{1-4}$$

holds uniformly in the range $q < \log^A x$, for any fixed A. This is a uniform version of the prime number theorem in arithmetic progressions. This theorem is in general noneffective. The asymptotic formula is only known to be effective if A is chosen to be smaller than 2.

In [9], by adapting a method of Bombieri [2, 3], Friedlander and Iwaniec [10] proved (1-3) uniformly in the range

$$\log q < \varepsilon(x)\log x.$$

In the same paper, by using the L-function (analytic) techniques Friedlander proved (1-3) uniformly in a smaller range

$$\log q < \varepsilon(x)\frac{\log x}{\log\log x},$$

where $\varepsilon(x)$ is a fixed positive function, tending to 0 as $x \to \infty$. For $k \ge 2$, the presence of an extra $\log x$ in the residue coming from the principal character allows for improvement of the length of $\log q$ even in (1-4). In other words, effects due to the hypothetical Siegel (or exceptional) zero can be reduced in this case.

In [12], Knafo proved that

$$\sum_{n\le x} a(n)\Lambda_k(n) \sim \frac{kx}{\phi(q)}\log^{k-1} x,$$

for $k \geq 2$ and

$$\log q < \varepsilon(x)^{1/(k-1)} \frac{\log x}{\log\log x}.$$

Let $j, n \geq 1$ be integers. Then an analogue of the Möbius function is

$$\mu_j(n) := \begin{cases} 1 & \text{if } n = 1, \\ 0 & \text{if } p^{j+1} \mid n \text{ for some prime } p, \\ (-1)^{\sum \alpha} & \text{if } p^{\alpha} \parallel n \text{ implies } \alpha \leq j \text{ for some prime } p. \end{cases} \tag{1-5}$$

If $j = 1$, then this function coincides with the Möbius function $\mu(n)$; and if $j \to \infty$ then this function coincides with the Liouville function $\lambda(n)$.

Analogously to (1-1) we define

$$\Lambda_{j,k}(n) := \sum_{d \mid n} \mu_j(d) \log^k \frac{n}{d}$$

for $j, k \geq 1$. Here we consider a sum which is taken over $(j+1)$-free divisors of n. If j is an odd integer, then $\Lambda_{j,k}$ is supported on $n = ab$, where b has at most k prime factors and $p^{\alpha} \parallel a$ implies α is even and $\alpha < j$. If j is an even integer, then $\Lambda_{j,k}$ is supported on $n = ab$, where b has at most k prime factors and $p^{\alpha} \parallel a$ and if $\alpha \leq j$ then α is even. It is clear that if $j = k = 1$, then we recover the usual von Mangoldt function $\Lambda(n)$. If $j = 1$ and $k \geq 1$, then $\Lambda_{1,k}(n) = \Lambda_k(n)$. Recent applications of these functions can be found in [14, 15] where they were used to improve the proportion of zeros of the Riemann zeta function on the critical line. In [17], the function Λ_k is an important ingredient in the mollifier to obtain a zero-density result of the derivative of the completed Riemann zeta function.

We shall also define

$$L_k(n) := \sum_{d \mid n} \lambda(d) \log^k \frac{n}{d},$$

for $k \geq 1$ integer.

Consider the following two generalizations of the Chebyshev function in arithmetic progressions:

$$\vartheta_k(x; q, a) := \sum_{n \leq x} a(n) L_k(n)$$

for $k \geq 1$ integer, and

$$\psi_{j,k}(x; q, a) := \sum_{n \leq x} a(n) \Lambda_{j,k}(n) \tag{1-6}$$

for $j, k \geq 1$ integers. Calderón [4] obtained an asymptotic formula for (1-6) when a, q are fixed positive integers with $(a, q) = 1$. We will prove the following results.

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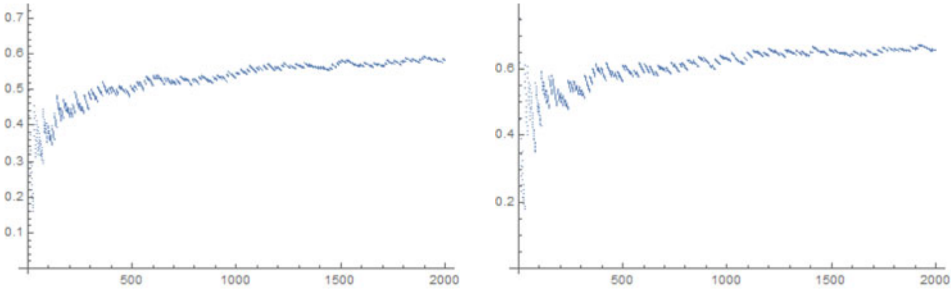


(a) (b)

FIGURE 1. (a) Plot of left-hand side/right-hand side of (1-7) for $j = k = 2$, $q = 11$ and $a = 7$ for $1 \le x \le 2000$. (b) Plot of left-hand side/right-hand side of (1-7) for $j = 3$, $k = 2$, $q = 13$ and $a = 5$ for $1 \le x \le 2000$.

THEOREM 1.1. *Let $j, k \ge 1$ be integers. Then the asymptotic formula*

$$\psi_{j,k}(x; q, a) \sim k\frac{c(j,q)}{\phi(q)} x \log^{k-1} x \tag{1-7}$$

holds uniformly in

$$\log q < \varepsilon_k(x)\frac{\log x}{\log\log x},$$

where $\varepsilon_k(x)$ be a fixed positive function, such that $\varepsilon_k(x) = o(1)$ as $x \to \infty$. Here

$$c(j,q) = \begin{cases} (-1)^{j+3/2}\dfrac{(j+1)!}{12B_{j+1}(2\pi)^{j-1}}\displaystyle\prod_{p|q}\frac{1-1/p^2}{1-1/p^{j+1}} & \text{if } j \ge 1 \text{ odd},\\ (-1)^{j}\dfrac{\zeta(j+1)(2(j+1))!}{12B_{2(j+1)}(2\pi)^{2j}}\displaystyle\prod_{p|q}\frac{1-1/p^2}{1+1/p^{j+1}} & \text{if } j \ge 2 \text{ even}, \end{cases}$$

and B_n is the $(n+1)$th Bernoulli number. Here p denotes a prime.

One should note that the product over primes in the representation of $c(j, q)$ can be expressed as Jordan totient functions.

Figure 1 gives a comparison between the left-hand side and the right-hand side of (1-7). Figure 2 illustrates the distribution of $\phi(q)/c(j, q)$ for odd and even values of j.

Let

$$\psi_{j,k}(x) = \sum_{n \le x} \Lambda_{j,k}(n).$$

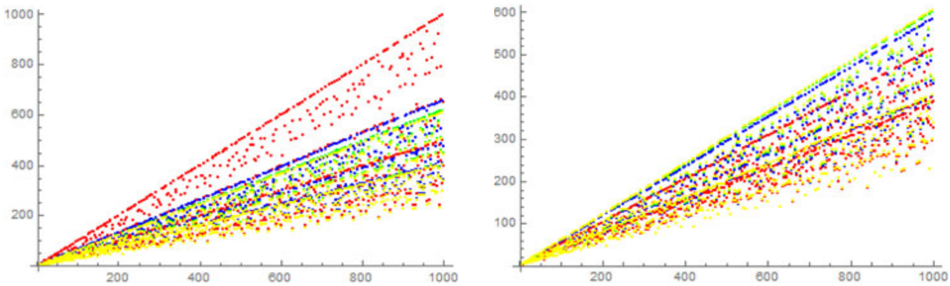
At the end of the proof of Theorem 1.1 we find that

$$\psi_{j,k}(x) \sim kc(j, 1)x \log^{k-1} x.$$

Then for any residue class one should expect

$$\psi_{j,k}(x; q, a) \sim k\frac{c(j,1)}{\phi(q)} x \log^{k-1} x.$$

But Theorem 1.1 produces an extra factor $c(j, q)/c(j, 1) < 1$ or $c(j, q)/c(j, 1) > 1$, which shows that the average value of $\Lambda_{j,k}(n)$ increases or decreases (see Figure 3), depending



(a) (b)

FIGURE 2. (a) Plot of $\phi(q)/c(j,q)$ for $j = 1$ (red/dark grey), $j = 3$ (blue/black), $j = 5$ (green/grey) $j = 7$ (yellow/light grey) for $2 \le q \le 1000$. (b) Plot of $\phi(q)/c(j,q)$ for $j = 2$ (red/dark grey), $j = 4$ (blue/black), $j = 6$ (green/grey) $j = 8$ (yellow/light grey) for $2 \le q \le 1000$ (colour available online).

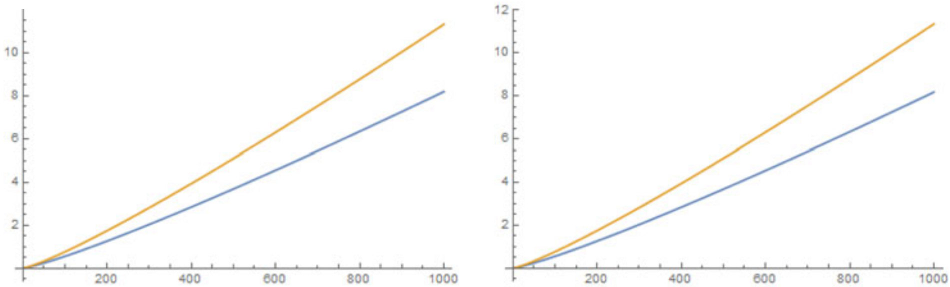


FIGURE 3. (a) Plot of right-hand side of (1-7) for $j = 11$, $k = 2$, $a = 5$, $q = 5000$ (blue/black) and $kc(j,1)x\log^{k-1} x/\phi(q)$ (orange/grey) for $1 \le x \le 1000$. (b) Plot of right-hand side of (1-7) for $j = 12$, $k = 2$, $a = 7$, $q = 5000$ (blue/black) and $kc(j,1)x\log^{k-1} x/\phi(q)$ (orange/grey) for $1 \le x \le 1000$ (colour available online).

on j, in any given residue class compared to its expected value. This is a strange phenomenon and this occurrence cannot be seen in the case of $j = 1$; in other words, it cannot be seen for Λ_k (see Friedlander [9], Knafo [12]) and most of the other arithmetic functions.

The case $\lambda(n)$ is treated below.

THEOREM 1.2. *Let $k \ge 1$ be an integer. Then the asymptotic formula*

$$\vartheta_k(x; q, a) \sim k\frac{c(q)}{\phi(q)} x \log^{k-1} x \tag{1-8}$$

holds uniformly in

$$\log q < \beta_k(x)\frac{\log x}{\log\log x},$$

where $\beta_k(x)$ is a fixed positive function, such that $\beta_k(x) = o(1)$ as $x \to \infty$. Here

$$c(q) = \frac{\pi^2}{6}\prod_{p \mid q}\Big(1 - \frac{1}{p^2}\Big),$$

and p denotes a prime.

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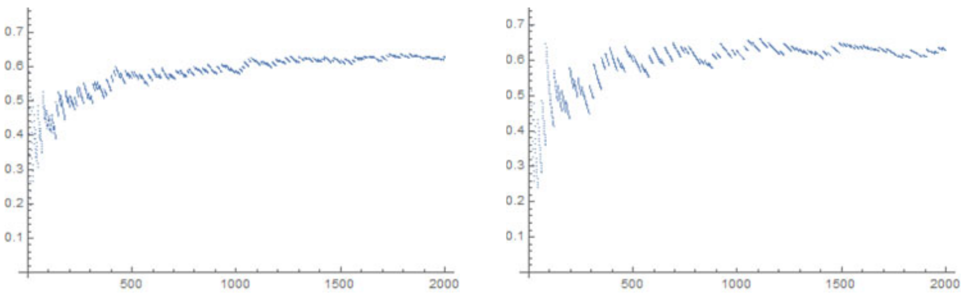

(a) (b)

FIGURE 4. (a) Plot of left-hand side/right-hand side of (1-8) for $k = 2$, $q = 11$ and $a = 5$ for $1 \leq x \leq 2000$. (b) Plot of left-hand side/right-hand side of (1-8) for $k = 2$, $q = 19$ and $a = 7$ for $1 \leq x \leq 2000$.

Figure 4 gives a comparison between the left-hand side and the right-hand side of (1-8).

The explicit formula for $\Lambda(n)$ was derived by Riemann and later by von Mangoldt [6, Ch. 17]. It is given by

$$\sum_{n \leq x} \Lambda(n) = x - \sum_{\rho} \frac{x^{\rho}}{\rho} - \log(2\pi) - \frac{1}{2}\log(1 - x^{-2}),$$

for $x > 1$ and $x \neq p^m$, where p is again a prime and m is an integer. The sum over ρ is performed over all nontrivial zeros of the Riemann zeta function. This is a cornerstone result in the *analytic* proof of the prime number theorem.

The Weil explicit formula is a generalization of the Riemann explicit formula for more general test functions. The Weil explicit formula also links the zeros of the Riemann zeta function and the von Mangoldt function as follows. Suppose that f is a compactly supported C^2 function and let

$$F(s) = \int_0^{\infty} f(x) x^{s-1}\, dx$$

be the Mellin transform of f. Weil [24] proved that

$$\sum_{\rho} F(\rho) + \sum_{n \geq 1} F(-2n) = F(1) + \sum_{n \geq 1} \Lambda(n) f(n). \tag{1-9}$$

This is in fact a specific case of a more general set-up studied by Weil [24] who treated general L-functions associated with a Grössencharakter χ. These are representations of the group of idèle classes of an algebraic number field $\mathbb{K}$ into the multiplicative group of nonzero complex numbers.

We now provide the Weil explicit formula analogue of the function $\Lambda_k(n)$.

THEOREM 1.3. *Suppose that $h \in C^2(0, \infty)$ and is compactly supported. Suppose that the nontrivial zeros of $\zeta(s)$ are simple. Let $\hat{h}$ be the Mellin transform of h. Then, for any*

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positive integer $k \geq 1$, we have

$$\sum_{n=1}^{\infty} \Lambda_k(n)h(n) = \Phi(k) + (-1)^k \sum_{\rho} \frac{\zeta^{(k)}}{\zeta'}(\rho)\hat{h}(\rho) + (-1)^k \sum_{m=1}^{\infty} \frac{\zeta^{(k)}}{\zeta'}(-2m)\hat{h}(-2m),$$

where

$$\Phi(k) := \frac{(-1)^k}{(k-1)!} \lim_{s\to 1} \frac{d^{k-1}}{ds^{k-1}}\Big((s-1)^k \frac{\zeta^{(k)}}{\zeta}(s)\hat{h}(s)\Big).$$

The first few values of $\Phi(k)$ are given by

$$\Phi(1) = \hat{h}(1), \quad \Phi(2) = 2(\hat{h}'(1) - \gamma_0\hat{h}(1)),$$

and

$$\Phi(3) = 3(\hat{h}''(1) - 2\gamma_0\hat{h}'(1) + 2\gamma_0^2\hat{h}(1) + 2\gamma_1\hat{h}(1)).$$

Here γ_n are the Stieltjes constants given by the limit

$$\gamma_n = \lim_{m\to\infty}\Big(\sum_{k=1}^{m} \frac{\log^n k}{k} - \frac{\log^{n+1} m}{n+1}\Big),$$

with the case 0^0 taken to be 1. In particular, $\gamma_0 = \gamma = 0.577\cdots$ is Euler's constant. For simplicity we have supposed that all the nontrivial zeros ρ of $\zeta(s)$ are simple, which is harmless in our proofs. This assumption can be lifted at the cost of adding extra terms.

Recently some arithmetic properties of the generalized von Mangoldt function have been studied in the literature. In order to obtain the pair correlation of zeros of derivatives of the completed Riemann zeta function, Gonek, Farmer and Lee [7] first deduced certain asymptotics involving Λ_k. To improve the positive proportion zeros of the Riemann zeta function on the critical line, the present authors, along with Zaharescu [16], have exploited the combinatorial properties of $\Lambda_k(n)$.

2. Preliminary results

The following tools will be needed in the proofs of our results.

Lemma 2.1. *For each real number $T \geq 2$ there is a T_1, $T \leq T_1 \leq T+1$, such that*

$$\frac{\zeta^{(k)}}{\zeta}(\sigma + iT_1) \ll_k \log^{2k} T$$

uniformly for $-1 \leq \sigma \leq 2$.

Proof. Set $s = \sigma + it$. From [22, page 217] we have

$$\frac{\zeta'}{\zeta}(s) = \sum_{|t-\gamma|\leq 1} \frac{1}{s-\rho} + O(\log t),$$

uniformly for $-1 \leq \sigma \leq 2$, where $\rho = \beta + i\gamma$ runs through zeros of $\zeta(s)$. By Cauchy's integral formula one finds that

$$\Big(\frac{\zeta'}{\zeta}(s)\Big)^{(k-1)} = \sum_{|t-\gamma|\leq 1} \frac{(-1)^{k-1}(k-1)!}{(s-\rho)^k} + O(\log^k t)$$

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uniformly for $-1 \le \sigma \le 2$. If $N(T)$ denotes the number of zeros of $\zeta(s)$ in the critical strip up to height T, then

$$N(T+1) - N(T) = O(\log T)$$

as $T \to \infty$ (see [22, page 221]). Hence, there exist zeros whose imaginary parts lie in the interval $[T, T+1]$ and the gap between them is at least $1/\log T$. Therefore

$$\left(\frac{\zeta'}{\zeta}(\sigma + iT_1)\right)^{(k-1)} \ll_k \log^{k+1} T, \tag{2-1}$$

for some $T \le T_1 \le T+1$ and uniformly for $-1 \le \sigma \le 2$. Now, an application of the Faà di Bruno formula [8, page 188] allows us to write

$$\frac{f^{(n)}}{f}(s) = n! \sum_{\substack{\mu_1 + 2\mu_2 + \cdots + k\mu_k = n \\ \mu_i \ge 0}} \prod_{i=1}^{k} \frac{1}{\mu_i!(i!)^{\mu_i}} \left(\left(\frac{f'}{f}\right)^{(i-1)}(s) \right)^{\mu_i}, \tag{2-2}$$

for any analytic function f with $f(s) \ne 0$. Setting $f(s) = \zeta(s)$, and using equations (2-1) and (2-2) yields the desired result. □

Lemma 2.2. *Let $\mathcal{A}$ denote the set of those points $s \in \mathbb{C}$ such that $\sigma \le -1$ and $|s + 2m| \ge \frac{1}{4}$ for every positive integer m. Then*

$$\frac{\zeta^{(k)}}{\zeta}(s) \ll_k \log^k(|s| + 1)$$

uniformly for $s \in \mathcal{A}$.

Proof. From the functional equation of $\zeta(s)$ we obtain

$$\frac{\zeta'}{\zeta}(s) = -\frac{\zeta'}{\zeta}(1-s) + \log 2\pi - \frac{\Gamma'}{\Gamma}(1-s) + \frac{\pi}{2}\cot\frac{\pi s}{2};$$

see [22, page 20]. Hence

$$\left(\frac{\zeta'}{\zeta}(s)\right)^{(k)} = (-1)^{k-1}\left(\frac{\zeta'}{\zeta}(1-s)\right)^{(k)} + (-1)^{(k-1)}\left(\frac{\Gamma'}{\Gamma}(1-s)\right)^{(k)} + Q\left(\cot\frac{\pi s}{2}\right), \tag{2-3}$$

where Q is a polynomial of degree $k+1$. Since s is away from integers,

$$\cot\frac{\pi s}{2} = i\frac{e^{\pi i s} + 1}{e^{\pi i s} - 1} = i + \frac{2i}{e^{\pi i s} - 1} \ll 1. \tag{2-4}$$

From the definition of the logarithmic derivative of the gamma function we have

$$\frac{\Gamma'}{\Gamma}(s) = -\frac{1}{s} + \Gamma'(1) - \sum_{n=1}^{\infty}\left(\frac{1}{s+n} - \frac{1}{n}\right). \tag{2-5}$$

It can be shown that

$$\frac{\Gamma'}{\Gamma}(s) = \log s + O\left(\frac{1}{|s|}\right) \tag{2-6}$$

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for $|s| > \delta$, and $|\arg s| < \pi - \delta$ for any $\delta > 0$ (see [6]). By differentiation of (2-5) we get

$$\left(\frac{\Gamma'}{\Gamma}(s)\right)^{(k)} = (-1)^{k-1} \sum_{n=0}^{\infty} \frac{k!}{(s+n)^{k+1}}.$$

Therefore for $k \geq 1$ we see that

$$\left(\frac{\Gamma'}{\Gamma}(s)\right)^{(k)} \ll_k \frac{1}{|s|^k}. \tag{2-7}$$

Combining (2-2), (2-3), (2-4), (2-6), and (2-7), we conclude the proof. □

Let $q > 1$ and let χ be a character modulo q. Let $L(s,\chi)$ be the associated Dirichlet L-function. From [6, Section 14], there is a positive absolute constant A_4 (which we take to be less than $\frac{1}{12}$), such that if

$$\sigma \geq 1 - \frac{A_4}{\log(q(|t|+1))}, \tag{2-8}$$

then there is at most one zero of $L(s,\chi)$. If such a zero exists, then it is real and simple, χ is real and nonprincipal, and $L(s,\psi)$ has no zeros in the above region for any other character ψ of the modulus q.

If such a zero β exists and if $\beta > 1 - (A_4/9 \log 2q)$, then we shall call χ an exceptional character, β an exceptional zero, and the modulus q an exceptional modulus.

Next, from [12] we have the following result.

Lemma 2.3. *Let $2 \leq T \leq x$ and define the contour C_χ to consist of $\sigma = 1 - (A_4/B\log(q(|t|+2)))$, $t \leq |T|$, together with the line segments*

$$t = \pm T, \quad 1 - \frac{A_4}{B\log(q(|T|+2))} \leq \sigma \leq 1 + \frac{1}{\log x},$$

where we take $B = 8$ if χ is exceptional and $B = 10$ otherwise. Let $k \geq 1$. Then on the contour C_χ,

$$\frac{L^{(k)}}{L}(s,\chi) \ll_k \log(q(|T|+2))^{k+4}.$$

3. Proof of Theorems 1.1 and 1.2

First we prove the following theorem.

Theorem 3.1. *Let $j,k \geq 1$ be integers. Let $2 \leq T \leq x$, $q \leq x$, and A_4 be as in (2-8). For each character χ mod q, we have*

$$\begin{aligned}\psi_{j,k}(x,\chi) &= \sum_{n \leqslant x} \chi(n)\Lambda_{j,k}(n)\\ &= W_{j,k}(x,\chi) + O_{k,j}\left(\frac{x}{T}\log^{k+3} x\right) + O_{k,j}\left(x \log^{k+5}(qT) \exp\left(-\frac{A_4 \log x}{20 \log qT}\right)\right).\end{aligned}$$

Here $W_{j,k}(x,\chi)$ is given as follows:

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(1) *if χ is a principal character, then*

$$W_{j,k}(x,\chi) = xkc(j,q)\log^{k-1} x + O_{j,k}\bigg(x\sum_{n=0}^{k-2}\log^n(x)(\log\log q)^{k-n-1}\bigg),$$

for all $k \geq 2$;

(2) *if χ is an exceptional character and β is the exceptional zero, then*

$$W_{j,k}(x,\chi) \ll_{k,j} x(\log q\log\log q)^{k-1},$$

for all $k \geq 2$;

(3) *otherwise*

$$W_{j,k}(x,\chi) = 0.$$

Proof. Suppose that χ is a Dirichlet character mod q. From Equation (1-5) we find that

$$\sum_{n=1}^{\infty}\frac{\chi(n)\mu_j(n)}{n^s} = \prod_p\sum_{k=0}^{j}(-1)^k\frac{\chi(p^k)}{p^{ks}} \tag{3-1}$$

for $\mathrm{Re}(s) > 1$. If $j \geq 2$ is an even integer, then the right-hand side of (3-1) can be written as

$$\begin{aligned}\prod_p\sum_{k=0}^{j}(-1)^k\frac{\chi(p^k)}{p^{ks}} &= \prod_p\frac{1+\frac{\chi(p^{j+1})}{p^{(j+1)s}}}{1+\frac{\chi(p)}{p^s}}\\ &= \prod_p\frac{1-\frac{\chi^{2(j+1)}(p)}{p^{2(j+1)s}}}{1-\frac{\chi^2(p)}{p^{2s}}}\,\frac{1-\frac{\chi(p)}{p^s}}{1-\frac{\chi^{j+1}(p)}{p^{(j+1)s}}}\\ &= \frac{1}{L(s,\chi)}\,\frac{L(2s,\chi^2)L((j+1)s,\chi^{j+1})}{L(2(j+1)s,\chi^{2(j+1)})}\end{aligned}$$

for $\mathrm{Re}(s) > 1$. On the other hand, if $j \geq 1$ is an odd integer, then the right-hand side of (3-1) is

$$\prod_p\sum_{k=0}^{j}(-1)^k\frac{\chi(p^k)}{p^{ks}} = \prod_p\frac{1-\frac{\chi(p^{j+1})}{p^{(j+1)s}}}{1+\frac{\chi(p)}{p^s}} = \frac{1}{L(s,\chi)}\,\frac{L(2s,\chi^2)}{L((j+1)s,\chi^{j+1})}$$

for $\mathrm{Re}(s) > 1$. For convenience we define

$$F(j,s,\chi) := \begin{cases}\dfrac{L(2s,\chi^2)}{L((j+1)s,\chi^{j+1})} & \text{if } j \geq 1 \text{ is odd},\\[2ex] \dfrac{L(2s,\chi^2)L((j+1)s,\chi^{j+1})}{L(2(j+1)s,\chi^{2(j+1)})} & \text{if } j \geq 2 \text{ is even}.\end{cases}$$

For $\mathrm{Re}(s) > 1$ we have

$$\sum_{n=1}^{\infty}\frac{\chi(n)\mu_j(n)}{n^s} = \frac{1}{L(s,\chi)}F(j,s,\chi).$$

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This formula appeared, for example, in [5, page 465] for the simpler case of the Riemann zeta function. By the properties of the convolution we have

$$\begin{aligned}((\chi\cdot\mu_j)*(\chi\cdot\log^k))(n) &= \sum_{d\mid n}(\chi\cdot\mu_j)(d)(\chi\cdot\log^k)\Big(\frac{n}{d}\Big)\\ &= \sum_{d\mid n}\chi(d)\mu_j(d)\chi\Big(\frac{n}{d}\Big)\log^k\Big(\frac{n}{d}\Big) = \chi(n)\sum_{d\mid n}\mu_j(d)\log^k\Big(\frac{n}{d}\Big)\\ &= \chi(n)\Lambda_{j,k}(n).\end{aligned}$$

Therefore the generating Dirichlet series for $\chi(n)\Lambda_{j,k}(n)$ for $\mathrm{Re}(s) > 1$ is

$$\Big(\sum_{n=1}^{\infty}\frac{\chi(n)\mu_j(n)}{n^s}\Big)\Big(\sum_{n=1}^{\infty}\frac{\chi(n)\log^k(n)}{n^s}\Big) = (-1)^k\frac{L^{(k)}}{L}(s,\chi)F(j,s,\chi).$$

We remark that $\Lambda_{j,k}(n) \ll \log^k n$. By [22, Lemma 3.12] with $c = 1 + (1/\log x)$ we obtain

$$\sum_{n\leqslant x}\chi(n)\Lambda_{j,k}(n) = \frac{1}{2\pi i}\int_{c-iT}^{c+iT}(-1)^k\frac{L^{(k)}}{L}(s,\chi)\frac{x^s}{s}F(j,s,\chi)\,ds + O_k\Big(\frac{x}{T}\log^{k+1}x\Big).$$

Let C_χ be the contour given in Lemma 2.3. Clearly $F(j,s,\chi)$ is bounded on C_χ. Now applying Lemma 2.3 when we encounter the residues at the poles of the integrand we get

$$\begin{aligned}\sum_{n\leqslant x}\chi(n)\Lambda_{j,k}(n) &= R_{j,k}(x,\chi) + \frac{1}{2\pi i}\int_{C_\chi}(-1)^k\frac{L^{(k)}}{L}(s,\chi)\frac{x^s}{s}F(j,s,\chi)\,ds + O_k\Big(\frac{x}{T}\log^{k+1}x\Big)\\ &= R_{j,k}(x,\chi) + O_k\Big(\frac{x}{T}\log^{k+1}x\Big)\\ &\quad + O_k\Big(\frac{x}{T}\log^{k+4}(q(T+2))\Big(\frac{1}{\log q(T+2)} + \frac{1}{\log x}\Big)\Big)\\ &\quad + O_k\Big(x\log^{k+5}(qT)\exp\Big(-\Big(\frac{A_4}{20}\frac{\log x}{\log qT}\Big)\Big)\Big),\end{aligned}$$

where $R_{j,k}(x,\chi)$ is the aggregate of the residues of the poles of the integrand in C_χ. Now we compute the residue. By the use of the fact that

$$\frac{d^n}{ds^n}\frac{x^s}{s}\Big|_{s=1} = n!x\sum_{i=0}^{n}\frac{(-1)^{n-i}\log^i x}{i!},$$

we see that

$$\begin{aligned}\frac{d^n}{ds^n}\Big(\frac{x^s}{s}F(j,s,\chi)\Big)\Big|_{s=1} &= \sum_{l=0}^{n}\binom{n}{l}\Big(\frac{d^{n-l}}{ds^{n-l}}\frac{x^s}{s}\Big)\Big(\frac{d^l}{ds^l}F(j,s,\chi)\Big)\Big|_{s=1}\\ &= \sum_{l=0}^{n}\binom{n}{l}x(n-l)!\sum_{i=0}^{n-l}\frac{(-1)^{n-l-i}\log^i x}{i!}F^{(l)}(j,1,\chi)\\ &= xn!\sum_{l=0}^{n}\frac{(-1)^l F^{(l)}(j,1,\chi)}{l!}\sum_{i=0}^{n-l}\frac{(-1)^{n-i}\log^i x}{i!}. \qquad (3\text{-}2)\end{aligned}$$

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Now consider the fact that

$$L(s,\chi_q^0) = \zeta(s)h_q(s), \tag{3-3}$$

for $\mathrm{Re}(s) > 1$ with χ_q^0 the principal character, and where

$$h_q(s) := \prod_{p|q}\Big(1 - \frac{1}{p^s}\Big).$$

Clearly

$$\frac{h_q'(s)}{h_q(s)} = \sum_{p|q}\frac{\log p}{p^s - 1} \quad \text{and} \quad \Big(\frac{h_q'(s)}{h_q(s)}\Big)' = -\sum_{p|q}\frac{\log^2 p}{p^s - 1} + \sum_{p|q}\frac{\log^2 p}{(p^s-1)^2}.$$

Therefore

$$\Big(\frac{h_q'(1)}{h_q(1)}\Big)' \ll \sum_{p|q}\frac{\log^2 p}{p-1} \quad \text{and similarly} \Big(\frac{h_q'(1)}{h_q(1)}\Big)^{(n)} \ll_n \sum_{p|q}\frac{\log^{n+1} p}{p-1}.$$

Now

$$\begin{aligned}\sum_{p|q}\frac{\log^{n+1} p}{p-1} \ll \sum_{p\le V}\frac{\log^{n+1} p}{p-1} + \sum_{\substack{p|q\\ p>V}}\frac{\log^{n+1} p}{p-1} &\ll \log^n V\sum_{p\le V}\frac{\log p}{p} + \frac{\log^{n+1} V}{V}\sum_{\substack{p|q\\ p>V}} 1\\ &\ll \log^{n+1} V + \frac{\log q\log^n V}{V}\\ &\ll (\log\log q)^{n+1},\end{aligned}$$

where we chose $V = \log q$ in the penultimate step. Therefore, by (2-2),

$$\frac{h_q^{(n)}(1)}{h_q(1)} \ll (\log\log q)^n \tag{3-4}$$

for $n \ge 0$. For $|s-1| < 1/2$, we have

$$\zeta(s) = \frac{1}{s-1} + \sum_{n=0}^{\infty} c_0(s-1)^n,$$

where the c_n are constants and

$$h_q(s) = \sum_{n=0}^{\infty}\frac{h_q^{(n)}(1)}{n!}(s-1)^n.$$

Therefore the Laurent series of $L(s,\chi_q^0)$ at $s = 1$ is given by

$$L(s,\chi_q^0) = \frac{h_q(1)}{s-1} + \sum_{n=0}^{\infty} a_n(s-1)^n.$$

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Hence

$$(-1)^k \frac{L^{(k)}}{L}(s,\chi_q^0) = \frac{\frac{k!h_q(1)}{(s-1)^k} + \sum_{n=k}^{\infty}(n)_k a_n (s-1)^{n-k}}{h_q(1) + \sum_{n=0}^{\infty} a_n (s-1)^{n+1}},$$

where $(n)_k = n(n-1)\cdots(n-k+1)$. Let

$$G(s,\chi_q^0) := (-1)^k (s-1)^k \frac{L^{(k)}}{L}(s,\chi_q^0) = \frac{k! + \sum_{n=k}^{\infty}(n)_k b_n (s-1)^n}{1 + \sum_{n=0}^{\infty} b_n (s-1)^{n+1}}$$
$$= k!(1 + d_1(s-1) + d_2(s-1)^2 + \cdots).$$

Then, by (3-4), $d_n \ll_k (\log\log q)^n$ for $n \le k$. Now we compute the residue for the principal character

$$R_{j,k}(x,\chi_q^0) = \frac{1}{(k-1)!} \lim_{s\to 1} \frac{d^{k-1}}{ds^{k-1}}\Big(G(s,\chi_q^0)\frac{x^s}{s}F(j,s,\chi_q^0)\Big).$$

Invoking (3-2) and the fact $F^{(l)}(j,1,\chi_q^0) \ll 1$, we find

$$R_{j,k}(x,\chi_q^0) = \frac{x}{(k-1)!}\sum_{n=0}^{k-1}\binom{k-1}{n} G^{(n)}(1,\chi_q^0)$$
$$\times \sum_{l=0}^{k-1-n} \frac{(-1)^l (k-n)! F^{(l)}(j,1,\chi_q^0)}{l!} \sum_{i=0}^{k-1-n-l} \frac{(-1)^{k-1-n-i}\log^i x}{i!}$$
$$= xkF(j,1,\chi_q^0)\log^{k-1} x + O_{j,k}\Big(x\sum_{n=0}^{k-2}\log^n(x)(\log\log q)^{k-n-1}\Big).$$

Next we consider the case where χ_q is an exceptional character. By the density lemma [1, page 42] and following similar lines as in [9], we have

$$\frac{L'}{L}(s,\chi_q) = \frac{1}{s-\beta} + O(\log q \log\log q),$$

where

$$|s-\beta| \le \frac{A_5}{\log q}.$$

Here β is the exceptional zero. Then, by Cauchy's integral formula, we find

$$\Big(\frac{L'}{L}(s,\chi_q)\Big)^{(n)} = \frac{(-1)^n n!}{(s-\beta)^{n+1}} + O((\log q \log\log q)^{n+1}). \tag{3-5}$$

Let $g_n(\beta)$ be the residue of $L^{(n)}/L(s,\chi_q)$ at $s=\beta$. Since $s=\beta$ is a simple pole,

$$\frac{L^{(n)}}{L}(s,\chi_q) = \frac{g_n(\beta)}{s-\beta} + \cdots.$$

Now, from (2-2) and (3-5),

$$g_n(\beta) \ll_n (\log q\log\log q)^{\mu_1 - 1 + 2\mu_2 + 3\mu_+ \cdots + k\mu_k} \ll_n (\log q \log\log q)^{n-1}.$$

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Therefore

$$R_{j,k}(x,\chi_q) = \lim_{s\to\beta}(s-\beta)(-1)^k \frac{L^{(k)}}{L}(s,\chi_q)\frac{x^s}{s}F(j,s,\chi_q) = (-1)^k g_k(\beta)\frac{x^\beta}{\beta}F(j,\beta,\chi_q).$$

Since β is the exceptional zero, $x^\beta/\beta \ll x$ and $F(j,\beta,\chi_q) \ll 1$. Hence

$$R_{j,k}(x,\chi_q) \ll_k x(\log q \log\log q)^{k-1}.$$

Now, from the definition of F,

$$F(j,1,\chi_q^0) = \frac{L(2,\chi_q^0)}{L(1+j,\chi_q^0)}, \quad F(j,1,\chi_q^0) = \frac{L(2,\chi_q^0)L(1+j,\chi_q^0)}{L(2(1+j),\chi_q^0)}$$

for $j \geq 1$ odd and $j \geq 2$ even, respectively. We know that

$$\zeta(2n) = (-1)^{n+1}\frac{B_{2n}(2\pi)^{2n}}{2(2n)!},$$

where B_n denotes the Bernoulli numbers and n is a nonnegative integer. From (3-3) and for $j \geq 1$ odd, we have

$$F(j,1,\chi_q^0) = (-1)^{(j+3)/2}\frac{(j+1)!}{12B_{j+1}(2\pi)^{j-1}}\prod_{p|q}\frac{1-1/p^2}{1-1/p^{j+1}},$$

and for $j \geq 2$ even,

$$F(j,1,\chi_q^0) = (-1)^j\frac{\zeta(j+1)(2(j+1))!}{12B_{2(j+1)}(2\pi)^{2j}}\prod_{p|q}\frac{1-1/p^2}{1+1/p^{j+1}}.$$

This completes the proof of the theorem. □

Finally, we can now prove Theorem 1.1. This follows from the orthogonal relation of Dirichlet characters, Theorem 3.1 with $T = \log^{k+5} x$, and the fact that

$$\psi_{j,k}(x;q,a) = \sum_{\substack{m\leqslant x\\ m\equiv a \bmod q}}\Lambda_{j,k}(m) = \frac{1}{\phi(q)}\sum_\chi \bar{\chi}(a)\sum_{m\leqslant x}\chi(m)\Lambda_{j,k}(m).$$

Thus, by Theorem 3.1,

$$\psi_{j,k}(x;q,a) \sim \frac{k}{\phi(q)}xc(j,q)\log^{k-1} x,$$

for

$$\log q = o\Big(\frac{\log x}{\log\log x}\Big).$$

Define

$$\mathfrak{W}(j,s) := \begin{cases} 1/\zeta(s) & \text{if } j \geq 1 \text{ is odd,}\\ \zeta(s)/\zeta(2s) & \text{if } j \geq 2 \text{ is even.}\end{cases}$$

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For $\mathrm{Re}(s) > 1$ we may write

$$\sum_{n=1}^{\infty} \frac{\Lambda_{j,k}(n)}{n^s} = (-1)^k \frac{\zeta(2s)}{\zeta(s)} \mathfrak{W}(j,(j+1)s)\zeta^{(k)}(s).$$

Lemma 2.3 can be modified to read

$$\frac{\zeta^{(k)}}{\zeta}(s) \ll_k \log((|T|+2))^{k+4}$$

on a similar contour C, which is simpler than Lemma 2.3 because of the absence of the exceptional zero. Now if we proceed along lines similar to the proof of Theorem 1.1 then

$$\sum_{n \le x} \Lambda_{j,k}(n) \sim kc(j,1)x \log^{k-1} x.$$

The proof of Theorem 1.2 is also similar. The only modification that is needed is that

$$\sum_{n=1}^{\infty} \frac{\chi(n)L_k(n)}{n^s} = (-1)^k \frac{L^{(k)}}{L}(s,\chi)L(2s,\chi)$$

for $\mathrm{Re}(s) > 1$ and $L_k(n) \ll \log^k x$.

4. Proof of Theorem 1.3

First, for a large positive number T, let T_1 be the number supplied by Lemma 2.1 and consider the positively oriented contour C determined by the line segments

$$[c - iT_1, c + iT_1], \quad [c + iT_1, \lambda + iT_1], \quad [-K + iT_1, -K - iT_1], \quad [-K - iT_1, c + iT_1]$$

with some $K > 0$. Let us assume that the horizontal line segments do not pass through any poles of $\zeta^{(k)}/\zeta$. We then have

$$\hat{h}(s) = \int_0^{\infty} h(x)x^{s-1}\, ds. \tag{4-1}$$

Let h be supported on the subinterval $[J_0, J]$ of $(0,\infty)$. Now we observe from (4-1) that

$$\hat{h}(s) = \int_{J_0}^{J} h(x)x^{s-1}\, ds \ll \frac{J^{\sigma}}{|s|}, \tag{4-2}$$

for $|s| > \delta$. Therefore

$$\begin{aligned}\sum_{n=1}^{\infty} \Lambda_k(n)h(n) &= \sum_{n=1}^{\infty} \Lambda_k(n) \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \hat{h}(s)n^{-s}\, ds = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \hat{h}(s) \sum_{n=1}^{\infty} \frac{\Lambda_k(n)}{n^s}\, ds \\ &= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} (-1)^k \frac{\zeta^{(k)}}{\zeta}(s)\hat{h}(s)\, ds,\end{aligned}$$

with $c = 1 + (1/\log J)$ so that the interchange is justified. The poles of the integrand are located at $s = 1$, $s = \rho$ and $s = -2m$. Here ρ runs over the nontrivial zeros of $\zeta(s)$

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and m runs over the positive integers. By Cauchy's theorem we have

$$\frac{1}{2\pi i}\oint_C (-1)^k \frac{\zeta^{(k)}}{\zeta}(s)\hat{h}(s)\,ds = R_1(k) + \sum_{-T<\operatorname{Im}\rho<T} R_2(k,\rho) + \sum_{1\le m\le K} R_3(k,m),$$

where R_1, R_2 and R_3 are the residues at $s = 1$, $s = \rho$ and $s = -2m$ respectively, that is,

$$R_1(k) = \operatorname*{res}_{s=1}(-1)^k\frac{\zeta^{(k)}}{\zeta}(s) = \lim_{s\to 1}\frac{(-1)^k}{(k-1)!}\frac{d^{k-1}}{ds^{k-1}}\Big((s-1)^k\frac{\zeta^{(k)}}{\zeta}(s)\hat{h}(s)\Big) =: \Phi(k),$$

as well as

$$R_2(k,\rho) = \operatorname*{res}_{s=\rho}(-1)^k\frac{\zeta^{(k)}}{\zeta}(s) = (-1)^k\frac{\zeta^{(k)}}{\zeta'}(\rho)\hat{h}(\rho),$$

and finally,

$$R_3(k,m) = \operatorname*{res}_{s=-2m}(-1)^k\frac{\zeta^{(k)}}{\zeta}(s) = (-1)^k\frac{\zeta^{(k)}}{\zeta'}(-2m)\hat{h}(-2m).$$

Next, we can make the horizontal and far-left integrals tend to zero as $K \to \infty$ and $T \to \infty$ using the well-chosen sequence that T_1 obeys. In particular, by Lemma 2.1 and (4-2), we have

$$\begin{aligned}\int_{-1\pm iT_1}^{c\pm iT_1}(-1)^k\frac{\zeta^{(k)}}{\zeta}(s)\hat{h}(s)\,ds &\ll_\varepsilon \log^{2k}T\int_{-1}^{c}|\hat{h}(\sigma+T_1)|\,d\sigma\\ &\ll \log^{2k}T\int_{-1}^{c}\frac{J^\sigma}{|\sigma+iT_1|}\,d\sigma.\end{aligned}$$

Using the fact that $|\sigma + iT_1| \gg T$, we arrive at

$$\int_{-1\pm iT_1}^{c\pm iT_1}(-1)^k\frac{\zeta^{(k)}}{\zeta}(s)\hat{h}(s)\,ds \ll \frac{J\log^{2k}T}{T\log J}.$$

By Lemma 2.2, we find

$$\int_{-1\pm iT_1}^{-K\pm iT_1}(-1)^k\frac{\zeta^{(k)}}{\zeta}(s)\hat{h}(s)\,ds \ll \int_{-K}^{-1}\frac{\log^k|\sigma+iT_1|}{|\sigma+iT_1|}J^\sigma\,d\sigma \ll \frac{\log^k T}{TJ\log J}.$$

Similarly, for the vertical line at the far left, we get

$$\int_{-K-iT_1}^{-K+iT_1}(-1)^k\frac{\zeta^{(k)}}{\zeta}(s)\hat{h}(s)\,ds \ll \frac{\log^k|K+iT|}{|K+iT|}J^{-K}\int_{-T_1}^{T_1}1\,dt \ll \frac{T\log^k(KT)}{KJ^K} \to 0$$

as $K \to \infty$, by Lemma 2.2. Thus as $T \to \infty$ we obtain

$$\sum_{n=1}^{\infty}\Lambda_k(n)h(n) = \Phi(k) + (-1)^k\sum_\rho\frac{\zeta^{(k)}}{\zeta'}(\rho)\hat{h}(\rho) + (-1)^k\sum_{m=1}^{\infty}\frac{\zeta^{(k)}}{\zeta'}(-2m)\hat{h}(-2m),$$

as was to be shown. If $k = 1$, then we obtain the Weil explicit formula (1-9).

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