

# SIGNS OF THE SECOND COEFFICIENTS OF HECKE POLYNOMIALS

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ABSTRACT. Let  $T_m(N, k, \chi)$  be the  $m$ -th Hecke operator of level  $N$ , weight  $k \geq 2$ , and nebentypus  $\chi$ , where  $N$  is coprime to  $m$ . We first show that for any given  $m \geq 1$ , the second coefficient of the characteristic polynomial of  $T_m(N, k, \chi)$  is nonvanishing for all but finitely many triples  $(N, k, \chi)$ . Furthermore, for  $\chi$  trivial and any fixed  $m$ , we determine the sign of the second coefficient for all but finitely many pairs  $(N, k)$ . Finally, for  $\chi$  trivial and  $m = 3, 4$ , we compute the sign of the second coefficient for all pairs  $(N, k)$ .

## 1. INTRODUCTION

Let  $k \geq 2$ ,  $N \geq 1$  be integers and let  $\chi$  be a Dirichlet character modulo  $N$  such that  $\chi(-1) = (-1)^k$ . The space of cuspforms of level  $N$ , weight  $k$ , and nebentypus  $\chi$  is denoted by  $S_k(\Gamma_0(N), \chi)$  [3, Section 7.2]. For  $m \geq 1$ , let  $T_m(N, k, \chi)$  be the  $m$ -th Hecke operator on  $S_k(\Gamma_0(N), \chi)$  [3, Chapter 10]. When the character  $\chi$  is trivial, we will drop  $\chi$  and simply write  $T_m(N, k)$  and  $S_k(\Gamma_0(N))$ , respectively. Several interesting questions about these Hecke operators  $T_m(N, k, \chi)$  have been studied. For instance, let

$$\Delta(z) = q \prod_{n \geq 1} (1 - q^n)^{24} = \sum_{n \geq 1} \tau(n) q^n$$

be the discriminant function, which is the unique normalized cuspform of weight 12, level one, and trivial nebentypus. Lehmer [6] conjectured that  $\tau(m) \neq 0$  for all  $m \geq 1$ . Let  $\text{Tr } T_m(N, k)$  denote the trace of  $T_m(N, k)$  on the space  $S_k(\Gamma_0(N))$ . The Lehmer Conjecture can then be reinterpreted as follows:  $\text{Tr } T_m(1, 12) \neq 0$  for all  $m \geq 1$ . More broadly, Rouse [10] gave the Generalized Lehmer Conjecture, which predicts that  $\text{Tr } T_m(N, k) \neq 0$  for even  $k \geq 16$  or  $k = 12$  and  $\gcd(m, N) = 1$ . He also proved this result for  $m = 2$ . Recently, the nonvanishing of  $\text{Tr } T_3(1, k)$  was also established in [1].

Now, let us write the characteristic polynomial for  $T_m(N, k, \chi)$ , the so-called Hecke polynomial, as

$$T_m(N, k, \chi)(x) = x^n - a_1(m, N, k, \chi)x^{n-1} + a_2(m, N, k, \chi)x^{n-2} - \cdots + (-1)^n a_n(m, N, k, \chi),$$

where  $n = \dim S_k(\Gamma_0(N), \chi)$ . Here, we will refer to  $a_i(m, N, k, \chi)$  as the  $i$ -th coefficient of the Hecke polynomial. To ease notation we will simply write  $a_i(m, N, k)$  if  $\chi$  is trivial. Using this

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notation, the Generalized Lehmer Conjecture concerns the nonvanishing of the first coefficient  $a_1(m, N, k)$  of  $T_m(N, k)(x)$ . One may also consider the nonvanishing of the other coefficients, in particular the second coefficient,  $a_2(m, N, k, \chi)$ . Most recently, for trivial characters  $\chi$ , Clayton et al. [2, Theorems 1.1 and 1.3] computed the complete list of pairs  $(N, k)$  for which the second coefficient of  $T_2(N, k)(x)$  vanishes. In this paper, we shall first extend the results of [2] to study the nonvanishing of  $a_2(m, N, k, \chi)$  for general  $m$ ,  $N$ ,  $k$ , and  $\chi$ . More precisely, we have the following result.

**Theorem 1.1.** *Let  $m \geq 1$  be fixed. Suppose  $\gcd(N, m) = 1$ ,  $k \geq 2$ , and  $\chi$  is a Dirichlet character modulo  $N$  such that  $\chi(-1) = (-1)^k$ . Then  $a_2(m, N, k, \chi)$  vanishes for only finitely many triples  $(N, k, \chi)$ .*

When  $\chi$  is trivial, we also explicitly determine the sign of the second coefficient.

**Theorem 1.2.** *Let  $m \geq 1$  be fixed. Suppose  $\gcd(N, m) = 1$  and  $k \geq 2$  is even.*

- (1): *If  $m$  is not a perfect square, then  $a_2(m, N, k)$  is negative for all but finitely many pairs  $(N, k)$ .*
- (2): *If  $m$  is a perfect square, then  $a_2(m, N, k)$  is positive for all but finitely many pairs  $(N, k)$ .*

We show these two theorems by first expressing  $a_2(m, N, k, \chi)$  in terms of traces of various Hecke operators (Lemma 2.1). These traces can each be evaluated by the Eichler-Selberg trace formula (2.1). From this formula, we can then identify the dominant terms for these traces, coming from the Hecke operators with perfect square index (Lemma 4.2). This allows us to determine the asymptotic growth of  $a_2(m, N, k, \chi)$ , which then yields Theorems 1.1 and 1.2.

In fact, our method is effective: for any given  $m$ , these exceptional pairs can be computed explicitly. As an illustration of the two cases in Theorem 1.2, when  $\chi$  is trivial and  $m = 3, 4$ , we carry out the details to compute all the exceptional pairs.

**Theorem 1.3.** *Suppose that  $\gcd(N, 3) = 1$  and that  $k \geq 2$  is even. Then  $a_2(3, N, k)$  is positive or zero only for the pairs  $(N, k)$  given in Table 5.4.*

**Theorem 1.4.** *Suppose that  $\gcd(N, 4) = 1$  and that  $k \geq 2$  is even. Then  $a_2(4, N, k)$  is negative or zero only for the pairs  $(N, k)$  given in [9, Table  $m = 4$ ].*

The paper is organized as follows. In Section 2, following the idea in [2], we express the second coefficient  $a_2(m, N, k, \chi)$  in terms of traces of Hecke operators. We also state the Eichler-Selberg trace formula to compute these traces. Section 3 is preparatory and establishes estimates on certain terms in the Eichler-Selberg trace formula. In Section 4, we prove Theorems 1.1 and 1.2. In Sections 5 and 6 we apply the techniques developed in Section 4 to the cases of  $m = 3$  and  $m = 4$ , and prove Theorems 1.3 and 1.4, respectively. Section 7 discusses some related questions.

## 2. SECOND COEFFICIENTS IN TERMS OF TRACES

Following [2, Proposition 2.1], we first derive a formula for  $a_2(m, N, k, \chi)$  in terms of traces of Hecke operators.

**Lemma 2.1.** *For convenience of notation, let  $T_m$  denote  $T_m(N, k, \chi)$ . Then*

$$a_2(m, N, k, \chi) = \frac{1}{2} \left[ (\operatorname{Tr} T_m)^2 - \sum_{d|m} \chi(d) d^{k-1} \operatorname{Tr} T_{m^2/d^2} \right].$$

*Proof.* Let  $\lambda_1 \dots \lambda_n$  be the eigenvalues of  $T_m$ . By the definition of characteristic polynomial, we have

$$\begin{aligned} a_2(m, N, k, \chi) &= \sum_{1 \leq i < j \leq n} \lambda_i \lambda_j \\ &= \frac{1}{2} \left[ \left( \sum_{1 \leq i \leq n} \lambda_i \right)^2 - \sum_{1 \leq i \leq n} \lambda_i^2 \right] \\ &= \frac{1}{2} [(\operatorname{Tr} T_m)^2 - \operatorname{Tr} T_m^2]. \end{aligned}$$

On the other hand, recall the following formula [3, Theorem 10.2.9] for Hecke operators:

$$T_m^2 = \sum_{d|m} \chi(d) d^{k-1} T_{m^2/d^2}.$$

Thus,

$$\begin{aligned} a_2(m, N, k, \chi) &= \frac{1}{2} [(\operatorname{Tr} T_m)^2 - \operatorname{Tr} T_m^2] \\ &= \frac{1}{2} \left[ (\operatorname{Tr} T_m)^2 - \sum_{d|m} \chi(d) d^{k-1} \operatorname{Tr} T_{m^2/d^2} \right], \end{aligned}$$

as desired.  $\square$

Next, we state the Eichler-Selberg trace formula in order to give an explicit formula for the traces appearing in Lemma 2.1. Let  $m \geq 1$ ,  $N \geq 1$ ,  $k \geq 2$ , and  $\chi$  be a Dirichlet character modulo  $N$  such that  $\chi(-1) = (-1)^k$ . From [5, pp. 370-371], and borrowing some notation from [3, 24.4.11], the Eichler-Selberg trace formula is given by

$$\operatorname{Tr} T_m(N, k, \chi) = A_{1,m} - A_{2,m} - A_{3,m} + A_{4,m}, \quad (2.1)$$

where

$$A_{1,m} = \chi(\sqrt{m}) \frac{k-1}{12} \psi(N) m^{k/2-1}, \quad (2.2)$$

$$A_{2,m} = \frac{1}{2} \sum_{t^2 < 4m} U_{k-1}(t, m) \sum_n h_w \left( \frac{t^2 - 4m}{n^2} \right) \mu(t, n, m), \quad (2.3)$$

$$A_{3,m} = \frac{1}{2} \sum_{d|m} \min(d, m/d)^{k-1} \sum_{\tau} \phi(\gcd(\tau, N/\tau)) \chi(y_{\tau}), \quad (2.4)$$

$$A_{4,m} = \begin{cases} \sum_{\substack{c|m \\ (N, m/c)=1}} c & \text{if } k = 2 \text{ and } \chi = \chi_0, \\ 0 & \text{if } k > 2 \text{ or } \chi \neq \chi_0. \end{cases} \quad (2.5)$$

Here, we have the following notation.

- $\chi(\sqrt{m})$  is interpreted as 0 if  $m$  is not a perfect square.
- $\psi(N) = [\mathrm{SL}_2(\mathbb{Z}) : \Gamma_0(N)] = N \prod_{p|N} \left(1 + \frac{1}{p}\right)$ .
- The outer summation in  $A_{2,m}$  runs over all  $t \in \mathbb{Z}$  such that  $t^2 < 4m$ . Note that the terms corresponding to  $t = t_0$  and  $t = -t_0$  coincide.
- $U_{k-1}(t, m)$  denotes the Lucas sequence of the first kind. In particular,  $U_{k-1}(t, m) = \frac{\rho^{k-1} - \bar{\rho}^{k-1}}{\rho - \bar{\rho}}$  where  $\rho, \bar{\rho}$  are the two roots of the polynomial  $X^2 - tX + m$ .
- The inner summation in  $A_{2,m}$  runs through all positive integers  $n$  such that  $n^2 | (t^2 - 4m)$  and  $\frac{t^2 - 4m}{n^2} \equiv 0, 1 \pmod{4}$ .
- $h_w\left(\frac{t^2 - 4m}{n^2}\right)$  is the weighted class number of the imaginary quadratic order with discriminant  $\frac{t^2 - 4m}{n^2}$ . This is the usual class number, divided by 2 (respectively 3) if the discriminant is  $-4$  (respectively  $-3$ ). For our purposes, the first few of them are given explicitly in Table 2.2 below.
- $\mu(t, n, m) = \frac{\psi(N)}{\psi(N/N_n)} \sum'_{c \bmod N} \chi(c)$ , where  $N_n = \gcd(N, n)$ , and the primed summation runs through all elements  $c$  of  $(\mathbb{Z}/N\mathbb{Z})^\times$  which lift to solutions of  $c^2 - tc + m \equiv 0 \pmod{NN_n}$ .
- The outer summation for  $A_{3,m}$  runs through all positive divisors  $d$  of  $m$ . Note that the terms corresponding to  $d = d_0$  and  $d = m/d_0$  coincide.
- The inner summation for  $A_{3,m}$  runs over all positive divisors  $\tau$  of  $N$  such that  $\gcd(\tau, N/\tau)$  divides  $\gcd(N/N_\chi, d - m/d)$ . Here  $N_\chi$  is the conductor of  $\chi$ .
- $\phi$  is the Euler totient function.
- $y_\tau$  is the unique integer modulo  $\mathrm{lcm}(\tau, N/\tau)$  determined by the congruences  $y_\tau \equiv d \pmod{\tau}$  and  $y_\tau \equiv \frac{m}{d} \pmod{\frac{N}{\tau}}$ .
- $\chi_0$  denotes the trivial character modulo  $N$ .
- Throughout, remember that  $\chi$  is a character modulo  $N$ , so  $\chi(a) = 0$  if  $\gcd(a, N) > 1$ , even in the trivial character case.

**Table 2.2** (Weighted class numbers; [5, p. 345], [8, A014600]).

$n$	-3	-4	-7	-8	-11	-12	-15	-16	-19	-20	-23
$h_w(n)$	$\frac{1}{3}$	$\frac{1}{2}$	1	1	1	1	2	1	1	2	3
$n$	-24	-27	-28	-31	-32	-35	-36	-39	-40	-43	-44
$h_w(n)$	2	1	1	3	2	2	2	4	2	1	3
$n$	-47	-48	-51	-52	-55	-56	-59	-60	-63	-64	-67
$h_w(n)$	5	2	2	2	4	4	3	2	4	2	1

## 3. ESTIMATES ON TERMS IN THE TRACE FORMULA

In this section we give estimates on the  $A_{i,m}$  trace terms (2.2), (2.3), (2.4), and (2.5). First, we introduce some arithmetic functions that will be used to express these estimates.

**Lemma 3.1.** *Recall that  $\psi(N) = N \prod_{p|N} \left(1 + \frac{1}{p}\right)$ , and let  $\omega(N)$  denote the number of distinct prime divisors of  $N$ . Define*

$$\theta_1(N) := \frac{2^{\omega(N)} \sqrt{N}}{\psi(N)}, \quad \theta_2(N) := \frac{(2^{\omega(N)})^2}{\psi(N)}, \quad \theta_3(N) := \frac{2^{\omega(N)}}{\psi(N)}.$$

Then each  $\theta_i(N) \rightarrow 0$  as  $N \rightarrow \infty$ .

In particular, we have the bounds given in the following table.

$N \geq$	1	43	571	8,800	150,000	2,700,000	63,000,000
$\theta_1(N) \leq$	1.00	0.465	0.257	0.133	0.0607	0.0265	0.0106
$\theta_2(N) \leq$	1.34	0.445	0.149	0.0424	0.00941	0.00189	0.000314
$\theta_3(N) \leq$	1.00	0.0556	0.00926	0.00133	0.000147	0.000015	0.000015

*Proof.* Note that every prime other than 2, 3, 5, 7 is  $\geq 8$ . Thus  $\omega(N) \leq 4 + \log_8(N)$  and so  $2^{\omega(N)} \leq 2^{4+\log_8(N)} \leq 16 \cdot N^{1/3}$ . Since  $\psi(N) \geq N$ , it is clear that

$$\theta_1(N) = \frac{2^{\omega(N)} \sqrt{N}}{\psi(N)}, \quad \theta_2(N) = \frac{(2^{\omega(N)})^2}{\psi(N)}, \quad \theta_3(N) = \frac{2^{\omega(N)}}{\psi(N)} \rightarrow 0 \text{ as } N \rightarrow \infty.$$

To prove the specific numerical bounds given above, we will first show that

$$\theta_1(N) \leq 0.0106, \quad \theta_2(N) \leq 0.000314, \quad \theta_3(N) \leq 0.000015 \quad (3.1)$$

for all  $N \geq 584,000,000$ . Then we will verify each of the claimed bounds in the table by exhaustive computer check over all  $N < 584,000,000$ .

Let  $p_n$  denote the  $n$ -th prime number, and let  $P_n := p_1 \cdots p_n$ . For all  $N$  with  $\omega(N) \geq 9$ , we show that  $\theta_i(N) \leq \theta_i(P_9)$ . For such  $N$ , let  $N = q_1^{e_1} \cdots q_m^{e_m}$  be its prime factorization. Then

$$\begin{aligned}
\frac{\psi(N)}{\sqrt{N}} &= \frac{(q_1 + 1)q_1^{e_1-1} \cdots (q_m + 1)q_m^{e_m-1}}{q_1^{e_1/2} \cdots q_m^{e_m/2}} \\
&\geq \frac{(q_1 + 1) \cdots (q_m + 1)}{q_1^{1/2} \cdots q_m^{1/2}} \\
&\geq \frac{(p_1 + 1) \cdots (p_m + 1)}{p_1^{1/2} \cdots p_m^{1/2}} \quad \left( \text{since } \frac{x+1}{x^{1/2}} \text{ is increasing for } x \geq 1 \right) \\
&= \frac{\psi(P_9) (p_{10} + 1) \cdots (p_m + 1)}{\sqrt{P_9} p_{10}^{1/2} \cdots p_m^{1/2}} \\
&\geq \frac{\psi(P_9)}{\sqrt{P_9}} 2^{m-9}.
\end{aligned}$$

This means that  $\theta_1(N) = \frac{2^m \sqrt{N}}{\psi(N)} \leq \frac{2^m \sqrt{P_9}}{2^{m-9} \psi(P_9)} = \theta_1(P_9) \leq 0.0106$ .

By an identical argument,  $\psi(N) \geq 4^{m-9} \psi(P_9)$ , which means that  $\theta_2(N) \leq \theta_2(P_9) \leq 0.000314$  and  $\theta_3(N) \leq \theta_3(P_9) \leq 0.000015$ . This verifies the three bounds in (3.1) for all  $N$  with  $\omega(N) \geq 9$ .

For  $N$  with  $\omega(N) \leq 8$  and  $N \geq 584,000,000$ , we have

$$\begin{aligned}
\theta_1(N) &= \frac{2^{\omega(N)} \sqrt{N}}{\psi(N)} \leq \frac{2^8 \sqrt{N}}{N} \leq 0.00915, \\
\theta_2(N) &= \frac{(2^{\omega(N)})^2}{\psi(N)} \leq \frac{2^{16}}{N} \leq 0.000314, \\
\theta_3(N) &= \frac{2^{\omega(N)}}{\psi(N)} \leq \frac{2^8}{N} \leq 0.000015.
\end{aligned}$$

This verifies the three bounds in (3.1) for all  $N$  with  $N \geq 584,000,000$ .

Then via exhaustive computer check over all  $N < 584,000,000$ , we obtain the claimed bounds from the table. See [9] for the code.  $\square$

Next, we bound the inner summation for  $A_{2,m}$  in (2.3).

**Lemma 3.2.** *For  $t, n, m$  given in (2.3),*

$$|U_{k-1}(t, m) \cdot \mu(t, n, m)| \leq 2\psi(n)2^{\omega(N)}m^{(k-1)/2}.$$

*Proof.* Recall that  $m \geq 1$ ,  $t \in \mathbb{Z}$  such that  $4m - t^2 > 0$ , and  $n \geq 1$  such that  $n^2 \mid (t^2 - 4m)$  and  $\frac{t^2 - 4m}{n^2} \equiv 0, 1 \pmod{4}$ . And recall that  $U_{k-1}(t, m) = \frac{\rho^{k-1} - \bar{\rho}^{k-1}}{\rho - \bar{\rho}}$  where  $\rho, \bar{\rho}$  are the two roots of the polynomial  $X^2 - tX + m$ . Finally, recall that  $\mu(t, n, m) = \frac{\psi(N)}{\psi(N/N_n)} \sum'_{c \bmod N} \chi(c)$ , where  $N_n = \gcd(N, n)$ , and the primed summation runs through all elements  $c$  of  $(\mathbb{Z}/N\mathbb{Z})^\times$  which lift to solutions of  $c^2 - tc + m \equiv 0 \pmod{NN_n}$ .

So,

$$|U_{k-1}(t, m) \cdot \mu(t, n, m)| = \left| \frac{\rho^{k-1} - \bar{\rho}^{k-1}}{\rho - \bar{\rho}} \right| \cdot \frac{\psi(N)}{\psi(N/N_n)} \cdot \left| \sum'_{c \bmod N} \chi(c) \right|. \quad (3.2)$$

We give bounds on each of these three factors.

First, since

$$|\rho| = \sqrt{m} \quad \text{and} \quad |\rho - \bar{\rho}| = \sqrt{4m - t^2},$$

we have

$$\left| \frac{\rho^{k-1} - \bar{\rho}^{k-1}}{\rho - \bar{\rho}} \right| \leq \frac{|\rho^{k-1}| + |\bar{\rho}^{k-1}|}{|\rho - \bar{\rho}|} = \frac{2m^{(k-1)/2}}{\sqrt{4m - t^2}}. \quad (3.3)$$

Second, note that for every prime  $p \mid N$ , we will either have  $p \mid N_n$  or  $p \mid N/N_n$ . Thus

$$\begin{aligned} \psi(N) &= N \prod_{p \mid N} \left(1 + \frac{1}{p}\right) \\ &\leq N_n \prod_{p \mid N_n} \left(1 + \frac{1}{p}\right) \cdot N/N_n \prod_{p \mid N/N_n} \left(1 + \frac{1}{p}\right) \\ &= \psi(N_n) \psi(N/N_n), \end{aligned}$$

which yields

$$\frac{\psi(N)}{\psi(N/N_n)} \leq \psi(N_n) \leq \psi(n), \quad (3.4)$$

where the second inequality comes from the fact that  $N_n \mid n$ .

Third, note for every term  $c$  in the sum of (3.2),  $c^2 - tc + m \equiv 0 \pmod{NN_n}$  means that  $c^2 - tc + m \equiv 0 \pmod{N}$  as well. By [11, Lemma 2], the congruence  $x^2 - tx + m \equiv 0 \pmod{N}$  has at most  $2^{\omega(N)} \sqrt{4m - t^2}$  solutions. Thus

$$\left| \sum'_{c \bmod N} \chi(c) \right| \leq 2^{\omega(N)} \sqrt{4m - t^2}. \quad (3.5)$$

Combining the bounds (3.3), (3.4), and (3.5), we obtain

$$|U_{k-1}(t, m) \cdot \mu(t, n, m)| \leq 2\psi(n) 2^{\omega(N)} m^{(k-1)/2},$$

which completes the proof.  $\square$

Next, we bound the inner summation for  $A_{3,m}$  in (2.4).

**Lemma 3.3.** *Let*

$$\Sigma(N, m, d) := \sum_{\tau} \phi(\gcd(\tau, N/\tau)) \chi(y_{\tau})$$

*denote the inner summation for  $A_{3,m}$  in (2.4). Then*

$$|\Sigma(N, m, d)| \leq \begin{cases} \left|d - \frac{m}{d}\right| \cdot 2^{\omega(N)} & \text{if } d \neq \sqrt{m}, \\ \sqrt{N} \cdot 2^{\omega(N)} & \text{in general.} \end{cases}$$

*Proof.* Recall that the summation  $\sum_{\tau}$  runs over all positive divisors  $\tau$  of  $N$  such that  $\gcd(\tau, N/\tau)$  divides  $\gcd(N/N_{\chi}, d - m/d)$ . Additionally,  $y_{\tau}$  is the unique integer modulo  $\text{lcm}(\tau, N/\tau)$  determined by the congruences  $y_{\tau} \equiv d \pmod{\tau}$  and  $y_{\tau} \equiv m/d \pmod{N/\tau}$ .

Let  $h := |d - \frac{m}{d}|$ . Then

$$\begin{aligned}
|\Sigma(N, m, d)| &= \left| \sum_{\substack{\tau|N \\ (\tau, N/\tau) | (h, N/N_{\chi})}} \phi(\gcd(\tau, N/\tau)) \chi(y_{\tau}) \right| \\
&\leq \sum_{\substack{\tau|N \\ (\tau, N/\tau) | (h, N/N_{\chi})}} \phi(\gcd(\tau, N/\tau)) \\
&\leq \sum_{\substack{\tau|N \\ (\tau, N/\tau) | h}} \phi(\gcd(\tau, N/\tau)) \\
&= \sum_{\delta|h} \sum_{\substack{\tau|N \\ (\tau, N/\tau) = \delta}} \phi(\delta) \\
&= \sum_{\delta|h} \phi(\delta) \cdot \#\{\tau \mid N : \gcd(\tau, N/\tau) = \delta\}.
\end{aligned}$$

In the case of  $d \neq \sqrt{m}$ , we have  $h \neq 0$ , and so using Lemma 3.4 below, we have

$$\begin{aligned}
|\Sigma(N, m, d)| &\leq \sum_{\delta|h} \phi(\delta) \cdot \#\{\tau \mid N : \gcd(\tau, N/\tau) = \delta\} \\
&\leq \sum_{\delta|h} \phi(\delta) \cdot 2^{\omega(N)} \\
&= h \cdot 2^{\omega(N)}.
\end{aligned}$$

Here, we used the well-known formula  $\sum_{\delta|h} \phi(\delta) = h$ .

In the general case, write  $N = DM^2$  where  $D$  is squarefree. Then for any  $\delta$  such that  $\gcd(\tau, N/\tau) = \delta$  for some  $\tau$ , note  $\delta \mid \tau$  and  $\delta \mid N/\tau$  imply  $\delta^2 \mid N$ , which means that  $\delta \mid M$ . Hence by Lemma 3.4 again,

$$\begin{aligned}
|\Sigma(N, m, d)| &\leq \sum_{\delta|h} \phi(\delta) \cdot \#\{\tau \mid N : (\tau, N/\tau) = \delta\} \\
&\leq \sum_{\delta|M} \phi(\delta) \cdot \#\{\tau \mid N : (\tau, N/\tau) = \delta\} \\
&\leq \sum_{\delta|M} \phi(\delta) \cdot 2^{\omega(N)} \\
&= M \cdot 2^{\omega(N)}
\end{aligned}$$



$$\leq \sqrt{N} \cdot 2^{\omega(N)},$$

which completes the proof.  $\square$

**Lemma 3.4.** *Let  $N$  and  $\delta$  be positive integers. Then*

$$\#\{\tau \mid N : \gcd(\tau, N/\tau) = \delta\} \leq 2^{\omega(N)}.$$

*Proof.* Without loss of generality, we can assume that  $\delta \mid N$  (otherwise, the inequality holds trivially). Consider the possible  $\tau$  that would yield  $\gcd(\tau, N/\tau) = \delta$ . For each prime  $p \mid N$ , let  $v_p(\cdot)$  denote  $p$ -adic valuation, and let  $r_p := v_p(\delta)$ . Note that  $\gcd(\tau, N/\tau) = \delta$  precisely for  $\tau$  such that  $v_p(\gcd(\tau, N/\tau)) = r_p$  for each  $p \mid N$ . On the other hand,  $v_p(\gcd(\tau, N/\tau)) = r_p$  means that either  $v_p(\tau) = r_p$  and  $v_p(N/\tau) \geq r_p$ , or  $v_p(N/\tau) = r_p$  and  $v_p(\tau) \geq r_p$ . This yields only two possible values for  $v_p(\tau)$ :  $r_p$  and  $v_p(N) - r_p$ . Thus, since there are at most two possible options for  $v_p(\tau)$  for each prime  $p \mid N$ , we have that  $\#\{\tau \mid N : \gcd(\tau, N/\tau) = \delta\} \leq 2^{\omega(N)}$ .  $\square$

#### 4. PROOF OF THEOREMS 1.1 AND 1.2

In this section, we will show Theorems 1.1 and 1.2. We split the proof into the case when  $m$  is not a perfect square (Proposition 4.3), and the case when  $m$  is a perfect square (Proposition 4.4).

Recall what big  $O$  notation means in terms of two variables  $N$  and  $k$ . A function  $f(N, k)$  is  $O(g(N, k))$  if there exists a constant  $C$  such that  $|f(N, k)| \leq C \cdot g(N, k)$  for  $N + k$  sufficiently large. In other words, for any fixed value of  $N$ , this can be interpreted as big  $O$  notation with respect to  $k$ , and for any fixed value of  $k$ , this can be interpreted as big  $O$  notation with respect to  $N$ .

Now, we give a bound on the trace  $\text{Tr } T_m(N, k, \chi)$  when  $m$  is not a perfect square.

**Lemma 4.1.** *Let  $m \geq 1$  be fixed such that  $m$  is not a perfect square. For all  $N \geq 1$ ,  $k \geq 2$ , and  $\chi$  a Dirichlet character modulo  $N$  with  $\chi(-1) = (-1)^k$ , we have*

$$\text{Tr } T_m(N, k, \chi) = O(2^{\omega(N)} m^{k/2}).$$

*Proof.* We examine each of the  $A_{i,m}$  terms in (2.1) separately.

First, since  $m$  is not a perfect square and  $\chi(\sqrt{m}) = 0$ , we have that  $A_{1,m} = 0$  by (2.2).

Second, observe that all the  $t$  and  $n$  from (2.3) are bounded by the fixed value of  $2\sqrt{m}$ . Thus by Lemma 3.2,

$$|U_{k-1}(t, m) \cdot \mu(t, n, m)| = O(2^{\omega(N)} m^{k/2}),$$

so by (2.3)

$$\begin{aligned} A_{2,m} &= \frac{1}{2} \sum_{t^2 < 4m} \sum_n h_w \left( \frac{t^2 - 4m}{n^2} \right) U_{k-1}(t, m) \mu(t, n, m) \\ &= O(2^{\omega(N)} m^{k/2}). \end{aligned}$$

Third, since  $m$  is not a perfect square, only the first case of Lemma 3.3 applies. Thus each inner summation  $\Sigma(N, m, d)$  for  $A_{3,m}$  is  $O(2^{\omega(N)})$ . And also note that  $\min(d, m/d) \leq m^{1/2}$ . So by (2.4),

$$\begin{aligned} A_{3,m} &= \frac{1}{2} \sum_{d|m} \min(d, m/d)^{k-1} \Sigma(N, m, d) \\ &= O(2^{\omega(N)} m^{k/2}). \end{aligned}$$

Fourth,  $A_{4,m} \leq \sum_{c|m} c = O(1)$  by (2.5).

Combining the above bounds, we obtain

$$\begin{aligned} \text{Tr } T_m(N, k, \chi) &= A_{1,m} - A_{2,m} - A_{3,m} + A_{4,m} \\ &= O(2^{\omega(N)} m^{k/2}), \end{aligned}$$

which completes the proof.  $\square$

Next, we estimate the trace  $\text{Tr } T_m(N, k, \chi)$  when  $m$  is a perfect square.

**Lemma 4.2.** *Let  $m$  be fixed such that  $m$  is a perfect square. Then for all  $N \geq 1$ ,  $k \geq 2$ , and  $\chi$  a Dirichlet character modulo  $N$  with  $\chi(-1) = (-1)^k$ , we have*

$$\text{Tr } T_m(N, k, \chi) = \chi(\sqrt{m}) \frac{k-1}{12} \psi(N) m^{k/2-1} + O(\sqrt{N} 2^{\omega(N)} m^{k/2}).$$

*Proof.* We examine each of the  $A_{i,m}$  terms in (2.1) separately.

First,  $A_{1,m} = \chi(\sqrt{m}) \frac{k-1}{12} \psi(N) m^{k/2-1}$  from (2.2).

Second, like in the previous Lemma,  $A_{2,m} = O(2^{\omega(N)} m^{k/2})$ .

Third, from Lemma 3.3, each inner summation  $\Sigma(N, m, d)$  in  $A_{3,m}$  is  $O(\sqrt{N} 2^{\omega(N)})$ . So by (2.4) and the fact that  $\min(d, m/d) \leq m^{1/2}$ ,

$$\begin{aligned} A_{3,m} &= \frac{1}{2} \sum_{d|m} \min(d, m/d)^{k-1} \Sigma(N, m, d) \\ &= O(\sqrt{N} 2^{\omega(N)} m^{k/2}). \end{aligned}$$

Fourth, we have  $A_{4,m} = O(1)$  by (2.5).

Combining the above bounds, we obtain

$$\begin{aligned} \text{Tr } T_m(N, k, \chi) &= A_{1,m} - A_{2,m} - A_{3,m} + A_{4,m} \\ &= \chi(\sqrt{m}) \frac{k-1}{12} \psi(N) m^{k/2-1} + O(\sqrt{N} 2^{\omega(N)} m^{k/2}), \end{aligned}$$

concluding the proof.  $\square$

Next, we prove Theorems 1.1 and 1.2 in the case when  $m$  is not a perfect square.

**Proposition 4.3.** *Let  $m \geq 1$  be fixed and not a perfect square. Suppose that  $\gcd(N, m) = 1$ ,  $k \geq 2$ , and  $\chi$  is a Dirichlet character modulo  $N$  with  $\chi(-1) = (-1)^k$ . Then  $a_2(m, N, k, \chi)$  is nonvanishing for all but finitely many triples  $(N, k, \chi)$ . Furthermore, when  $\chi$  is trivial,  $a_2(m, N, k)$  is negative for all but finitely many pairs  $(N, k)$ .*

*Proof.* By Lemma 2.1, we have

$$a_2(m, N, k, \chi) = \frac{1}{2} \left[ (\text{Tr } T_m)^2 - \sum_{d|m} \chi(d) d^{k-1} \text{Tr } T_{m^2/d^2} \right].$$

Now, observe that every term inside the sum has  $m^2/d^2$  a perfect square. Thus for each term in the sum, we have by Lemma 4.2,

$$\begin{aligned} & \chi(d) d^{k-1} \text{Tr } T_{m^2/d^2} \\ &= \chi(d) d^{k-1} \left[ \chi \left( \sqrt{\frac{m^2}{d^2}} \right) \frac{k-1}{12} \psi(N) \left( \frac{m^2}{d^2} \right)^{k/2-1} + O \left( \sqrt{N} 2^{\omega(N)} \left( \frac{m^2}{d^2} \right)^{k/2} \right) \right] \\ &= \chi(d) d^{k-1} \left[ \chi \left( \frac{m}{d} \right) \frac{k-1}{12} \psi(N) \frac{m^{k-2}}{d^{k-2}} + O \left( \sqrt{N} 2^{\omega(N)} \frac{m^k}{d^k} \right) \right] \\ &= \chi(m) d \frac{k-1}{12} \psi(N) m^{k-2} + O(\sqrt{N} 2^{\omega(N)} m^k). \end{aligned}$$

This yields

$$\begin{aligned} a_2(m, N, k, \chi) &= \frac{1}{2} \left[ (\text{Tr } T_m)^2 - \sum_{d|m} \chi(d) d^{k-1} \text{Tr } T_{m^2/d^2} \right] \\ &= \frac{1}{2} \left[ (\text{Tr } T_m)^2 - \sum_{d|m} \left[ \chi(m) d \frac{k-1}{12} \psi(N) m^{k-2} + O(\sqrt{N} 2^{\omega(N)} m^k) \right] \right] \\ &= \frac{1}{2} \left[ (\text{Tr } T_m)^2 - \chi(m) \frac{k-1}{12} \psi(N) m^{k-2} \sigma_1(m) + O(\sqrt{N} 2^{\omega(N)} m^k) \right]. \end{aligned}$$

Since  $m$  is not a perfect square, we apply Lemma 4.1 to  $\text{Tr } T_m$  and obtain

$$\begin{aligned} a_2(m, N, k, \chi) &= \frac{1}{2} \left[ O(2^{\omega(N)} m^{k/2})^2 - \chi(m) \frac{k-1}{12} \psi(N) m^{k-2} \sigma_1(m) - O(\sqrt{N} 2^{\omega(N)} m^k) \right] \\ &= \frac{1}{2} \left[ -\chi(m) \frac{k-1}{12} \psi(N) m^{k-2} \sigma_1(m) + O(\sqrt{N} 2^{\omega(N)} m^k) \right] \\ &= \frac{\psi(N) m^{k-2} \sigma_1(m)}{2} \left[ -\chi(m) \frac{k-1}{12} + O(\theta_1(N)) \right]. \end{aligned} \tag{4.1}$$

Here we used the fact that  $2^{\omega(N)} = O(\sqrt{N})$  (from the proof of Lemma 3.1) and the definition  $\theta_1(N) = \frac{\sqrt{N} 2^{\omega(N)}}{\psi(N)}$  (also from Lemma 3.1).

Now,  $\gcd(m, N) = 1$  means that  $|\chi(m)| = 1$ , and hence  $|\chi(m) \frac{k-1}{12}| \geq \frac{1}{12}$  for all  $k \geq 2$ . But for sufficiently large  $N$  (independent of  $k$ ), the  $O(\theta_1(N))$  term will be  $< \frac{1}{12}$  in magnitude since

$\theta_1(N) \rightarrow 0$  according to Lemma 3.1. Thus  $a_2(m, N, k, \chi)$  will be nonvanishing for sufficiently large  $N$ .

This leaves only finitely many  $N$  to check. For these values of  $N$ , the  $O(\theta_1(N))$  term will be bounded by a constant. So for  $k$  sufficiently large,  $|\chi(m)\frac{k-1}{12}| = \frac{k-1}{12}$  will be larger than that constant, and  $a_2(m, N, k, \chi)$  will be nonvanishing.

This shows that  $a_2(m, N, k, \chi)$  is nonvanishing for all but finitely many triples  $(N, k, \chi)$ .

Furthermore, note that when  $\chi$  is trivial,  $a_2(m, N, k)$  will be real. In this case, the expression inside the brackets of (4.1) becomes  $-\frac{k-1}{12} + O(\theta_1(N))$ . So in particular,  $a_2(m, N, k)$  will be negative for all but finitely many pairs  $(N, k)$ .  $\square$

Finally, we prove Theorems 1.1 and 1.2 in the case when  $m$  is a perfect square.

**Proposition 4.4.** *Let  $m \geq 1$  be fixed and a perfect square. Suppose that  $\gcd(N, m) = 1$ ,  $k \geq 2$ , and  $\chi$  is a Dirichlet character modulo  $N$  with  $\chi(-1) = (-1)^k$ . Then  $a_2(m, N, k, \chi)$  is nonvanishing for all but finitely many triples  $(N, k, \chi)$ . Furthermore, when  $\chi$  is trivial,  $a_2(m, N, k)$  is positive for all but finitely many pairs  $(N, k)$ .*

*Proof.* By the same argument as in Proposition 4.3,

$$a_2(m, N, k, \chi) = \frac{1}{2} \left[ (\text{Tr } T_m)^2 - \chi(m) \frac{k-1}{12} \psi(N) m^{k-2} \sigma_1(m) + O(\sqrt{N} 2^{\omega(N)} m^k) \right].$$

Then using the fact that  $\sqrt{N} 2^{\omega(N)} = O(\psi(N))$  from Lemma 3.1, this yields

$$a_2(m, N, k, \chi) = \frac{1}{2} \left[ (\text{Tr } T_m)^2 + O(k\psi(N)m^k) \right].$$

Since  $m$  is a perfect square, we apply Lemma 4.2 to  $\text{Tr } T_m$ , and we have

$$\begin{aligned} (\text{Tr } T_m)^2 &= \left( \chi(\sqrt{m}) \frac{k-1}{12} \psi(N) m^{k/2-1} + O(\sqrt{N} 2^{\omega(N)} m^{k/2}) \right)^2 \\ &= \chi(m) \frac{(k-1)^2}{144} \psi(N)^2 m^{k-2} + O\left(k\psi(N)m^{k/2} \cdot \sqrt{N} 2^{\omega(N)} m^{k/2}\right) + O\left(\sqrt{N} 2^{\omega(N)} m^{k/2}\right)^2 \\ &= \chi(m) \frac{(k-1)^2}{144} \psi(N)^2 m^{k-2} + O\left(k\psi(N)\sqrt{N} 2^{\omega(N)} m^k\right). \end{aligned}$$

Here, we again used the fact that  $\sqrt{N} 2^{\omega(N)} = O(\psi(N))$ . Then

$$\begin{aligned} a_2(m, N, k, \chi) &= \frac{1}{2} \left[ (\text{Tr } T_m)^2 + O(k\psi(N)m^k) \right] \\ &= \frac{1}{2} \left[ \chi(m) \frac{(k-1)^2}{144} \psi(N)^2 m^{k-2} + O\left(k\psi(N)\sqrt{N} 2^{\omega(N)} m^k\right) \right] \\ &= \frac{k\psi(N)^2 m^{k-2}}{2} \left[ \chi(m) \frac{(k-1)^2}{144k} + O(\theta_1(N)) \right]. \end{aligned} \tag{4.2}$$

Now,  $\left| \chi(m) \frac{(k-1)^2}{144k} \right| \geq \frac{1}{288}$  for all  $k \geq 2$ . But for sufficiently large  $N$ , the  $O(\theta_1(N))$  term will be  $< \frac{1}{288}$  in magnitude, according to Lemma 3.1. Thus  $a_2(m, N, k, \chi)$  will be nonvanishing for sufficiently large  $N$ .

Again, this leaves only finitely many  $N$  to check. For these values of  $N$ , the  $O(\theta_1(N))$  term will be bounded by a constant, by Lemma 3.1. So for  $k$  sufficiently large,  $\left| \chi(m) \frac{(k-1)^2}{144k} \right| = \frac{(k-1)^2}{144k}$  will be larger than that constant, and  $a_2(m, N, k, \chi)$  will be nonvanishing.

This shows that  $a_2(m, N, k, \chi)$  is nonvanishing for all but finitely many triples  $(N, k, \chi)$ .

Furthermore, note that when  $\chi$  is trivial, the expression inside the brackets of (4.2) becomes  $\frac{(k-1)^2}{144k} + O(\theta_1(N))$ . So in particular,  $a_2(m, N, k)$  will be positive for all but finitely many pairs  $(N, k)$ .  $\square$

Propositions 4.3 and 4.4 combine to imply Theorems 1.1 and 1.2.

In these two proofs, we needed  $\gcd(m, N) = 1$  to use the fact that  $|\chi(m)| = 1$ . It is worth noting that this is the first place that we need this coprimality assumption. In particular, all of the trace bounds given above still work even when  $\gcd(m, N) > 1$ .

Note that all of the bounds given here are explicitly computable. So in Section 5, we compute all of these bounds for  $m = 3$ , and give the complete list of pairs  $(N, k)$  for which  $a_2(3, N, k)$  is positive or zero. In Section 6, we compute the bounds for  $m = 4$ , and give the complete list of pairs  $(N, k)$  for which  $a_2(4, N, k)$  is negative or zero.

## 5. PROOF OF THEOREM 1.3

In this section, we show Theorem 1.3: for  $N$  coprime to 3 and  $k \geq 2$  even,  $a_2(3, N, k)$  is positive or zero only for the pairs  $(N, k)$  given in Table 5.4.

Observe that in the notation of Lemma 2.1, for  $\gcd(N, 3) = 1$  and  $k \geq 2$  even, we have

$$a_2(3, N, k) = \frac{1}{2} \left[ (\text{Tr } T_3)^2 - \text{Tr } T_9 - 3^{k-1} \text{Tr } T_1 \right]. \quad (5.1)$$

We bound the terms of (5.1) separately in the following three lemmas. Each of these bounds will be expressed in terms of the  $\theta_i(N)$  defined in Lemma 3.1.

**Lemma 5.1.** *Let  $N \geq 1$  and  $k \geq 2$  be even. Then*

$$\frac{(\text{Tr } T_3)^2}{\psi(N)3^k} \leq \frac{448 + 160\sqrt{3}}{27} \theta_2(N).$$

*Proof.* We examine each of the  $A_{i,3}$  terms from (2.1) separately.

First, by (2.2),

$$A_{1,3} = \chi_0(\sqrt{3}) \frac{k-1}{12} \psi(N) 3^{k/2-1} = 0.$$

Second, by (2.3) (recalling that the  $t = t_0$  and  $t = -t_0$  terms coincide) and Table 2.2,

$$\begin{aligned}
A_{2,3} &= \frac{1}{2} \sum_{t^2 < 12} U_{k-1}(t, 3) \sum_n h_w \left( \frac{t^2 - 12}{n^2} \right) \mu(t, n, 3) \\
&= \frac{1}{2} U_{k-1}(0, 3) \sum_n h_w \left( \frac{-12}{n^2} \right) \mu(0, n, 3) \\
&\quad + U_{k-1}(1, 3) \sum_n h_w \left( \frac{-11}{n^2} \right) \mu(1, n, 3) \\
&\quad + U_{k-1}(2, 3) \sum_n h_w \left( \frac{-8}{n^2} \right) \mu(2, n, 3) \\
&\quad + U_{k-1}(3, 3) \sum_n h_w \left( \frac{-3}{n^2} \right) \mu(3, n, 3) \\
&= \frac{1}{2} U_{k-1}(0, 3) [h_w(-12)\mu(0, 1, 3) + h_w(-3)\mu(0, 2, 3)] \\
&\quad + U_{k-1}(1, 3) [h_w(-11)\mu(1, 1, 3)] \\
&\quad + U_{k-1}(2, 3) [h_w(-8)\mu(2, 1, 3)] \\
&\quad + U_{k-1}(3, 3) [h_w(-3)\mu(3, 1, 3)] \\
&= \frac{1}{2} U_{k-1}(0, 3) [\mu(0, 1, 3) + \frac{1}{3}\mu(0, 2, 3)] \\
&\quad + U_{k-1}(1, 3) [\mu(1, 1, 3)] \\
&\quad + U_{k-1}(2, 3) [\mu(2, 1, 3)] \\
&\quad + U_{k-1}(3, 3) [\frac{1}{3}\mu(3, 1, 3)].
\end{aligned}$$

So by Lemma 3.2,

$$\begin{aligned}
|A_{2,3}| &\leq 2^{\omega(N)} 3^{(k-1)/2} \cdot 2 \left[ \frac{1}{2} \left( 1 + \frac{1}{3} \cdot 3 \right) + (1) + (1) + \left( \frac{1}{3} \right) \right] \\
&= \frac{20}{3\sqrt{3}} 2^{\omega(N)} 3^{k/2}.
\end{aligned}$$

Third, by (2.4) (recalling that the  $d = d_0$  and  $d = m/d_0$  terms coincide) and Lemma 3.3,

$$\begin{aligned}
A_{3,3} &= \frac{1}{2} \sum_{d|3} \min(d, 3/d)^{k-1} \Sigma(N, 3, d) \\
&= \Sigma(N, 3, 1) \\
&\leq |-2| \cdot 2^{\omega(N)} \\
&= 2 \cdot 2^{\omega(N)}.
\end{aligned}$$

Fourth, by (2.5),

$$A_{4,3} \leq \sum_{c|3} c = 1 + 3 = 4.$$

Now, note that  $A_{3,3}$  and  $A_{4,3}$  here are both positive and  $\leq 4 \cdot 2^{\omega(N)}$ . So putting all this together, we obtain

$$\begin{aligned} |\operatorname{Tr} T_3| &= |A_{1,3} - A_{2,3} - A_{3,3} + A_{4,3}| \\ &\leq |A_{2,3}| + |A_{3,3} - A_{4,3}| \\ &\leq \frac{20}{3\sqrt{3}} \cdot 2^{\omega(N)} 3^{k/2} + 4 \cdot 2^{\omega(N)} \\ &\leq \frac{20}{3\sqrt{3}} \cdot 2^{\omega(N)} 3^{k/2} + \frac{4}{3} \cdot 3^{k/2} 2^{\omega(N)} \\ &= \left( \frac{20}{3\sqrt{3}} + \frac{4}{3} \right) 2^{\omega(N)} 3^{k/2}, \end{aligned}$$

which yields

$$\begin{aligned} \frac{(\operatorname{Tr} T_3)^2}{\psi(N) 3^k} &\leq \frac{\left( \frac{20}{3\sqrt{3}} + \frac{4}{3} \right)^2 (2^{\omega(N)})^2 3^k}{\psi(N) 3^k} \\ &= \frac{448 + 160\sqrt{3}}{27} \theta_2(N), \end{aligned}$$

as desired. □

Next, we bound the  $\operatorname{Tr} T_9$  term from (5.1).

**Lemma 5.2.** *Let  $N \geq 1$  with  $\gcd(N, 3) = 1$  and  $k \geq 2$  be even. Then*

$$\left| \frac{\operatorname{Tr} T_9 - A_{1,9}}{\psi(N) 3^k} \right| \leq \frac{65}{6} \theta_3(N) + \frac{1}{6} \theta_1(N),$$

where

$$A_{1,9} = \frac{k-1}{108} \psi(N) 3^k.$$

*Proof.* We examine each of the  $A_{i,9}$  terms from (2.1) separately.

First, by (2.2),

$$A_{1,9} = \chi_0(\sqrt{9}) \frac{k-1}{12} \psi(N) 9^{k/2-1} = \frac{k-1}{108} \psi(N) 3^k,$$

as claimed.

Second, similarly to the proof of Lemma 5.1, we compute

$$A_{2,9} = \frac{1}{2} \sum_{t^2 < 36} U_{k-1}(t, 9) \sum_n h_w \left( \frac{t^2 - 36}{n^2} \right) \mu(t, n, 9)$$

$$\begin{aligned}
&= \frac{1}{2} U_{k-1}(0, 9) \sum_n h_w \left( \frac{-36}{n^2} \right) \mu(0, n, 9) \\
&\quad + U_{k-1}(1, 9) \sum_n h_w \left( \frac{-35}{n^2} \right) \mu(1, n, 9) \\
&\quad + U_{k-1}(2, 9) \sum_n h_w \left( \frac{-32}{n^2} \right) \mu(2, n, 9) \\
&\quad + U_{k-1}(3, 9) \sum_n h_w \left( \frac{-27}{n^2} \right) \mu(3, n, 9) \\
&\quad + U_{k-1}(4, 9) \sum_n h_w \left( \frac{-20}{n^2} \right) \mu(4, n, 9) \\
&\quad + U_{k-1}(5, 9) \sum_n h_w \left( \frac{-11}{n^2} \right) \mu(5, n, 9) \\
&= \frac{1}{2} U_{k-1}(0, 9) [h_w(-36)\mu(0, 1, 9) + h_w(-4)\mu(0, 3, 9)] \\
&\quad + U_{k-1}(1, 9) [h_w(-35)\mu(1, 1, 9)] \\
&\quad + U_{k-1}(2, 9) [h_w(-32)\mu(2, 1, 9) + h_w(-8)\mu(2, 2, 9)] \\
&\quad + U_{k-1}(3, 9) [h_w(-27)\mu(3, 1, 9) + h_w(-3)\mu(3, 3, 9)] \\
&\quad + U_{k-1}(4, 9) [h_w(-20)\mu(4, 1, 9)] \\
&\quad + U_{k-1}(5, 9) [h_w(-11)\mu(5, 1, 9)] \\
&= \frac{1}{2} U_{k-1}(0, 9) [2\mu(0, 1, 9) + \frac{1}{2}\mu(0, 3, 9)] \\
&\quad + U_{k-1}(1, 9) [2\mu(1, 1, 9)] \\
&\quad + U_{k-1}(2, 9) [2\mu(2, 1, 9) + \mu(2, 2, 9)] \\
&\quad + U_{k-1}(3, 9) [\mu(3, 1, 9) + \frac{1}{3}\mu(3, 3, 9)] \\
&\quad + U_{k-1}(4, 9) [2\mu(4, 1, 9)] \\
&\quad + U_{k-1}(5, 9) [\mu(5, 1, 9)].
\end{aligned}$$

So by Lemma 3.2,

$$\begin{aligned}
|A_{2,9}| &\leq 2^{\omega(N)} 9^{(k-1)/2} \cdot 2 \left[ \frac{1}{2} \left( 2 + \frac{1}{2} \cdot 4 \right) + (2) + (2+3) + \left( 1 + \frac{1}{3} \cdot 4 \right) + (2) + (1) \right] \\
&= \frac{86}{9} \cdot 2^{\omega(N)} 3^k.
\end{aligned}$$

Third, by (2.4) and Lemma 3.3,

$$A_{3,9} = \frac{1}{2} \sum_{d|9} \min(d, 9/d)^{k-1} \Sigma(N, 9, d)$$



$$\begin{aligned}
&= \Sigma(N, 9, 1) + \frac{1}{2} \cdot 3^{k-1} \Sigma(N, 9, 3) \\
&\leq |-8| \cdot 2^{\omega(N)} + \frac{1}{2} \cdot 3^{k-1} \sqrt{N} 2^{\omega(N)} \\
&= \frac{1}{6} \cdot 3^k \sqrt{N} 2^{\omega(N)} + 8 \cdot 2^{\omega(N)}.
\end{aligned}$$

Fourth, by (2.5),

$$A_{4,9} \leq \sum_{c|9} c = 1 + 3 + 9 = 13.$$

Now, note that  $A_{3,9}$  and  $A_{4,9}$  here are both positive and  $\leq \frac{1}{6} \cdot 3^k \sqrt{N} 2^{\omega(N)} + \frac{23}{2} \cdot 2^{\omega(N)}$ . So putting this all together, we obtain

$$\begin{aligned}
|\mathrm{Tr} T_9 - A_{1,9}| &= |-A_{2,9} - A_{3,9} + A_{4,9}| \\
&\leq |A_{2,9}| + |A_{3,9} - A_{4,9}| \\
&\leq \frac{86}{9} \cdot 2^{\omega(N)} 3^k + \frac{1}{6} \cdot 3^k \sqrt{N} 2^{\omega(N)} + \frac{23}{2} \cdot 2^{\omega(N)} \\
&\leq \frac{86}{9} \cdot 2^{\omega(N)} 3^k + \frac{1}{6} \cdot 3^k \sqrt{N} 2^{\omega(N)} + \frac{23}{18} \cdot 3^k 2^{\omega(N)} \\
&= \frac{65}{6} \cdot 2^{\omega(N)} 3^k + \frac{1}{6} \cdot 3^k \sqrt{N} 2^{\omega(N)},
\end{aligned}$$

which yields

$$\left| \frac{\mathrm{Tr} T_9 - A_{1,9}}{\psi(N) 3^k} \right| \leq \frac{65}{6} \theta_3(N) + \frac{1}{6} \theta_1(N),$$

as desired. □

Finally, we bound the  $\mathrm{Tr} T_1$  term from (5.1).

**Lemma 5.3.** *Let  $N \geq 1$  and  $k \geq 2$  be even. Then*

$$\left| \frac{\mathrm{Tr} T_1 - A_{1,1}}{\psi(N)} \right| \leq \frac{5}{3} \theta_3(N) + \frac{1}{2} \theta_1(N),$$

where

$$A_{1,1} = \frac{k-1}{12} \psi(N).$$

*Proof.* We examine each of the  $A_{i,1}$  terms from (2.1) separately.

First, by (2.2),

$$A_{1,1} = \chi_0(\sqrt{1}) \frac{k-1}{12} \psi(N) 1^{k/2-1} = \frac{k-1}{12} \psi(N),$$

as claimed.

Second, by (2.3),

$$\begin{aligned}
A_{2,1} &= \frac{1}{2} \sum_{t^2 < 4} U_{k-1}(t, 1) \sum_n h_w \left( \frac{t^2 - 4}{n^2} \right) \mu(t, n, 1) \\
&= \frac{1}{2} U_{k-1}(0, 1) \sum_n h_w \left( \frac{-4}{n^2} \right) \mu(0, n, 1) + U_{k-1}(1, 1) \sum_n h_w \left( \frac{-3}{n^2} \right) \mu(1, n, 1) \\
&= \frac{1}{2} U_{k-1}(0, 1) h_w(-4) \mu(0, 1, 1) + U_{k-1}(1, 1) h_w(-3) \mu(1, 1, 1) \\
&= \frac{1}{2} \cdot \frac{1}{2} U_{k-1}(0, 1) \mu(0, 1, 1) + \frac{1}{3} U_{k-1}(1, 1) \mu(1, 1, 1).
\end{aligned}$$

So by Lemma 3.2,

$$|A_{2,1}| \leq \frac{1}{4} \cdot 2 \cdot 2^{\omega(N)} + \frac{1}{3} \cdot 2 \cdot 2^{\omega(N)} = \frac{7}{6} \cdot 2^{\omega(N)}.$$

Third, by (2.4) and Lemma 3.3,

$$\begin{aligned}
A_{3,1} &= \frac{1}{2} \sum_{d|1} \min(d, 1/d)^{k-1} \Sigma(N, 1, d) \\
&= \frac{1}{2} \Sigma(N, 1, 1) \\
&\leq \frac{1}{2} \sqrt{N} 2^{\omega(N)}.
\end{aligned}$$

Fourth, by (2.5),

$$A_{4,1} \leq \sum_{c|1} c = 1.$$

Now, note that  $A_{3,1}$  and  $A_{4,1}$  are both positive and  $\leq \frac{1}{2} \sqrt{N} 2^{\omega(N)} + \frac{1}{2} \cdot 2^{\omega(N)}$ . So putting all this together, we obtain

$$\begin{aligned}
|\mathrm{Tr} T_1 - A_{1,1}| &= |-A_{2,1} - A_{3,1} + A_{4,1}| \\
&\leq |A_{2,1}| + |A_{3,1} - A_{4,1}| \\
&\leq \frac{7}{6} \cdot 2^{\omega(N)} + \frac{1}{2} \sqrt{N} 2^{\omega(N)} + \frac{1}{2} \cdot 2^{\omega(N)} \\
&= \frac{5}{3} \cdot 2^{\omega(N)} + \frac{1}{2} \sqrt{N} 2^{\omega(N)},
\end{aligned}$$

which yields

$$\left| \frac{\mathrm{Tr} T_1 - A_{1,1}}{\psi(N)} \right| \leq \frac{5}{3} \theta_3(N) + \frac{1}{2} \theta_1(N),$$

completing the proof.  $\square$

Note that  $\mathrm{Tr} T_1$  is just the dimension of  $S_k(\Gamma_0(N))$ . So Lemma 5.3 is just a dimension estimate. And in fact, one can also derive the bounds in this lemma from the dimension formula given in [3, p. 264].

We are now ready to prove Theorem 1.3.

**Theorem 1.3.** *Suppose that  $\gcd(N, 3) = 1$  and that  $k \geq 2$  is even. Then the second coefficient  $a_2(3, N, k)$  is positive or zero only for the pairs  $(N, k)$  given in Table 5.4.*

*Proof.* By (5.1) and Lemmas 5.2 and 5.3,

$$\begin{aligned}
& a_2(3, N, k) \\
&= \frac{1}{2} \left[ (\text{Tr } T_3)^2 - \text{Tr } T_9 - 3^{k-1} \text{Tr } T_1 \right] \\
&= \frac{1}{2} \left[ (\text{Tr } T_3)^2 - A_{1,9} - (\text{Tr } T_9 - A_{1,9}) - 3^{k-1} A_{1,1} - 3^{k-1} (\text{Tr } T_1 - A_{1,1}) \right] \\
&= \frac{1}{2} \left[ -\frac{k-1}{108} \psi(N) 3^k - \frac{k-1}{12} \psi(N) 3^{k-1} + (\text{Tr } T_3)^2 - (\text{Tr } T_9 - A_{1,9}) - 3^{k-1} (\text{Tr } T_1 - A_{1,1}) \right] \\
&= \frac{\psi(N) 3^k}{2} \left[ -\frac{k-1}{27} + \frac{(\text{Tr } T_3)^2}{\psi(N) 3^k} - \left( \frac{\text{Tr } T_9 - A_{1,9}}{\psi(N) 3^k} \right) - \frac{1}{3} \left( \frac{\text{Tr } T_1 - A_{1,1}}{\psi(N)} \right) \right] \\
&= \frac{\psi(N) 3^k}{2} \left[ -\frac{k-1}{27} + E(N, k) \right], \tag{5.2}
\end{aligned}$$

where  $E(N, k)$  denotes the three error terms above. In particular, from Lemmas 5.1, 5.2, and 5.3,

$$\begin{aligned}
|E(N, k)| &= \left| \frac{(\text{Tr } T_3)^2}{\psi(N) 3^k} - \left( \frac{\text{Tr } T_9 - A_{1,9}}{\psi(N) 3^k} \right) - \frac{1}{3} \left( \frac{\text{Tr } T_1 - A_{1,1}}{\psi(N)} \right) \right| \\
&\leq \frac{448 + 160\sqrt{3}}{27} \theta_2(N) + \left( \frac{65}{6} \theta_3(N) + \frac{1}{6} \theta_1(N) \right) + \frac{1}{3} \left( \frac{5}{3} \theta_3(N) + \frac{1}{2} \theta_1(N) \right) \\
&= \frac{448 + 160\sqrt{3}}{27} \theta_2(N) + \frac{205}{18} \theta_3(N) + \frac{1}{3} \theta_1(N).
\end{aligned}$$

For  $N \geq 63,000,000$ , we have the bounds  $\theta_1(N) \leq 0.0106$ ,  $\theta_2(N) \leq 0.000314$ , and  $\theta_3(N) \leq 0.000015$  given in Lemma 3.1. Thus

$$\begin{aligned}
|E(N, k)| &\leq \frac{448 + 160\sqrt{3}}{27} 0.000314 + \frac{205}{18} 0.000015 + \frac{1}{3} 0.0106 \\
&\leq 0.0122,
\end{aligned}$$

which is  $< \frac{k-1}{27}$  for all  $k \geq 2$ . By (5.2), this shows that  $a_2(3, N, k) < 0$  for  $N \geq 63,000,000$  and  $k \geq 2$ .

Utilizing the table in Lemma 3.1, an identical argument using 2,700,000, 150,000, 8,800, 571, 43, and 1 as the bounds for  $N$ , shows that  $a_2(3, N, k) < 0$  for  $N \geq 2,700,000, k \geq 4$ ;  $N \geq 150,000, k \geq 10$ ;  $N \geq 8,800, k \geq 34$ ;  $N \geq 571, k \geq 116$ ;  $N \geq 43, k \geq 346$ ; and  $N \geq 1, k \geq 1290$ .

We then check the finite number of cases left by computer, which yields the complete list given in Table 5.4. See [9] for the code.  $\square$

**Table 5.4.**

<i>All pairs <math>(N, k)</math> for which <math>a_2(3, N, k)</math> is positive or zero, along with <math>\dim S_k(\Gamma_0(N))</math> and the actual value of <math>a_2(3, N, k)</math>.</i>											
$(N, k)$	dim	$a_2$	$(N, k)$	dim	$a_2$	$(N, k)$	dim	$a_2$	$(N, k)$	dim	$a_2$
(1, 2)	0	0	(8, 2)	0	0	(4, 6)	1	0	(4, 8)	2	144
(1, 4)	0	0	(10, 2)	0	0	(5, 4)	1	0	(22, 2)	2	1
(1, 6)	0	0	(13, 2)	0	0	(5, 6)	1	0	(28, 2)	2	4
(1, 8)	0	0	(16, 2)	0	0	(7, 4)	1	0	(34, 2)	3	0
(1, 10)	0	0	(25, 2)	0	0	(8, 4)	1	0	(40, 2)	3	4
(1, 14)	0	0	(1, 12)	1	0	(11, 2)	1	0	(64, 2)	3	0
(2, 2)	0	0	(1, 16)	1	0	(14, 2)	1	0	(38, 2)	4	3
(2, 4)	0	0	(1, 18)	1	0	(17, 2)	1	0	(44, 2)	4	0
(2, 6)	0	0	(1, 20)	1	0	(19, 2)	1	0	(56, 2)	5	0
(4, 2)	0	0	(1, 22)	1	0	(20, 2)	1	0	(67, 2)	5	1
(4, 4)	0	0	(1, 26)	1	0	(32, 2)	1	0	(80, 2)	7	0
(5, 2)	0	0	(2, 8)	1	0	(49, 2)	1	0	(140, 2)	19	0
(7, 2)	0	0	(2, 10)	1	0	(2, 12)	2	63504	(280, 2)	41	0

Now, in the case of  $m = 2$ , Clayton et al. [2, Theorems 1.1 and 1.3] already gave the complete list of  $(N, k)$  for which  $a_2(2, N, k)$  vanishes. But for completeness, we extend their result slightly and give the complete list of  $(N, k)$  for which  $a_2(2, N, k)$  is positive or zero. We forgo repeating all of the exact same details for the  $m = 2$  case, and just give the corresponding bounds that our method would yield.

**Proposition 5.5** (c.f. [2, Theorems 1.1 and 1.3]). *Suppose that  $\gcd(N, 2) = 1$  and that  $k \geq 2$  is even. Then the second coefficient  $a_2(2, N, k)$  is positive or zero only for the pairs  $(N, k)$  given in Table 5.6.*

*Proof.* From Lemma 2.1, we have

$$a_2(2, N, k) = \frac{1}{2} \left[ (\text{Tr } T_2)^2 - \text{Tr } T_4 - 2^{k-1} \text{Tr } T_1 \right].$$

Then by an identical method as in Lemmas 5.1, 5.2, and 5.3, we obtain the bounds

$$\begin{aligned} \frac{(\text{Tr } T_2)^2}{\psi(N)2^k} &\leq \frac{41 + 24\sqrt{2}}{4}\theta_2(N), \\ \left| \frac{\text{Tr } T_4 - A_{1,4}}{\psi(N)2^k} \right| &\leq \frac{17}{2}\theta_3(N) + \frac{1}{4}\theta_1(N), \quad \text{where} \quad A_{1,4} = \frac{k-1}{48}\psi(N)2^k, \\ \left| \frac{\text{Tr } T_1 - A_{1,1}}{\psi(N)} \right| &\leq \frac{5}{3}\theta_3(N) + \frac{1}{2}\theta_1(N), \quad \text{where} \quad A_{1,1} = \frac{k-1}{12}\psi(N). \end{aligned}$$

As done in Theorem 1.3, combining these three bounds gives

$$a_2(2, N, k) = \frac{\psi(N)2^k}{2} \left[ -\frac{k-1}{16} + E(N, k) \right],$$

where

$$|E(N, k)| \leq \frac{41 + 24\sqrt{2}}{4}\theta_2(N) + \frac{28}{3}\theta_3(N) + \frac{1}{2}\theta_1(N).$$

This yields  $a_2(2, N, k) < 0$  for  $N \geq 2,700,000, k \geq 2$ ;  $N \geq 150,000, k \geq 6$ ;  $N \geq 8,800, k \geq 16$ ;  $N \geq 571, k \geq 50$ ;  $N \geq 43, k \geq 148$ ; and  $N \geq 1, k \geq 562$ .

We then check the finite number of cases left by computer, which yields the complete list given in Table 5.6. See [9] for the code.  $\square$

**Table 5.6.**

<i>All pairs <math>(N, k)</math> for which <math>a_2(2, N, k)</math> is positive or zero, along with <math>\dim S_k(\Gamma_0(N))</math> and the actual value of <math>a_2(2, N, k)</math>.</i>											
$(N, k)$	dim	$a_2$	$(N, k)$	dim	$a_2$	$(N, k)$	dim	$a_2$	$(N, k)$	dim	$a_2$
(1, 2)	0	0	(7, 2)	0	0	(1, 26)	1	0	(17, 2)	1	0
(1, 4)	0	0	(9, 2)	0	0	(3, 6)	1	0	(19, 2)	1	0
(1, 6)	0	0	(13, 2)	0	0	(3, 8)	1	0	(21, 2)	1	0
(1, 8)	0	0	(25, 2)	0	0	(5, 4)	1	0	(27, 2)	1	0
(1, 10)	0	0	(1, 12)	1	0	(5, 6)	1	0	(49, 2)	1	0
(1, 14)	0	0	(1, 16)	1	0	(7, 4)	1	0	(37, 2)	2	0
(3, 2)	0	0	(1, 18)	1	0	(9, 4)	1	0	(33, 2)	3	0
(3, 4)	0	0	(1, 20)	1	0	(11, 2)	1	0	(57, 2)	5	0
(5, 2)	0	0	(1, 22)	1	0	(15, 2)	1	0			

## 6. PROOF OF THEOREM 1.4

In this section, we show Theorem 1.4: for  $N$  coprime to 4 and  $k \geq 2$  even,  $a_2(4, N, k)$  is negative or zero only for the pairs  $(N, k)$  given in [9, Table  $m = 4$ ].

Observe that in the notation of Lemma 2.1, for  $\gcd(N, 4) = 1$  and  $k \geq 2$  even, we have

$$a_2(4, N, k) = \frac{1}{2} \left[ (\text{Tr } T_4)^2 - \text{Tr } T_{16} - 2^{k-1} \text{Tr } T_4 - 4^{k-1} \text{Tr } T_1 \right]. \quad (6.1)$$

We bound the four terms of (6.1) separately in Lemmas 6.1 - 6.4.

**Lemma 6.1.** *Let  $N \geq 1$  with  $\gcd(N, 4) = 1$  and  $k \geq 2$  be even such that  $\frac{k-1}{48} \geq 7\theta_3(N) + \frac{1}{4}\theta_1(N)$ . Then*

$$\frac{(\text{Tr } T_4)^2}{(k-1)4^k\psi(N)^2} \geq \frac{k-1}{2304} - \frac{7}{24}\theta_3(N) - \frac{1}{96}\theta_1(N).$$

*Proof.* We examine each of the  $A_{i,4}$  terms from (2.1) separately.

First, by (2.2),

$$A_{1,4} = \chi_0(\sqrt{4}) \frac{k-1}{12} \psi(N) 4^{k/2-1} = \frac{k-1}{48} \psi(N) 2^k.$$

Second, summing over  $t$  with  $t^2 < 16$  and positive  $n$  such that  $n^2 \mid (t^2 - 16)$  and  $(t^2 - 16)/n^2 \equiv 0, 1 \pmod{4}$ , we get

$$\begin{aligned} A_{2,4} &= \frac{1}{2} \sum_{t^2 < 16} U_{k-1}(t, 4) \sum_n h_w \left( \frac{t^2 - 16}{n^2} \right) \mu(t, n, 4) \\ &= \frac{1}{2} U_{k-1}(0, 4) [\mu(0, 1, 4) + \frac{1}{2} \mu(0, 2, 4)] \\ &\quad + U_{k-1}(1, 4) [2\mu(1, 1, 4)] \\ &\quad + U_{k-1}(2, 4) [\mu(2, 1, 4) + \frac{1}{3} \mu(2, 2, 4)] \\ &\quad + U_{k-1}(3, 4) [\mu(3, 1, 4)]. \end{aligned}$$

So by Lemma 3.2,

$$\begin{aligned} |A_{2,4}| &\leq 2^{\omega(N)} 4^{(k-1)/2} \cdot 2 \left[ \frac{1}{2} \left( 1 + \frac{1}{2} \cdot 3 \right) + (2) + \left( 1 + \frac{1}{3} \cdot 3 \right) + (1) \right] \\ &= \frac{25}{4} \cdot 2^k 2^{\omega(N)}. \end{aligned}$$

Third, by (2.4) (recalling that the  $d = d_0$  and  $d = m/d_0$  terms coincide) and Lemma 3.3,

$$\begin{aligned} A_{3,4} &= \frac{1}{2} \sum_{d|4} \min(d, 4/d)^{k-1} \Sigma(N, 4, d) \\ &= \Sigma(N, 4, 1) + \frac{1}{2} \cdot 2^{k-1} \Sigma(N, 4, 2) \end{aligned}$$

$$\begin{aligned}
&\leq |-3| \cdot 2^{\omega(N)} + \frac{1}{2} \cdot 2^{k-1} \sqrt{N} 2^{\omega(N)} \\
&= 3 \cdot 2^{\omega(N)} + \frac{1}{4} \cdot 2^k \sqrt{N} 2^{\omega(N)}.
\end{aligned}$$

Putting this all together, and using the fact that  $A_{4,16} \geq 0$ , we obtain

$$\begin{aligned}
\text{Tr } T_4 &= A_{1,4} - A_{2,4} - A_{3,4} + A_{4,4} \\
&\geq A_{1,4} - |A_{2,4}| - A_{3,4} \\
&\geq \frac{k-1}{48} \psi(N) 2^k - \frac{25}{4} \cdot 2^k 2^{\omega(N)} - 3 \cdot 2^{\omega(N)} - \frac{1}{4} \cdot 2^k \sqrt{N} 2^{\omega(N)} \\
&\geq \frac{k-1}{48} \psi(N) 2^k - \frac{25}{4} \cdot 2^k 2^{\omega(N)} - \frac{3}{4} \cdot 2^k 2^{\omega(N)} - \frac{1}{4} \cdot 2^k \sqrt{N} 2^{\omega(N)} \\
&= \psi(N) 2^k \left( \frac{k-1}{48} - 7\theta_3(N) - \frac{1}{4} \theta_1(N) \right).
\end{aligned}$$

Thus if  $\frac{k-1}{48} \geq 7\theta_3(N) + \frac{1}{4} \theta_1(N)$ , then we have

$$\begin{aligned}
\frac{(\text{Tr } T_4)^2}{(k-1)4^k \psi(N)^2} &\geq \frac{\left( \frac{k-1}{48} - 7\theta_3(N) - \frac{1}{4} \theta_1(N) \right)^2}{k-1} \\
&\geq \frac{\left( \frac{k-1}{48} \right)^2 - 2 \frac{k-1}{48} (7\theta_3(N) + \frac{1}{4} \theta_1(N))}{k-1} \\
&= \frac{k-1}{2304} - \frac{7}{24} \theta_3(N) - \frac{1}{96} \theta_1(N),
\end{aligned}$$

as desired. □

Next, we bound the  $\text{Tr } T_{16}$  term from (6.1).

**Lemma 6.2.** *Let  $N \geq 1$  with  $\gcd(N, 4) = 1$  and  $k \geq 2$  be even. Then*

$$\frac{\text{Tr } T_{16}}{(k-1)4^k \psi(N)^2} \leq \frac{4309}{192N}.$$

*Proof.* We examine each of the  $A_{i,16}$  terms from (2.1) separately.

First, by (2.2),

$$A_{1,16} = \chi_0(\sqrt{16}) \frac{k-1}{12} \psi(N) 16^{k/2-1} = \frac{k-1}{192} \psi(N) 4^k.$$

Second, summing over  $t$  with  $t^2 < 64$  and positive  $n$  such that  $n^2 \mid (t^2 - 64)$  and  $(t^2 - 64)/n^2 \equiv 0, 1 \pmod{4}$ , we get

$$\begin{aligned}
A_{2,16} &= \frac{1}{2} \sum_{t^2 < 64} U_{k-1}(t, 16) \sum_n h_w \left( \frac{t^2 - 64}{n^2} \right) \mu(t, n, 16) \\
&= \frac{1}{2} U_{k-1}(0, 16) [2\mu(0, 1, 16) + \mu(0, 2, 16) + \frac{1}{2} \mu(0, 4, 16)]
\end{aligned}$$

$$\begin{aligned}
& + U_{k-1}(1, 16) [4\mu(1, 1, 16) + \mu(1, 3, 16)] \\
& + U_{k-1}(2, 16) [2\mu(2, 1, 16) + 2\mu(2, 2, 16)] \\
& + U_{k-1}(3, 16) [4\mu(3, 1, 16)] \\
& + U_{k-1}(4, 16) [2\mu(4, 1, 16) + \mu(4, 2, 16) + \frac{1}{3}\mu(4, 4, 16)] \\
& + U_{k-1}(5, 16) [4\mu(5, 1, 16)] \\
& + U_{k-1}(6, 16) [\mu(6, 1, 16) + \mu(6, 2, 16)] \\
& + U_{k-1}(7, 16) [2\mu(7, 1, 16)].
\end{aligned}$$

Thus, by Lemma 3.2,

$$\begin{aligned}
|A_{2,16}| & \leq 2^{\omega(N)} 16^{(k-1)/2} \cdot 2 \left[ \frac{1}{2} \left( 2 + 3 + \frac{1}{2} \cdot 6 \right) + (4 + 4) + (2 + 2 \cdot 3) \right. \\
& \quad \left. + (4) + \left( 2 + 3 + \frac{1}{3} \cdot 6 \right) + (4) + (1 + 3) + (2) \right] \\
& = \frac{41}{2} \cdot 2^{\omega(N)} 4^k.
\end{aligned}$$

Third, by (2.5),

$$A_{4,16} \leq \sum_{c|16} c = 1 + 2 + 4 + 8 + 16 = 31.$$

Putting this all together, and using the fact that  $A_{3,16} \geq 0$ , we obtain

$$\begin{aligned}
\text{Tr } T_{16} & = A_{1,16} - A_{2,16} - A_{3,16} + A_{4,16} \\
& \leq A_{1,16} + |A_{2,16}| + A_{4,16} \\
& \leq \frac{k-1}{192} \psi(N) 4^k + \frac{41}{2} \cdot 2^{\omega(N)} 4^k + 31 \\
& \leq \frac{k-1}{192} \psi(N) 4^k + \frac{41}{2} \psi(N) 4^k (k-1) + \frac{31}{16} \psi(N) 4^k (k-1) \\
& = \frac{4309}{192} \cdot \psi(N) 4^k (k-1).
\end{aligned}$$

This yields

$$\frac{\text{Tr } T_{16}}{(k-1)4^k \psi(N)^2} \leq \frac{4309}{192 \psi(N)} \leq \frac{4309}{192N},$$

as desired. □

**Lemma 6.3.** *Let  $N \geq 1$  with  $\gcd(N, 4) = 1$  and  $k \geq 2$  be even. Then*

$$\frac{\text{Tr } T_4}{(k-1)2^k \psi(N)^2} \leq \frac{385}{48N}.$$



*Proof.* We examine each of the  $A_{i,4}$  terms from (2.1) separately.

From the computations in the proof of Lemma 6.1, we have

$$A_{1,4} = \frac{k-1}{48}\psi(N)2^k \quad \text{and} \quad |A_{2,4}| \leq \frac{25}{4}2^k 2^{\omega(N)}.$$

Also, by (2.5),

$$A_{4,4} \leq \sum_{c|4} c = 1 + 2 + 4 = 7.$$

Putting all this together, and noticing that  $A_{3,4} \geq 0$ , we obtain

$$\begin{aligned} \text{Tr } T_4 &= A_{1,4} - A_{2,4} - A_{3,4} + A_{4,4} \\ &\leq A_{1,4} + |A_{2,4}| + A_{4,4} \\ &\leq \frac{k-1}{48}\psi(N)2^k + \frac{25}{4} \cdot 2^k 2^{\omega(N)} + 7 \\ &\leq \frac{k-1}{48}\psi(N)2^k + \frac{25}{4} \cdot 2^k \psi(N)(k-1) + \frac{7}{4} \cdot 2^k \psi(N)(k-1) \\ &= \frac{385}{48} \cdot \psi(N)2^k(k-1). \end{aligned}$$

This yields

$$\frac{\text{Tr } T_4}{(k-1)2^k \psi(N)^2} \leq \frac{385}{48\psi(N)} \leq \frac{385}{48N},$$

as desired. □

**Lemma 6.4.** *Let  $N \geq 1$  and  $k \geq 2$  be even. Then*

$$\frac{\text{Tr } T_1}{(k-1)\psi(N)^2} \leq \frac{9}{4N}.$$

*Proof.* We examine each of the  $A_{i,1}$  terms from (2.1) separately.

By the calculations in the proof of Lemma 5.3, we have

$$A_{1,1} = \frac{k-1}{12}\psi(N), \quad |A_{2,1}| \leq \frac{7}{6}2^{\omega(N)}, \quad \text{and} \quad A_{4,1} \leq 1.$$

Putting all this together, and noticing that  $A_{3,1} \geq 0$ , we obtain

$$\begin{aligned} \text{Tr } T_1 &= A_{1,1} - A_{2,1} - A_{3,1} + A_{4,1} \\ &\leq A_{1,1} + |A_{2,1}| + A_{4,1} \\ &\leq \frac{k-1}{12}\psi(N) + \frac{7}{6}2^{\omega(N)} + 1 \\ &\leq \frac{k-1}{12}\psi(N) + \frac{7}{6}\psi(N)(k-1) + \psi(N)(k-1) \\ &= \frac{9}{4} \cdot \psi(N)(k-1), \end{aligned}$$

which yields

$$\frac{\operatorname{Tr} T_1}{(k-1)\psi(N)^2} \leq \frac{9}{4\psi(N)} \leq \frac{9}{4N},$$

completing the proof.  $\square$

We are now ready to prove Theorem 1.4.

**Theorem 1.4.** *Suppose that  $\gcd(N, 4) = 1$  and that  $k \geq 2$  is even. Then  $a_2(4, N, k)$  is negative or zero only for the pairs  $(N, k)$  given in [9, Table  $m = 4$ ].*

*Proof.* Assume that the condition  $\frac{k-1}{48} \geq 7\theta_3(N) + \frac{1}{4}\theta_1(N)$  from Lemma 6.1 is satisfied. Then by (6.1) and Lemma 6.1,

$$\begin{aligned} & a_2(4, N, k) \\ &= \frac{1}{2} \left[ (\operatorname{Tr} T_4)^2 - \operatorname{Tr} T_{16} - 2^{k-1} \operatorname{Tr} T_4 - 4^{k-1} \operatorname{Tr} T_1 \right] \\ &= \frac{(k-1)4^k\psi(N)^2}{2} \left[ \frac{(\operatorname{Tr} T_4)^2}{(k-1)4^k\psi(N)^2} - \frac{\operatorname{Tr} T_{16}}{(k-1)4^k\psi(N)^2} - \frac{1}{2} \frac{\operatorname{Tr} T_4}{(k-1)2^k\psi(N)^2} - \frac{1}{4} \frac{\operatorname{Tr} T_1}{(k-1)\psi(N)^2} \right] \\ &\geq \frac{(k-1)4^k\psi(N)^2}{2} \left[ \frac{k-1}{2304} - \frac{7}{24}\theta_3(N) - \frac{1}{96}\theta_1(N) - \frac{\operatorname{Tr} T_{16}}{(k-1)4^k\psi(N)^2} \right. \\ &\quad \left. - \frac{1}{2} \frac{\operatorname{Tr} T_4}{(k-1)2^k\psi(N)^2} - \frac{1}{4} \frac{\operatorname{Tr} T_1}{(k-1)\psi(N)^2} \right] \\ &= \frac{(k-1)4^k\psi(N)^2}{2} \left[ \frac{k-1}{2304} - E(N, k) \right], \end{aligned} \tag{6.2}$$

where  $E(N, k)$  denotes the five error terms above. In particular, from Lemmas 6.2, 6.3, and 6.4,

$$\begin{aligned} E(N, k) &= \frac{7}{24}\theta_3(N) + \frac{1}{96}\theta_1(N) + \frac{\operatorname{Tr} T_{16}}{(k-1)4^k\psi(N)^2} + \frac{1}{2} \frac{\operatorname{Tr} T_4}{(k-1)2^k\psi(N)^2} + \frac{1}{4} \frac{\operatorname{Tr} T_1}{(k-1)\psi(N)^2} \\ &\leq \frac{7}{24}\theta_3(N) + \frac{1}{96}\theta_1(N) + \frac{4309}{192N} + \frac{1}{2} \cdot \frac{385}{48N} + \frac{1}{4} \cdot \frac{9}{4N} \\ &= \frac{7}{24}\theta_3(N) + \frac{1}{96}\theta_1(N) + \frac{1729}{64N}. \end{aligned}$$

For  $N \geq 2,700,000$ , we have the bounds  $\theta_1(N) \leq 0.0265$  and  $\theta_3(N) \leq 0.000015$  given in Lemma 3.1. Note for such  $N$ , the condition  $\frac{k-1}{48} \geq 7\theta_3(N) + \frac{1}{4}\theta_1(N)$  from Lemma 6.1 is satisfied for all  $k \geq 2$ . Additionally,

$$\begin{aligned} E(N, k) &\leq \frac{7}{24} \cdot 0.000015 + \frac{1}{96} \cdot 0.0265 + \frac{1729}{64 \cdot 2,700,000} \\ &\leq 0.000291, \end{aligned}$$

which is  $< \frac{k-1}{2304}$  for all  $k \geq 2$ . By (6.2), this shows that  $a_2(4, N, k) > 0$  for  $N \geq 2,700,000$  and  $k \geq 2$ .

Utilizing the table in Lemma 3.1, an identical argument using 150,000, 8,800, 571, 43, and 1 as the bounds for  $N$ , shows that  $a_2(4, N, k) > 0$  for  $N \geq 150,000, k \geq 4$ ;  $N \geq 8,800, k \geq 14$ ;  $N \geq 571, k \geq 124$ ;  $N \geq 43, k \geq 1498$ ; and  $N \geq 1, k \geq 62942$ .

We then check the finite number of cases left by computer, which yields the complete list given in [9, Table  $m = 4$ ]. (The table contains 164 pairs, and was too large to include here.) See [9] for the code.  $\square$

Now, the same methods here would also work for the perfect square case of  $m = 1$ . But this would just be proving a result that is already known.  $T_1(N, k)$  is just the identity operator, so  $a_2(1, N, k)$  will necessarily be positive for all  $(N, k)$  with  $\dim S_k(\Gamma_0(N)) \geq 2$ . And for the finitely many pairs  $(N, k)$  where  $\dim S_k(\Gamma_0(N)) = 0$  or 1, we will trivially have  $a_2(1, N, k) = 0$ .

## 7. DISCUSSION

We first make some observations about the proofs of Propositions 4.3 and 4.4. One of the last steps in these two proofs was to show that for any given  $(m, N, \chi)$ , the  $a_2$  coefficient is nonvanishing for sufficiently large  $k$ . It is worth noting that is also what one would expect from the well-known Skolem-Mahler-Lech theorem [4, Section 2.1]. For any fixed  $(m, N, \chi)$ ,  $\text{Tr } T_m(N, k, \chi)$  satisfies a linear recurrence in  $k$ ; this fact follows from the Eichler-Selberg trace formula (2.1). So by Lemma 2.1,  $a_2(m, N, k, \chi)$  also satisfies a linear recurrence in  $k$ . Thus by Skolem-Mahler-Lech, one would expect that for any given  $(m, N, \chi)$ ,  $a_2(m, N, k, \chi)$  only vanishes for finitely many  $k$ .

Now, one might ask if the same result holds including  $m$  as well, i.e. if  $a_2(m, N, k, \chi)$  only vanishes for finitely many  $(m, N, k, \chi)$ . It turns out this is not true for a trivial reason. When  $\dim S_k(\Gamma_0(N), \chi) < 2$ , the characteristic polynomial for  $T_m(N, k, \chi)$  will have degree less than 2. Thus the second coefficient will necessarily be 0 for all  $m$  in this case.

So one might instead ask if  $a_2(m, N, k, \chi)$  vanishes only for finitely many  $(m, N, k, \chi)$  when we restrict to the case of  $\dim S_k(\Gamma_0(N), \chi) \geq 2$ . It turns out this is not true either. For example,  $S_2(\Gamma_0(23))$  has dimension 2. And the two Hecke eigenforms for  $S_2(\Gamma_0(23))$  both happen to have 43rd Fourier coefficient vanish [7]. Thus for any  $m$  with exactly one factor of 43, these two eigenforms will both have  $m$ -th Fourier coefficient vanish. So for such  $m$ ,  $T_m(23, 2)$  will have two eigenvalues of 0, and hence will have characteristic polynomial  $x^2$ . This gives an infinite family of vanishing  $a_2$  coefficients.

One could also ask if the result still holds if we allow  $N$  not coprime to  $m$ . In fact, this appears to not be true either. For example, it appears that for  $j \geq 2$ , all the eigenvalues of  $T_3(3^j, 4)$  vanish. This would give an infinite family of  $N$  for which  $a_2(3, N, 4)$  vanishes. One can find many other similar examples.

Next, we make some remarks about Table 5.4, Table 5.6, and [9, Table  $m = 4$ ]. In principle, one could run the same computations for general character  $\chi$  and calculate the finitely many triples  $(N, k, \chi)$  for which  $a_2(m, N, k, \chi)$  vanishes. However, the number of  $(N, k, \chi)$  to check makes this computationally infeasible. Even with only considering trivial character, we used the Clemson University PALMETTO cluster, and it took several hours to check all the possible pairs  $(N, k)$ .

Additionally, observe that many of the entries in these three tables come from  $(N, k)$  for which  $\dim S_k(\Gamma_0(N))$  is 0 or 1 (so the  $a_2$  coefficient trivially vanishes). For  $m = 2$ , 32 out of 35 entries in Table 5.6 come from  $(N, k)$  for which  $\dim S_k(\Gamma_0(N)) = 0$  or 1. All of the remaining 3 nontrivial entries have  $a_2$  coefficient vanish. For  $m = 3$ , 38 out of 52 entries in Table 5.4 come from  $(N, k)$  for which  $\dim S_k(\Gamma_0(N)) = 0$  or 1. Of the remaining 14 nontrivial entries, 7 have positive  $a_2$  coefficient and 7 have vanishing  $a_2$  coefficient. For  $m = 4$ , 32 out of 164 entries in [9, Table  $m = 4$ ] come from  $(N, k)$  for which  $\dim S_k(\Gamma_0(N)) = 0$  or 1. Of the remaining 132 nontrivial entries, 129 have negative  $a_2$  coefficient and 3 have vanishing  $a_2$  coefficient.

Looking at the  $(N, k)$  given in these three tables, one might ask if  $a_2(m, N, k)$  is non-trivially vanishing (i.e. is vanishing when  $\dim S_k(\Gamma_0(N)) \geq 2$ ) only for  $k = 2$ . In fact, this is not true: for  $m = 7, N = 12, k = 4$ ,  $a_2(7, 12, 4) = 0$ . However this is the only counter-example that we could find, and we speculate that it is the only such counter-example.

One might also ask if the  $a_2$  coefficient never non-trivially vanishes in the level one case. In fact, a more general result was conjectured in [2].

**Conjecture 7.1** ([2, Conjecture 5.1]). *Let  $m \geq 1$ ,  $k \geq 2$  be even, and  $n := \dim S_k(\Gamma_0(1))$ . Write the characteristic polynomial for  $T_m(1, k)$  as*

$$T_m(1, k)(x) = x^n - a_1(m, 1, k)x^{n-1} + a_2(m, 1, k)x^{n-2} - \dots + (-1)^n a_n(m, 1, k).$$

*Then  $a_i(m, 1, k) \neq 0$  for  $1 \leq i \leq n$ .*

## REFERENCES

- [1] Liubomir Chiriac, Daphne Kurzenhauser, and Eric Williams. The nonvanishing of the trace of T3. *Involve*, 17(2):263–272, 2024.
- [2] Archer Clayton, Helen Dai, Tianyu Ni, Hui Xue, and Jake Zummo. Nonvanishing of second coefficients of Hecke polynomials. *J. Number Theory*, 262:186–221, 2024.
- [3] Henri Cohen and Fredrik Strömberg. *Modular forms: A classical approach*, volume 179 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI, 2017.
- [4] Graham Everest, Alf van der Poorten, Igor Shparlinski, and Thomas Ward. *Recurrence sequences*, volume 104 of *Mathematical Surveys and Monographs*. American Mathematical Society, Providence, RI, 2003.
- [5] Andrew Knightly and Charles Li. *Traces of Hecke operators*, volume 133 of *Mathematical Surveys and Monographs*. American Mathematical Society, Providence, RI, 2006.
- [6] D. H. Lehmer. The vanishing of Ramanujan’s function  $\tau(n)$ . *Duke Math. J.*, 14:429–433, 1947.

- [7] The LMFDB Collaboration. The L-functions and modular forms database. Home page of the newform 23.2.a.a. <https://www.lmfdb.org/ModularForm/GL2/Q/holomorphic/23/2/a/a/>, 2024. [Online; accessed 17 May 2024].
- [8] OEIS Foundation Inc. The On-Line Encyclopedia of Integer Sequences, 2024. Published electronically at <http://oeis.org>.
- [9] Erick Ross. Nonvanishing  $a_2$  coefficient. <https://github.com/eross156/nonvanishing-a2-coefficient>, 2024.
- [10] Jeremy Rouse. Vanishing and non-vanishing of traces of Hecke operators. *Trans. Amer. Math. Soc.*, 358(10):4637–4651, 2006.
- [11] Jean-Pierre Serre. Répartition asymptotique des valeurs propres de l'opérateur de Hecke  $T_p$ . *J. Amer. Math. Soc.*, 10(1):75–102, 1997.

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