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EXPLICIT BOUNDS FOR SUMS OF SQUARES

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Abstract. For an even integer k, let $r_{2k}(n)$ be the number of representations of n as a sum of $2k$ squares. The quantity $r_{2k}(n)$ is approximated by the classical singular series $\rho_{2k}(n) \asymp n^{k-1}$. Deligne's bound on the Fourier coefficients of Hecke eigenforms gives that $r_{2k}(n) = \rho_{2k}(n) + O(d(n)n^{\frac{k-1}{2}})$. We determine the optimal implied constant in this estimate provided that either $k/2$ or n is odd. The proof requires a delicate positivity argument involving Petersson inner products.

1. Introduction and statement of results

In Hardy's book on Ramanujan [1], he states the following (Chapter 9, p. 132).

> The problem of the representations of an integer n as the sum of a given number k of integral squares is one of the most celebrated in the theory of numbers. Its history may be traced back to Diophantus, but begins effectively with Girard's (or Fermat's) theorem that a prime $4m + 1$ is the sum of two squares. Almost every arithmetician of note since Fermat has contributed to the solution of the problem, and it has its puzzles for us still.

If n is a non-negative integer, let

$$r_s(n) = \#\{(x_1, x_2, \ldots, x_s) \in \mathbb{Z}^s : x_1^2 + x_2^2 + \cdots + x_s^2 = n\}$$

be the number of representations of n as a sum of s squares.

The classical work that Hardy refers to includes the results of Jacobi giving the following exact formulae. Let n be a positive integer and write $n = 2^\alpha m$, where m is odd. Then

$$r_4(n) = \begin{cases} 8\sigma_1(m), & \text{if } \alpha = 0, \\ 24\sigma_1(m), & \text{if } \alpha \geq 1, \end{cases} \qquad r_8(n) = \begin{cases} 16\sigma_3(m), & \text{if } \alpha = 0, \\ 16 \cdot \dfrac{2^{3\alpha+3} - 15}{7}\sigma_3(m), & \text{if } \alpha \geq 1. \end{cases}$$

The search for higher exact formulae (each involving more complicated arithmetic functions) for was carried out by many mathematicians. Glaisher [2] and Rankin [3] were interested in these formulae where the arithmetic functions involved were multiplicative.

In a different direction, Hardy [4] and Mordell [5] applied the circle method to give an approximation

$$r_s(n) = \rho_s(n) + R_s(n)$$

where $\rho_s(n)$ is the "singular series" and $R_s(n)$ is an error term. Here $\rho_s(n)$ can be expressed as a divisor sum if s is even, and $\rho_s(n) \asymp n^{\frac{s}{2}-1}$ provided $s > 4$. The

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contribution $R_s(n)$ is more mysterious, and Deligne's proof of the Weil conjectures (see [6]) implies an estimate of the form

$$R_s(n) = O(d(n)n^{\frac{s}{4}-\frac{1}{2}}) \tag{1.1}$$

provided s is even. The phenomena of exact formulae for $r_s(n)$ of the form $r_s(n) = \rho_s(n)$ only occurs for small s. In [7], Rankin shows that $R_s(n)$ is identically zero if and only if $s \leq 8$. Exact formulae of a different nature were given by Milne in [8] when $s = 4n^2$ and $s = 4n(n+1)$.

The problem we study is the implied constant in equation (1.1) above. This is a natural question, and in [9–11], the author has studied the corresponding problem for powers of the Δ function, p-core partitions (joint work with Byungchan Kim), and arbitrary level 1 cusp forms (joint work with Paul Jenkins), respectively. To prove their now famous "290-theorem" Bhargava and Hanke [12] compute this implied constant for about 6000 quadratic forms in four variables and use this to determine precisely which integers these forms represent.

Returning to our problem, if $s = 2k$ and k is even, we have that

$$\begin{aligned}\rho_{2k}(n) \\ &= \frac{2k(-1)^{k/2+1}}{(2^k-1)B_k}\Big(\sigma_{k-1}(n) + (-1+(-1)^{k/2+1})\sigma_{k-1}(n/2) + (-1)^{k/2}2^k\sigma_{k-1}(n/4)\Big),\end{aligned}$$

where B_k is the kth Bernoulli number and $\sigma_{k-1}(n)$ is the sum of the $(k-1)$st powers of the positive integer divisors of n (and is hence zero if n is not an integer). Our main result is the following.

Theorem 1.1. *Suppose that k is even. If either $k/2$ is odd or n is odd, then we have*

$$|r_{2k}(n) - \rho_{2k}(n)| \leq \left(4k + \frac{2k(-1)^{k/2}}{(2^k-1)B_k}\right) d(n)n^{\frac{k-1}{2}}.$$

Remark 1.1. If $2k = 4$ or $2k = 8$, the right hand side is zero, and we recover the exact formulae of Jacobi. For arbitrary even k, we have $r_{2k}(1) = 4k$ and $\rho_{2k}(1) = \frac{2k(-1)^{k/2+1}}{(2^k-1)B_k}$. Thus, the inequality above becomes an equality when $n = 1$. This shows that the implied constant

$$4k + \frac{2k(-1)^{k/2}}{(2^k-1)B_k}$$

in (1.1) is best possible. The error term is smaller than the main term provided $n \gg k^2$.

Our approach to proving Theorem 1.1 is as follows. If

$$\theta(z) = 1 + 2\sum_{n=1}^{\infty} q^{n^2}, \quad q = \mathrm{e}^{2\pi \mathrm{i} z}$$

is the classical Jacobi theta function, then

$$\theta^{2k}(z) = \sum_{n=0}^{\infty} r_{2k}(n)q^n$$

is a modular form of weight k on $\Gamma_0(4)$. If k is even, we can decompose

(1.2)
$$\theta^{2k}(z) = a_1 E_k(z) + a_2 E_k(2z) + a_3 E_k(4z) + \sum_i c_i g_i(z) + \sum_i d_i g_i(2z) + \sum_i e_i g_i(4z)$$

where
$$E_k(z) = 1 - \frac{2k}{B_k} \sum_{n=1}^{\infty} \sigma_{k-1}(n) q^n$$
is the classical level 1 Eisenstein series, and the $g_i(z)$ are normalized newforms of level 1, 2 or 4. We prove the following.

Theorem 1.2. *Assume the notation above. Then for all i, $c_i \geq 0$.*

Theorem 1.2 allows us to read off
$$\sum_i |c_i| = \sum_i c_i = 4k + \frac{2k(-1)^{k/2}}{(2^k - 1)B_k}$$
from the coefficient of q on both sides of (1.2), using that $a_1 = \frac{(-1)^{k/2}}{(2^k-1)B_k}$.

To prove Theorem 1.2 we use properties of the Petersson inner product on $M_k(\Gamma_0(4))$ (see Section 2 for precise definitions). If $g_i(z)$ is a newform of level 4, then $g_i(z)$ is orthogonal to every other term in the expansion (1.2). It follows that
$$\langle \theta^{2k}, g_i \rangle = c_i \langle g_i, g_i \rangle.$$
It suffices to prove that $\langle \theta^{2k}, g_i \rangle \geq 0$. This Petersson inner product consists of a contribution from each of the three cusps of $\Gamma_0(4)$: ∞, 0 and 1/2. The contribution from ∞ is
$$\frac{2}{(4\pi)^k} \sum_{n=1}^{\infty} \frac{r_{2k}(n) a(n)}{n^{k-1}} \int_{4\pi n}^{\infty} u^{k-2} \mathrm{e}^{-u}\, du.$$
Here $g_i(z) = \sum_{n=1}^{\infty} a(n) q^n$. Our approach is to show that the main term in the above sum comes from $n = 1$. If n is fixed, $r_{2k}(n)$ is a polynomial of degree $2k$ in n. We compute these polynomials explicitly, and use this to the bound the terms when $2 \leq n \leq 2500$. Next, we use a simple induction bound on $r_{2k}(n)$ to show that the terms with $2500 \leq n \leq \frac{k}{2\pi} \log(k)$ are small enough. Finally, we use the exponential decay of $\int_{4\pi n}^{\infty} u^{k-2} \mathrm{e}^{-u}\, du$ when $n \geq \frac{k}{2\pi} \log(k)$.

The cusp at zero behaves in an essentially identical way to the cusp at ∞, and the contribution from the cusp at 1/2 is very small, since $\theta(z)$ vanishes there.

Remark 1.2. This result can be thought of as a refined form of the circle method. The Eisenstein series is the contribution of the major arcs, while Deligne's result, and the bounds we give on the constants c_i can be thought of as explicit, uniform minor arc estimates. Further, it is plausible that the Fourier coefficients of distinct newforms are independent (an assertion that could be justified under the assumption of the holomorphy of certain Rankin–Selberg convolutions). This combined with the recent proof of the Sato–Tate conjecture (see [13]) suggests that for any $\epsilon > 0$, there are infinitely many primes p so that
$$|r_{2k}(p) - \rho_{2k}(p)| > \left(4k + \frac{2k(-1)^{k/2}}{(2^k - 1)B_k} - \epsilon\right) d(p) p^{\frac{k-1}{2}}.$$

Remark 1.3. The proof gives more detailed information about the constants c_i in (1.2). In particular, if $g_i(z)$ is a newform of level 4 and $k \equiv 2 \pmod 4$, then

$$c_i = 16k \cdot \frac{(k-2)!}{(4\pi)^k \langle g_i, g_i \rangle}(1 + O(\alpha^k)),$$

where $\alpha \approx 0.918$. If $k \equiv 0 \pmod 4$, then $c_i = 0$. Similar, but more complicated results are true for the constants c_i associated with levels 1 and 2 newforms.

An outline of the paper is as follows. In Section 2, we give precise definitions and review necessary background information. In Section 3, we prove a number of auxiliary results that will be used in the proof of Theorem 1.2. In Section 4, we prove Theorem 1.2 and use this to deduce Theorem 1.1. Finally in Section 5, we address other values of k and n.

2. Background

In this section, we give definitions and review necessary background. For $N \geq 1$, let $M_k(\Gamma_0(N))$ denote the $\mathbb{C}$-vector space of modular forms of weight k on $\Gamma_0(N) := \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}_2(\mathbb{Z}) : N | c \right\}$. Let $S_k(\Gamma_0(N))$ denote the subspace of cusp forms.

If f is a modular form of weight k, and $\alpha = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \in \mathrm{GL}_2(\mathbb{Q})$ and has positive determinant, define the usual slash operator by

$$f|\alpha = (ad - bc)^{k/2}(cz + d)^{-k} f\left(\frac{az + b}{cz + d}\right).$$

For a positive integer d, define the operator $V(d)$ by $f(z)|V(d) = f(dz)$. It is well-known (see [14], p. 107 for a proof) that $V(d)$ maps $M_k(\Gamma_0(N))$ to $M_k(\Gamma_0(dN))$ and $S_k(\Gamma_0(N))$ to $S_k(\Gamma_0(dN))$. For a positive integer d, define the operator $U(d)$ by

$$\sum_{n=0}^{\infty} a(n)q^n | U(d) = \sum_{n=0}^{\infty} a(dn)q^n.$$

If $d|N$, then $U(d)$ maps $M_k(\Gamma_0(N))$ to itself and $S_k(\Gamma_0(N))$ to itself. If p is a prime with $p \nmid N$, define the usual Hecke operator $T(p)$ by $T(p) = U(p) + p^{k-1}V(p)$.

If $f, g \in M_k(\Gamma_0(N))$ and at least one of f or g is a cusp form, let

$$\langle f, g \rangle = \frac{3}{\pi[\mathrm{SL}_2(\mathbb{Z}) : \Gamma_0(N)]} \iint_{\mathbb{H}/\Gamma_0(N)} f(x + iy)\overline{g(x + iy)} y^k \, \frac{dx\, dy}{y^2}$$

denote the usual Petersson inner product. If $p \nmid N$, then the Hecke operators $T(p)$, acting on $S_k(\Gamma_0(N))$, are self-adjoint with respect to the Petersson inner product. Moreover, if $\alpha \in \mathrm{GL}_2(\mathbb{Q})$ and has positive determinant, then $\langle f|\alpha, g|\alpha \rangle = \langle f, g \rangle$.

Let $S_k^{\mathrm{new}}(\Gamma_0(N))$ denote the orthogonal complement under this inner product of the space spanned by all forms

$$f(z)|V(d), \text{ where } f(z) \in S_k(\Gamma_0(M)),$$

and we have $M|N$, $M < N$, and d is a divisor of N/M. A *newform* of level N is a form

$$f(z) = \sum_{n=1}^{\infty} a(n)q^n \in S_k^{\mathrm{new}}(\Gamma_0(N))$$

that is a simultaneous eigenform of the Hecke operators $T(p)$, normalized so that $a(1) = 1$. We have the Deligne bound

$$|a(n)| \leq d(n)n^{\frac{k-1}{2}},$$

where $d(n)$ is the number of divisors of n (for a detailed proof of this inequality, see the new book by Brian Conrad [15]). A newform $f(z)$ of level N is also an eigenform of the Atkin–Lehner operator $W_N = \begin{bmatrix} 0 & -1 \\ N & 0 \end{bmatrix}$. This operator commutes with the Hecke operators $T(p)$ for primes $p \nmid N$. One has more information about the coefficient $a(p)$ if $p|N$. If $N = p$, then $a(p) = -\lambda p^{\frac{k}{2}-1}$, where λ is the eigenvalue of f under W_N. If $p^2|N$, then $a(p) = 0$ (see [16], Theorem 3).

The multiplicity-one theorem states that the joint eigenspaces of all $T(p)$ (with $p \nmid N$) in $S_k^{\text{new}}(\Gamma_0(N))$ are one-dimensional. It follows from this, and the self-adjointness of the Hecke operators, that if f_1 and f_2 are two distinct newforms, then $\langle f_1, f_2 \rangle = 0$. It is known (see Section 5.11 of [17]) that the Eisenstein series $E_k(z)$ (and $E_k(z)|V(d)$) are orthogonal to cusp forms under the Petersson inner product.

Finally, let $\eta(z)$ denote as usual the Dedekind eta function

$$\eta(z) = q^{1/24} \prod_{n=1}^{\infty} (1 - q^n), \quad q = \mathrm{e}^{2\pi \mathrm{i} z}.$$

We have the following well-known identities:

$$\begin{aligned} \theta(z) &= \frac{\eta^5(2z)}{\eta^2(z)\eta^2(4z)}, \\ \frac{\eta^8(4z)}{\eta^4(2z)} &= \sum_{n=0}^{\infty} \sigma(2n+1) q^{2n+1}, \\ (2z+1)^{-2}\theta^4\left(\frac{z}{2z+1}\right) &= 16\frac{\eta^8(4z)}{\eta^4(2z)} \end{aligned}$$

(see the exercises on page 145 of [18], solutions are on p. 234).

3. Preliminary results

In this section, we prove three lemmas that will be used in the proof of the main results. Our first lemma proves some simple bounds on $r_s(n)$.

Lemma 3.1. (1) *Suppose that n is a non-negative integer. There are non-negative constants $c_{i,n}$ $(0 \leq i \leq n)$ so that*

$$r_s(n) = \sum_{i=0}^{n} c_{i,n} \binom{s}{i}, \textit{ for all } s \geq 0.$$

(2) *If n is fixed, $\frac{r_{2s}(n)}{n^{\frac{s-1}{2}}}$ is a decreasing function of s, provided $2s \geq n + \frac{n}{\sqrt[4]{n}-1}$.*

(3) *If n is a positive integer and $s \geq 6$, then*

$$r_s(n) \leq \frac{3(4.11)^s}{25\sqrt{s!}}(n+s)^{\frac{s}{2}-1}.$$

Proof. We prove the first statement by strong induction on n. For $n = 0$, we have $r_s(0) = 1 = 1 \cdot \binom{s}{0}$. Thus, $c_{0,0} = 1$ and the result holds.

Assume the result is true for all $m < n$. Let t be a positive integer with $t \leq s$. Then

$$r_t(n) - r_{t-1}(n) = 2 \sum_{r=1}^{\lfloor \sqrt{n} \rfloor} r_{t-1}(n - r^2)$$
$$= 2 \sum_{r=1}^{\lfloor \sqrt{n} \rfloor} \sum_{i=0}^{n-r^2} c_{i,n-r^2} \binom{t-1}{i}.$$

Summing both sides over all t, $1 \leq t \leq s$ and using that $\sum_{t=1}^{s} \binom{t-1}{i} = \binom{s}{i+1}$ gives

$$r_s(n) = \sum_{r=1}^{\lfloor \sqrt{n} \rfloor} \sum_{i=0}^{n-r^2} 2c_{i,n-r^2} \binom{s}{i+1}$$
$$= 2 \sum_{i=1}^{n} \left(\sum_{r=1}^{\lfloor \sqrt{n-i} \rfloor} c_{i-1,n-r^2} \right) \binom{s}{i}.$$

Since the $c_{i-1,n-r^2}$ are non-negative, by the induction hypothesis, it follows that their sum is non-negative, and this proves that the result is true for n.

To prove the second statement, it suffices to prove that each term in the expression

$$\frac{r_{2s}(n)}{n^{\frac{s-1}{2}}} = \sum_{i=0}^{n} c_{i,n} \frac{\binom{2s}{i}}{n^{\frac{s-1}{2}}}$$

is a decreasing function of s. Let $f(s) = \binom{2s}{i} \cdot n^{(1-s)/2}$. Then,

$$\frac{f(s+1)}{f(s)} = \frac{1}{\sqrt{n}} \cdot \frac{(2s+2)(2s+1)}{(2s+2-i)(2s+1-i)}$$
$$\leq \frac{1}{\sqrt{n}} \frac{(2s+2)(2s+1)}{(2s+2-n)(2s+1-n)}$$
$$< \frac{1}{\sqrt{n}} \left(1 + \frac{n}{2s-n} \right)^2.$$

This is a decreasing function of s, and if we take $s = n + \frac{n}{\sqrt[4]{n}-1}$, then $2s - n = \frac{n}{\sqrt[4]{n}-1}$ and so

$$\frac{1}{\sqrt{n}} \left(1 + \frac{n}{2s-n} \right)^2 = \frac{1}{\sqrt{n}} \left(1 + (\sqrt[4]{n} - 1) \right)^2 = 1.$$

This proves that $f(s+1) < f(s)$, as desired.

We prove the third statement by induction on s. Our base case is $s = 6$ and in this case, we use the exact formula:

$$r_6(n) = \sum_{d \mid n} d^2 \left(-4\chi_{-1}(d) + 16\chi_{-1}(n/d) \right),$$

where

$$\chi_{-1}(n) = \begin{cases} 1, & \text{if } n \equiv 1 \pmod 4, \\ -1, & \text{if } n \equiv 3 \pmod 4, \\ 0, & \text{if } n \text{ is even.} \end{cases}$$

We rewrite this as

$$r_6(n) = n^2 \sum_{d|n} \frac{16\chi_{-1}(n/d) - 4\chi_{-1}(d)}{(n/d)^2}.$$

If n is even, then $r_6(n)/n^2 \leq 8\zeta(2) \leq 13.2$. On the other hand if n is odd, then $16\chi_{-1}(n/d) - 4\chi_{-1}(d)$ is negative if $n/d \equiv 3 \pmod 4$ and $16\chi_{-1}(n/d) - 4\chi_{-1}(d) \leq 20$ if $n/d \equiv 1 \pmod 4$. Thus,

$$\frac{r_6(n)}{n^2} \leq 20 \sum_{\substack{d|n \\ d \equiv 1 \pmod 4}} \frac{1}{d^2} \leq 20 \sum_{n=0}^{\infty} \frac{1}{(4n+1)^2}.$$

One can show that the right-hand side above is about $21.4966613 \leq \frac{6449}{300}$. We denote by C_s a constant so that $r_s(n) \leq C_s(n+s)^{\frac{s}{2}-1}$, and we take $C_6 = \frac{6449}{300}$. This proves the base case.

Assume now that $s \geq 6$. We have

$$\begin{aligned} r_{s+1}(n) &= r_s(n) + 2\sum_{m=1}^{\lfloor \sqrt{n} \rfloor} r_s(n - m^2) \\ &\leq C_s(n+s)^{\frac{s}{2}-1} + 2C_s \sum_{m=1}^{\lfloor \sqrt{n} \rfloor} (n + s - m^2)^{\frac{s}{2}-1} \\ &\leq C_s(n+s)^{\frac{s}{2}-1} + 2C_s \int_0^{\sqrt{n+s+1}} (n+s+1-x^2)^{\frac{s}{2}-1}\, dx \\ &\leq C_s(n+s)^{\frac{s}{2}-1} + 2C_s(n+s+1)^{\frac{s+1}{2}-1} \int_0^1 (1-u^2)^{\frac{s}{2}-1}\, du. \end{aligned}$$

We have

$$(1-u^2)^{\frac{s}{2}-1} = \mathrm{e}^{\left(\frac{s}{2}-1\right)\log(1-u^2)} \leq \mathrm{e}^{-(s/2-1)u^2}.$$

Thus

$$2\int_0^1 (1-u^2)^{\frac{s}{2}-1}\, du \leq 2\int_0^{\infty} \mathrm{e}^{-(s/2-1)u^2}\, du = \sqrt{\frac{\pi}{\frac{s}{2}-1}}$$

and

$$\begin{aligned} r_{s+1}(n) &\leq C_s(n+s)^{\frac{s}{2}-1} + C_s(n+s+1)^{\frac{s+1}{2}-1} \left[\sqrt{\frac{2\pi}{s-2}}\right] \\ &\leq C_s(n+s+1)^{\frac{s+1}{2}-1} \left[\sqrt{\frac{2\pi}{s-2}} + \frac{(n+s)^{(s/2)-1}}{(n+s+1)^{\frac{s+1}{2}-1}}\right]. \end{aligned}$$

Note that the second term inside the brackets above is a decreasing function of n and is relevant only for $n \geq 1$. It follows that

$$r_{s+1}(n) \leq C_s(n+s+1)^{\frac{s+1}{2}-1} \cdot \frac{1}{\sqrt{s+1}} \left[\sqrt{2\pi}\sqrt{\frac{s+1}{s-2}} + \left(\frac{s+1}{s+2}\right)^{s/2-1} \right]$$
$$\leq \frac{C_s \cdot 4.11}{\sqrt{s+1}}(n+s+1)^{\frac{s+1}{2}-1}.$$

Hence, we may take $C_{s+1} = \frac{4.11}{\sqrt{s+1}} C_s$ and so

$$C_s = \frac{6449}{300} \cdot \frac{4.11^{s-6}}{\sqrt{s!/6!}} \leq \frac{3(4.11)^s}{25\sqrt{s!}}.$$

□

Next, we use Deligne's bound on the Fourier coefficients of a newform to bound its value.

Lemma 3.2. *Suppose that $k \geq 7$, $y \geq \frac{1}{2\pi}$, and $g(z) = \sum_{n=1}^{\infty} a(n)q^n$ with $|a(n)| \leq d(n)n^{\frac{k-1}{2}}$. Then*

$$|g(x+\mathrm{i}y)| \leq \frac{1}{(2\pi y)^{\frac{k+1}{2}}}\Gamma\left(\frac{k+1}{2}\right)\left[\log\left(\frac{k+1}{2}\right)+\gamma+1\right],$$

where γ is Euler's constant.

Proof. Since the nth Fourier coefficient of $g(z)$ is bounded by $d(n)n^{\frac{k-1}{2}}$, we have that

$$|g(x+\mathrm{i}y)| \leq \sum_{n=1}^{\infty} d(n)n^{\frac{k-1}{2}}\mathrm{e}^{-2\pi n y}.$$

If $D(x) = \sum_{n \leq x} d(n)$, then $D(x) \leq x\log(x) + \gamma x + 1 \leq x\log(x) + (\gamma+1)x$. By partial summation, we have

$$\sum_{n=1}^{\infty} d(n)n^{\frac{k-1}{2}}\mathrm{e}^{-2\pi n y} = \int_1^{\infty} D(x)\left[2\pi y x^{\frac{k-1}{2}} - \left(\frac{k-1}{2}\right)x^{\frac{k-3}{2}}\right]\mathrm{e}^{-2\pi x y}\,dx$$
$$\leq 2\pi y \int_{\frac{k-1}{4\pi y}}^{\infty} (\log(x) + (\gamma+1))x^{\frac{k+1}{2}}\mathrm{e}^{-2\pi x y}\,dx.$$

Now, we set $u = 2\pi x y$, $du = 2\pi y\,dx$. We get

$$2\pi y \int_{\frac{k-1}{2}}^{\infty}\left(\log\left(\frac{u}{2\pi y}\right) + (\gamma+1)\right)\left(\frac{u}{2\pi y}\right)^{\frac{k+1}{2}}\mathrm{e}^{-u}\,\frac{du}{2\pi y}$$
$$= \frac{1}{(2\pi y)^{\frac{k+1}{2}}}\int_{\frac{k-1}{2}}^{\infty}(\log(u) - \log(2\pi y) + \gamma + 1)\,u^{\frac{k+1}{2}}\mathrm{e}^{-u}\,du.$$

Since $y \geq \frac{1}{2\pi}$, $\log(2\pi y) > 0$ and so we neglect the term involving it. We get

$$\frac{1}{(2\pi y)^{\frac{k+1}{2}}}\left[\int_{\frac{k-1}{2}}^{\infty}\log(u)u^{\frac{k+1}{2}}\mathrm{e}^{-u}\,du + (\gamma+1)\int_{\frac{k-1}{2}}^{\infty}u^{\frac{k+1}{2}}\mathrm{e}^{-u}\,du\right].$$

If we extend the integrals down to zero, then the negative contribution of $\int_0^1 \log(u)$ $u^{\frac{k+1}{2}} \mathrm{e}^{-u}\,du$ is cancelled by that of $[1.5, 2]$ for $k \geq 7$. Thus, we get the bound

$$|g(z)| \leq \frac{1}{(2\pi y)^{\frac{k+1}{2}}} \Gamma\left(\frac{k+1}{2}\right)\left[\psi\left(\frac{k+1}{2}\right) + \gamma + 1\right],$$

where $\Gamma'(z) = \int_0^\infty \log(u) u^{z-1} \mathrm{e}^{-u}\,du$ and $\psi(z) = \frac{\Gamma'(z)}{\Gamma(z)}$. The formula (see equation 6.3.21 on p. 258 of [19])

$$\psi(z) = \log(z) - \frac{1}{2z} - \int_0^\infty \frac{2t\,dt}{(z^2+t^2)(\mathrm{e}^{2\pi t}-1)}$$

shows that $\psi(z) \leq \log(z)$. Thus, we obtain the bound

$$\frac{1}{(2\pi y)^{\frac{k+1}{2}}} \Gamma\left(\frac{k+1}{2}\right)\left[\log\left(\frac{k+1}{2}\right) + \gamma + 1\right].$$

□

Finally, we will need to understand Petersson inner products of newforms f with their images under $V(d)$. This is the subject of the next result.

Lemma 3.3. *Suppose that $f(z) = \sum_{n=1}^{\infty} a(n)q^n \in S_k^{\mathrm{new}}(\Gamma_0(N))$ is a newform. If $p \nmid N$, then*

$$\langle f, f|V(p)\rangle = \frac{a(p)}{p^{k-1}(p+1)}\langle f, f\rangle.$$

Note that the assumption that f has trivial character implies that the Fourier coefficients of f are real. This fact will be used frequently in what follows.

Proof. Rankin proved in [20] that if $f = \sum a(n)q^n$ and $g = \sum b(n)q^n$ are cusp forms of weight k, then

$$\sum_{n \leq x} \frac{a(n)\overline{b(n)}}{n^{k-1}} = \frac{(4\pi)^k}{(k-1)!}\langle f, g\rangle x + O(x^{3/5}).$$

We will use this formula to prove the results above. We start by letting $c = \frac{(4\pi)^k}{(k-1)!}$, and p be a prime number with $p \nmid N$. Then,

$$\begin{aligned}
\langle f, f|V(p)\rangle &= \lim_{x\to\infty} \frac{1}{c}\cdot\frac{1}{x}\sum_{n\leq x} \frac{a(n)a(n/p)}{n^{k-1}} \\
&= \lim_{x\to\infty} \frac{1}{c}\cdot\frac{1}{x}\sum_{pn\leq x} \frac{a(pn)a(n)}{(pn)^{k-1}} \\
&= \lim_{x\to\infty} \frac{1}{c}\cdot\frac{1}{p^k}\cdot\frac{1}{\frac{x}{p}}\sum_{n\leq \frac{x}{p}} \frac{a(pn)a(n)}{n^{k-1}} \\
&= \frac{1}{p^k}\langle f, f|U(p)\rangle.
\end{aligned}$$

Now, $a(p)f = f|T(p) = f|U(p) + p^{k-1}f|V(p)$. It follows that

$$\begin{aligned} a(p)\langle f, f\rangle &= \langle f, f|T(p)\rangle = \langle f, f|U(p)\rangle + p^{k-1}\langle f, f|V(p)\rangle \\ &= p^k\langle f, f|V(p)\rangle + p^{k-1}\langle f, f|V(p)\rangle \\ &= p^{k-1}(p+1)\langle f, f|V(p)\rangle. \end{aligned}$$

Thus,

$$\langle f, f|V(p)\rangle = \frac{a(p)}{p^{k-1}(p+1)}\langle f, f\rangle.$$

□

4. Proof of Theorems 1.1 and 1.2

In this section, we will prove the main results. We will first prove Theorem 1.2 and then deduce Theorem 1.1 from it.

Proof of Theorem 1.2. First, for each newform g of level 1, 2 or 4, we will find a form $\tilde{g}$ with the property that the coefficient of g in the representation of θ^{2k} is positive if and only if $\langle \theta^{2k}, \tilde{g}\rangle > 0$. Each $\tilde{g}$ will be an eigenform of T_p for all odd primes p, and will also be an eigenform of W_4 with the same eigenvalue as that of θ^{2k}.

Recall the decomposition

$$\theta^{2k}(z) = a_1E_k(z) + a_2E_k(2z) + a_3E_k(4z) + \sum_i c_ig_i(z) + \sum_i d_ig_i(2z) + \sum_i e_ig_i(4z),$$

where the g_i are newforms of levels 1, 2 or 4, and the $c_i, d_i, e_i \in \mathbb{R}$. If V is an eigenspace for all T_n (with n odd), then V is also stable under W_4. Since $\theta^{2k}|W_4 = (-1)^{\frac{k}{2}}\theta^{2k}$, it follows that the projection of θ^{2k} onto V must also have eigenvalue $(-1)^{\frac{k}{2}}$ under W_4.

If V is an eigenspace coming from a newform g_i of level 4, then $\dim V = 1$. If $c_i \neq 0$, then $g_i|W_4 = (-1)^{\frac{k}{2}}$. In this case, we have $\langle \theta^{2k}, g\rangle = \langle c_ig_i, g_i\rangle = c_i\langle g_i, g_i\rangle$ and thus $c_i > 0$ if and only if $\langle \theta^{2k}, g_i\rangle > 0$, and so we set $\tilde{g}_i = g_i$. Part (i) of Theorem 7 of [16] shows that for any newform of level 4, $g_i|W_4 = -g_i$, and hence $c_i = 0$, if $k \equiv 0 \pmod 4$.

If V is an eigenspace coming from a newform g_i of level 2, then $\dim V = 2$. This vector space decomposes into one-dimensional plus and minus eigenspaces under the action of W_4. It follows that the projection of θ^{2k} onto V is $c_i(g_i + (-2)^{\frac{k}{2}}\lambda g_i|V(2))$, where λ is the Atkin–Lehner eigenvalue of g_i. Thus, we set $\tilde{g}_i = g_i + (-2)^{\frac{k}{2}}\lambda g_i|V(2)$. This form will be orthogonal to any element in the opposite W_4 eigenspace, since W_4 is an isometry with respect to the Petersson inner product. It follows that $c_i > 0$ if and only if $\langle \theta^{2k}, \tilde{g}_i\rangle > 0$.

If V is an eigenspace coming from a newform g_i of level 1, then $\dim V = 3$ and

$$\begin{aligned} g_i|W_4 &= 2^kg_i|V(4), \\ g_i|V(2)|W_4 &= g_i|V(2), \\ g_i|V(4)|W_4 &= 2^{-k}g_i. \end{aligned}$$

We have that $V = V^+ \oplus V^-$, where V^+ and V^- are the plus and minus eigenspaces for W_4. Then $\dim V^+ = 2$ and it is spanned by $g_i + 2^kg_i|V(4)$ and $g_i|V(2)$. Also $\dim V^- = 1$ and it is spanned by $g_i - 2^kg_i|V(4)$. If $k \equiv 0 \pmod 4$, then the Atkin–Lehner sign is $+1$. If $k \equiv 2 \pmod 4$, the Atkin–Lehner sign is -1.

When $k \equiv 2 \pmod 4$, we set $\tilde{g}_i = g_i - 2^k g_i|V(4)$. This form satisfies $\tilde{g}_i|W_4 = -\tilde{g}_i$, and is again orthogonal to the form spanning the plus eigenspace for W_4.

When $k \equiv 0 \pmod 4$, we set $\tilde{g}_i = g_i - \frac{4}{3}a(2)g_i|V(2) + 2^k g_i|V(4)$. This form satisfies $\tilde{g}_i|W_4 = \tilde{g}_i$, and is hence orthogonal to $g_i - 2^k g_i|V(4)$. By Lemma 3.3 it is orthogonal to $g_i|V(2)$.

We have

$$\begin{aligned}\langle \theta^{2k}, \tilde{g}_i \rangle &= \frac{1}{2\pi} \iint_{\mathbb{H}/\Gamma_0(4)} \theta^{2k}(z)\overline{\tilde{g}_i(z)} y^k \, \frac{dx\,dy}{y^2} \\ &= \frac{1}{2\pi} \sum_{j=1}^{6} \int_{-1/2}^{1/2} \int_{\sqrt{1-x^2}}^{\infty} \left(\theta^{2k}|_k\gamma_j\right)(x+\mathrm{i}y)\overline{\tilde{g}_i|_k\gamma_j(x+\mathrm{i}y)} y^{k-2}\, dy\, dx.\end{aligned}$$

Here, the matrices

$$\gamma_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \gamma_2 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad \gamma_3 = \begin{bmatrix} 0 & -1 \\ 1 & 1 \end{bmatrix},$$
$$\gamma_4 = \begin{bmatrix} 0 & -1 \\ 1 & 2 \end{bmatrix}, \quad \gamma_5 = \begin{bmatrix} 0 & -1 \\ 1 & 3 \end{bmatrix}, \quad \gamma_6 = \begin{bmatrix} 1 & 0 \\ 2 & 1 \end{bmatrix}$$

are a set of representatives for the right cosets of $\Gamma_0(4)$ in $\mathrm{SL}_2(\mathbb{Z})$.

Term 1. This is the contribution from the cusp at infinity. In particular, it is the $j=1$ term in the above sum. We split this term into two parts: $\{x+\mathrm{i}y : -1/2 \le x \le 1/2, y \ge 1\}$, and $\{x + \mathrm{i}y : -1/2 \le x \le 1/2, \sqrt{1-x^2} \le y \le 1\}$.

Write

$$\tilde{g}_i(z) = \sum_{n=1}^{\infty} a(n) q^n.$$

Applying the Deligne bound to each of the various possible forms of $\tilde{g}_i$, we see that in all cases $|a(n)| \le \frac{17}{3} d(n) n^{\frac{k-1}{2}}$.

The first part is

$$\frac{1}{2\pi} \int_1^{\infty} \int_{-1/2}^{1/2} \left(\sum_{m=0}^{\infty} r_{2k}(m)\, \mathrm{e}^{-2\pi m y}\, \mathrm{e}^{2\pi i m x} \right) \left(\sum_{n=1}^{\infty} \overline{a(n)}\, \mathrm{e}^{-2\pi n y} \mathrm{e}^{-2\pi \mathrm{i} n x} \right) y^{k-2}\, dx\, dy.$$

Since the Fourier series representations converge uniformly on compact subsets of these regions, we can invert the summations and the integrals and obtain

$$\frac{1}{2\pi} \sum_{m=0}^{\infty} \sum_{n=1}^{\infty} r_{2k}(m)\overline{a(n)} \int_{-1/2}^{1/2} \int_1^{\infty} y^{k-2} \mathrm{e}^{-2\pi(m+n)y} \mathrm{e}^{2\pi i(m-n)x}\, dy\, dx.$$

The integral over $-1/2 \le x \le 1/2$ is zero unless $m = n$, in which case it is 1. We set $u = 4\pi n y$, $du = 4\pi n\, dy$ and this gives

$$\frac{2}{(4\pi)^k} \sum_{n=1}^{\infty} \frac{r_{2k}(n)\overline{a(n)}}{n^{k-1}} \int_{4\pi n}^{\infty} u^{k-2}\, \mathrm{e}^{-u}\, du.$$

We now split this sum into several ranges. The main contribution comes from $n = 1$. We have $a(1) = 1$ and $r_{2k}(1) = 4k$. This term is

$$\frac{8k}{(4\pi)^k}\int_{4\pi}^{\infty} u^{k-2}\mathrm{e}^{-u}\,du = \frac{8k}{(4\pi)^k}\left[\int_0^{\infty} u^{k-2}\mathrm{e}^{-u}\,du - \int_0^{4\pi} u^{k-2}\mathrm{e}^{-u}\,du\right]$$
$$\geq \frac{8k}{(4\pi)^k}\left[(k-2)! - (4\pi)^{k-1}\mathrm{e}^{-4\pi}\right],$$

for $k \geq 15$, since if $k > 4\pi + 2$, $u^{k-2}\mathrm{e}^{-u}$ is increasing on $[0, 4\pi]$.

The second range is $2 \leq n \leq 2500$. Here we explicitly compute the polynomials $r_{2k}(n)$ (using the algorithm in the proof of part 1 of Lemma 3.1). Part 2 of Lemma 3.1 shows that $\frac{r_{2k}(n)}{n^{\frac{k-1}{2}}}$ is a decreasing function of k, provided $k \geq 1456$.

The third range is $2500 \leq n \leq \frac{k}{2\pi}\log(2k)$. In this range, we use the bound from part 3 of Lemma 3.1, the Deligne bound, $d(n) \leq 2\sqrt{n}$, and we obtain that

$$\left|\frac{r_{2k}(n)\overline{a(n)}}{n^{k-1}}\right| \leq \frac{34(4.11)^{2k}}{25\sqrt{(2k)!}} \cdot \sqrt{n} \cdot \frac{(n+2k)^{k-1}}{n^{\frac{k-1}{2}}}$$
$$\leq \frac{34}{25}\frac{(4.11)^{2k}}{\sqrt{(2k)!}} \cdot \sqrt{\frac{k}{2\pi}\log(2k)} \cdot \left(\sqrt{n} + \frac{2k}{\sqrt{n}}\right)^{k-1}.$$

The function $f(x) = \left(x + \frac{2k}{x}\right)^{k-1}$ is decreasing for $x < \sqrt{2k}$ and increasing after that. We have that $f(50) = f(\frac{2k}{50})$ and $\frac{2k}{50} \geq \sqrt{\frac{k}{2\pi}\log(2k)}$ if $k \geq 724$. Thus, we have the bound

$$\frac{68}{25}\frac{(4.11)^{2k}}{(4\pi)^k\sqrt{(2k)!}} \cdot \frac{k^{3/2}}{(2\pi)^{3/2}}\log^{3/2}(2k) \cdot \left(50 + \frac{2k}{50}\right)^{k-1} \cdot (k-2)!,$$

valid provided $k \geq 724$. For $k \leq 724$, we use the larger of the values of f at $x = 50$ and $x = \sqrt{\frac{k}{2\pi}\log(2k)}$.

The fourth and final range is $n \geq \frac{k}{2\pi}\log(2k)$. In this range we use the decay of the integral $\int_{4\pi n}^{\infty} u^{k-2}\mathrm{e}^{-u}\,du$. We have that $u \geq 2k\log(2k)$ and so $u^{k-2}\mathrm{e}^{-u} \leq \mathrm{e}^{-u/2}$ and so the integral is bounded by $2\,\mathrm{e}^{-2\pi n}$. Bounding $\overline{a(n)}$ and $r_{2k}(n)$ as before, we have that the contribution from this range is at most

$$\frac{34}{3(4\pi)^k}\sum_{n=\frac{k}{2\pi}\log(2k)}^{\infty} \frac{2n^{\frac{k}{2}}}{n^{k-1}} \cdot \left(\frac{3}{25} \cdot \frac{(4.11)^{2k}}{\sqrt{(2k)!}}\right)(n+2k)^{k-1} \cdot 2\,\mathrm{e}^{-2\pi n}.$$

We write $\frac{(n+2k)^{k-1}}{n^{k-1}}$ as $\left(1 + \frac{2k}{n}\right)^{k-1}$. If $k \geq 40$, $1 + \frac{2k}{n} \leq 3.87$ and we get

$$\frac{136}{25(4\pi)^k} \cdot \frac{(4.11)^{2k}(3.87)^{k-1}}{\sqrt{(2k)!}}\sum_{n=\frac{k}{2\pi}\log(2k)}^{\infty} n^{\frac{k}{2}}\,\mathrm{e}^{-2\pi n}.$$

If $a_n = n^{\frac{k}{2}}\,\mathrm{e}^{-2\pi n}$, then we have

$$\frac{a_{n+1}}{a_n} \leq \left(1 + \frac{1}{n}\right)^{\frac{k}{2}}\mathrm{e}^{-2\pi} \leq \mathrm{e}^{\frac{k}{2n} - 2\pi} \leq \mathrm{e}^{-2\pi + \frac{\pi}{\log(2k)}} \leq \mathrm{e}^{-5.6}.$$

Thus, we get the bound

$$\frac{136}{25(4\pi)^k} \cdot \frac{(4.11)^{2k}(3.87)^{k-1}}{\sqrt{(2k)!}} \cdot \left(\frac{k}{2\pi}\log(2k)\right)^{\frac{k}{2}} (2k)^{-k} \cdot \frac{1}{1-\mathrm{e}^{-5.6}},$$

valid if $k \geq 40$.

The second part of the contribution from the cusp at infinity is

$$\frac{1}{2\pi}\int_{-1/2}^{1/2}\int_{\sqrt{1-x^2}}^{1} \theta^{2k}(x+\mathrm{i}y)\overline{g(x+\mathrm{i}y)}y^{k-2}\,dy\,dx.$$

In this region we use Lemma 3.2 to bound $g(x+\mathrm{i}y)$, and we use that

$$|\theta(z)| \leq 1 + 2\sum_{n=1}^{\infty} \mathrm{e}^{-2\pi n^2 y} \leq 1.008667$$

for $y \geq \sqrt{3}/2$. This gives the bound

$$\frac{\Gamma\left(\frac{k+1}{2}\right)\left[\log\left(\frac{k+1}{2}\right)+\gamma+1\right](1.008667)^{2k}}{(2\pi)^{\frac{k+3}{2}}}\int_{-1/2}^{1/2}\int_{\sqrt{1-x^2}}^{1} y^{\frac{k-5}{2}}\,dy\,dx.$$

The double integral above is less than or equal to $\int_{-1/2}^{1/2}\int_0^1 y^{\frac{k-5}{2}}\,dy\,dx = \frac{2}{k-3}$. Hence, we get the bound

$$\frac{34\Gamma\left(\frac{k+1}{2}\right)\left[\log\left(\frac{k+1}{2}\right)+\gamma+1\right](1.008667)^{2k}}{3(k-3)(2\pi)^{\frac{k+3}{2}}},$$

valid for $k \geq 7$.

Term 2. This is the contribution of the cusp at zero, and in particular the contributions from the terms involving γ_2, γ_3, γ_4, and γ_5. We have

$$\theta^{2k}|W_4 = (-1)^{\frac{k}{2}}\theta^{2k} \quad \text{and} \quad \tilde{g}_i|W_4 = (-1)^{\frac{k}{2}}\tilde{g}_i.$$

Translating this into Fourier expansions gives

$$\theta^{2k}|\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix} = \frac{(-1)^{\frac{k}{2}}}{2^k}\theta^{2k}\left(\frac{z}{4}\right), \quad \tilde{g}_i|\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix} = \frac{(-1)^{\frac{k}{2}}}{2^k}\tilde{g}_i\left(\frac{z}{4}\right).$$

Thus, the contribution from these four terms is

$$\frac{1}{(2\pi)\cdot 4^k}\sum_{j=0}^{3}\int_{-1/2}^{1/2}\int_{\sqrt{1-x^2}}^{\infty}\theta^{2k}\left(\frac{x+j+\mathrm{i}y}{4}\right)\overline{\tilde{g}_i\left(\frac{x+j+\mathrm{i}y}{4}\right)}y^{k-2}\,dy\,dx.$$

We set $u = x/4$ and $v = y/4$ in the integrand and obtain

$$\frac{1}{2\pi}\sum_{j=0}^{3}\int_{-1/8}^{1/8}\int_{\frac{\sqrt{1-16u^2}}{4}}^{\infty}\theta^{2k}\left(u+\mathrm{i}v+\frac{j}{4}\right)\overline{\tilde{g}_i\left(u+\mathrm{i}v+\frac{j}{4}\right)}v^{k-2}\,dv\,du.$$

We break this into two terms. The first term consists of those pieces with $v \leq 1$. The smallest value v takes on this piece is $\sqrt{3}/8$ and since $\sqrt{3}/8 > \frac{1}{2\pi}$, we may use Lemma 3.2 to bound the contribution. This yields

$$|\tilde{g}_i(u+iv)| \leq \frac{17}{3\cdot(2\pi v)^{\frac{k+1}{2}}}\Gamma\left(\frac{k+1}{2}\right)\left[\log\left(\frac{k+1}{2}\right)+\gamma+1\right].$$

We also have

$$|\theta(u+\mathrm{i}v)| \leq 1 + 2\sum_{n=1}^{\infty} \mathrm{e}^{-2\pi n^2 v} \leq 1.52182$$

for $v \geq \sqrt{3}/8$. The contribution of these terms is therefore bounded by

$$\frac{17\cdot(1.52182)^{2k}}{3\cdot(2\pi)^{\frac{k+3}{2}}}\Gamma\left(\frac{k+1}{2}\right)\left[\log\left(\frac{k+1}{2}\right)+\gamma+1\right]\sum_{j=0}^{3}\int_{-1/8}^{1/8}\int_{\frac{\sqrt{1-16u^2}}{4}}^{1} v^{\frac{k-5}{2}}\,dv\,du$$

The sum of double integrals is bounded by $\int_{-1/2}^{1/2}\int_0^1 v^{\frac{k-5}{2}}\,dv = \frac{2}{k-3}$ and we get the bound

$$\frac{34\cdot(1.52182)^{2k}}{3\cdot(2\pi)^{\frac{k+3}{2}}\cdot(k-3)}\Gamma\left(\frac{k+1}{2}\right)\left[\log\left(\frac{k+1}{2}\right)+\gamma+1\right],$$

on the part where $v \leq 1$, valid for $k \geq 7$.

The second term consists of those pieces with $v \geq 1$. This gives

$$\frac{1}{2\pi}\int_{-1/2}^{1/2}\int_1^{\infty}\theta^{2k}(u+\mathrm{i}v)\overline{\tilde{g}_i(u+\mathrm{i}v)}v^{k-2}\,dv\,du.$$

This is exactly the same as the contribution of the first part of the cusp at infinity!

Term 3. This is the contribution of the cusp at $1/2$ corresponding to the matrix γ_6. We must understand the Fourier expansion of $\tilde{g}_i|\gamma_6$. Since $\gamma_6 \in \Gamma_0(2)$, terms of level 1 or 2 are not affected.

If g is a newform of level 4, then since γ_6 is not in $\Gamma_0(4)$, we have that $g \mapsto g + g|\gamma_6$ is the trace map from $S_k(\Gamma_0(4))$ to $S_k(\Gamma_0(2))$. Since newforms are in the kernel of the trace map (by Theorem 4 of [21]), it follows that $g + g|\gamma_6 = 0$ and so $g|\gamma_6 = -g$.

If g is a newform of level 2, we have

$$g|V(2)|\gamma_6 = 2^{-k/2}g|\begin{bmatrix}2 & 0\\0 & 1\end{bmatrix}\begin{bmatrix}1 & 0\\2 & 1\end{bmatrix} = 2^{-k/2}g|\begin{bmatrix}0 & -1\\2 & 0\end{bmatrix}\begin{bmatrix}1 & 0\\-2 & 1\end{bmatrix}\begin{bmatrix}1 & 1/2\\0 & 1\end{bmatrix}.$$

The first matrix is the Atkin–Lehner involution of level 2, of which g is an eigenform. The second matrix is in $\Gamma_0(2)$ and the third matrix does not affect the size of the Fourier coefficients at infinity. It follows that the nth Fourier coefficient of $g|V(2)|\gamma_6$ is bounded by $2^{-k/2}d(n)n^{\frac{k-1}{2}}$.

If g is a newform of level 1, we have

$$g|V(4)|\gamma_6 = 2^{-k}g\begin{bmatrix}4 & 0\\0 & 1\end{bmatrix}\begin{bmatrix}1 & 0\\2 & 1\end{bmatrix} = 2^{-k}g|\begin{bmatrix}2 & 1\\1 & 1\end{bmatrix}\begin{bmatrix}2 & -1\\0 & 2\end{bmatrix} = 2^{-k}g(z-1/2).$$

Thus, the nth Fourier coefficient of $g|V(4)|\gamma_6$ is bounded by $2^{-k}d(n)n^{\frac{k-1}{2}}$. It follows that for any $\tilde{g}_i$, the nth coefficient of $\tilde{g}_i|\gamma_6$ is bounded by $\frac{14}{3}d(n)n^{\frac{k-1}{2}}$.

Now, $\theta^{2k}|\gamma_6 = 2^{2k}\frac{\eta(4z)^{4k}}{\eta(2z)^{4k}}$. The form $F(z) = \frac{\eta(4z)^8}{\eta(2z)^4} \in M_2(\Gamma_0(4))$ and satisfies

$$F(z) = \sum_{n \text{ odd}} \sigma(n)q^n.$$

Thus, for $y \geq \sqrt{3}/2$, $|F(z)| \leq \mathrm{e}^{-2\pi y}\left(\sum_{n \text{ odd}} \sigma(n)\,\mathrm{e}^{-2\pi(n-1)y}\right) \leq 1.0001\,\mathrm{e}^{-2\pi y}$ and so

$$|\theta^{2k}|\gamma_6| \leq 2^{2k}(1.0001)^{k/2}\mathrm{e}^{-k\pi y}$$

for $y \geq \sqrt{3}/2$. The contribution of the cusp at $1/2$ is therefore

$$\frac{1}{2\pi}\int_{-1/2}^{1/2}\int_{\sqrt{1-x^2}}^{\infty}\theta^{2k}|\gamma_6(x+\mathrm{i}y)\overline{\tilde{g}_i|\gamma_6(x+\mathrm{i}y)}y^{k-2}\,dy\,dx.$$

By Lemma 3.2, we have

$$|\tilde{g}_i|\gamma_6(x+\mathrm{i}y)| \leq \frac{14}{3}\frac{1}{(2\pi)^{\frac{k+1}{2}}}\Gamma\left(\frac{k+1}{2}\right)\left[\log\left(\frac{k+1}{2}\right)+\gamma+1\right]\cdot\frac{1}{y^{\frac{k+1}{2}}}.$$

This gives the bound

$$\frac{14\cdot 2^{2k}\cdot(1.0001)^{k/2}}{3(2\pi)^{\frac{k+3}{2}}}\Gamma\left(\frac{k+1}{2}\right)\left[\log\left(\frac{k+1}{2}\right)+\gamma+1\right]\int_0^\infty y^{\frac{k-5}{2}}\mathrm{e}^{-k\pi y}\,dy.$$

The integral above is $\frac{1}{(k\pi)^{\frac{k-3}{2}}}\Gamma\left(\frac{k-3}{2}\right)$, and so the bound on this term is

$$\frac{14\cdot 2^{2k}\cdot(1.0001)^{k/2}}{3(2\pi)^{\frac{k+3}{2}}(k\pi)^{\frac{k-3}{2}}}\Gamma\left(\frac{k+1}{2}\right)\Gamma\left(\frac{k-3}{2}\right)\left[\log\left(\frac{k+1}{2}\right)+\gamma+1\right]$$

and is valid for $k \geq 7$.

After dividing each term above by $\frac{(k-2)!}{(4\pi)^k}$, the main term is increasing linearly (it is about $16k$), and each other term decreases exponentially. The most troublesome term is the term from the third range of values of n from the cusp at infinity, and (after dividing by $\frac{(k-2)!}{(4\pi)^k}$) is asymptotic to $c_1c_2^k k^{1/4}\ln(k)^{3/2}$, where $c_2 \approx 0.918$, but $c_1 \approx 1.69\times 10^{543}$. This term is smaller than the main term only when $k \geq 14{,}000$.

For this reason, we must explicitly calculate our bounds for $k < 14,000$. In this range, we refine our estimate of the troublesome term by using the exact values of the incomplete Γ-function $\int_{4\pi n}^{\infty}u^{k-2}\,\mathrm{e}^{-u}\,du$. Also, for $k \leq 2550$, we compute the values of $r_{2k}(n)$ explicitly for $2 \leq n \leq 2500$ and use these in our bounds. For $k \geq 2552$, we use part 2 of Lemma 3.1.

Finally, for $k \leq 194$, our numerical bounds are not sufficient and we use Magma to explicitly compute the decomposition of θ^{2k} as in equation (1.2) and find that the constants c_i are non-negative. □

Proof of Theorem 1.1. First, assume that n is odd. Considering the coefficient of q on both sides of (1.2), we obtain

$$r_{2k}(1) = 4k = \frac{2k(-1)^{k/2}}{(2^k-1)B_k}+\sum_i c_i.$$

By Theorem 1.2, we have

$$\sum_i |c_i| = \sum_i c_i = 4k - \frac{2k(-1)^{k/2}}{(2^k-1)B_k}.$$

Deligne's bound on the nth coefficient of $g_i(z)$ is bounded by $d(n)n^{\frac{k-1}{2}}$. Plugging this bound into the decomposition and using the fact that the coefficients of q^n in $g_i(2z)$ and $g_i(4z)$ are zero if n is odd gives the desired bound on the cusp form contribution to $\theta^{2k}(z)$.

Now, suppose that $k/2$ is odd and n is even. Then $k \equiv 2 \pmod 4$. We represent the decomposition of the cusp form part of $\theta^{2k}(z)$ as

$$C(z) = \sum_i r_i \left(f_i(z) - 2^k f_i(z)|V(4)\right) + \sum_i s_i \left(g_i(z) - 2^{\frac{k}{2}} \lambda_i g_i(z)|V(2)\right) + \sum_i t_i h_i(z).$$

Here, the $f_i(z)$, $g_i(z)$ and $h_i(z)$ are the newforms of levels 1, 2 and 4, respectively, and λ_i is the Atkin–Lehner eigenvalue of $g_i(z)$. One can see that the nth coefficients of $f_i(z) - 2^k f_i(z)|V(4)$ and $g_i(z) - 2^{\frac{k}{2}}\lambda_i g_i(z)|V(2)$ are bounded by $3d(n)n^{\frac{k-1}{2}}$. Thus, for even n, we obtain the bound

$$\left(\sum_i 3r_i + 3s_i\right) d(n)n^{\frac{k-1}{2}}.$$

We will show that $\sum_i 3r_i + 3s_i < 4k - \frac{2k}{(2^k-1)B_k}$.

To compute the constant $\sum_i 3r_i + 3s_i$, we will compute the trace of $C(z)$ to $S_k(\Gamma_0(2))$, given by $\mathrm{Tr}(C) := C(z) + C(z)|\begin{bmatrix} 1 & 0 \\ 2 & 1 \end{bmatrix}$. Straightforward, but somewhat lengthy computations show that

$$\begin{aligned} \mathrm{Tr}(f_i(z) - 2^k f_i(z)|V(4)) &= 3f_i(z) - 2a_i(2)f_i(z)|V(2), \\ \mathrm{Tr}(g_i(z) - 2^{\frac{k}{2}}\lambda_i g_i(z)|V(2) &= 3g_i(z), \\ \mathrm{Tr}(h_i(z)) &= 0. \end{aligned}$$

It follows from these formulae that $\sum_i 3r_i + 3s_i$ is the coefficient of q in $\mathrm{Tr}(C)$. We have that

$$\begin{aligned} C &= \theta^{2k} + \frac{1}{2^k-1}E_k(z) - \frac{2^k}{2^k-1}E_k(4z), \\ \mathrm{Tr}(C) &= \mathrm{Tr}(\theta^{2k}) - \frac{(-1)^{k/2}}{2^k-1}\mathrm{Tr}(E_k(z)) - \frac{2^k}{2^k-1}\mathrm{Tr}(E_k(4z)), \\ &= \left(\theta^{2k} + 4^k \frac{\eta^{4k}(4z)}{\eta^{2k}(2z)}\right) + \frac{2}{2^k-1}E_k(z) \\ &\quad - \frac{2^k}{2^k-1}\left((1+2^{1-k})E_k(z)|V(2) - 2^{-k}E_k(z)\right). \end{aligned}$$

Taking the coefficient of q on both sides of the preceding equation gives

$$\sum_i 3r_i + 3s_i = 4k - \frac{6k}{(2^k-1)B_k} < 4k - \frac{2k}{(2^k-1)B_k}$$

since $k \equiv 2 \pmod 4$ and hence $B_k > 0$. This proves Theorem 1.1 in the case that $k \equiv 2 \pmod 4$ and n is even. □

5. Final remarks

It is natural to consider if Theorem 1.1 is true in other cases. When $k \equiv 0 \pmod 4$ and n is even, the main issue is that if g_i is a level 1 eigenform and

$$\tilde{g}_i = g_i - \frac{4}{3}a(2)g_i|V(2) + 2^k g_i|V(4) = \sum_{n=1}^{\infty} c(n)q^n,$$

then the best possible bound on the Fourier coefficients of $\tilde{g}_i$ is $|c(n)| \leq 2d(n)n^{\frac{k-1}{2}}$. In order for this bound to come close to being achieved, it is necessary for $|a(2)|$, the absolute value of the second coefficient in g_i, to be close to $2^{\frac{k+1}{2}}$. Serre proved in 1997 (see [22]) that if p is a fixed prime, the pth coefficients of newforms become equidistributed (along any sequence of weights and levels whose sum tends to infinity, where the levels are not multiples of p). It follows from this that there will be level 1 eigenforms with $|a(2)|$ arbitrarily close to $2^{\frac{k+1}{2}}$, but also that there will be few such forms. One approach to extending Theorem 1.1 to the case when $k \equiv 0 \pmod 4$ is to use the equidistribution of the numbers $|a(2)|$.

It is also natural to consider the problem of deriving a sharp bound in the case that k is odd. In the case when k is even, the contribution from the cusp at zero is (up to a fairly small error) the same as the contribution at the cusp at infinity, since both θ^{2k} and the newforms are eigenforms of the Atkin–Lehner involution W_4. However, when k is odd, the newforms are not eigenforms of W_4 any longer. This means that the contribution of the cusp at zero is (up to some small error) the contribution of the cusp at infinity times some complex number λ of absolute value 1. This complex number is related to the coefficient of q^4 of the relevant eigenform g_i. A similar result could be proven provided one could rule out the possibility that λ is close to -1. In fact, the analogue of Theorem 1.2 is false for $k = 17$, although this seems to be a consequence of the smallness of the weight, rather than a value of λ too close to -1.

For half-integral values of k (corresponding to representations of n as the sum of an odd number of squares), the question is still interesting. In this case, the coefficients of the cusp forms involve square roots of central critical L-values of quadratic twists of forms of level 1 and level 2. The analogue of Deligne's theorem in this case would be optimal subconvexity bounds on these L-values, currently attainable only under the assumption of the generalized Riemann hypothesis.

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