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EXACT FORMULAS FOR TRACES OF SINGULAR MODULI OF PRIME SQUARE LEVEL MODULAR FUNCTIONS

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Abstract. We find exact formulas for traces of singular moduli of prime square level modular functions and give their applications.

1. Introduction and statement of result

The modular j-invariant is defined for z in the complex upper half plane $\mathbb{H}$ by

$$j(z) = q^{-1} + 744 + 196884q + \cdots ,$$

where $q = e(z) = e^{2\pi iz}$. The values of j-function at imaginary quadratic arguments in $\mathbb{H}$ are known as *singular moduli* and they are algebraic integers that play important roles in number theory. For example, $j(\frac{-1+\sqrt{-23}}{2})$ is an algebraic integer of degree $h(-23)$, the class number of the imaginary quadratic field $K = \mathbb{Q}(\frac{-1+\sqrt{-23}}{2})$ and generates the Hilbert class field of K. In fact, $j(\frac{-1+\sqrt{-23}}{2})$ is the real root of $x^3 + 3491750x^2 - 5151296875x + 23375^3 = 0$.

The trace of a singular modulus, that is the sum of the conjugates of $j(z)$, also has an interesting arithmetic property. D. Zagier [9] proved that the traces of $J(z) = j(z) - 744$, the Hauptmodul for the group $\Gamma(1) = PSL_2(\mathbb{Z})$, are Fourier coefficients of

$$g(z) := -q^{-1}+2+\sum_{\substack{D>0\\ D\equiv 0,3 (\mathrm{mod} 4)}} \mathbf{t}_J(D)q^D = -q^{-1}+2-248q^3+492q^4-4119q^7+7256q^8-\cdots ,$$

which is a weakly holomorphic (holomorphic away from the cusps) modular form of weight 3/2 on $\Gamma_0(4)$. We note that $\mathbf{t}_J(23) = -3491750 - 3 \times 744$.

Recently, Bruinier, Jenkins, and Ono [2] obtained an explicit formula for the Fourier coefficients of $g(z)$ in terms of Kloosterman sums and Duke [5] derived their exact formulas in terms of Salié sums $S_D(c)$ that is defined for any positive integer c by $S_D(c) = \sum_{x^2 \equiv -D (\mathrm{mod}\, c)} e(2x/c)$. The exact formulas lead to the following nice asymptotic result [5, eq.(3)]

$$\frac{1}{h(-D)}\left(\mathbf{t}_J(D) - \frac{1}{2}\sum_{\substack{0<c<2\sqrt{D}\\ c\equiv 0 (\mathrm{mod}\ 4)}} S_D(c)\sinh\left(\frac{4\pi\sqrt{D}}{c}\right)\right) \to -24 \tag{1.1}$$

as $D \to \infty$, with $-D$ a fundamental discriminant. These results are special cases of more general theorems for the traces of the values of f of any $f \in \mathbb{C}[j]$.

For a higher level case, an exact formula for traces of singular values of modular functions of any prime level p is derived in [4]. As a matter of fact, we always can find an exact formula for traces of singular moduli in the same line with the one in [4] whatsoever the level is as long as the modular function is completely determined by its principal part at ∞..

In order to make this more precise, let $\Gamma_0^*(N)$ denote the group generated by $\Gamma_0(N)$ and the Fricke involution. For a positive integer D congruent to 0 or 3 modulo 4, we let $\mathcal{Q}_{D,N}$ denote the set of positive definite integral binary quadratic forms

$$Q(x, y) = [a, b, c] = Nax^2 + bxy + cy^2$$

with discriminant $-D = b^2 - 4Nac$ on which $\Gamma_0^*(N)$ acts. We choose an integer $\beta \pmod{2N}$ with $\beta^2 \equiv -D \pmod{4N}$ and consider the set $\mathcal{Q}_{D,N,\beta} = \{[a, b, c] \in \mathcal{Q}_{D,N} \mid b \equiv \beta \pmod{2N}\}$ on which $\Gamma_0(N)$ acts. For each quadratic form Q, we let z_Q be the corresponding Heegner point in $\mathbb{H}$, the unique root of $Q(x, 1)$ in $\mathbb{H}$.

For a modular function f for $\Gamma_0^*(N)$, we define the class number $H_N(D)$ (resp. $H_N^*(D)$) and the trace $\mathbf{t}_f(D)$ (resp. $\mathbf{t}_f^*(D)$) by

$$H_N(D) = \sum_{Q\in\mathcal{Q}_{D,N,\beta}/\Gamma_0(N)} \frac{1}{|\Gamma_0(N)_Q|}; \qquad \mathbf{t}_f(D) = \sum_{Q\in\mathcal{Q}_{D,N,\beta}/\Gamma_0(N)} \frac{1}{|\Gamma_0(N)_Q|} f(z_Q)$$

$$H_N^*(D) = \sum_{Q\in\mathcal{Q}_{D,N}/\Gamma_0^*(N)} \frac{1}{|\Gamma_0^*(N)_Q|}; \qquad \mathbf{t}_f^*(D) = \sum_{Q\in\mathcal{Q}_{D,N}/\Gamma_0^*(N)} \frac{1}{|\Gamma_0^*(N)_Q|} f(z_Q),$$

where $\Gamma_0(N)_Q$ and $\Gamma_0^*(N)_Q$ are the stabilizers of Q in $\Gamma_0(N)$ and $\Gamma_0^*(N)$, respectively. When $N = 1$ and $f = J$, we recover the Hurwitz-Kronecker class number $H(D)$ and the Zagier trace $t_J(D)$. It is easy to see that

$$H_N^*(D) = \begin{cases} \frac{1}{2}H_N(D), & \text{if } \beta \equiv 0 \text{ or } N \pmod{2N}, \\ H_N(D), & \text{otherwise,} \end{cases} \tag{1.2}$$

and

$$\mathbf{t}_f^*(D) = \begin{cases} \frac{1}{2}\mathbf{t}_f(D), & \text{if } \beta \equiv 0 \text{ or } N \pmod{2N}, \\ \mathbf{t}_f(D), & \text{otherwise.} \end{cases} \tag{1.3}$$

In [4], the following exact formula for traces of singular moduli of prime level is given: If f is a modular function for $\Gamma_0^*(p)$ with principal part $\sum_{m=1}^{N} a_m e(-mz)$ at $i\infty$, then

$$\mathbf{t}_f^*(D) = \sum_{m=1}^{N} a_m \left[c_m H_p^*(D) + \sum_{\substack{c>0 \\ c\equiv 0 \,(\mathrm{mod}\, 4p)}} S_D(m,c) \sinh\left(\frac{4\pi m\sqrt{D}}{c}\right) \right], \tag{1.4}$$

where

$$c_m = -24\left(\frac{-p^{\alpha+1}}{p+1}\sigma(m/p^\alpha) + \sigma(m)\right) \quad \text{with} \quad p^\alpha || m \tag{1.5}$$

and

$$S_D(m,c) = \sum_{x^2 \equiv -D (\mathrm{mod}\, c)} e(2mx/c) \quad \text{for any positive integers } m \text{ and } c. \tag{1.6}$$

However, we can find that using Niebur's Poincaré series [8] as in [5], [4], we can easily obtain more general theorem:

Theorem 1. *Suppose that f is a modular function for $\Gamma_0^*(N)$ whose poles are supported only at $i\infty$, and f has principal part $\sum_{m=1}^{j} a_m e(-mz)$ at $i\infty$. If we define $S_D(m,c)$ as in (1.6), then for some constants c_m depending on m and the level N, we have*

$$\mathbf{t}_f^*(D) = \sum_{m=1}^{j} a_m \left[c_m H_N^*(D) + \sum_{\substack{c>0 \\ c\equiv 0 \,(mod\, 4N)}} S_D(m,c) \sinh\left(\frac{4\pi m\sqrt{D}}{c}\right) \right]. \tag{1.7}$$

If $f = j_m$, the unique modular function such that $j_m(z) - q^{-m}$ has a zero at $i\infty$, then $c_m = -24\sigma(m)$ and when $N = p$ the constants c_m are given by (1.5). If N is the square of a prime, then the precise formula for c_m is given

Theorem 2. *Suppose that f is a modular function for $\Gamma_0^*(p^2)$ whose poles are supported only at $i\infty$, and f has principal part $\sum_{m=1}^{j} a_m e(-mz)$ at $i\infty$. Then $\mathbf{t}_f^*(D)$ is given by (1.7) with $N = p^2$ and*

$$c_m = -24 \times \begin{cases} \frac{\sigma(m)}{p^2-1}, & \text{if } p \nmid m, \\ \sigma(m) - p^\alpha \sigma(m/p^\alpha)\frac{p+2}{p+1}, & \text{if } p^\alpha \| m. \end{cases} \tag{1.8}$$

Let $F_{\lambda,N}(-m;\tau)$ be the Maass-Poincaré series defined in [7]. Using theta lifts we can find a Harmonic weak Maass form $G_N(\tau)$ whose holomorphic part is given by $\sum_D H_N^*(D)q^D$. Let

$$F_{1,N}^*(-m,\tau) := F_{1,N}(-m,\tau) + (-c_1)\delta_{\Box,m} G_N(\tau)$$

and denote the coefficient of q^n in the holomorphic part of $F_{1,N}^*(-m,\tau)$ by $B_{1,N}(-m;n)$. On the other hand, we define

$$F_{0,N}^*(-m,\tau) := F_{0,N}(-m,\tau) + H_N^*(m)\cdot c_1\theta(\tau)/2$$

and denote the coefficient of q^n in the holomorphic part of $F_{0,N}^*(-m,\tau)$ by $B_{0,N}(-m;n)$.

Theorem 3. *Assume the notation above. Suppose that m is a positive integer for which $m \equiv \Box (\mathrm{mod}\, 4N)$. For every positive integer n with $-n \equiv \Box (\mathrm{mod}\, 4N)$ we have*

$$B_{1,N}(-m;n) = -B_{0,N}(-n;m).$$

Theorem 4. *Uniform Distribution*

2. Exact Formulas: the proofs of Theorems 1 and 2

Proof of Theorem 1. Recall Niebur's Poincaré series in [8]: for a positive integer m,

$$\mathcal{F}_m(z,s) = \sum_{M\in\Gamma_\infty\backslash\Gamma} e(-m\mathrm{Re}Mz)(\mathrm{Im}Mz)^{1/2} I_{s-1/2}(2\pi m\mathrm{Im}Mz), \tag{2.1}$$

where $I_{s-1/2}$ is the modified Bessel function of the first kind. Then $\mathcal{F}_m(z,s)$ converges absolutely for $\mathrm{Re}\, s > 1$ and satisfies

$$\mathcal{F}_m(Mz,s) = \mathcal{F}_m(z,s) \text{ for } M\in\Gamma \tag{2.2}$$

and

$$\triangle\mathcal{F}_m(z,s) = s(1-s)\mathcal{F}_m(z,s), \tag{2.3}$$

where $\triangle$ is the hyperbolic Laplacian $\triangle = -y^2(\partial_x^2 + \partial_y^2)$ for $z = x+iy$. Niebur showed that $\mathcal{F}_m(z,s)$ has an analytic continuation to $s=1$ [8, Theorem 5] and that $\mathcal{F}_m(z,s)$ has the following Fourier expansion [8, Theorem 1]; for $\mathrm{Re}\, s>1$,

$$\mathcal{F}_m(z,s) = e(-mx)y^{1/2}I_{s-1/2}(2\pi my) + \sum_{n=-\infty}^{\infty} b_n(y,s;-m)e(nx), \tag{2.4}$$

where $b_n(y,s;-m) \to 0$ $(n\neq 0)$ exponentially as $y\to i\infty$. Hence the pole of $\mathcal{F}_m(z,1)$ at $i\infty$ may occur only in $e(-mx)y^{1/2}I_{1/2}(2\pi my)$, which is equal to

$$\frac{1}{\pi y^{1/2}m^{1/2}}\sinh(2\pi my)y^{1/2}e(-mx) = \frac{1}{2\pi m^{1/2}}(e(-mz) - e(-m\bar{z})). \tag{2.5}$$

We normalize $\mathcal{F}_m(z,1)$ by multiplying with $2\pi m^{1/2}$, so that the coefficient of $e(-mz)$ is normalized.

Now we define

$$\mathcal{F}_m^*(z,s) = (2\pi m^{1/2})\mathcal{F}_m(z,s) + c_m,$$

where $-c_m$ is the constant term in $(2\pi m^{1/2})\mathcal{F}_m(z,1)$. Then by (2.3), (2.4), and (2.5), $\mathcal{F}_m^*(z,1)$ is a Γ-invariant harmonic function and $\mathcal{F}_m^*(z,1) - e(-mz)$ has a zero at $i\infty$. Hence it follows from [8, Theorem 6] that

$$f(z) = \sum_{m=1}^{N} a_m \mathcal{F}_m^*(z,1)$$

for any modular function f for $\Gamma_0^*(N)$ whose poles are only supported at $i\infty$ and whose principal part is given by $\sum_{m=1}^{N} a_m e(-mz)$. Hence

$$\mathbf{t}_f^*(D) = \sum_{m=1}^{N} a_m \left(\sum_{Q\in\mathcal{Q}_{D,N}/\Gamma} \frac{1}{|\Gamma_Q|}\mathcal{F}_m^*(z_Q,1) \right). \tag{2.6}$$

In order to complete the proof of Theorem 1, it suffices to determine the value $\sum_{Q\in\mathcal{Q}_{D,N}/\Gamma} \frac{1}{|\Gamma_Q|}\mathcal{F}_m^*(z_Q,1)$ which is given in the lemma below. As its proof is very similar to that of Lemma 2 in [4], we omit the proof here.

Lemma 1. *Let $\mathcal{F}_m^*(z,s) = (2\pi m^{1/2})\mathcal{F}_m(z,s) + c_m$, where $\mathcal{F}_m(z,s)$ is defined in (2.1) and $-c_m$ is the constant term in $(2\pi m^{1/2})\mathcal{F}_m(z,1)$. Then the trace of CM values of $\mathcal{F}_m^*$ is given by*

$$\sum_{Q\in\mathcal{Q}_{D,N}/\Gamma} \frac{1}{|\Gamma_Q|}\mathcal{F}_m^*(z_Q,1) = c_m H_N^*(D) + \sum_{\substack{c>0 \\ c\equiv 0\,(mod\,4N)}} S_D(m,c)\sinh\left(\frac{4\pi m\sqrt{D}}{c}\right).$$

This completes the proof of Theorem 1. □

Proof of Theorem 2. Now we restrict N to the square of a prime p.

It follows from [8, Theorem 1] that $b_0(y,s,-m) = a_m(s)y^{1-s}/(2s-1)$. Here

$$a_m(s) = 2\pi^s m^{s-1/2}\phi_m(s)/\Gamma(s) \quad \text{and} \quad \phi_m(s) = \sum_{c>0} S(m,0;c)c^{-2s}, \tag{2.7}$$

where $S(m,n;c)$ is the general Kloosterman sum $\sum_{0\le d<|c|} e((ma+nd)/c)$ for $\left(\begin{smallmatrix} a & * \\ c & d \end{smallmatrix}\right) \in \Gamma$. Note that if $M = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \in \Gamma = \Gamma_0^*(p^2)$, then $M \in \Gamma_0(p^2)$ or M is of the form $\left(\begin{smallmatrix} px & y/p \\ pz & pw \end{smallmatrix}\right)$ with $x,y,z,w \in \mathbb{Z}$. In the former case, c is a multiple of p^2 and in the latter case, $c = pz$ with $p \nmid z$. Let $u_m(c)$ denote the sum of m-th powers of primitive c-th roots of unity. We define

$$u_m^*(c) = \begin{cases} u_m(c), & \text{if } p^2 \mid c, \\ u_m(c/p), & \text{if } p \| c, \\ 0, & \text{if } p \nmid c. \end{cases}$$

We then observe that

$$S(m,0;c) = \sum_{0\le d<|c|} e(ma/c),\ \left(\begin{smallmatrix} a & * \\ c & d \end{smallmatrix}\right) \in \Gamma_0^*(p^2)$$
$$= u_m^*(c)$$

and

$$\phi_m(s)\zeta(2s) = \sum_{c>0} S(m,0;c)c^{-2s} \sum_{c'>0} {c'}^{-2s}$$
$$= \sum_{c>0} u_m^*(c)c^{-2s} \sum_{c'>0} {c'}^{-2s} = \sum_{k\ge 1}\left(\sum_{c|k} u_m^*(c)\right) k^{-2s}. \tag{2.8}$$

Note that if $p \nmid k$, then

$$\sum_{c|k} u_m^*(c) = 0. \tag{2.9}$$

If $p||k$, then we write $k = pk'$ with $p \nmid k'$. We then come up with

$$\sum_{c|k} u_m^*(c) = \sum_{d|k'} u_m^*(d) + \sum_{d|k'} u_m^*(pd) = \sum_{d|k'} u_m(d) = \begin{cases} k', & \text{if } k' \mid m, \\ 0, & \text{if } k' \nmid m \end{cases} \tag{2.10}$$

since $\sum_{d|k'} u_m(d)$ is equal to the sum of m-th powers of k'-th roots of unity. If $k = p^l k'$ with $l \ge 2$ and $p \nmid k'$, then

$$\sum_{c|k} u_m^*(c) = \sum_{d|k'} u_m^*(d) + \sum_{d|k'} u_m^*(pd) + \sum_{\substack{c|k \\ p^2|c}} u_m^*(c) = 0 + \sum_{d|k'} u_m(d) + \sum_{\substack{c|k \\ p^2|c}} u_m(c). \tag{2.11}$$

By adding $\sum_{c|pk'} u_m(c)$ on both sides of (2.11), we obtain

$$\sum_{c|k} u_m^*(c) + \sum_{c|pk'} u_m(c) = \sum_{d|k'} u_m(d) + \sum_{c|k} u_m(c).$$

Since $\sum_{d|k'} u_m(d) = \begin{cases} k', & \text{if } k' \mid m, \\ 0, & \text{if } k' \nmid m \end{cases}$ and $\sum_{c|k} u_m(c) = \begin{cases} k, & \text{if } k \mid m, \\ 0, & \text{if } k \nmid m \end{cases}$,
we find that

(2.12)

$$\sum_{c|k} u_m^*(c) = \sum_{d|k'} u_m(d) + \sum_{c|k} u_m(c) - \sum_{c|pk'} u_m(c) = \begin{cases} k + k' - pk', & \text{if } k \mid m, \\ k' - pk', & \text{if } k \nmid m \text{ and } pk' \mid m, \\ k', & \text{if } k \nmid m,\ p \nmid m \text{ and } k' \mid m, \\ 0, & \text{if } k' \nmid m. \end{cases}$$

Writing $m = p^\alpha m'$ and $k = p^l k'$ with $p \nmid m'k'$, we obtain from (2.9), (2.10) and (2.12) the following tables on the values of $\sum_{c|k} u_m^*(c)$:

Table 1. Values of $\sum_{c|k} u_m^*(c)$ when $\alpha = 0$

	$l = 0$	$l > \alpha = 0$
$k' \mid m'$	0	k'
$k' \nmid m'$	0	0

Table 2. Values of $\sum_{c|k} u_m^*(c)$ when $\alpha \geq 1$

	$l = 0$	$1 \leq l \leq \alpha$	$l > \alpha$
$k' \mid m'$	0	$(p^l + 1 - p)k'$	$(1 - p)k'$
$k' \nmid m'$	0	0	0

When $\alpha = 0$, utilizing (2.8) and Table 1 one has

$$\begin{aligned} \phi_m(s)\zeta(2s) &= \sum_{k\geq 1}\left(\sum_{c|k} u_m^*(c)\right)k^{-2s} \\ &= \sum_{l\geq 1}\sum_{\substack{k' \\ p\nmid k'}}\left(\sum_{c|p^lk'} u_m^*(c)\right)(p^lk')^{-2s} = \sum_{l=1}^{\infty}(\sum_{k'|m'} k')(p^lk')^{-2s} \\ &= \sum_{l=1}^{\infty}\sum_{k'|m'} {k'}^{1-2s}(p^{-2s})^l = \sigma_{1-2s}(m')\frac{p^{-2s}}{1-p^{-2s}}, \end{aligned} \tag{2.13}$$

which tends to $\frac{\sigma_{-1}(m)}{p^2-1}$ as $s \to 1$.

Meanwhile if $\alpha \geq 1$, then if follows from (2.8) and Table 2 that

$$\begin{aligned} \phi_m(s)\zeta(2s) &= \sum_{k\geq 1}\left(\sum_{c|k} u_m^*(c)\right)k^{-2s} = \sum_{l\geq 1}\sum_{\substack{k' \\ p\nmid k'}}\left(\sum_{c|p^lk'} u_m^*(c)\right)(p^lk')^{-2s} \\ &= \sum_{l=1}^{\alpha}(\sum_{k'|m'}(p^l+1-p)k')(p^lk')^{-2s} + \sum_{l>\alpha}(\sum_{k'|m'}(1-p)k')(p^lk')^{-2s} \\ &= \sum_{l=1}^{\alpha}(\sum_{k'|m'}(p^lk')^{1-2s} + \sum_{l=1}^{\infty}(\sum_{k'|m'}(1-p)k')(p^lk')^{-2s} \\ &= \sigma_{1-2s}(m) - \sigma_{1-2s}(m') + (1-p)\sigma_{1-2s}(m')\frac{p^{-2s}}{1-p^{-2s}}, \end{aligned} \tag{2.14}$$

which tends to $\sigma_{-1}(m) - \sigma_{-1}(m')\frac{p+2}{p+1}$ as $s \to 1$.

Recall that the constant term in $(2\pi m^{1/2})\mathcal{F}_m(z,1)$ is

$$\lim_{s\to 1} 2\pi m^{1/2} b_0(y,s,-m) = \lim_{s\to 1} 2\pi m^{1/2} a_m(s) y^{1-s}/(2s-1).$$

By the definition of $a_m(s)$ in (2.7), it is equal to

$$\lim_{s\to 1} 2\pi m^{1/2}(2\pi^s m^{s-1/2}\phi_m(s)/\Gamma(s))y^{1-s}/(2s-1) = 4\pi^2 m \lim_{s\to 1}\frac{\phi_m(s)\zeta(2s)}{\Gamma(s)\zeta(2s)}.$$

It follows from (2.13) and (2.14) that this limit goes to

$$\frac{4\pi^2 m}{\zeta(2)} \times \begin{cases} \frac{\sigma_{-1}(m)}{p^2-1}, & \text{if } p \nmid m, \\ \sigma_{-1}(m) - \sigma_{-1}(m/p^\alpha)\frac{p+2}{p+1}, & \text{if } p^\alpha \mid m \end{cases}.$$

Now simple calculations lead us to have the constant term of $(2\pi m^{1/2})\mathcal{F}_m(z,1)$ in (1.8). □

3. Proof of Theorem 3

Let $b_{\lambda,N}(-m;n)$ denote the coefficients of q^n in the Fourier development of $F_{\lambda,N}(-m;\tau)$. According to [7, Theorem 2.1], the coefficient $b_{1,N}(-m;n)$ is given by

$$-\pi\sqrt{2}(n/m)^{1/4}(1+i)\sum_{\substack{c>0\\4N|c}}(1+\delta_{odd}(c/4))\frac{K_1(-m,n,c)}{c}I_{1/2}\left(\frac{4\pi\sqrt{nm}}{c}\right).$$

Applying [3, Proposition 3.1] we find that $b_{1,N}(-m;n)$ is equal to

$$-\pi\sqrt{2}(n/m)^{1/4}(1+i)\sum_{\substack{c>0\\4N|c}}(1+\delta_{odd}(c/4))(-i)\frac{K_0(-m,n,c)}{c}I_{1/2}\left(\frac{4\pi\sqrt{nm}}{c}\right).$$

Again by [7, Theorem 2.1] we see

$$b_{1,N}(-m;n) = -b_{0,N}(-n;m). \tag{3.1}$$

It follows from definition of $B_{\lambda,N}(-m;n)$ that

$$B_{1,N}(-m;n) = -c_1\delta_{\square,m}H_N^*(n) + b_{1,N}(-m;n) \tag{3.2}$$

and

$$B_{0,N}(-m;n) = c_1\delta_{\square,n}H_N^*(m) + b_{0,N}(-m;n). \tag{3.3}$$

Now by (3.1), (3.2) and (3.3) the assertion is proved.

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