EXACT FORMULAS FOR TRACES OF SINGULAR MODULI OF HIGHER LEVEL MODULAR FUNCTIONS

DOHOON CHOI, DAEYEOL JEON, SOON-YI KANG AND CHANG HEON KIM

Abstract. Zagier proved that the traces of singular values of the classical $j$-invariant are the Fourier coefficients of a weight $\frac{3}{2}$ modular form and Duke provided a new proof of the result by establishing an exact formula for the traces using Niebur’s work on a certain class of non-holomorphic modular forms. In this short note, by utilizing Niebur’s work again, we generalize Duke’s result to exact formulas for traces of singular moduli of higher level modular functions.

1. Introduction and statement of result

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

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

where $q = e(z) = e^{2\pi iz}$ and $J(z) = j(z) - 744$ is its normalized Hauptmodul for the group $\Gamma(1) = \text{PSL}_2(\mathbb{Z})$. All the modular groups discussed in this paper are subgroups of $\Gamma(1)$. For a positive integer $D$ congruent to 0 or 3 modulo 4, we denote by $Q_D$ the set of positive definite integral binary quadratic forms

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

with discriminant $-D = b^2 - 4ac$. For each $Q \in Q_D$, we let

$$z_Q = \frac{-b + i\sqrt{D}}{2a},$$

the corresponding CM point in $\mathcal{H}$. The group $\Gamma(1)$ acts on $Q_D$ and we write $\Gamma(1)_Q$ for the stabilizer of $Q$ in $\Gamma(1)$. The trace of $J$ singular moduli of
discriminant $-D$ is defined as

$$ t_J(D) = \sum_{Q \in \mathcal{Q}_D/\Gamma(1)} \frac{1}{|\Gamma(1)Q|} J(z_Q). $$

In [7, Theorem 1], Zagier proved the generating series for the traces of singular moduli

$$ g(z) := q^{-1} - 2 - \sum_{D>0 \atop D \equiv 0,3 \pmod{4}} t_J(D)q^D = q^{-1} - 2 + 248q^3 - 492q^4 + \cdots $$

is a weakly holomorphic modular form of weight $3/2$ on $\Gamma_0(4)$. Recently, Bruinier, Jenkins, and Ono [2] obtained an explicit formula for the Fourier coefficients of $g(z)$ in terms of Kloosterman sums and Duke [3] derived an exact formula for $t_J(D)$ as follows;

$$ t_J(D) = -24H(D) + \sum_{c>0 \atop c \equiv 0 \pmod{4}} S_D(c) \sinh \left( \frac{4\pi\sqrt{D}}{c} \right), $$

where $H(D) = \sum_{Q \in \mathcal{Q}_D/\Gamma(1)} \frac{1}{|\Gamma(1)Q|}$ is the Hurwitz class number and

$$ S_D(c) = \sum_{x^2 \equiv -D \pmod{c}} e(2x/c). $$

Using these two results together, Duke [3] reestablished Zagier's trace formula [7, Theorem 1].

The purpose of this paper is to give a generalization of (1) to traces of singular values of modular functions of any prime level $p$. For prime $p$, let $\Gamma_0(p)$ be the group generated by $\Gamma_0(p)$ and the Fricke involution $W_p = \frac{1}{\sqrt{p}} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. Let $\mathcal{Q}_{D,p}$ denote the set of quadratic forms $Q \in \mathcal{Q}_D$ such that $a \equiv 0$ (mod $p$) on which $\Gamma_0(p)$ acts. Then the discriminant $-D$ is congruent to a square modulo $4p$. We choose an integer $\beta$ (mod $2p$) with $\beta^2 \equiv -D$ (mod $4p$) and consider the set $\mathcal{Q}_{D,p,\beta} = \{ [a,b,c] \in \mathcal{Q}_{D,p} \mid b \equiv \beta$ (mod $2p$)$\}$ on which $\Gamma_0(p)$ acts. For a modular function $f$ for $\Gamma_0^*(p)$, we define the class number $H_p(D)$ (resp. $H_p^*(D)$) and the trace $t_f(D)$ (resp. $t_f^*(D)$) by

$$ H_p(D) = \sum_{Q \in \mathcal{Q}_{D,p,\beta}/\Gamma_0(p)} \frac{1}{|\Gamma_0(p)Q|}; \quad t_f(D) = \sum_{Q \in \mathcal{Q}_{D,p,\beta}/\Gamma_0(p)} \frac{1}{|\Gamma_0(p)Q|} f(z_Q) $$

$$ H_p^*(D) = \sum_{Q \in \mathcal{Q}_{D,p}/\Gamma_0^*(p)} \frac{1}{|\Gamma_0^*(p)Q|}; \quad t_f^*(D) = \sum_{Q \in \mathcal{Q}_{D,p}/\Gamma_0^*(p)} \frac{1}{|\Gamma_0^*(p)Q|} f(z_Q). $$
Here $\Gamma_0(p)Q$ and $\Gamma^*_0(p)Q$ are the stabilizers of $Q$ in $\Gamma_0(p)$ and $\Gamma^*_0(p)$, respectively. It is easy to see that

\[
H^*_p(D) = \begin{cases} 
\frac{1}{2}H_p(D), & \text{if } \beta \equiv 0 \text{ or } p \pmod{2p}, \\
H_p(D), & \text{otherwise},
\end{cases}
\]

and

\[
t^*_f(D) = \begin{cases} 
\frac{1}{2}t_f(D), & \text{if } \beta \equiv 0 \text{ or } p \pmod{2p}, \\
t_f(D), & \text{otherwise}.
\end{cases}
\]

The modularity for traces $t_f(D)$ was established by one of the authors in [4], [5] when $\Gamma^*_0(p)$ is of genus zero. If $f$ is the Hauptmodul for such $\Gamma^*_0(p)$ and if we define $t_f(-1) = -1$, $t_f(0) = 2$ and $t_f(D) = 0$ for $D < -1$, then the series $\sum_{n \geq 1} t_f(4pn - r^2)q^n \zeta^r$, where $\zeta = e(w)$ for a complex number $w$, is a weak Jacobi form of weight 2 and index $p$. Meanwhile, using theta correspondence, Bruinier and Funke [1] generalized Zagier's trace formula to traces of CM values of modular functions of arbitrary level. In particular, they showed that if $p$ is an odd prime and $f = \sum a(n)q^n$ is a modular function for $\Gamma^*_0(p)$ with $a(0) = 0$, then

\[
\sum_{D \equiv \Box \pmod{4p}} t^*_f(D)q^D + \sum_{n \geq 1} (\sigma(n) + p\sigma(n/p))a(-n) - \sum_{m \geq 1} \sum_{n \geq 1} ma(-mn)q^{-m^2}
\]

is a weakly holomorphic modular form of weight $3/2$ and level $4p$.

We will obtain in the next section, the following exact formula for $t^*_f(D)$ which is a generalization of (1).

**Theorem 1.1.** Suppose $f$ is a modular function for $\Gamma^*_0(p)$ with principal part $\sum_{m=1}^N a_m e(-mz)$ at $i\infty$ and define for any positive integers $m$ and $c$,

\[
S_D(m, c) = \sum_{x^2 \equiv -D \pmod{c}} e(2mx/c).
\]

Then

\[
t^*_f(D) = \sum_{m=1}^N a_m \left[ c_m H^*_p(D) + \sum_{c > 0 \pmod{4p}} \quad \sum_{c \equiv 0 \pmod{4p}} S_D(m, c) \sinh \left( \frac{4\pi m\sqrt{D}}{c} \right) \right],
\]

where $c_m = -24 \left( \frac{-p^{\alpha+1}}{p+1} \sigma(m/p^\alpha) + \sigma(m) \right)$ with $p^\alpha || m$. 


As an example, consider
\[ f = \left( \frac{\eta(z)}{\eta(37z)} \right)^2 - 2 + 37 \left( \frac{\eta(37z)}{\eta(z)} \right)^2, \]
where \( \eta(z) \) is the Dedekind eta function defined by \( \eta(z) = q^{1/24} \prod_{n=1}^{\infty} (1 - q^n) \).
Then \( f \) is a modular function for \( \Gamma^*_0(37) \) which is of genus 1 and has a Fourier expansion of the form \( q^{-3} - 2q^{-2} - q^{-1} + 0 + O(q) \). Since the representatives for \( \mathcal{Q}_{148,37,0}/\Gamma_0(37) \) are given by \([37, 0, 1]\) and \([74, -74, 19]\), we find from equations (2), (3), and Theorem 1.1 that
\[
24 \cdot \frac{3}{38} + \sum_{c > 0, \, c \equiv 0 \pmod{148}} \left[ S_D(3, c) \sinh \left( \frac{12\pi \sqrt{D}}{c} \right) - 2S_D(2, c) \sinh \left( \frac{8\pi \sqrt{D}}{c} \right) \right] - S_D(1, c) \sinh \left( \frac{4\pi \sqrt{D}}{c} \right) = \frac{1}{2} \left[ f \left( \frac{\sqrt{37}i}{37} \right) + f \left( \frac{37 + \sqrt{37}i}{74} \right) \right],
\]
where the latter is known to be \(-2\).

2. Proof of Theorem 1.1

Throughout this section, \( \Gamma \) denotes \( \Gamma^*_0(p) \). For a positive integer \( m \) we consider Niebur’s Poincaré series [6]
\[
F_m(z, s) = \sum_{M \in \Gamma \setminus \Gamma^*_0} e(-mReMz)(ImMz)^{1/2}I_{s-1/2}(2\pi m\Im Mz),
\]
where \( I_{s-1/2} \) is the modified Bessel function of the first kind. Then \( F_m(z, s) \) converges absolutely for \( \Re s > 1 \) and satisfies
\[
F_m(Mz, s) = F_m(z, s) \text{ for } M \in \Gamma \text{ and } \Delta F_m(z, s) = s(1 - s)F_m(z, s),
\]
where \( \Delta \) is the hyperbolic Laplacian \( \Delta = -y^2(\partial_x^2 + \partial_y^2) \) for \( z = x + iy \). Niebur showed that \( F_m(z, s) \) has an analytic continuation to \( s = 1 \) [6, Theorem 5] and that \( F_m(z, s) \) has the following Fourier expansion [6, Theorem 1]; for \( \Re s > 1 \),
\[
F_m(z, s) = e(-mx)y^{1/2}I_{s-1/2}(2\pi my) + \sum_{n=-\infty}^{\infty} b_n(y, s; -m)e(nx),
\]
where \( b_n(y, s; -m) \to 0 \) (\( n \neq 0 \)) exponentially as \( y \to i\infty \). Hence the pole of \( F_m(z, 1) \) at \( i\infty \) may occur only in \( e(-mx)y^{1/2}I_{1/2}(2\pi my) \), which is equal
to
\[
\frac{1}{\pi y^{1/2}m^{1/2}} \sinh(2\pi my)y^{1/2}e(-mx) = \frac{1}{2\pi m^{1/2}} (e(-mz) - e(-m\bar{z})).
\]

So if we multiply \( F_m(z, 1) \) by \( 2\pi m^{1/2} \), then the coefficient of \( e(-mz) \) is normalized. Now we need to compute the constant term in \( (2\pi m^{1/2})F_m(z, 1) \).

It follows from [6, Theorem 1] that \( b_0(y, s, -m) = a_m(s)y^{1-s}/(2s - 1) \). Here
\[
a_m(s) = 2\pi^s m^{s-1/2} \phi_m(s)/\Gamma(s) \quad \text{and} \quad \phi_m(s) = \sum_{c > 0} S(m, 0; c) c^{-2s},
\]

where \( S(m, n; c) \) is the general Kloosterman sum \( \sum_{0 \leq d < (n/c)} e((ma + nd)/c) \) for \((a \ b \ c \ d) \in \Gamma \). Note that if \( M = (a \ b \ c \ d) \in \Gamma = \Gamma_0(p) \), then \( M \in \Gamma_0(p) \) or \( M \) is of the form \((\sqrt{p} y/\sqrt{p}) \) with \( x, y, z, w \in \mathbb{Z} \). In the former case, \( c \) is a multiple of \( p \) and in the latter case, \( c = \sqrt{p}z \) with \( p \nmid z \). For \( n \in \mathbb{Z}^+ \), let \( u_m(n) \) denote the sum of \( m \)-th powers of primitive \( n \)-th roots of unity. We observe that
\[
S(m, 0; c) = \begin{cases} u_m(c), & \text{if } p \mid c, \\ u_m(z), & \text{if } c = \sqrt{p}z \text{ with } p \nmid z. \end{cases}
\]

If we define \( u_m^*(n) = \begin{cases} u_m(n), & \text{if } p \mid n, \\ p^{-s}u_m(n), & \text{if } p \nmid n. \end{cases} \), then
\[
p^s \phi_m(s)\zeta(2s) = p^s \sum_{c > 0} S(m, 0; c)c^{-2s} \sum_{c' \in \mathbb{Z}^+} c'^{-2s}
\]
\[
= \sum_{c \in \mathbb{Z}^+} (p^s u_m^*(c))^{-2s} \sum_{c' \in \mathbb{Z}^+} c'^{-2s} = \sum_{k \in \mathbb{Z}^+} \left( \sum_{c \mid k} p^s u_m^*(c) \right) k^{-2s}.
\]

Note that if \( p \nmid k \), then
\[
\sum_{c \mid k} p^s u_m^*(c) = \sum_{c \mid k} u_m(c) = \begin{cases} k, & \text{if } k \mid m, \\ 0, & \text{if } k \nmid m. \end{cases}
\]

and if \( k = p^l k' \) with \( l \geq 1 \) and \( p \nmid k' \), then
\[
\sum_{c \mid k} p^s u_m^*(c) = \sum_{d \mid k'} p^s u_m^*(c) = \sum_{d \mid k'} u_m(d) + \sum_{c \mid k} p^s u_m(c).
\]

By adding \( (p^s - 1) \sum_{d \mid k'} u_m(d) \) on both sides of (11), we obtain
\[
(p^s - 1) \sum_{d \mid k'} u_m(d) + \sum_{c \mid k} p^s u_m^*(c) = \sum_{c \mid k} p^s u_m(c).
\]
Thus simple calculations lead us to have the constant term of \((2 \pi m^{1/2})F_m(z, 1)\) as

\[
\sum_{c \mid k} p^s u_m(c) = \begin{cases} 
p^s k, & \text{if } k \mid m, \\
0, & \text{if } k \nmid m,
\end{cases}
\]

we find that

\[
\sum_{c \mid k} p^s u_m(c) = \begin{cases} 
p^s k + (1 - p^s)k', & \text{if } k \mid m, \\
(1 - p^s)k', & \text{if } k \nmid m \text{ and } k' \mid m, \\
0, & \text{if } k \nmid m \text{ and } k' \nmid m.
\end{cases}
\]

Writing \(m = p^{\alpha} m'\) with \(p \nmid m'\), we can deduce from (10) and (12) that

\[
\sum_{k \in \mathbb{Z}_+} (\sum_{c \mid k} p^s u_m(c)) k^{-2s} = \sum_{k' \mid m'} \sum_{l = 1}^{\infty} (1 - p^s)k'(p^l k')^{-2s}
\]

\[
+ \sum_{l = 1}^{\infty} \sum_{k' \mid m'} p^s(p^l k')^{-2s} = \sigma_{1-2s}(m') + (1 - p^s)\sigma_{1-2s}(m') \sum_{l = 1}^{\infty} (p^{-2s})^l + p^s \sum_{1 \leq l \leq \alpha} k' \mid m' (p^l k')^{-1-2s}
\]

\[
= \sigma_{1-2s}(m') \left[ 1 + (1 - p^s) \frac{p^{-2s}}{1 - p^{-2s}} \right] + p^s(\sigma_{1-2s}(m) - \sigma_{1-2s}(m'))
\]

\[
\sum_{k \in \mathbb{Z}_+} (\sum_{c \mid k} p^s u_m(c)) k^{-2s} = \sigma_{1-2s}(m) - \sigma_{1-2s}(m')
\]

Recall the constant term in \((2 \pi m^{1/2})F_m(z, 1)\) 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 (8), it is equal to

\[
\lim_{s \to 1} 2\pi m^{1/2} (2\pi m^{-1/2} \phi_m(s)/\Gamma(s)) y^{1-s}/(2s - 1).
\]

It follows from (9) and (13) that this limit goes to

\[
\frac{4\pi^2 m}{\pi \zeta(2)} \left( \frac{-p^2}{1 + p} \sigma_{-1}(m/p^\alpha) + p \sigma_{-1}(m) \right)
\]

Thus simple calculations lead us to have the constant term of \((2 \pi m^{1/2})F_m(z, 1)\) as

\[
24 \left( \frac{-p^{\alpha+1}}{1 + p} \sigma(m/p^\alpha) + \sigma(m) \right) = -c_m.
\]

Now we define

\[
F_m^*(z, s) = (2 \pi m^{1/2})F_m(z, s) + c_m.
\]
Then by (5), (6), and (7), $F_m^*(z, 1)$ is $\Gamma$-invariant harmonic function and $F_m^*(z, 1) - e(-mz)$ has a zero at $i\infty$. Hence it follows from [6, Theorem 6] that

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

for any modular function $f$ for $\Gamma_0^*(p)$ with principal part $\sum_{m=1}^{N} a_m e(-mz)$ at $i\infty$. Hence (15)

$$t^*_f(D) = \sum_{m=1}^{N} a_m \left( \sum_{Q \in \mathbb{Q}_{D,p} / \Gamma} \frac{1}{|\Gamma_Q|} F_m^*(z_Q, 1) \right).$$

In order to determine the value $\sum_{Q \in \mathbb{Q}_{D,p} / \Gamma} \frac{1}{|\Gamma_Q|} F_m^*(z_Q, 1)$, we first compute for $\text{Re } s > 1$,

(16)

$$\sum_{Q \in \mathbb{Q}_{D,p} / \Gamma} \frac{1}{|\Gamma_Q|} F_m^*(z_Q, s) = c_m H_p^*(D) + 2\pi \sqrt{m} \sum_{Q \in \mathbb{Q}_{D,p} / \Gamma} \frac{1}{|\Gamma_Q|} F_m(z_Q, s).$$

By Poincaré series expansion of $F_m(z_Q, s)$ in (4),

$$2\pi \sqrt{m} \sum_{Q \in \mathbb{Q}_{D,p} / \Gamma} \frac{F_m(z_Q, s)}{|\Gamma_Q|} = 2\pi \sqrt{m} \sum_{Q \in \mathbb{Q}_{D,p} / \Gamma} e(-m \text{Re } z_Q)(\text{Im } z_Q)^{1/2} I_{s-1/2}(2\pi m \text{Im } z_Q).$$

The series in the latter is equal to

$$\sum_{\substack{a=1 \atop x \equiv \pm d \pmod{4ap}}}^{\infty} e \left( \frac{2mb}{4pa} \right) \left( \frac{2\sqrt{D}}{4pa} \right)^{1/2} I_{s-1/2} \left( 2\pi m \frac{2\sqrt{D}}{4pa} \right)$$

$$= \sum_{c>0 \atop c \equiv 0 \pmod{4p}} S_D(m, c) \left( \frac{2\sqrt{D}}{c} \right)^{1/2} I_{s-1/2} \left( 2\pi m \frac{2\sqrt{D}}{c} \right),$$

which converges uniformly for $s \in [1, 2]$. Therefore, by (16),

$$\sum_{Q \in \mathbb{Q}_{D,p} / \Gamma} \frac{1}{|\Gamma_Q|} F_m^*(z_Q, 1) = c_m H_p^*(D) + \sum_{c>0 \atop c \equiv 0 \pmod{4p}} S_D(m, c) \sinh \left( \frac{4\pi m \sqrt{D}}{c} \right).$$

This combined with (15) completes the proof.
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Dohoon Choi, School of Mathematics, Korea Institute for Advanced Study, Seoul 130-722, Korea
E-mail address: choija@kias.re.kr

Daeyeol Jeon, Department of Mathematics Education, Kongju National University, Kongju 314-701, Chungnam, Korea
E-mail address: dyjeon@kongju.ac.kr

Soon-Yi Kang, School of Mathematics, Korea Institute for Advanced Study, Seoul 130-722, Korea
E-mail address: sykang@kias.re.kr

Chang Heon Kim, Department of Mathematics, Seoul Women’s University, Seoul, 139-774, Korea
E-mail address: chkim@swu.ac.kr