Modular forms and $q$-analogues of modified double zeta values

Henrik Bachmann

Abstract
We present explicit formulas for Hecke eigenforms as linear combinations of $q$-analogues of modified double zeta values. As an application, we obtain period polynomial relations and sum formulas for these modified double zeta values. These relations have similar shapes as the period polynomial relations of Gangl, Kaneko, and Zagier and the usual sum formulas for classical double zeta values.

Keywords Modular forms · Double zeta values · Period polynomials · Hecke operators

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1 Introduction

In [4] Gangl, Kaneko and Zagier gave an explicit connection between cusp forms for the full modular group of weight $r + s$ and $\mathbb{Q}$-linear relations among the double zeta values

$$\zeta(r, s) = \sum_{0 < m < n} \frac{1}{m^r n^s}, \quad (r \geq 1, s \geq 2).$$

For example, one of the consequences of their work (see Remark 4.9) is that the first non-trivial cusp form $\Delta(q) = q \prod_{n>0}(1 - q^n)^{24}$ in weight 12 gives rise to the relation

$$14\zeta(3, 9) + 42\zeta(4, 8) + 75\zeta(5, 7) + 95\zeta(6, 6) + 84\zeta(7, 5) + 42\zeta(8, 4) = \frac{6248}{691}\zeta(12). \quad (1.1)$$

The connection of this relation to the cusp form $\Delta$ is given by the fact that the coefficients on the left-hand side are obtained by the even period polynomial of $\Delta$.

In this note we will show a similar result for the following modified version of the double zeta values

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\[ \zeta(r, s) = \sum_{0 < n < \frac{1}{m+n}^{-r-s}} \frac{1}{(m+n)^{r+s}}, \quad (r \geq 1, s \geq 2), \]

and give an even more direct connection between cusp forms and linear relation among them. The values (1.2) are special cases of Apostol-Vu double zeta values or Witten zeta functions for \( \mathfrak{so}(5) \) (see [8, 10]). As an analogue of the relation (1.1) we obtain

\[ 14\zeta(3, 9) + 42\zeta(4, 8) + 75\zeta(5, 7) + 95\zeta(6, 6) + 84\zeta(7, 5) + 42\zeta(8, 4) = \frac{1639}{176896}\zeta(12), \]

which is not a trivial consequence of (1.1), since it is expected that \( \zeta(r, s) \) is in general not a linear combination of \( \zeta(r, s) \) and \( \zeta(r+s) \). We will see in Eq. (4.6) that \( \zeta(r, s) \) can be written in terms of alternating multiple zeta values, which conjecturally are not expressible in terms of ordinary multiple zeta values. The connection of relation (1.3) and the cusp form \( \Delta \) will be made explicit by writing \( \Delta \) as a linear combination of \( q \)-analogues of the modified double zeta values \( \zeta(r, s) \) and the Riemann zeta value \( \zeta(k) \). These are \( q \)-series \( \zeta_q(r, s), \zeta_q(k) \in \mathbb{Q}[[q]] \) which degenerate to \( \zeta(r, s) \) and \( \zeta(k) \) respectively, as \( q \to 1 \) (see Lemma 2.2). In general we will write any Hecke eigenform as a linear combination of this \( q \)-analogue and a “lower-weight” \( q \)-series, which vanishes after normalization as \( q \to 1 \).

We denote by \( M_k \) and \( S_k \) the spaces of modular forms and cusp forms of weight \( k \) for the full modular group. The first result of this work is the following.

**Theorem 1.1** Let \( f \in S_k \) be a cuspidal Hecke eigenform with restricted even period polynomial \( P_f^{\nu, 0} \) (see (4.1) for the definition). Define the coefficients \( q_{f, rs} \in \mathbb{C} \) by

\[ P_f^{\nu, 0}(X + Y, X) = \sum_{\substack{r + s = k \\ \text{odd} \\ r, s \geq 1}} \binom{k-2}{r-1} q_{f, rs} X^{r-1} Y^{s-1} \quad \text{(1.4)} \]

Then

\[ \frac{L_f^*(1)}{2(k-2)!} f(q) = \sum_{\substack{r + s = k \\ \text{odd} \\ r, s \geq 2}} q_{f, rs} \zeta_q(r, s) - \lambda_f \zeta_q(k) - R_f(q), \]

where \( L_f^* \) is the completed L-function of \( f \) (see (3.2)), \( R_f(q) \in \mathbb{C}[[q]] \) is an explicitly given “lower weight” \( q \)-series (see Lemma 4.6) and

\[ \lambda_f = \frac{k-1}{2} \left( \sum_{\substack{r + s = k \\ r, s \geq 3 \ \text{odd}}} \frac{(-1)^{r-1}}{r 2^{r-1}} \binom{k-2}{s-1} L_f^*(s) - L_f^*(1) \right). \quad \text{(1.5)} \]

We will see that, for a cusp form \( f \in S_k \), the terms \( (1-q)^k R_f(q) \) and \( (1-q)^k f(q) \) vanish as \( q \to 1 \). As a corollary of our result we therefore obtain the following analog of the result of Gangl, Kaneko and Zagier for the values \( \zeta(r, s) \).

**Corollary 1.2** For any cusp form \( f \in S_k \) the following relation holds

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where the coefficients $d_{r,s}^f$ and $\lambda_f$ are given by (1.4) and (1.5) respectively.

By the work of Kohnen and Zagier [5] it is known that there exists a basis of cusp forms $\{f_i\}$ for $S_k$ such that $P_{f_i,0}^{ev}(X,Y) \in \mathbb{Q}[X,Y]$. Therefore, Corollary 1.2 gives $(\dim S_k)$-many $\mathbb{Q}$-linear relations among the modified double zeta values. As the second result of this work we will write the $q$-analogue $\hat{\zeta}(k)$, which is just the Eisenstein series of weight $k$ without constant term, as a sum over all $\hat{\zeta}(r,s)$ with $r + s = k$ and another explicitly given “lower-weight” $q$-series $E_k(q)$.

**Theorem 1.3** For all even $k \geq 4$ we have

$$\zeta_q(k) = 2^{k-1} \sum_{r + s = k, \ r \geq 1, \ s \geq 2} \hat{\zeta}(r,s) - E_k(q),$$

where the $q$-series $E_k(q) \in \mathbb{Q}[[q]]$ is given by (4.5).

Again by considering $q \to 1$ the term $(1 - q^k)E_k(q)$ vanishes and we get, for the even weight case (the odd weight case will be proven separately), the following sum formula.

**Theorem 1.4** For all $k \geq 3$ we have

$$\zeta(k) = 2^{k-1} \sum_{r + s = k, \ r \geq 1, \ s \geq 2} \hat{\zeta}(r,s).$$

**Remark 1.5** Numerically also Theorem 1.3 holds for any $k \geq 3$ and Theorem 1.4 should be a Corollary of this general version. But since we are using the period polynomials of the Eisenstein series, our proof of Theorem 1.3 is just valid for even $k \geq 4$. One might get a proof of Theorem 1.3 for all $k \geq 3$ by trying to adapt the proof of Theorem 1.4 for the $q$-versions of the appearing objects.

The contents of this paper are as follows. In Section 2 we start by giving the definition of the $q$-analogues of the modified double zeta values $\hat{\zeta}(r,s)$. For the proof of Theorems 1.1 and 1.3, we need the theory of Hecke operators for period polynomials of modular forms, which we will introduce in Section 3. Finally, we write any modular form as a linear combination of $q$-analogues in Section 4 and give the proofs of our main results.

## 2 $q$-analogues of modified double zeta values

In this section we will introduce $q$-analogues of the modified double zeta value $\hat{\zeta}(r,s)$. For classical double (or multiple) zeta values there are various works on different models of $q$-analogues in the literature. An easy way to obtain a $q$-analogue of a zeta value is to
replace the appearing natural numbers \( n \) in the definition by their \( q \)-analogues \( [n]_q = \frac{1 - q^n}{1 - q} \), which satisfy \( \lim_{q \to 1} [n]_q = n \). In general a sum of the form

\[
\sum_{0 < m < n} \frac{Q_r(q^{m+n})}{[m+n]^q} \frac{Q_s(q^n)}{[n]_q},
\]

where \( Q_r(t), Q_s(t) \in t\mathbb{Q}[t] \) are polynomials satisfying \( Q_r(1) = Q_s(1) = 1 \), gives a \( q \)-analogue of \( \hat{\zeta}(r,s) \). In the context of modular forms it is convenient to remove the global factor \((1 - q)^{r+s}\) from the definition of these \( q \)-analogues and to use the polynomials \( Q_k(t) \in t\mathbb{Q}[t] \) defined for \( k \geq 1 \) by

\[
\frac{Q_1(t)}{(1 - t)^k} = \frac{1}{(k-1)!} \sum_{d > 0} d^{k-1} t^d.
\] (2.1)

We have \( Q_1(t) = t \) and for \( k \geq 2 \) the \( Q_k(t) \) are polynomials of degree \( k - 1 \) satisfying \( Q_k(1) = 1 \). These are, up to the factorial factor, the so-called Eulerian polynomials (c.f. [1, Remark 2.6]).

**Definition 2.1** For \( k, r, s \geq 1 \) define the \( q \)-analogues of \( \zeta(k) \) and \( \hat{\zeta}(r,s) \) by

\[
\zeta_q(k) = \sum_{n > 0} \frac{Q_r(q^n)}{(1 - q^n)^k},
\]
\[
\hat{\zeta}_q(r,s) = \sum_{0 < m < n} \frac{Q_r(q^{m+n})}{(1 - q^{m+n})^r} \frac{Q_s(q^n)}{(1 - q^n)^s},
\]

where the polynomials \( Q_j(t) \) for \( j \geq 1 \) are defined by (2.1).

**Lemma 2.2**

(i) For \( k \geq 2 \) and \( r \geq 1, s \geq 2 \) we have

\[
\lim_{q \to 1} (1 - q)^k \zeta_q(k) = \zeta(k), \quad \lim_{q \to 1} (1 - q)^{r+s} \hat{\zeta}_q(r,s) = \hat{\zeta}(r,s).
\]

In particular \( \lim_{q \to 1} (1 - q)^k \zeta_q(k') = \lim_{q \to 1} (1 - q)^k \hat{\zeta}_q(r,s) = 0 \) if \( k', r + s < k \).

(ii) If \( f(q) = \sum_{n \geq 0} a_n q^n \in M_k \) is a modular form of weight \( k \), then

\[
\lim_{q \to 1} (1 - q)^k f(q) = (-2\pi i)^k a_0.
\]

In particular,

\[
\lim_{q \to 1} (1 - q)^k f(q) = 0
\]

if \( f \in S_k \).

**Proof** This follows from Proposition 6.4 and Corollary 6.5 in [1], where the notation \([k] = \zeta_q(k)\) is used. The result for \( \hat{\zeta}_q(r,s) \) follows along a similar argument as given there for the \( q \)-series \([r,s]\). \( \square \)
3 Period polynomials and Hecke operators

We recall the definition and results on period polynomials as they are presented in [14, 15] and [16]. For even $k \geq 4$, denote by $V_k \subset \mathbb{C}[X,Y]$ the space of homogeneous polynomials in two indeterminates of degree $k - 2$. The group $\text{SL}_2(\mathbb{Z})$ acts on the space $V_k$ by

$$ (P|\gamma)(X,Y) = P(aX + bY, cX + dY) \quad \left( P \in V_k, \gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \text{SL}_2(\mathbb{Z}) \right). \quad (3.1) $$

Denote by $S$ and $U$ the following elements in $\text{SL}_2(\mathbb{Z})$:

$$ S = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad U = \begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix}. $$

For a modular form $f(\tau) = \sum_{n \geq 0} a_n q^n \in M_k$, where as usual $\tau$ is an element in the complex upper-half plane, i.e. $\Im(\tau) > 0$, and $q = \exp(2\pi i \tau)$, define the even (extended) period polynomial of $f$ by

$$ P_{f}^{ev}(X,Y) = \sum_{s \geq 1} \left(-1\right)^{s-1} \left( \frac{s}{2} \right) L_f^{-s}(s) X/y^{s-1} \in V_k. $$

Here the $L_f^{-s}(s)$ denotes the normalized $L$-series $L_f(s) = \sum_{n \geq 1} a_n n^{-s}$ of $f$ multiplied by its gamma-factor

$$ L_f^{-s}(s) = \int_0^\infty (f(iy) - a_0) y^{s-1} dy = (2\pi)^{-s} \Gamma(s) L(f,s). \quad (\text{for } \Re(s) > 0) \quad (3.2) $$

The function $L_f^{-s}(s)$ has a meromorphic continuation to the entire complex plane, with possible simple poles at $s = 0$ and $s = k$, and satisfies the functional equation $L_f^{-s}(s) = (-1)^s L_f^{-k-s}(k-s)$. Using the modular transformation of $f$, one can check that $P_f^{\text{ev}}$ vanishes under the action of $1 + S$ and $1 + U + U^2$ and therefore it is an element of the space

$$ W_k = \left\{ P \in V_k \mid P(1 + S) = P(1 + U + U^2) = 0 \right\}. $$

We decompose $W_k = W_k^{\text{ev}} \oplus W_k^{\text{od}}$ into the even and odd polynomials and therefore have $P_f^{\text{ev}} \in W_k^{\text{ev}}$. As a generalization of the classical Eichler–Shimura isomorphism, which deals with the case of a cusp form $f$, Zagier proved the following.

**Theorem 3.1** [15] The map $f \mapsto P_f^{\text{ev}}$ is an isomorphism from $M_k$ to $W_k^{\text{ev}}$. 

One of the most important structures on the space $M_k$ is the action of the Hecke algebra. For $n \in \mathbb{Z}_{\geq 1}$ denote by $T_n \in \text{End}(M_k)$ the $n$-th Hecke operator. A natural question is, if there is an operator on $W_k^{\text{ev}}$, which corresponds, with respect to the isomorphism in Theorem 3.1, to the operator $T_n$ on $M_k$. One such operator was first given in [14]; to define it, we first write $M_n = \{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \mid a, b, c, d \in \mathbb{Z}, ad - bc = n \}$ and extend the action (3.1) by linearity to an action of the algebra $\bigoplus_{n \geq 1} \mathbb{Q}[M_n]$ on $V_k$. For $n \in \mathbb{Z}_{\geq 1}$ we then define the element
Theorem 3.2 The action of $\tilde{T}_n$ on $W_{k}^\text{ev}$ corresponds to the action of $T_n$ on $W_k$, i.e. we have for all $f \in M_k$

$$P_{T_n}^\text{ev}(X, Y) = P_f^\text{ev}|\tilde{T}_n(X, Y).$$

(3.3)

Proof This is Theorem 2 in [14] or Theorem 3 in [3].

4 Modular forms as $q$-analogues of double zeta values

To simplify our notation, define the following pairing of a polynomial $P(X, Y) \in \mathbb{C}[X, Y]$ and an element $T = \sum_{\gamma} t_{\gamma} \in \mathbb{Q}[M_n]$:

$$\langle P, T \rangle := \sum_{\gamma = \left(\begin{array}{cc} a & b \\ c & d \end{array}\right)} t_{\gamma} P(b, d).$$

With this we obtain the following consequence of Theorem 3.2, which gives an explicit formula for the Fourier coefficients of Hecke eigenforms.

Lemma 4.1 Let $f = \sum_{n \geq 0} a_n q^n \in M_k$ be a Hecke eigenform, i.e. $T_n f = a_n f$. Then for $n \geq 1$,

$$a_n = -\frac{1}{L_f^*(1)} \langle P_f^\text{ev}, \tilde{T}_n \rangle.$$ 

Proof It is is well-known that zeros of $L_f^*(s)$, for a cuspidal Hecke eigenform $f$, can only occur inside the critical strip $\frac{k-1}{2} < \Re(s) < \frac{k+1}{2}$; in particular, $L_f^*(1) \neq 0$. Also $L_{G_k}^*(1) \neq 0$ for the normalized Eisenstein series $G_k$. Setting $(X, Y) = (0, 1)$ in (3.3), the left-hand side becomes $P_{T_n}^\text{ev}(0, 1) = a_n P_f^\text{ev}(0, 1) = a_n(-1)^{\frac{k-1}{2}} L_f^*(k-1) = -a_n L_f^*(1)$ and the right-hand side is $P_f^\text{ev}|\tilde{T}_n(1, 0) = \langle P_f^\text{ev}, \tilde{T}_n \rangle$ by the definition of the pairing, from which the statement follows.

Remark 4.2 A similar formula as in Lemma 4.1 for the Fourier coefficients of cusp forms was already given by Manin in [7, Section 1.3].

Corollary 4.3 For even $k \geq 4$ and $n \geq 1$ we have

$$\sigma_{k-1}(n) = \sum_{d|n} d^{k-1} = \langle Y^{k-2} - X^{k-2}, \tilde{T}_n \rangle.$$ 

Proof This follows directly from Lemma 4.1, since the normalized Eisenstein series $G_k(\tau) = -\frac{B_k}{2k} + \sum_{n \geq 0} \sigma_{k-1}(n) q^n$ is a Hecke eigenform with the period polynomial $P_{G_k}^\text{ev} = L_{G_k}^*(1)(X^{k-2} - Y^{k-2})$ (see the first proposition in Section 2 of [15]).

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To prove Theorem 1.1 we will calculate $\langle P_{ev}^0, \hat{T}_n \rangle$ explicitly. First we define the even restricted period polynomial $P_{ev}^0$ of a modular form $f \in M_k$ by

$$P_{ev}^0(X, Y) = P_{e}^0(X, Y) - L_f^*(1)(X^{k-2} - Y^{k-2}) = \sum_{r + s = k, r, s \geq 3 \text{ odd}} (-1)^{\frac{k+1}{2}} \binom{k-2}{s-1} L_f^*(s) X^{r-1} Y^{s-1}. \quad (4.1)$$

**Lemma 4.4** For a cuspidal Hecke eigenform $f \in S_k$ we have

$$f(q) = (k-1)! \zeta_q(k) - \frac{1}{L_f^*(1)} \sum_{n>0} \langle P_{ev}^0, \hat{T}_n \rangle q^n. \quad \text{Proof} \quad \text{This follows from Corollary 4.3 together with (4.1) and the fact that the coefficients of } \zeta_q(k) \text{ are given by the divisor-sum } \sigma_{k-1}(n):$$

$$\zeta_q(k) = \sum_{n>0} \frac{Q_k(q^n)}{(1-q^n)^k} = \frac{1}{(k-1)!} \sum_{n>0} \sum_{d>0} d^{k-1} q^d = \frac{1}{(k-1)!} \sum_{n>0} \sigma_{k-1}(n) q^n. \quad \square$$

It remains to evaluate $\langle P_{ev}^0, \hat{T}_n \rangle$. For this we write $\hat{T}_n = \hat{T}_n^{(1)} + \hat{T}_n^{(2)} + \hat{T}_n^{(3)}$ with

$$\hat{T}_n^{(1)} = \sum_{ad-bc=n, a>c>0, d>-b>0} \left( \begin{array}{cc} a & b \\ c & d \end{array} \right), \quad \hat{T}_n^{(2)} = \sum_{ad=n, -\frac{d}{2} < b \leq \frac{d}{2}} \left( \begin{array}{cc} a & b \\ 0 & d \end{array} \right), \quad \hat{T}_n^{(3)} = \sum_{ad=n, \frac{a}{2} < c \leq \frac{a}{2}, c \neq 0} \left( \begin{array}{cc} a & 0 \\ c & d \end{array} \right).$$

In the following we will calculate $\sum_{n>0} \langle P_{ev}^0, \hat{T}_n^{(j)} \rangle q^n$ individually for $j = 1, 2, 3$, before combining them in the end for the proof of Theorem 1.1.

**Lemma 4.5** For a cusp form $f \in S_k$ we have

$$\sum_{n>0} \langle P_{ev}^0, \hat{T}_n^{(1)} \rangle q^n = -2(k-2)! \sum_{r+s=k, r, s \geq 2} q_{r,s} \zeta_q(r,s),$$

where the coefficients $q_{r,s}$ are given by (1.4).

**Proof** By direct calculation and the fact that $P_{ev}^0$ is an even polynomial, we obtain
The limits of \( P_{f}^{\text{ev},0}(X + Y, X) \) are always zero. The even and odd \( P_{f}^{\text{ev},0}(b + d, b) \) and odd \( P_{f}^{\text{ev},0}(b + d + b) \) and odd variants will just appear in lower weights and their limits will always vanish.

By Definition 2.1 we have
\[
\zeta_{q}(r, s) = \sum_{a > c > 0} \frac{Q_{r}(q^{a+c})}{(1 - q^{a+c})^{r}} \frac{Q_{s}(q^{a})}{(1 - q^{a})^{s}} = \sum_{a > c > 0} \frac{b^{r-1} d^{s-1}}{(r-1)! (s-1)!} q^{(a+c)b+ad}.
\]

Since \( P_{f}^{\text{ev},0}(X, 0) = P_{f}^{\text{ev},0}(0, Y) = 0 \) and \( P_{f}^{\text{ev},0}((1 + U + U^{2}) = 0 \) it follows that \( q_{r,1}^{f} = q_{1,s}^{f} = 0 \). Combining this together with (4.2) and (4.3) we obtain the desired result.

To evaluate \( \sum_{n>0} (P_{f}^{\text{ev},0}, \tilde{T}_{n}^{(1)}) q^{n} \) we will introduce some further notation. For \( k \geq 1 \) we define the even and odd \( q \)-analogues of the single zeta value by
\[
\zeta_{q}^{\text{e}}(k) = \sum_{a, d > 0 \atop d \text{ even}} \frac{d^{k-1}}{(k-1)!} q^{ad}, \quad \zeta_{q}^{\text{o}}(k) = \sum_{a, d > 0 \atop d \text{ odd}} \frac{d^{k-1}}{(k-1)!} q^{ad}.
\]

The limits of \((1 - q)^{h} \zeta_{q}^{\text{e}}(k)\) and \((1 - q)^{h} \zeta_{q}^{\text{o}}(k)\) as \( q \to 1 \) both are given by rational multiples of \( \zeta(k) \). In the following these even and odd variants will just appear in lower weights and therefore their limits will always vanish.

Lemma 4.6 For a cusp form \( f \in S_{k} \) with even restricted period polynomial
\[
P_{f}^{\text{ev},0}(X, Y) = \sum_{r + s = k \atop r, s \geq 3 \text{ odd}} c_{r,s} X^{r-1} Y^{s-1},
\]
we have
\[ \sum_{n>0} \langle P_f^{e_{n}}, \tilde{T}_n \rangle q^n = \left( \sum_{r+s = k} r+3 \text{ odd} \right) \left( \sum_{r+s = k} \frac{c_{r,s}}{r2^{r-1}} \right) (k-1)!\zeta_q(k) + 2(k-2)!R_f(q), \]

where the q-series \( R_f(q) \) is given by

\[ R_f(q) = \sum_{r+s = k} c_{r,s} \left( \sum_{j=1}^{r-1} \left( \begin{array}{c} r \\ j \end{array} \right) \right) \frac{B_j \cdot (k-j-1)!}{r2^{r-j}(k-2)!} \zeta_q(k-j) - \frac{1}{2r} \zeta_q^e(k-1). \]

**Proof** Again by using the fact that \( P_f^{e_{n}} \) is even and \( P_f^{e_{n}}(0, Y) = 0 \) we obtain

\[ \sum_{n>0} \langle P_f^{e_{n}}, \tilde{T}_n \rangle q^n = \sum_{r+s = k} c_{r,s} \left( \sum_{a, d > 0} 2 \sum_{0 < b \leq \frac{d}{2}} b^{r-1} d^{r-1} q^{ad} \right) \frac{1}{2^{r-1}} \sum_{a, d > 0} d^{k-2} q^{ad}. \]

Now by using the well-known formula

\[ \sum_{b=1}^{N} b^{r-1} = \frac{1}{r} \sum_{j=0}^{r-1} \left( \begin{array}{c} r \\ j \end{array} \right) B_j N^{r-j}, \]

for the Bernoulli numbers \( B_j \) of the first kind, i.e. \( B_1 = \frac{1}{2} \), we deduce by a straightforward calculation for \( r+s = k \) that

\[ \sum_{a, d > 0} 2 \sum_{0 < b \leq \frac{d}{2}} b^{r-1} d^{r-1} q^{ad} = \frac{(k-1)!}{r2^{r-1}} \zeta_q(k) \sum_{j=1}^{r-1} \left( \begin{array}{c} r \\ j \end{array} \right) \frac{B_j \cdot (k-j-1)!}{r2^{r-j}} \zeta_q(k-j) \]

\[ + \sum_{0 \leq j \leq r-1} \sum_{1 \leq l \leq r-j} \left( \begin{array}{c} r \\ j \end{array} \right) \frac{(-1)^j B_j \cdot (k-j-l-1)!}{r2^{r-j}} \zeta_q^e(k-j-l). \]

Combining this with (4.4) implies the result stated. \( \square \)

**Proof of Theorem 1.1** The statement of Theorem 1.1 follows from Lemma 4.4, 4.5, 4.6 and the fact that \( \sum_{n>0} \langle P_f^{e_{n}}, \tilde{T}_n \rangle q^n = 0. \) \( \square \)

**Proof of Corollary 1.2** In [1, Proposition 7.2] it was shown that for a q-series \( f(q) = \sum_{n>0} a_n q^n \) with \( a_n = O(n^{K-1}) \) and \( K < k \) one has \( \lim_{q \to 1} (1-q)^{k} f(q) = 0. \) The coefficients of \( \zeta_q(K), \zeta_q^e(K) \) and \( \zeta_q^o(K) \) are all in \( O(n^{K-1}) \) and since in the definition of \( R_f \) just the cases \( K < k \) (where \( k \) is the weight of \( f \)) appear, we get \( \lim_{q \to 1} (1-q)^{k} R_f(q) = 0. \) Corollary 1.2 therefore follows from Lemma 2.2, Theorem 1.1 and the fact that any cusp form can be written as a linear combination of Hecke eigenforms. \( \square \)
Example 4.7 We give one example for Theorem 1.1. The period polynomial of \( f = (45L_\Delta(9))^{-1} \Delta \) is given by
\[
P_f^{\omega}(X, Y) = \frac{36}{691} (X^{10} - Y^{10}) - X^2 Y^2 (X^2 - Y^2)^3.
\]
In this case the \( q \)-series \( R_f(q) \) can be written as
\[
R_f(q) = \frac{1}{5} \zeta_q(4) + \frac{40}{21} \zeta_q(6) + 21 \zeta_q(8) - \frac{51}{128} \zeta_q^o(4) - \frac{15}{4} \zeta_q^o(6) - \frac{315}{8} \zeta_q^o(8).
\]
By Theorem 1.1 we therefore obtain the following expression for \( \Delta \) from which relation (1.3) follows after multiplying both sides by \( (1 - q)^{12} \) and taking the limit as \( q \to 1 \).

Proof of Theorem 1.3 By Corollary 4.3 we have
\[
(k - 1)! \zeta_q(k) = \sum_{n > 0} \langle Y^{k-2} - X^{k-2}, \tilde{T}_n \rangle q^n.
\]
Using similar calculations as in Lemma 4.5 and 4.6 one can give explicit formulas for \( \sum_{n > 0} \langle Y^{k-2} - X^{k-2}, \tilde{T}_n^{(1)} \rangle q^n \) and \( \sum_{n > 0} \langle Y^{k-2} - X^{k-2}, \tilde{T}_n^{(2)} \rangle q^n \). Together with
\[
\sum_{n > 0} \langle Y^{k-2} - X^{k-2}, \tilde{T}_n^{(3)} \rangle q^n = (k - 3)! q \frac{d}{dq} \zeta_q(k - 2) - (k - 2)! \zeta_q(k - 1)
\]
one then can check that Theorem 1.3 holds with the \( q \)-series \( E_k(q) \) given by
\[
E_k(q) = 2^{k-2} \zeta_q(k - 1) - \frac{2^{k-2}}{(k - 2)!} q \frac{d}{dq} \zeta_q(k - 2) + \sum_{j=2}^{k-2} \frac{2^j B_j}{j!} \zeta_q(k - j) + \sum_{\substack{0 \leq j \leq k - 2 \\ 1 \leq l \leq k - j - 1 \\ (l, j) \neq (1, 0)}} \frac{(-1)^j 2^j B_j}{j! l!} \zeta_q^o(k - j - l).
\]

Proof of Theorem 1.4 For even weight \( k \) Theorem 1.4 follows from Theorem 1.3 with the same arguments as given for Corollary 1.2. But we will give an alternative prove which works also for the odd weight case. First observe that the modified double zeta value can be written as
\[
\zeta(r, s) = \sum_{0 < m < n} \frac{1}{(m + n)^{r+s}} = \sum_{0 < m < n} \frac{1}{m^{r+s}} = \left( \sum_{0 < m < n} - \sum_{0 < m < n} - \sum_{0 < m = n} \right) \frac{1}{m^{r+s}} \tag{4.6}
\]

where \( \text{Li}_{r,s}(z) = \sum_{0 < m < n} \frac{z^m}{m^{r+s}} \) denotes the double polylogarithm. When \( k = r + s \) is odd, it is known, due to the parity result for double polylogarithms (see [2, (75)]), that \( \text{Li}_{r,s}(z) \) can be written explicitly in terms of single polylogarithms. From this one can deduce together with \( \text{Li}_k(1) + \text{Li}_k(-1) = \frac{1}{2^{k-1}} \text{Li}_k(1) = \frac{1}{2^{k-1}} \zeta(k) \), that

\[
\sum_{r + s = k, r \geq 1, s \geq 2} 2^{s-1} \text{Li}_{r,s}(-1) = \frac{1}{2^{k-1}} \zeta(k) + \frac{k-3}{2} \zeta(k). \tag{4.7}
\]

But formula (4.7) holds for all \( k \geq 3 \), as it was shown in [13, Theorem 3.6]. Now using the following sum formulas for double zeta values (see [11])

\[
\sum_{r + s = k, r \geq 1, s \geq 2} \zeta(r, s) = \zeta(k), \quad \sum_{r + s = k, r \geq 1, s \geq 2} 2^{s-1} \zeta(r, s) = \frac{(k + 1)}{2} \zeta(k),
\]

we obtain together with (4.6)

\[
\sum_{r + s = k, r \geq 1, s \geq 2} \zeta(r, s) = \frac{1}{2^{k-1}} \zeta(k) + \frac{k-3}{2} \zeta(k) + \frac{(k + 1)}{2} \zeta(k) - (k - 1) \zeta(k) = \frac{1}{2^{k-1}} \zeta(k).
\]

We end this note by giving examples for Theorem 1.3 and some general remarks.

**Example 4.8** For \( k = 4, 6 \) Theorem 1.3 gives the following expressions for \( \zeta_q(k) \).

\[
\zeta_q(4) = 8(\hat{\zeta}_q(1, 3) + \hat{\zeta}_q(2, 2)) - \frac{1}{3} \zeta_q(2) - 4 \zeta_q(3) + \frac{1}{2} \hat{\zeta}_q(2) + 2q \frac{d}{dq} \zeta_q(2),
\]

\[
\zeta_q(6) = 32(\hat{\zeta}_q(1, 5) + \hat{\zeta}_q(2, 4) + \hat{\zeta}_q(3, 3) + \hat{\zeta}_q(4, 2)) + \frac{1}{45} \zeta_q(2) - \frac{1}{3} \zeta_q(4) - 16 \zeta_q(5)
\]

\[
- \frac{1}{24} \hat{\zeta}_q(2) + \frac{1}{2} \hat{\zeta}_q(4) + 4q \frac{d}{dq} \zeta_q(4).
\]

**Remark 4.9** The result for the classical case of double zeta values, given in [4, Theorem 3], focuses on relations among \( \zeta(r, s) \), where \( r \) and \( s \) are both odd. Their result is that for a cusp forms \( f \in S_k \) the following relation holds

\[
\sum_{r + s = k, r, s \geq 3; \text{odd}} q^f_{r,s} \zeta(r, s) = \beta_f \zeta(k), \tag{4.8}
\]

where the coefficients \( q^f_{r,s} \) are given by (1.4) and the coefficient \( \beta_f \) (first explicitly written down by Ma and Tasaka in [6, Corollary 2.3]) is given by
\begin{equation}
\beta_f = -\frac{1}{2} \left( \frac{k-1}{2} L^*_f(1) + \sum_{r+s = k, r, s \geq 3: \text{odd}} q^f_{r,s} \right) .
\end{equation}

For integers \( a, b \in \mathbb{Z}_{\geq 1} \) the coefficients \( q^f_{r,s} \) satisfy \( q^f_{2a,2b} = q^f_{2b,2a} \). Together with the well-known fact that \( \zeta(2a)\zeta(2b) \in \zeta(2(a + b))\mathbb{Q} \) and the harmonic product formula

\[ \zeta(2a)\zeta(2b) = \zeta(2a, 2b) + \zeta(2b, 2a) + \zeta(2(a + b)), \]

one obtains that also \( \sum_{r+s = k} q^f_{r,s} \zeta(r,s) \) is a multiple of \( \zeta(k) \). This gives the relation (1.1) in the introduction as a consequence of the famous relation

\[ 28\zeta(3, 9) + 150\zeta(5, 7) + 168\zeta(7, 5) = \frac{5197}{691} \zeta(12), \]

which follows from (4.8) by taking for \( f \) a certain multiple of \( \Delta \). For the modified double zeta values the harmonic product formula does not hold and therefore it is not clear if one can reduce our result to the case where \( r \) and \( s \) are both odd.

**Remark 4.10** In [9] the authors introduced (using a different order) double zeta values of level 2 given for \( r \geq 1, s \geq 2 \) by

\[ \zeta^{oe}(r, s) = \sum_{0 < m < n} \frac{1}{m^r n^s}, \]

\[ m \text{ odd}, \ n \text{ even} \]

\[ \zeta^{ee}(r, s) = \sum_{0 < m < n} \frac{1}{m^r n^s}, \]

\[ m \text{ even}, \ n \text{ even} \]

These are related to the modified and usual double zeta values by [see (4.6)]

\[ \hat{\zeta}(r, s) = 2^s (\zeta^{oe}(r, s) + \zeta^{ee}(r, s)) - \zeta(r, s) - \zeta(r+s). \]

Combining Corollary 1.2 and the period polynomial relations for classical double zeta values (Remark 4.9), one could therefore also explicitly write down period polynomial relations and sum formulas for the values \( 2^s (\zeta^{oe}(r, s) + \zeta^{ee}(r, s)) \).

**Remark 4.11** After the first version of the current work appeared, Tasaka also gave a nice analogue of Theorem 1.1 for the classical double zeta values \( \zeta(r, s) \) in [12].

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