ON A FAMILY OF POLYNOMIALS RELATED TO $\zeta(2, 1) = \zeta(3)$

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Abstract. We give a new proof of the identity $\zeta(\{2, 1\}^l) = \zeta(\{3\}^l)$ of the multiple zeta values, where $l = 1, 2, \ldots$, using generating functions of the underlying generalized polylogarithms. In the course of study we arrive at (hypergeometric) polynomials satisfying 3-term recurrence relations, whose properties we examine and compare with analogous ones of polynomials originated from an (ex-) conjectural identity of Borwein, Bradley and Broadhurst.

1. Introduction

The first thing one normally starts with, while learning about the multiple zeta values (MZVs)

$$\zeta(s) = \zeta(s_1, s_2, \ldots, s_l) = \sum_{n_1 > n_2 > \ldots > n_l \geq 1} \frac{1}{n_1^{s_1} n_2^{s_2} \ldots n_l^{s_l}},$$

is Euler’s identity $\zeta(2, 1) = \zeta(3)$ — see [3] for an account of proofs and generalizations of the remarkable equality. One such generalization reads

$$\zeta(\{2, 1\}^l) = \zeta(\{3\}^l) \quad \text{for} \quad l = 1, 2, \ldots, \quad (1)$$

where the notation $\{s\}^m$ denotes the multi-index with $m$ consecutive repetitions of the same index $s$. The only known proof of (1) available in the literature makes use of the duality relation of MZVs, originally conjectured in [6] and shortly after established in [12]. The latter relation is based on a simple iterated-integral representation of MZVs (see [12] but also [3, 4, 14] for details) but, unfortunately, it is not capable of establishing similar-looking identities

$$\zeta(\{3, 1\}^l) = \frac{2\pi^{4l}}{(4l + 2)!} \quad \text{for} \quad l = 1, 2, \ldots. \quad (2)$$

The equalities (2) were proven in [4] using a simple generating series argument.

The principal goal of this note is to give a proof of (1) via generating functions and to discuss, in this context, a related ex-conjecture of the alternating MZVs. An interesting outcome of this approach is a family of (hypergeometric) polynomials that satisfy a 3-term recurrence relation; a shape of the relation and (experimentally...
observed) structure of the zeroes of the polynomials suggest their bi-orthogonality origin \([7, 8, 11]\).

2. MULTIPLE POLYLOGARITHMS

For \(l = 1, 2, \ldots\), consider the generalized polylogarithms

\[
\text{Li}_{\{3\}}(z) = \sum_{n_1 > n_2 > \cdots > n_l \geq 1} \frac{z^{n_1}}{n_1^3 n_2^3 \cdots n_l^3},
\]

\[
\text{Li}_{\{2,1\}}(z) = \sum_{n_1 > m_1 > n_2 > m_2 > \cdots > n_l > m_l \geq 1} \frac{z^{n_1}}{n_1^2 m_1^2 n_2^2 m_2^2 \cdots n_l^2 m_l^2},
\]

\[
\text{Li}_{\{\overline{3},1\}}(z) = \sum_{n_1 > m_1 > n_2 > m_2 > \cdots > n_l > m_l \geq 1} \frac{z^{n_1} (-1)^{n_1 + n_2 + \cdots + n_l}}{n_1^2 m_1^2 n_2^2 m_2^2 \cdots n_l^2 m_l^2};
\]

if \(l = 0\) we set all these functions to be 1. Then at \(z = 1\),

\[
\zeta(\{3\}) = \text{Li}_{\{3\}}(1) \quad \text{and} \quad \zeta(\{2,1\}) = \text{Li}_{\{2,1\}}(1),
\]

and we also get the related alternating MZVs

\[
\zeta(\{\overline{3},1\}) = \text{Li}_{\{\overline{3},1\}}(1)
\]

from the specialization of the third polylogarithm.

Since

\[
\left( (1 - z) \frac{d}{dz} \right)^2 \left( z \frac{d}{dz} \right) \text{Li}_{\{3\}}(z) = \text{Li}_{\{3\}}(1 - z),
\]

\[
\left( (1 - z) \frac{d}{dz} \right)^2 \left( z \frac{d}{dz} \right) \text{Li}_{\{2,1\}}(z) = \text{Li}_{\{2,1\}}(1 - z),
\]

\[
\left( (1 + z) \frac{d}{dz} \right)^2 \left( z \frac{d}{dz} \right) \text{Li}_{\{\overline{3},1\}}(z) = \text{Li}_{\{\overline{3},1\}}(-z)
\]

for \(l = 1, 2, \ldots\), the generating series

\[
C(z; t) = \sum_{l=0}^{\infty} \text{Li}_{\{3\}}(z) t^{3l},
\]

\[
B(z; t) = \sum_{l=0}^{\infty} \text{Li}_{\{2,1\}}(z) t^{3l} \quad \text{and} \quad A(z; t) = \sum_{l=0}^{\infty} \text{Li}_{\{\overline{3},1\}}(z) t^{3l}
\]
satisfy linear differential equations. Namely, we have

\[
\left( \left( (1 - z) \frac{d}{dz} \right)^2 \left( z \frac{d}{dz} \right) - t^3 \right) C(z; t) = 0, \quad \left( \left( (1 - z) \frac{d}{dz} \right)^2 \left( z \frac{d}{dz} \right) - t^3 \right) B(z; t) = 0
\]

and

\[
\left( \left( (1 - z) \frac{d}{dz} \right)^2 \left( z \frac{d}{dz} \right) \left( (1 + z) \frac{d}{dz} \right)^2 \left( z \frac{d}{dz} \right) - t^6 \right) A(z; t) = 0,
\]
At the same time, the differential equation for $C$ implying

$$\frac{1}{8^l} \zeta([2, 1]^l) = \zeta([2, 1])$$

for $l = 1, 2, \ldots$, conjectured in [4] and confirmed in [13] by means of a nice though sophisticated machinery of double shuffle relations and the 'distribution' relations (see also an outline in [2]), translate into

$$C(1; t) = B(1; t) = A(1; 2t).$$  \hspace{1cm} (3)

Note that

$$C(1; t) = \sum_{l=0}^{\infty} t^{3l} \sum_{n_1 > n_2 > \cdots > n_{l} \geq 1} \frac{1}{n_1!n_2! \cdots n_{l}!} = \prod_{j=1}^{\infty} \left(1 + \frac{t^3}{j^3}\right).$$  \hspace{1cm} (4)

At the same time, the differential equation for $C(z; t) = \sum_{n=0}^{\infty} C_n(t)z^n$ results in

$$-n^3 C_n + (n + 1)^3 C_{n+1} = t^3 C_n$$

implying

$$\frac{C_{n+1}}{C_n} = \frac{n^3 + t^3}{(n + 1)^3} \frac{(n + t)(n + e^{2\pi i/3}t)(n + e^{4\pi i/3}t)}{(n + 1)^3}$$

and leading to the hypergeometric form

$$C(z; t) = \binom{3}{1} F_2 \left( t, \omega t, \omega^2 t \div 1, 1 \div z \right),$$  \hspace{1cm} (5)

where $\omega = e^{2\pi i/3}$. We recall that

$$\binom{m+1}{n} F_m \left( a_0, a_1, \ldots, a_m \div b_1, \ldots, b_m \div z \right) = \sum_{n=0}^{\infty} \frac{(a_0)_n(a_1)_n \cdots (a_m)_n z^n}{n! (b_1)_n \cdots (b_m)_n},$$

where $(a)_n = \Gamma(a + n)/\Gamma(a)$ denotes the Pochhammer symbol (also known as the 'shifted factorial' because $(a)_n = a(a + 1) \cdots (a + n - 1)$ for $n = 1, 2, \ldots$). It is not hard to see that the sequences $A_n(t)$ and $B_n(t)$ from $A(z; t) = \sum_{n=0}^{\infty} A_n(t)z^n$ and $B(z; t) = \sum_{n=0}^{\infty} B_n(t)z^n$ do not satisfy 2-term recurrence relations with polynomial coefficients. Thus, no hypergeometric representations of the type (5) are available for them.

3. Special Polynomials

The differential equation for $B(z; t)$ translates into the 3-term recurrence relation

$$n^3 B_n - (n + 1)^2 (2n + 1) B_{n+1} + (n + 2)^2 (n + 1) B_{n+2} = t^3 B_n$$  \hspace{1cm} (6)

for the coefficients $B_n = B_n(t)$; the initial values are $B_0 = 1$ and $B_1 = 0$.

**Lemma 1.** We have

$$B_n(t) = \frac{1}{n!} \sum_{k=0}^{n} \frac{(\omega t)_k(\omega^2 t)_k(t)_{n-k}(-t + k)_{n-k}}{k!(n-k)!} = \frac{(t)_n(-t)_n}{n!^2} \binom{3}{1} F_2 \left( -n, \omega t, \omega^2 t \div -t, 1 - n - t \div 1 \right).$$  \hspace{1cm} (7)
Proof. The recursion (6) for the sequence in (7) follows from application of the Gosper–Zeilberger algorithm of creative telescoping. The initial values for \( n = 0 \) and 1 are straightforward. □

Remark. The hypergeometric form in (7) was originally prompted by [9, Theorem 3.4]: the change of variable \( z \mapsto 1 - z \) in the differential equation for \( B(z; t) \) shows that the function \( f(z) = B(1 - z; t) \) satisfies the hypergeometric differential equation with upper parameters \( -t, -\omega t, -\omega^2 t \) and lower parameters 0, 0.

It is not transparent from the formula (7) (but immediate from the recursion (6)) that \( B_n(t) \in t^3 \mathbb{Q}[t^3] \) for \( n = 0, 1, 2, \ldots \); the classical transformations of \( \genfrac{[}{]}{0pt}{}{3}{2} \) \( (-1) \) hypergeometric series (see [1]) do not shed a light on this belonging either.

Lemma 2. We have

\[
B(1; t) = \prod_{j=1}^{\infty} \left( 1 + \frac{t^3}{j^3} \right).
\]

Proof. This follows from the derivation

\[
B(1; t) = \sum_{n=0}^{\infty} B_n(t) = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{k=0}^{n} \frac{(\omega t)_k (\omega^2 t)_k (t)_n (-t + k)_n}{k! (n - k)!} \frac{(-t + k)_n}{n! (n + 1)_n} \\
= \sum_{k=0}^{\infty} \frac{(\omega t)_k (\omega^2 t)_k}{k!^2} \sum_{m=0}^{\infty} \frac{(t)_m (-t + k)_m}{m! (k + 1)_m} \\
= \sum_{k=0}^{\infty} \frac{(\omega t)_k (\omega^2 t)_k}{k!^2} \cdot \text{$_2F_1$} \left( t, -t + k \left| k + 1 \right. \right) \\
= \frac{1}{\Gamma(1 - t) \Gamma(1 + t)} \sum_{k=0}^{\infty} \frac{(\omega t)_k (\omega^2 t)_k}{k! (1 - t)_k} \\
= \frac{1}{\Gamma(1 - t) \Gamma(1 + t)} \cdot \text{$_2F_1$} \left( \omega t, \omega^2 t \left| 1 \right. \right) \\
= \frac{1}{\Gamma(1 - t) \Gamma(1 + t)} \cdot \frac{\Gamma(1 - t)}{\Gamma(1 - (1 + \omega t)) \Gamma(1 - (1 + \omega^2 t))} \\
= \frac{1}{\Gamma(1 + t) \Gamma(1 + \omega t) \Gamma(1 + \omega^2 t)} = \prod_{j=1}^{\infty} \left( 1 + \frac{t^3}{j^3} \right),
\]

where we applied twice Gauss’s summation [1, Section 1.3]

\[
\text{$_2F_1$} \left( a, b \left| c \right. \right) = \frac{\Gamma(c) \Gamma(c - a - b)}{\Gamma(c - a) \Gamma(c - b)}
\]

valid when \( \Re(c - a - b) > 0 \). □

Finally, we deduce from substituting (4) and (8) into (3),

Theorem 1. The identity \( \zeta(\{3\}_l) = \zeta(\{2, 1\}_l) \) is valid for \( l = 1, 2, \ldots \).
4. A general family of polynomials

It is not hard to extend Lemma 1 to the one-parameter family of polynomials

\[ B_n^\alpha(t) = \frac{1}{n!} \sum_{k=0}^{n} \frac{(\omega t)_k (\omega^2 t)_k (\alpha + t)_{n-k}(\alpha - t + k)_{n-k}}{k! (n-k)!} \]

\[ = \frac{1}{n!} \sum_{k=0}^{n} \frac{(\alpha + \omega t)_k (\alpha + \omega^2 t)_k (t)_{n-k}(\alpha - t + k)_{n-k}}{k! (n-k)!}. \quad (9) \]

**Lemma 3.** For each \( \alpha \in \mathbb{C} \), the polynomials (9) satisfy the 3-term recurrence relation

\[ ((n+\alpha)^2 - t^3)B_n^\alpha - (n+1)(2n^2 + 3n(\alpha+1) + \alpha^2 + 3\alpha + 1)B_{n+1}^\alpha + (n+2)^2(n+1)B_{n+2}^\alpha = 0 \]

and the initial conditions \( B_0^\alpha = 1, B_1^\alpha = \alpha^2 \). In particular, \( B_n^\alpha(t) \in \mathbb{C}[t^3] \) for \( n = 0, 1, 2, \ldots \).

In addition, we have \( B_n^\alpha \in t^3 \mathbb{Q}[t^3] \) for \( \alpha = 0, -1, \ldots, -n + 1 \) (in other words, \( B_n^\alpha(0) = 0 \) for these values of \( \alpha \)).

**Lemma 4.** \( B_n^{1-n-\alpha}(t) = B_n^\alpha(t) \).

**Proof.** This follows from the hypergeometric representation

\[ B_n^\alpha(t) = \frac{(\alpha + t)_n (\alpha - t)_n}{n!^2} \binom{-n}{\omega t, \omega^2 t} \binom{\alpha - t, 1 - \alpha - n - t}{1}. \]

Here is one more property of the polynomials that follows from Euler’s transformation [1 Section 1.2].

**Lemma 5.** We have

\[ \sum_{n=0}^{\infty} B_n^\alpha(t) z^n = (1 - z)^{1 - 2\alpha} \sum_{n=0}^{\infty} B_n^{1-\alpha}(t) z^n. \]

**Proof.** Indeed,

\[ \sum_{n=0}^{\infty} B_n^\alpha(t) z^n = \sum_{k=0}^{\infty} \frac{(\omega t)_k (\omega^2 t)_k}{k!^2} z^k \cdot \binom{\alpha + t, \alpha - t + k}{k+1} \binom{z}{1} \]

\[ = \sum_{k=0}^{\infty} \frac{(\omega t)_k (\omega^2 t)_k}{k!^2} z^k \cdot (1 - z)^{1 - 2\alpha} \binom{1 - \alpha + t, 1 - \alpha - t + k}{k+1} \binom{z}{1} \]

\[ = (1 - z)^{1 - 2\alpha} \sum_{n=0}^{\infty} B_n^{1-\alpha}(t) z^n. \]

**Alternative proof of Lemma 2** It follows from Lemma 5 that

\[ B_n^1(t) = \sum_{k=0}^{n} B_k(t), \]

hence \( B(1; t) = \lim_{n \to \infty} B_n^1(t) \) and the latter limit is straightforward from (9).
Note that, with the help of the standard transformations of $\,_{3}F_{2}(1)$ hypergeometric series, we can also write (9) as

$$B_{n}^{\alpha}(t) = \frac{(\alpha - \omega t)_{n}(\alpha - \omega^{2}t)_{n}}{n!^{2}}\,_{3}F_{2}\left(\begin{array}{c}
-n, \alpha + t, \alpha + t \\
\alpha - \omega t, \alpha - \omega^{2}t
\end{array} \mid 1\right),$$

so that the generating functions of the continuous dual Hahn polynomials lead to

$$\sum_{n=0}^{\infty} \frac{n!}{(\alpha - t)_{n}} B_{n}^{\alpha}(t)z^{n} = (1 - z)^{-t} {_{2}F_{1}}\left(\begin{array}{c}
\alpha + t, \alpha + t \\
\alpha - t
\end{array} \mid z\right)$$

and

$$\sum_{n=0}^{\infty} \frac{(\gamma)_{n} n!}{(\alpha - \omega t)_{n}(\alpha - \omega^{2}t)_{n}} B_{n}^{\alpha}(t)z^{n} = (1 - z)^{-\gamma} \,_{3}F_{2}\left(\begin{array}{c}
\gamma, \alpha + t, \alpha + t \\
\alpha - \omega t, \alpha - \omega^{2}t
\end{array} \mid z - 1\right),$$

where $\gamma$ is arbitrary.

Finally, numerical verification suggests that for real $\alpha$ the zeroes of $B_{n}^{\alpha}$ viewed as polynomials in $x = t^{3}$ lie on the real half-line $(-\infty, 0]$.

5. Polynomials related to the alternating MZV identity

Writing

$$A(z; t) = \sum_{n=0}^{\infty} A_{n}(t)z^{n}$$

$$= 1 + \frac{1}{4}t^{3}z^{2} - \frac{1}{6}t^{3}z^{3} + \left(\frac{1}{192}t^{3} + \frac{1}{96}\right)t^{3}z^{4} - \left(\frac{1}{720}t^{3} + \frac{1}{12}\right)t^{3}z^{5}$$

$$+ \left(\frac{1}{34560}t^{6} + \frac{23}{5760}t^{3} + \frac{137}{2160}\right)t^{3}z^{6} + O(z^{7})$$

and using the equation

$$\left((1 + z)\frac{d}{dz}\right)^{2} \left(z\frac{d}{dz}\right)A(z; t) = t^{3}A(-z; t),$$

we obtain

$$(n^{3} - T)A_{n} + (n + 1)^{2}(2n + 1)A_{n+1} + (n + 2)^{2}(n + 1)A_{n+2} = 0, \ (10)$$

where $T = (-1)^{n}t^{3}$. Producing two shifted copies of (10),

$$((n - 1)^{3} + T)A_{n-1} + n^{2}(2n - 1)A_{n} + (n + 1)^{2}nA_{n+1} = 0, \ (11)$$

$$((n - 2)^{3} - T)A_{n-2} + (n - 1)^{2}(2n - 3)A_{n-1} + n^{2}(n - 1)A_{n} = 0, \ (12)$$

then multiplying recursion (10) by $n(n - 1)^{2}(2n - 3)$, recursion (11) by $-(n - 1)^{2} \times (2n + 1)(2n - 3)$, recursion (12) by $(2n + 1)((n - 1)^{3} + T)$ and adding the three resulted equations we arrive at

$$2n + 1)((n - 1)^{3} + T)((n - 2)^{3} - T)A_{n-2}$$

$$- n(n - 1)(2n - 1)(2n(n - 1)(n^{2} - n - 1) - 3T)A_{n}$$

$$+ (n + 2)^{2}(n + 1)n(n - 1)^{2}(2n - 3)A_{n+2} = 0. \ (13)$$
This final recursion restricted to the subsequences $A'_n = A_{2n}$ and $A''_n = A_{2n+1}$
gives rise to two families of so-called Frobenius–Stickelberger–Thiele polynomials [10].
Unlike the case of $B(z;t)$ treated in Section 3 we cannot find closed form expressions for those subsequences.

Here is the case most closely related to the recursion (13) when $n$ is even (we replace $n$ there with $2n + 2$), that is, to
\[
(4n + 5)((2n)^3 - t^3)((2n + 1)^3 + t^3)A_{2n}
- (4n + 3)(2n + 1)(2n + 2)(2n + 1)(2n + 2)(4n^2 + 6n + 1) - 3t^2)A_{2n+2}
+ (4n + 1)(2n + 1)^2(2n + 2)(2n + 3)(2n + 4)^2A_{2n+4} = 0,
\]
and there is a similar version when $n$ is odd. We have
\[
(4n + 5) \frac{(2n)^3 - t^3 (2n + 1)^3 + t^3}{t - 2n} A'_n
- (4n + 3)(2n + 1)(2n + 2)(2n + 1)(2n + 2) + (8n^2 + 12n + 1)t + 3t^2)A'_{n+1}
+ (4n + 1)(2n + 1)^2(2n + 2)(2n + 3)(2n + 4)^2A'_{n+2} = 0,
\]
where
\[
A'_n = \frac{1}{2^n (1/2)_n n!} \sum_{k=0}^{n} \frac{(\omega t/2)(\omega^2 t/2)(\omega^3 t/2)_{n-k}}{k!(n-k)!} (-1)^k.
\]
The latter polynomials are not from $\mathbb{Q}[t^3]$.

If we consider $\Lambda_n(t) = \sum_{k=0}^{n} A_k(t)$ then (it is already known [5] [13] that)
\[
(n^3 - (-1)^n t^3)\Lambda_{n-1} + (2n + 1)n\Lambda_n - (n + 1)^2 n\Lambda_{n+1} = 0, \quad n = 1, 2, \ldots.
\]
As before, the standard elimination translates it into
\[
(2n + 3)((n - 1)^3 + T)(n^3 - T)\Lambda_{n-2}
- (2n + 1)n(n - 1)(2n^2 + n + 1)^2 - 6 - T)\Lambda_n
+ (2n - 1)(n + 2)^2(n + 1)^2(n - 1)\Lambda_{n+2} = 0,
\]
where $T = (-1)^n t^3$. One can easily verify that
\[
\Lambda_n(t) = 1 + \cdots + \frac{t^{3[n/2]}}{2^{[n/2]} [n/2]! n!}
\]
but we also lack an explicit representation for them.

We have checked numerically a fine behaviour (orthogonal-polynomial-like) of the zeroes of $A_n$ and $\Lambda_n$ viewed as polynomials in $x = t^3$ (both of degree $\lfloor n/2 \rfloor$ in $x$). Namely, all the zeroes lie on the real half-line ($-\infty, 0$]. This is in line with the property of the polynomials $B_n$ (see the last paragraph in Section 4).

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