Multiple Polylogarithms
and
Multiple Zeta Values:

Some Results and Conjectures

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The Dilogarithm

\[ \text{Li}_2(x) = \int_0^x \frac{t}{1-t} \log(1-t)^{-1} \, dt \]
\[ = \sum_{n=1}^\infty \frac{x^n}{n^2}, \quad |x| \leq 1. \]

- arises in the multiple integration of rational forms, eg.
  \[ \int_0^x \int_0^y \frac{adsdt}{1-ast} = \text{Li}_2(axy) \]
- QED, scattering of light
- connection with the Gaussian hypergeometric function:
  \[ \text{Li}_2(x) = \lim_{\varepsilon \to 0^+} e^{-2} [\text{F}_1(\varepsilon; \varepsilon; 1; x) - 1] \]

Polylogarithms

\[ \text{Li}_1(x) = \log(1-x)^{-1} \]
\[ = \sum_{n=1}^\infty \frac{x^n}{n}, \quad |x| < 1. \]

\[ \text{Li}_s(x) = \int_0^x t^{1-s} \log(1-t)^{-1} \, dt, \quad 1 < s \in \mathbb{Z} \]
\[ = \sum_{n=1}^\infty \frac{x^n}{n^s}, \quad |x| \leq 1. \]

\[ \text{Li}_s(1) = \sum_{n=1}^\infty \frac{1}{n^s} = \zeta(s). \]

Inverting Pascal Matrices

Let \( a \) be real and let \( P(a) \) be the matrix whose \((m, n)\) entry is \( \binom{m}{n} a^{m-n} \).

\[ P(a) := \begin{bmatrix}
  1 & 1 & 1 & \\
  a & 2a & 3a & \\
  a^2 & 3a^2 & 3a & \\
  \vdots & \vdots & \vdots & 
\end{bmatrix} \]

Then \( I = P(0) \) is the identity matrix and

\[ P(a)P(b) = P(a+b). \]

\textbf{Theorem 1 (Aggarwalla and Lamoureaux)} Let \( \lambda \neq 1 \). The inverse of \( I - \lambda P(a) \) has \((m, n)\) entry

\[ \begin{cases}
  \frac{1}{(1-\lambda)}, & \text{if } m = n; \\
  \binom{m}{n} a^{m-n} \text{Li}_{m-n}(\lambda), & \text{if } m \neq n.
\end{cases} \]
Multiple Polylogarithms

For positive integer $k$, let

\begin{align*}
  s_1, \ldots, s_k &\in \mathbb{Z}^+, \\
  z_1, \ldots, z_k &\in \mathbb{C}, \\
  |z_j| &\leq 1 \text{ for } 1 \leq j \leq k.
\end{align*}

\[ L_{s_1, \ldots, s_k}(z_1, \ldots, z_k) := \sum_{n_1, \ldots, n_k > 0} \prod_{j=1}^{k} z_j^{n_j} n_j^{-s_j}, \]

\[ \zeta(s_1, s_2, \ldots, s_k) := L_{s_1, s_2, \ldots, s_k}(1, 1, \ldots, 1). \]

\[ k = 1 : \begin{cases} 
  L_s(z) = \sum_{n=1}^{\infty} z^n n^{-s}, \\
  \zeta(s) = L_s(1).
\end{cases} \]

\[ k = 2 : \quad \zeta(s, t) = \sum_{n=1}^{\infty} n^{-s} \sum_{j=1}^{n-1} j^{-t} \]

One can also study $\zeta(s_1, \ldots, s_k)$ with complex arguments $s_1, \ldots, s_k \in \mathbb{C}$.

It can be shown that the multiple series is absolutely convergent if

\[ \sum_{j=1}^{m} \Re(s_j) > m, \quad m = 1, 2, \ldots, k. \]

It is then natural to inquire about

- analytic continuation,
- trivial zeros,
- values at the non-positive integers.

Multiple Zeta Functions

These are obtained when each $z_j = 1$ in the multiple polylogarithm.

\[ \zeta(s_1, \ldots, s_k) := \sum_{n_1, \ldots, n_k > 0} \prod_{j=1}^{k} n_j^{-s_j}. \]

Their study goes back to Euler ($k = 2$):

\[ 2\zeta(m, 1) = m\zeta(m + 1) - \sum_{j=1}^{m-2} \zeta(m - j)\zeta(j + 1), \]

where $2 \leq m \in \mathbb{Z}$.

An extremely difficult problem is to classify all relations that exist between values of multiple zeta functions ("multiple zeta values") at positive integer arguments.

Define the depth of a multiple polylogarithm or multiple zeta function to be the number $k$ of nested summations.

When can a nested sum of depth $k$ be expressed (say polynomially with rational coefficients) in terms of sums with depth less than $k$?

Settling this question in complete generality is currently a hopeless prospect.

eg. Is $\zeta(5, 3)/\zeta(5)\zeta(3)$ irrational?
Reductions at Arbitrary Depth

One of the earliest nontrivial successes at arbitrary depth was Broadhurst’s settling of Zagier’s conjecture

\[
\zeta(3,1,3,1,\ldots,3,1) = 4^{-n} \zeta(4,4,\ldots,4) \quad \text{for } 0 < n \in \mathbb{Z}.
\]

Abbreviate the first two members by \( \zeta(\{3,1\}^n) \) and \( 4^{-n} \zeta(\{4\}^n) \).

More generally, for real \( x \) with \( 0 \leq x \leq 1 \), let

\[
\zeta(x_1,\ldots,x_k) := \lim_{\varepsilon \to 0} \frac{\zeta(x_1,\ldots,x_k,1,\ldots,1)}{\pi^k} = \sum_{n_1 \geq \ldots \geq n_k > 0} x^{n_1} \prod_{j=1}^k n_j^{-s_j}.
\]


**Theorem 2**

\[
\sum_{n=0}^{\infty} \zeta(\{3,1\}^n) t^{4n} = 2F_1(z,-z;1;x)_{2F_1}(iz,-iz;1;z),
\]

where \( z = (1+i)t/2 \).

When \( x = 1 \), Theorem 2 reduces to

\[
\sum_{n=0}^{\infty} \zeta(\{3,1\}^n) t^{4n} = \frac{1}{\Gamma(1+z)\Gamma(1-z)} \cdot \frac{1}{\Gamma(1+iz)\Gamma(1-iz)} = \frac{\sin(\pi z) \cdot \sinh(\pi z)}{\pi z} \cdot \frac{\sinh(\pi z)}{\pi z} = \sum_{n=0}^{\infty} \frac{2(\pi t)^{4n}}{(4n+2)!}.
\]

Factoring Solutions to Differential Equations

**Theorem 3** Let \( f \) and \( g \) be suitably differentiable functions of a single variable, and let \( t \) be a free parameter. Define \( D_f = f(x) d/dx \), \( D_g = g(x) d/dx \) and suppose that

\[
(D_f D_g + t) u = 0 \quad (1)
\]

\[
(D_f D_g - t) v = 0. \quad (2)
\]

Then

\[
(D_f^2 D_g^2 + 4t^2) uv = 0. \quad (3)
\]

Moreover, if \( u_1 \) and \( u_2 \) are linearly independent solutions to (1) and if \( v_1 \) and \( v_2 \) are linearly independent solutions to (2) then \{\( u_1 v_1, u_1 v_2, u_2 v_1, u_2 v_2 \)\} are linearly independent solutions to (3).

**Proof Sketch.** Verify that \( u D_g^2 v + v D_g^2 u = 0 \), and then calculate

\[
D_f^2 D_g^2 (uv) = 2D_f^2 (D_g u)(D_g v) = 2t[v(D_f D_g u) - u(D_f D_g v)] = -4t^2 uv.
\]

Linear independence follows from the following modified Wronskian determinate identity:

\[
\begin{vmatrix}
D_g u_1 v_1 & D_g u_2 v_1 & D_g u_1 v_2 & D_g u_2 v_2 \\
D_g^2 u_1 v_1 & D_g^2 u_2 v_1 & D_g^2 u_1 v_2 & D_g^2 u_2 v_2 \\
D_f^2 u_1 v_1 & D_f^2 u_2 v_1 & D_f^2 u_1 v_2 & D_f^2 u_2 v_2 \\
D_f D_g^2 u_1 v_1 & D_f D_g^2 u_2 v_1 & D_f D_g^2 u_1 v_2 & D_f D_g^2 u_2 v_2
\end{vmatrix}
= 8t \begin{vmatrix}
D_g u_1 & u_2 \\
D_g u_2 & v_2
\end{vmatrix}^2 \begin{vmatrix}
v_1 & v_2 \\
v_1 & v_2
\end{vmatrix}^2.
\]

This identity follows by direct computation using the differential equations for \( u \) and \( v \).

\[ \square \]
Applications

For $0 \leq x \leq 1$ and complex $z = (1 + i)t/2$, let
\[
\psi(z) := \Gamma'(z)/\Gamma(z),
\]
\[
Y_1(x, z) := 2 F_1(z, -z; 1; x),
\]
\[
Y_2(x, z) := (1 - x)2 F_1(1 + z, 1 - z; 2; 1 - x),
\]
\[
G(z) := \frac{1}{i} \{\psi(1 + iz) + \psi(1 - iz) - \psi(1 + z) - \psi(1 - z)\}.
\]
Then (Trans. AMS)
\[
\sum_{n=0}^{\infty} t^{4n} \zeta_x(\{3, 1\}^n) = Y_1(x, z)Y_1(x, iz),
\]
and (Compositio Mathematica, to appear)
\[
z^2 \sum_{n=0}^{\infty} t^{4n} \zeta_x(3, \{1, 3\}^n) = G(z)Y_1(x, z)Y_1(x, iz)
\]
\[
- \frac{Y_1(x, iz)Y_2(x, z)}{4Y_1(1, z)} + \frac{Y_1(x, z)Y_2(x, iz)}{4Y_1(1, iz)}
\]
define entire functions of $z$.

Entirely in $z$ turns out to be a simple consequence of the identity
\[
\frac{(1 + \alpha)_n}{n!} 2 F_1 \left(-n, 1 + \alpha + \beta + n \left| \frac{1 - y}{2} \right. \right) = \frac{(-1)^n(1 + \beta)_n}{n!} 2 F_1 \left(-n, 1 + \alpha + \beta + n \left| \frac{1 + y}{2} \right. \right)
\]
for the Jacobi polynomials.

Here,
\[
(a)_n := \frac{\Gamma(a + n)}{\Gamma(a)} = \prod_{j=1}^{n} (a + j - 1)
\]
is the rising factorial (Pochhammer symbol).

Thus the apparent singularities in the generating functions are all removable.

More Applications

Let $s = (1 + z)/2$ and $z = (1 + i)t/2$,
\[
\zeta_x(\{1, 1\}^n) := Li_{1, \ldots, 1}(-x, 1, \{-1, 1\}^{n-1}),
\]
\[
\zeta_x(\{1, 1\}^n) := Li_{1, \ldots, 1}(-x, \{1, -1\}^n),
\]
\[
U(s, z) := 2 F_1(z, -z; 1; s)
\]
\[
- z(1 - s)2 F_1(1 + z, 1 - z; 2; 1 - s),
\]
\[
A(z) := \frac{\sqrt{\pi}}{\Gamma(1/2)\Gamma(1/2 - z/2)}.
\]

Then (Compositio Mathematica, to appear):
\[
\sum_{n=0}^{\infty} t^{2n} \zeta_x(\{1, 1\}^n) + t^{2n+1} \zeta_x(\{1, 1\}^n)
\]
\[
= \frac{U(s, -z)U(s, iz)}{A(-z)A(iz)}
\]
defines an entire function of $z$. 

Specialize $x = 1$. It follows that for all positive integers $n$,
\[
\zeta(\{3, 1\}^n) = 4^{-n} \zeta(\{4\}^n) = \frac{2\pi^{4n}}{(4n + 2)!},
\]
\[
\zeta(3, \{1, 3\}^n) = 4^{-n} \sum_{k=0}^{n} \zeta(4k + 3)\zeta(\{4\}^{n-k})
\]
\[
= \sum_{k=0}^{n} \frac{2\pi^{4k}}{(4k + 2)!} \left(\frac{1}{4}\right)^{n-k} \zeta(4n - 4k + 3),
\]
\[
\zeta(2, \{1, 3\}^n) = 4^{-n} \sum_{k=0}^{n} (-1)^k \zeta(\{4\}^{n-k}) \{4k + 1\}
\]
\[
\times \zeta(4k + 2) - 4 \sum_{j=1}^{k} \zeta(4j - 1)\zeta(4k - 4j + 3)\}.
\]

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Entirely in \( z \) is again a simple consequence of the identity

\[
\frac{(1 + \alpha)n}{n!} _2F_1\left( \begin{array}{c} -n, 1 + \alpha + \beta + n \\ 1 + \alpha \end{array} \left| \frac{1 - y}{2} \right. \right) = \frac{(-1)^n(1 + \beta)n}{n!} _2F_1\left( \begin{array}{c} -n, 1 + \alpha + \beta + n \\ 1 + \beta \end{array} \left| \frac{1 + y}{2} \right. \right)
\]

for the Jacobi polynomials.

Thus the apparent singularities in the generating functions are again all removable.

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The Simplex Integral

There is a representation, due to Kontsevich, for multiple zeta values in terms of a simplex integral. If \( s_1, \ldots, s_k \) are positive integers, then

\[
\zeta(s_1, \ldots, s_k) = \int \prod_{j=1}^{k} \left( \frac{t_{(j)}^{s_j-1}}{1 - t_{(j)}^{s_j}} \right) \frac{dt_{(j)}}{t_{(j)}^{s_j}},
\]

where the integral is over the simplex

\[ 1 > t_{(1)}^{(1)} > \cdots > t_{(1)}^{(s_1)} > \cdots > t_{(k)}^{(1)} > \cdots > t_{(k)}^{(s_k)} > 0, \]

and is abbreviated by

\[
\int_0^1 \prod_{j=1}^{k} a^{s_j-1} b, \quad a = dt/t, \quad b = dt/(1 - t).
\]
eg.
\[
\zeta(2, 1) = \sum_{n>m>0} n^{-2} m^{-1} \\
= \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} (k + j)^{-2} k^{-1} \\
= \sum_{k=1}^{\infty} k^{-1} \sum_{j=1}^{\infty} (k + j)^{-1} \int_0^1 t^{k+j-1} dt \\
= \sum_{k=1}^{\infty} k^{-1} \int_0^1 t^{-1} \sum_{j=1}^{\infty} \int_0^t u^{k+j-1} du dt \\
= \int_0^1 t^{-1} \int_0^t (1 - u)^{-1} \sum_{k=1}^{\infty} k^{-1} u^k du dt \\
= \int_0^1 t^{-1} \int_0^t (1 - u)^{-1} \sum_{k=1}^{\infty} \int_0^u v^{k-1} dv du dt \\
= \int_0^1 t^{-1} \int_0^t (1 - u)^{-1} \int_0^u (1 - v)^{-1} dv du dt \\
= \int \frac{dt}{t} \frac{du}{1 - u} \frac{dv}{1 - v} \\
= \int_0^1 ab^2. \]

Duality

Let \( s_j \) and \( r_j \) be non-negative integers (1 \( \leq j \leq k \)), and let
\[
m = \sum_{j=1}^{k} (s_j + 2 + r_j).
\]

Then
\[
\zeta(s_1 + 2, \{1\}^{r_1}, \ldots, s_k + 2, \{1\}^{r_k}) \\
= \int_0^1 \prod_{j=1}^{k} a^{s_j + 1} b^{r_j + 1} \\
= \int \prod_{1 > t_1 > \cdots > t_m > 0} \prod_{j=1}^{m} f_j(t_j) dt_j \\
= \int \prod_{1 > u_1 > \cdots > u_l > 0} \prod_{j=1}^{l} f_j(u_j) du_j, \quad u_j = 1 - t_j \\
= \int_0^1 \prod_{j=k}^{1} a^{r_j + 1} b^{s_j + 1} \\
= \zeta(r_k + 2, \{1\}^{s_k}, \ldots, r_1 + 2, \{1\}^{s_1}), \]
originally conjectured by Hoffman.

This is the only known non-trivial instance of an equivalence between two multiple zeta values.

A related integral representation enabled Y. Ohno to prove the following beautiful generalization of the duality identity. Let
\[
S(p, m) := \sum_{c_1 + \ldots + c_n = m} \zeta(p_1 + c_1, \ldots, p_n + c_n),
\]
where the sum is over all non-negative integers \( c_1, \ldots, c_n \) which sum to \( m \).

As in the duality identity, define the dual argument lists
\[
p := (s_1 + 2, \{1\}^{r_1}, \ldots, s_k + 2, \{1\}^{r_k})
\]
and
\[
p' := (r_k + 2, \{1\}^{s_k}, \ldots, r_1 + 2, \{1\}^{s_1}).
\]

Then \( S(p, m) = S(p', m) \).

When \( m = 0 \), Ohno’s result reduces to duality.

Another interesting specialization is obtained by taking \( p = (k + 1) \) and \( m = n - k - 1 \).

One then deduces Granville’s theorem, originally conjectured independently by Courtney Moen and Michael Schmidt:
\[
\sum_{s_1 + \ldots + s_k = n} \zeta(s_1, \ldots, s_k) = \zeta(n),
\]
where the sum is over all positive integers \( s_1, \ldots, s_k \) which sum to \( n \) and \( s_1 > 1 \).
The MacMahon Integral

Major Percy MacMahon's Omega operator discards terms with non-positive exponents from formal Laurent series in $\lambda_1, \ldots, \lambda_k$. Thus, if $0 \leq x_1, \ldots, x_k \leq 1$, then

$$\operatorname{Li}_{s_1, \ldots, s_k}(x_1, \ldots, x_k) = \sum_{n_1 > \cdots > n_k > 0} \frac{k}{\prod_{j=1}^k x_j n_j^{-s_j}}$$

$$= \sum_{n_1 > \cdots > n_k > 0} \frac{k}{\prod_{j=1}^k n_j^{-s_j}} (x_j \lambda_j \lambda_{j-1}^{-1})^{n_j}, \quad \lambda_0 := 1$$

$$= \frac{k}{\prod_{j=1}^k \Pi_{j=1}^{s_j-1} u_j^{(j)} \left( \prod_{r=1}^{u_j^{(j)}} \frac{y_j^m}{u_j^{(j)}} \right)}$$

Thus, we have

$$\operatorname{Li}_{s_1, \ldots, s_k}(x_1, \ldots, x_k) = \Omega \prod_{j=1}^k \frac{u_j^{(j)}}{u_j^{(j)}}$$

$$= \sum_{m_1 > \cdots > m_k > 0} \frac{k}{\prod_{j=1}^k u_j^{(j)}}$$

$$= \frac{1}{\Pi_{j=1}^k \frac{y_j}{1 - y_j}}$$

$$= \frac{1}{\Pi_{j=1}^k \frac{y_j}{1 - y_j}}$$

Shuffles

The simplex integral representation leads to a shuffle multiplication rule satisfied by multiple zeta values.

Suppose that $x, y \in \mathbb{R}$ and $f_j : [y, x] \to \mathbb{R}$ are integrable functions for $j = 1, 2, \ldots, n$.

It is customary to make the abbreviation

$$\int_y^x \prod_{j=1}^n \alpha_j := \prod_{x > t_1 > \cdots > t_n > y} \int_{x}^{t_1} \cdots \int_{t_n}^{t_{n-1}} f_j(t_j) dt_j$$

Contraction: the integral is equal to 1 if $n = 0$ regardless of the values of $x$ and $y$. 
Let \( \sigma \) be a permutation of \( \{1, 2, \ldots, m + n\} \) such that \( \sigma^{-1}(j) < \sigma^{-1}(k) \) for all \( 1 \leq j < k \leq m \) and \( m + 1 \leq j < k \leq m + n \).

Denote the set of all \( \binom{m+n}{n} \) such permutations \( \sigma \) by \( \text{Shuff}(m,n) \).

Then

\[
\left( \prod_{j=1}^{y} \prod_{j=m+1}^{x} a_j \right) \left( \prod_{j=1}^{y} \prod_{j=m+1}^{x} a_j \right) = \sum_{\sigma \in \text{Shuff}(m,n)} \prod_{j=1}^{m+n} a_{\sigma(j)},
\]

and so define the shuffle product \( \omega \) by

\[
\left( \prod_{j=1}^{m} a_j \right) \omega \left( \prod_{j=m+1}^{m+n} a_j \right) \overset{\text{def}}{=} \sum_{\sigma \in \text{Shuff}(m,n)} \prod_{j=1}^{m+n} a_{\sigma(j)}.
\]

### The Shuffle Algebra

Let \( A \) be a finite set and let \( A^* \) denote the free monoid generated by \( A \).

Regard \( A \) as an alphabet and the elements of \( A^* \) as words formed by concatenating any finite number of letters (repetitions permitted) from the alphabet \( A \).

By linearly extending the concatenation product to the set \( Q\{A\} \) of rational linear combinations of elements of \( A^* \), we obtain a non-commutative polynomial ring with indeterminates the elements of \( A \) and with multiplicative identity \( 1 \) denoting the empty word.

The shuffle product is alternatively defined first on words by the recursion

\[
\begin{align*}
1 \omega \omega & = \omega \omega 1 = \omega, \\
au \omega bv & = a(u \omega bv) + b(u \omega v),
\end{align*}
\]

\((\forall a, b \in A \text{ and } \forall u, v, w \in A^*)\) and then extended linearly to \( Q\{A\} \).

eg.

\[(ab - 2b) \omega c = ab \omega c - 2b \omega c = abc + abc + abc - 2bc - 2bc - 2cb\]

One checks that the shuffle product so defined is associative and commutative, and thus \( Q\{A\} \) equipped with the shuffle product becomes a commutative \( Q \)-algebra, denoted \( \text{Sh}_{Q}[A] \).

In what follows, if \( A \) is an alphabet and \( u, v \in A^* \), we’ll denote by \( \{u \omega v\} \) the multi-set of words appearing (with multiplicity) in the expansion of \( u \omega v \).

For example, suppose \( A = \{a, b\} \). Since \( ab \omega ab = 4aabb + 2abab \), we have

\[
\{ab \omega ab\} = \{abab, abab, aabb, aabb, aabb\},
\]

which, as a multi-set, properly contains \( \{abab, aabb\} \).

**Theorem 4 (Euro. J. Comb., to appear)** Let \( r \) be a positive integer, let \( A \) be an alphabet, and let \( a_1, a_2, \ldots \in A \) be such that \( a_r + m = a_m \) for all positive integers \( m \). Fix a positive integer \( n \), and define multi-sets \( S_0 = S_m = \{a_1 a_2 \cdots a_{2n}\} \), and

\[
S_k = \{a_1 a_2 \cdots a_k \omega a_1 a_2 \cdots a(2n-k)\},
\]

for \( k = 1, 2, \ldots, 2n - 1 \). Then \( S_{k-1} \subseteq S_k \) for \( k = 1, 2, \ldots, n \), and \( S_{k+1} \subseteq S_k \) for \( k = n, n+1, \ldots, 2n-1 \).
Corollary 1 Let \( n \) be a non-negative integer, and let \( \{a, b\} \) be an alphabet. Then
\[
\sum_{k=-n}^{n} (-1)^k [(ab)^{n+k} \omega (ab)^{n-k}] = (4a^2b^2)^n.
\]

Corollary 2 Let \( n \) be a non-negative integer. Then
\[
\sum_{k=-n}^{n} (-1)^k \zeta(\{2\}^{n+k}\zeta(\{2\}^{n-k}) = 4^n \zeta(3,1)^n).
\]

Proof of Corollary 1. We prove the trivially equivalent convolution formula
\[
\sum_{k=0}^{2n} (-1)^n (ab)^k \omega (ab)^{2n-k} = (4a^2b^2)^n.
\]
In Theorem 4, let \( A = \{a, b\} \) and \( r = 2 \). In view of the multi-set inclusions indicated by Theorem 4, there must be
\[
\sum_{k=0}^{2n} (-1)^n (ab)^k |_{S_k} = \sum_{k=0}^{2n} (-1)^n h_{2k} = 4^n
\]
terms on each side of (4), counting multiplicity. Furthermore, the word \((a^2b^2)^n\) occurs \( 4^n \) times in \( S_n \), since each \( a \) and each \( b \) can take two positions. Since \((a^2b^2)^n\) cannot occur in \( S_k \) for \( k \neq n \), (4) follows immediately.

One can similarly prove an intriguing shuffle factorization due to Broadhurst.

Let \( i^2 = -1 \). Then in the formal power series ring \((\text{Sh}Q[a,b])[\![z]\!]\), we have the identity
\[
A \left( \frac{z}{1-i} \right) \omega A \left( \frac{z}{1+i} \right) = M(z)
\]
where
\[
A(z) = \sum_{n=0}^{\infty} (cz)^n(1+cz)
\]
\[
= 1 + cz + cbz^2 + cbcz^3 + cbcz^4 + \ldots
\]
and
\[
M(z) = \sum_{n=0}^{\infty} (cz^3)^n(1 + cz + c^2 z^2 + c^2 b z^3)
\]
\[
= 1 + cz + c^2 z^2 + c^2 b z^3 + c^2 b^2 z^4 + \ldots
\]

Other shuffle convolution formulae can be established in a similar manner.

For example, if \( \{a, b\} \) is an alphabet and \( n \) is a positive integer, then
\[
2 \sum_{k=-n}^{n} (-1)^k [(ab)^{n+k} \omega (ba)^{n-k}] = (4abba)^n + (4baab)^n.
\]

With a little more work, one can also establish a shuffle convolution formula for
\[
\sum_{k=-n}^{n} (-1)^k [(a^2b)^{n+k} \omega (a^2b)^{n-k}], \quad 1 \leq n \in \mathbb{Z},
\]
and as a consequence, a corresponding identity for
\[
\zeta(\{5,1\}^n) := \zeta(\overbrace{5,1,\ldots,5,1}^{2n} \omega), \quad 1 \leq n \in \mathbb{Z}.
\]

In principle, it should be possible to extend this approach to \( \zeta(\{2p+1,1\}^n) \) for any positive integers \( n \) and \( p \), but the shuffle convolution formulae become prohibitively complicated as \( p \) increases.

Let \( n \) be a positive integer. Observe that in \((a^4 b^2)^n\), every occurrence of \( a^4 \) after the first is separated on both sides by \( b^2 \), and hence there are \( 2n-1 \) ways in which a single transposition of a letter \( b \) with an adjacent letter \( a \) can be performed. If we let \( \binom{2n-1}{k} \) denote the sum of the \( \binom{2n-1}{k} \) words obtained from \((a^4 b^2)^n\) by making \( k \) such transpositions, then we have the following result.

**Theorem 5** Let \( n \) be a positive integer. Then
\[
\sum_{k=0}^{n} (-1)^k (a^2b)^n \omega (a^2b)^{n+k} = \sum_{k=1}^{3n} 2k \left[ \binom{2n-1}{k} \right].
\]

**Example.** When \( n = 2 \), the right hand side of Theorem 5 is equal to
\[
18a^3 b^2 a^2 b a b + 144 a^4 b^2 a^4 b^2
+ 36(a^2 b a b a^3 b + a^3 b^2 b a^2 b^2 + a^4 b a b^2 b a b)
+ 72(a^4 b^2 a^3 b + a^5 b a b^2 a^2 b^2 + a^3 b a b^4 b^2).
\]
Definition 6 (EJC 5(1) 1998, #R38)  For integers \( m \geq n \geq 0 \) let

\[ S_{m,n} \]

denote the set of words occurring in the shuffle product

\[ (ab)^n \cup (ab)^{m-n} \]

in which the subword \( a^2 \) appears exactly \( n \) times.

Let

\[ T_{m,n} \]

be the sum of the \( \binom{m}{2n} \) distinct words in \( S_{m,n} \).

For all other pairs \( (m,n) \) define \( T_{m,n} := 0 \).

eg. \( S_{3,1} = \{a^2b^3ab,a^2bab^2,aba^2b^2\} \), \( T_{3,1} = a^2b^2ab + a^2bab^2 + aba^2b^2 \). Each word in \( S_{3,1} \) occurs 4 times in \( (ab) \cup (ab)^2 \).

Theorem 7 (JCTA 97 (2001) (1), 43–61)  Let \( x \) and \( y \) be commuting indeterminates, and let \( m \) be a non-negative integer. In the commutative polynomial ring \( (Sh\mathcal{Q}[a,b])[x,y] \) we have the shuffle convolution formula

\[
\sum_{k=0}^{m} \frac{x^k y^{m-k} [(ab)^k \cup (ab)^{m-k}]}{[m/2]!
= \sum_{n=0}^{m} \frac{(4xy)^n (x + y)^{m-2n} T_{m,n}}{[n/2]!}.
\]

Corollary 3  Let \( m \) be a non-negative integer. Then

\[
\sum_{k=-m}^{m} (-1)^k [(ab)^{m+k} \cup (ab)^{m-k}] = (4a^2b^2)^m.
\]

Corollary 4  Let \( m \) be a non-negative integer. Then

\[
\sum_{k=-m}^{m} (-1)^k \zeta((2)^{m+k})\zeta((2)^{m-k}) = 4^m \zeta(3,1)^m.
\]

Thus, if \( \tilde{s} = (m_0, m_1, \ldots, m_{2n}) \), then (following Broadhurst)

\[
Z(\tilde{s}) = \int_0^1 (ab)^{m_0} \prod_{k=1}^{n} (a^2b)((ab)^{m_{2k-1}}b(ab)^{m_{2k}})
= \zeta((2)^{m_0}, 3, (2)^{m_1}, 1, (2)^{m_2}, 3, (2)^{m_3}, 1, \ldots, 3, (2)^{m_{2n-1}}, 1, (2)^{m_{2n}}).
\]

The argument list consists of \( m_j \) consecutive twos inserted after the \( j \)th element of the string \( \{3,1\}^n \) for \( j = 0, 1, \ldots, 2n \).

It turns out that

\[
\sum_{\tilde{s} \in C_{2n+1}(m-2n)} Z(\tilde{s}) = \frac{2\pi^{2m}}{(2m+2)!} \left( \frac{m+1}{2n+1} \right),
\]

for all non-negative integers \( m \) and \( n \) with \( m \geq 2n \).
Theorem 8 Let $m$ and $n$ be non-negative integers with $m \geq 2n$. Then
\[
\sum_{\vec{s} \in C_{2n+1}(m-2n)} Z(\vec{s}) = \frac{2^{2m}}{(2m+2)!} \binom{m}{2n+1}.
\]

Corollary 5 Let $n$ be a non-negative integer. Then
\[
\zeta(\{3,1\}^n) = \frac{2^{4n}}{(4n+2)!}.
\]

Proof. Put $m = 2n$ in Theorem 8, and note that $Z(\{0\}^{2n+1}) = \zeta(\{3,1\}^n)$.

A more compelling formulation of Theorem 8 can be given as follows.

Again, let $\vec{s} = (m_0, m_1, \ldots, m_{2n})$ and put (following Broadhurst again)
\[
\mathcal{C}(\vec{s}) := Z(\vec{s}) + \sum_{j=1}^{2n} Z(m_j, m_{j+1}, \ldots, m_{2n}, m_0, \ldots, m_{j-1}).
\]

In other words, sum over all cyclic permutations of the argument list $\vec{s}$. Then
\[
\sum_{\vec{s} \in C_{2n+1}(m-2n)} \mathcal{C}(\vec{s}) = Z(m) \times |C_{2n+1}(m-2n)|
\]
\[
= \frac{\pi^{2m}}{(2m+1)!} \binom{m}{2n}
\]

is an equivalent formulation.

Theorem 9 Let $m$ and $n$ be non-negative integers with $m \geq 2n$. Then
\[
\sum_{\vec{s} \in C_{2n+1}(m-2n)} \mathcal{C}(\vec{s}) = Z(m) \times |C_{2n+1}(m-2n)|
\]
\[
= \frac{\pi^{2m}}{(2m+1)!} \binom{m}{2n}
\]

Corollary 6 If $n$ is a non-negative integer, then
\[
\mathcal{C}(1,\{0\}^{2n}) = Z(2n+1).
\]

Broadhurst’s cyclic insertion conjecture can be restated as the assertion that
\[
\mathcal{C}(\vec{s}) = Z(m), \quad \forall \vec{s} \in C_{2n+1}(m-2n)
\]
and integers $m \geq 2n \geq 0$.

Theorem 9 reduces the problem to proving that $\mathcal{C}(\vec{s})$ is invariant for $\vec{s} \in C_{2n+1}(m-2n)$.

Conjecture: The invariance can be proved using only the shuffle property of multiple zeta values plus the known values $\zeta(\{2n\}^k)$.

Theorem 8 Let $m$ and $n$ be non-negative integers with $m \geq 2n$. Then
\[
\sum_{\vec{s} \in C_{2n+1}(m-2n)} Z(\vec{s}) = \frac{2^{2m}}{(2m+2)!} \binom{m+1}{2n+1}.
\]

Proof. It suffices to prove that with $a = dt/t$, $b = dt/(1-t)$, we have
\[
\int_0^1 T_{m,n} = \frac{2^{2m}}{(2m+2)!} \binom{m+1}{2n+1}.
\]

Let
\[
J(z) := \sum_{k=0}^{\infty} z^{2k} \int_0^1 (ab)^k = \sum_{k=0}^{\infty} z^{2k} \zeta(\{2\}^k).
\]

Then [BBB]
\[
J(z) = \begin{cases} \frac{\sinh(\pi z)}{\pi z}, & \text{if } z \neq 0, \\ 1, & \text{if } z = 0. \end{cases}
\]
We have

\[ J(z \cos \theta) J(z \sin \theta) \]
\[ = \frac{\sinh(\pi z \cos \theta)}{\pi z \cos \theta} \cdot \frac{\sinh(\pi z \sin \theta)}{\pi z \sin \theta} \]
\[ = \frac{\cosh \pi z (\cos \theta + \sin \theta) - \cosh \pi z (\cos \theta - \sin \theta)}{2 \pi^2 z^2 \sin \theta \cos \theta} \]
\[ = \frac{\cosh \pi \sqrt{1 + \sin 2\theta} - \cosh \pi \sqrt{1 - \sin 2\theta}}{\pi^2 z^2 \sin 2\theta} \]
\[ = \sum_{m=1}^{\infty} \frac{(\pi z)^{2m}}{(2m)! \pi^2 z^2 \sin 2\theta} \left\{ (1 + \sin 2\theta)^m - (1 - \sin 2\theta)^m \right\} \]
\[ = \sum_{m=0}^{\infty} \frac{2(\pi z)^{2m}}{(2m + 2)!} \sum_{n=0}^{[m/2]} (m + 1 - 2n)(\sin 2\theta)^{2n}. \]

Now recall Theorem 7:

\[ \sum_{k=0}^{m} x^k y^{m-k} (ab)^k \omega (ab)^{m-k} \]
\[ = \sum_{n=0}^{[m/2]} (4xy)^n (x + y)^{m-2n} T_{m,n}. \]

Putting \( x = z^2 \cos \theta \) and \( y = z^2 \sin \theta \) yields

\[ J(z \cos \theta) J(z \sin \theta) \]
\[ = \left[ \sum_{k=0}^{\infty} (z \cos \theta)^2 k \int_0^1 (ab)^k \left[ \sum_{j=0}^{\infty} (z \sin \theta)^2 j \int_0^1 (ab)^j \right] \right] \]
\[ = \sum_{m=0}^{\infty} \sum_{n=0}^{[m/2]} (z \cos \theta)^{2n} (z \sin \theta)^{2m-2n} \]
\[ \times \int_0^1 (ab)^n \omega (ab)^{m-n} \]
\[ = \sum_{m=0}^{[m/2]} \sum_{n=0}^{[m/2]} (4z^4 \sin^2 \theta \cos^2 \theta)^n \]
\[ \times (z^2 \cos^2 \theta + z^2 \sin^2 \theta)^{m-2n} \int_0^1 T_{m,n} \]
\[ = \sum_{m=0}^{\infty} z^{2m} \sum_{n=0}^{[m/2]} (\sin 2\theta)^{2n} \int_0^1 T_{m,n}. \]

**Conjecture 10**

\[ Z(a_1, b_1, a_2, b_2, a_3) + Z(a_2, b_1, a_3, b_2, a_1) + Z(a_3, b_1, a_1, b_2, a_2) \]
\[ = Z(a_1, b_2, b_1, a_3) + Z(a_2, b_3, b_1, a_1) + Z(a_3, b_2, a_1, b_2, a_2) \]

**Conjecture 11** Let \( q_1 = q_2 = t^3 \), and for \( n \geq 1 \),
\[ n(n + 1)^2 q_{n+2} = n(2n + 1)q_{n+1} + (n^3 + (-1)^{n+1} t^3)q_n. \]

Then
\[ \lim_{n \to \infty} q_n = t^3 \prod_{n=1}^{\infty} \left( 1 + \frac{t^3}{3n^3} \right). \]

Equivalently, for all positive integers \( n \),
\[ \text{Li}_{[2,1]^n}((-1,1)^n) \geq 8^{-n} \text{Li}_{[2,1]^n}((1,1)^n) \]
\[ \iff \zeta((2,1)^n) \geq 8^{-n} \zeta((2,1)^n) = 8^{-n} \zeta((3)^n). \]

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