JOURNAL OF COMBINATORIAL THEORY, SERIES A ???, 2–22 (???)
ARTICLE NO. HA-00000

The Algebra and Combinatorics of Shuffles and Multiple Zeta Values

Douglas Bowman

Department of Mathematics, University of Illinois at Urbana-Champaign, Urbana, Illinois, U.S.A.
E-mail: bowman@math.uiuc.edu

and

David M. Bradley

Department of Mathematics and Statistics, University of Maine, Orono, Maine, U.S.A.
E-mail: bradley@gauss.umemat.maine.edu; dbradley@e-math.ams.org

Communicated by Bruce Rothschild

Received October 3, 2000; accepted April 11, 2001

The algebraic and combinatorial theory of shuffles, introduced by Chen and Ree, is further developed and applied to the study of multiple zeta values. In particular, we establish evaluations for certain sums of cyclically generated multiple zeta values. The boundary case of our result reduces to a former conjecture of Zagier. © ??? Academic Press

Key Words: Lie algebra, shuffle, multiple zeta value, iterated integral.

1. INTRODUCTION

We continue our study of nested sums of the form

$$\zeta(s_1, s_2, \ldots, s_k) := \sum_{n_1 > n_2 > \cdots > n_k > 0} \prod_{j=1}^{k} n_j^{-s_j}, \tag{1}$$

commonly referred to as multiple zeta values [2, 3, 4, 11, 12, 16, 19]. Here and throughout, $s_1, s_2, \ldots, s_k$ are positive integers with $s_1 > 1$ to ensure convergence.

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

There exist many intriguing results and conjectures concerning values of (1) at various arguments. For example,

$$\zeta(\{3,1\}^n) := \zeta(\underbrace{3,1,3,1,\ldots,3,1}_{2n}) = \frac{2\pi^{4n}}{(4n+2)!}, \qquad 0 \le n \in \mathbf{Z}, \tag{2}$$

was conjectured by Zagier [19] and first proved by Broadhurst et al [2] using analytic techniques. Subsequently, a purely combinatorial proof was given [3] based on the well-known shuffle property of iterated integrals, and it is this latter approach which we develop more fully here. For further and deeper results from the analytic viewpoint, see [4].

Our main result is a generalization of (2) in which twos are inserted at various places in the argument string $\{3,1\}^n$. Given a non-negative integer n, let $\vec{s} = (m_0, m_1, \ldots, m_{2n})$ be a vector of non-negative integers, and consider the multiple zeta value obtained by inserting m_j consecutive twos after the jth element of the string $\{3,1\}^n$ for each $j = 0, 1, 2, \ldots, 2n$:

$$\begin{aligned} &Z(\vec{s}) \\ &:= \zeta(\{2\}^{m_0}, 3, \{2\}^{m_1}, 1, \{2\}^{m_2}, 3, \{2\}^{m_3}, 1, \ldots, 3, \{2\}^{m_{2n-1}}, 1, \{2\}^{m_{2n}}). \end{aligned}$$

For non-negative integers k and r, let $C_r(k)$ denote the set of $\binom{k+r-1}{r-1}$ ordered non-negative integer compositions of k having r parts. For example, $C_3(2) = \{(2,0,0), (0,2,0), (0,0,2), (0,1,1), (1,0,1), (1,1,0)\}$. Our generalization of (2) states (see Corollary 5.1 of Section 5) that

$$\sum_{\vec{s} \in C_{2n+1}(m-2n)} Z(\vec{s}) = \frac{2\pi^{2m}}{(2m+2)!} \binom{m+1}{2n+1}, \tag{3}$$

for all non-negative integers m and n with $m \ge 2n$. Equation (2) is the special case of (3) in which $m = 2n$, since $Z(\{0\}^{2n+1}) = \zeta(\{3,1\}^n)$. If again $\vec{s} = (m_0, m_1, \ldots, m_{2n})$ and we put

$$\mathcal{C}(\vec{s}) := Z(\vec{s}) + \sum_{j=1}^{2n} Z(m_j, m_{j+1}, \ldots, m_{2n}, m_0, \ldots, m_{j-1}),$$

then (see Theorem 5.1 of Section 5)

$$\sum_{\vec{s} \in C_{2n+1}(m-2n)} \mathcal{C}(\vec{s}) = Z(m) \times |C_{2n+1}(m-2n)| = \frac{\pi^{2m}}{(2m+1)!} \binom{m}{2n} \tag{4}$$

is an equivalent formulation of (3). The cyclic insertion conjecture [3] can be restated as the assertion that $\mathcal{C}(\vec{s}) = Z(m)$ for all $\vec{s} \in C_{2n+1}(m-2n)$

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

and integers $m \geq 2n \geq 0$. Thus, our result reduces the problem to that of establishing the invariance of $\mathcal{C}(\vec{s})$ on $C_{2n+1}(m-2n)$.

The outline of the paper is as follows. Section 2 provides the essential background for our results. The theory is formalized and further developed in Section 3, in which we additionally give a simple proof of Ree's formula for the inverse of a Lie exponential. In Section 4 we focus on the combinatorics of two-letter words, as this is most directly relevant to the study multiple zeta values. In the final section, we establish the aforementioned results (3) and (4).

2. ITERATED INTEGRALS

As Kontsevich [19] observed, (1) admits an iterated integral representation

$$\zeta(s_1, s_2, \ldots, s_k) = \int_0^1 \prod_{j=1}^{k} a^{s_j-1}b \tag{5}$$

of depth $\sum_{j=1}^{k} s_j$. Here, the notation

$$\int_y^x \prod_{j=1}^{n} \alpha_j := \int_{x>t_1>t_2>\cdots>t_n>y} \prod_{j=1}^{n} f_j(t_j)\,dt_j, \qquad \alpha_j := f_j(t_j)\,dt_j \tag{6}$$

of [2] is used with a and b denoting the differential 1-forms dt/t and $dt/(1-t)$, respectively. Thus, for example, if $f_1 \neq f_2$, we write $\alpha_1^2\alpha_2\alpha_1$ for the integrand $f_1(t_1)f_1(t_2)f_2(t_3)f_1(t_4)\,dt_1\,dt_2\,dt_3\,dt_4$. Furthermore, we shall agree that any iterated integral of an empty product of differential 1-forms is equal to 1. This convention is mainly a notational convenience; nevertheless we shall find it useful for stating results about iterated integrals more concisely and naturally than would be possible otherwise. Thus (6) reduces to 1 when $n = 0$ regardless of the values of x and y.

Clearly the product of two iterated integrals of the form (6) consists of a sum of iterated integrals involving all possible interlacings of the variables. Thus if we denote the set of all $\binom{n+m}{n}$ permutations σ of the indices $\{1, 2, \ldots, n+m\}$ satisfying $\sigma^{-1}(j) < \sigma^{-1}(k)$ for all $1 \leq j < k \leq n$ and $n+1 \leq j < k \leq n+m$ by $\mathrm{Shuff}(n,m)$, then we have the self-evident formula

$$\Big(\int_y^x \prod_{j=1}^{n} \alpha_j\Big)\Big(\int_y^x \prod_{j=n+1}^{n+m} \alpha_j\Big) = \sum_{\sigma\in\mathrm{Shuff}(n,m)} \int_y^x \prod_{j=1}^{n+m} \alpha_{\sigma(j)},$$

???

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

and so define the shuffle product $\sqcup\!\sqcup$ by

$$\left(\prod_{j=1}^{n}\alpha_j\right)\sqcup\!\sqcup\left(\prod_{j=n+1}^{n+m}\alpha_j\right):=\sum_{\sigma\in\mathrm{Shuff}(n,m)}\prod_{j=1}^{n+m}\alpha_{\sigma(j)}. \tag{7}$$

Thus, the sum is over all non-commutative products (counting multiplicity) of length $n+m$ in which the relative orders of the factors in the products $\alpha_1\alpha_2\cdots\alpha_n$ and $\alpha_{n+1}\alpha_{n+2}\cdots\alpha_{n+m}$ are preserved. The term "shuffle" is used because such permutations arise in riffle shuffling a deck of $n+m$ cards cut into one pile of n cards and a second pile of m cards.

The study of shuffles and iterated integrals was pioneered by Chen [6, 7] and subsequently formalized by Ree [18]. A fundamental formula noted by Chen expresses an iterated integral of a product of two paths as a convolution of iterated integrals over the two separate paths. A second formula also due to Chen shows what happens when the underlying simplex (6) is re-oriented. Chen's proof in both cases is by induction on the number of differential 1-forms. Since we will make use of these results in the sequel, it is convenient to restate them here in the current notation and give direct proofs.

PROPOSITION 2.1 ([8, (1.6.2)]). *Let $\alpha_1,\alpha_2,\ldots,\alpha_n$ be differential 1-forms and let $x,y\in\mathbf{R}$. Then*

$$\int_y^x \alpha_1\alpha_2\cdots\alpha_n=(-1)^n\int_x^y\alpha_n\alpha_{n-1}\cdots\alpha_1.$$

Proof. Suppose $\alpha_j=f_j(t_j)\,dt_j$. Observe that

$$\begin{aligned}&\int_y^x f_1(t_1)\int_y^{t_1}f_2(t_2)\cdots\int_y^{t_{n-1}}f_n(t_n)\,dt_n\,dt_{n-1}\cdots dt_1\\&\quad=\int_y^x f_n(t_n)\int_{t_n}^x f_{n-1}(t_{n-1})\cdots\int_{t_2}^x f_1(t_1)\,dt_1\,dt_2\cdots dt_n.\end{aligned}$$

Now switch the limits of integration at each level. ∎

PROPOSITION 2.2 ([6, Lemma 1.1]). *Let $\alpha_1,\alpha_2,\ldots,\alpha_n$ be differential 1-forms and let $y\le z\le x$. Then*

$$\int_y^x\prod_{j=1}^{n}\alpha_j=\sum_{k=0}^{n}\left(\int_z^x\prod_{j=1}^{k}\alpha_j\right)\left(\int_y^z\prod_{j=k+1}^{n}\alpha_j\right).$$

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

Proof.

$$\begin{aligned}\big\{(t_1,t_2,\ldots,t_n)\in\mathbf{R}^n : x>t_1>t_2>\cdots>t_n>y\big\}\\ =\bigcup_{k=0}^{n}\big\{(t_1,\ldots,t_k)\in\mathbf{R}^k : x>t_1>\cdots>t_k>z\big\}\\ \times\big\{(t_{k+1},\ldots,t_n)\in\mathbf{R}^{n-k} : z>t_{k+1}>\cdots>t_n>y\big\}.\end{aligned}$$

∎

A related version of Proposition 2.2, "Hölder Convolution," is exploited in [2] to indicate how rapid computation of multiple zeta values and related slowly-convergent multiple polylogarithmic sums is accomplished. In Section 3.2, Proposition 2.2 is used in conjunction with Proposition 2.1 to give a quick proof of Ree's formula [18] for the inverse of a Lie exponential.

3. THE SHUFFLE ALGEBRA

We have seen how shuffles arise in the study of iterated integral representations for multiple zeta values. Following [15] (cf. also [3, 18]) let A be a finite set and let A^* denote the free monoid generated by A. We regard A as an alphabet, and the elements of A^* as words formed by concatenating any finite number of letters from this alphabet. By linearly extending the concatenation product to the set $\mathbf{Q}\langle A\rangle$ 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

$$\begin{cases}\forall w\in A^*, & 1\sqcup\!\sqcup w = w\sqcup\!\sqcup 1 = w,\\ \forall a,b\in A,\quad \forall u,v\in A^*, & au\sqcup\!\sqcup bv = a(u\sqcup\!\sqcup bv)+b(au\sqcup\!\sqcup v),\end{cases}\tag{8}$$

and then extended linearly to $\mathbf{Q}\langle A\rangle$. One checks that the shuffle product so defined is associative and commutative, and thus $\mathbf{Q}\langle A\rangle$ equipped with the shuffle product becomes a commutative $\mathbf{Q}$-algebra, denoted $\mathrm{Sh}_{\mathbf{Q}}[A]$. Radford [17] has shown that $\mathrm{Sh}_{\mathbf{Q}}[A]$ is isomorphic to the polynomial algebra $\mathbf{Q}[L]$ obtained by adjoining to $\mathbf{Q}$ the transcendence basis L of Lyndon words.

The recursive definition (8) has its analytical motivation in the formula for integration by parts—equivalently, the product rule for differentiation. Thus, if we put $a=f(t)\,dt$, $b=g(t)\,dt$ and

$$F(x) := \int_y^x (au\sqcup\!\sqcup bv) = \Big(\int_y^x f(t)\int_y^t u\,dt\Big)\Big(\int_y^x g(t)\int_y^t v\,dt\Big),$$

???

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

then writing $F(x) = \int_y^x F'(s)\,ds$ and applying the product rule for differentiation yields

$$\begin{aligned} F(x) &= \int_y^x \left(f(s)\int_y^s u\right)\left(\int_y^s g(t)\int_y^t v\,dt\right) ds \\ &\qquad + \int_y^x g(s)\left(\int_y^s f(t)\int_y^t u\,dt\right)\int_y^s v\,ds \\ &= \int_y^x \left[a(u \sqcup\!\sqcup bv) + b(au \sqcup\!\sqcup v)\right]. \end{aligned}$$

Alternatively, by viewing F as a function of y, we see that the recursion could equally well have been stated as

$$\begin{cases} \forall w \in A^*, & 1 \sqcup\!\sqcup w = w \sqcup\!\sqcup 1 = w, \\ \forall a, b \in A, \quad \forall u, v \in A^*, & ua \sqcup\!\sqcup vb = (u \sqcup\!\sqcup vb)a + (ua \sqcup\!\sqcup v)b. \end{cases} \tag{9}$$

Of course, both definitions are equivalent to (7).

3.1. Q-Algebra Homomorphisms on Shuffle Algebras

The following relatively straightforward results concerning $\mathbf{Q}$-algebra homomorphisms on shuffle algebras will facilitate our discussion of the Lie exponential in Section 3.2 and of relationships between certain identities for multiple zeta values and Euler sums [1, 2, 4]. To reduce the possibility of any confusion in what follows, we make the following definition explicit.

DEFINITION 3.1. Let R and S be rings with identity, and let A and B be alphabets. A ring anti-homomorphism $\psi : R\langle A\rangle \to S\langle B\rangle$ is an additive, R-linear, identity-preserving map that satisfies $\psi(u)\psi(v) = \psi(vu)$ for all $u, v \in A^*$ (and hence for all $u, v \in R\langle A\rangle$).

PROPOSITION 3.1. *Let A and B be alphabets. A ring anti-homomorphism $\psi : \mathbf{Q}\langle A\rangle \to \mathbf{Q}\langle B\rangle$ that satisfies $\psi(A) \subseteq B$ induces a $\mathbf{Q}$-algebra homomorphism of shuffle algebras $\psi : \mathrm{Sh}_{\mathbf{Q}}[A] \to \mathrm{Sh}_{\mathbf{Q}}[B]$ in the natural way.*

Proof. It suffices to show that $\psi(u \sqcup\!\sqcup v) = \psi(u) \sqcup\!\sqcup \psi(v)$ for all $u, v \in A^*$. The proof is by induction, and will require both recursive definitions of the shuffle product. Let $u, v \in A^*$ be words. For the base case, note that $\psi(1 \sqcup\!\sqcup u) = \psi(u) = 1 \sqcup\!\sqcup \psi(u)$ and likewise with the empty word on the right. For the inductive step, let $a, b \in A$ be letters and assume that $\psi(u \sqcup\!\sqcup bv) = \psi(u) \sqcup\!\sqcup \psi(bv)$ and $\psi(au \sqcup\!\sqcup v) = \psi(au) \sqcup\!\sqcup \psi(v)$ both hold.

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

Then as ψ is an anti-homomorphism of rings,

$$\begin{aligned}
\psi(au \sqcup\!\sqcup bv) &= \psi(a(u \sqcup\!\sqcup bv) + b(au \sqcup\!\sqcup v)) \\
&= \psi(a(u \sqcup\!\sqcup bv)) + \psi(b(au \sqcup\!\sqcup v)) \\
&= \psi(u \sqcup\!\sqcup bv)\psi(a) + \psi(au \sqcup\!\sqcup v)\psi(b) \\
&= [\psi(u) \sqcup\!\sqcup \psi(bv)]\psi(a) + [\psi(au) \sqcup\!\sqcup \psi(v)]\psi(b) \\
&= [\psi(u) \sqcup\!\sqcup \psi(v)\psi(b)]\psi(a) + [\psi(u)\psi(a) \sqcup\!\sqcup \psi(v)]\psi(b) \\
&= \psi(u)\psi(a) \sqcup\!\sqcup \psi(v)\psi(b) \\
&= \psi(au) \sqcup\!\sqcup \psi(bv).
\end{aligned}$$

∎

Of course, there is an analogous result for ring homomorphisms.

PROPOSITION 3.2. *Let A and B be alphabets. A ring homomorphism $\phi : \mathbf{Q}\langle A\rangle \to \mathbf{Q}\langle B\rangle$ that satisfies $\phi(A) \subseteq B$ induces a $\mathbf{Q}$-algebra homomorphism of shuffle algebras $\phi : \mathrm{Sh}_{\mathbf{Q}}[A] \to \mathrm{Sh}_{\mathbf{Q}}[B]$ in the natural way.*

Proof. The proof is similar to the proof of Proposition 3.1, and in fact is simpler in that it requires only one of the two recursive definitions of the shuffle product. Alternatively, one can put $u = a_1 a_2 \cdots a_n$, $v = a_{n+1}a_{n+2}\cdots a_{n+m}$ and verify the equation $\phi(u \sqcup\!\sqcup v) = \phi(u) \sqcup\!\sqcup \phi(v)$ using (7) and the hypothesis that ϕ is a ring homomorphism on $\mathbf{Q}\langle A\rangle$. ∎

Example 1. Let A be an alphabet and let $R : \mathbf{Q}\langle A\rangle \to \mathbf{Q}\langle A\rangle$ be the canonical ring anti-automorphism induced by the assignments $R(a) = a$ for all $a \in A$. Then $R(\prod_{j=1}^{n} a_j) = \prod_{j=1}^{n} a_{n-j+1}$ for all $a_1, \ldots, a_n \in A$, so that R is a string-reversing involution which induces a shuffle algebra automorphism of $\mathrm{Sh}_{\mathbf{Q}}[A]$. We shall reserve the notation R for this automorphism throughout.

Example 2. Let $A = \{a, b\}$ and let $S : \mathbf{Q}\langle A\rangle \to \mathbf{Q}\langle A\rangle$ be the ring automorphism induced by the assignments $S(a) = b$, $S(b) = a$. Then the composition $\psi := S \circ R$ is a letter-switching, string-reversing involution which induces a shuffle algebra automorphism of $\mathrm{Sh}_{\mathbf{Q}}[A]$. In the case $a = dt/t$, $b = dt/(1-t)$, this is the so-called Kontsevich duality [19, 1, 2, 16] for iterated integrals obtained by making the change of variable $t \mapsto 1 - t$ at each level of integration. Words which are invariant under ψ are referred to as *self-dual*. It is easy to see that a self-dual word must be of even length, and the number of self-dual words of length $2k$ is 2^k.

Example 3. Let $A = \{a, b\}, B = \{b, c\}$ and let $\psi : \mathbf{Q}\langle A\rangle \to \mathbf{Q}\langle B\rangle$ be the letter-shifting, string-reversing ring anti-homomorphism induced by

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

the assignments $\psi(a) = b$ and $\psi(b) = c$. Then ψ induces a shuffle algebra isomorphism $\psi : \mathrm{Sh}_{\mathbf{Q}}[A] \xrightarrow{\sim} \mathrm{Sh}_{\mathbf{Q}}[B]$. With the choice of differential 1-forms $a = dt/t$, $b = dt/(1-t)$, $c = -dt/(1+t)$, ψ maps shuffle identities for multiple zeta values to equivalent identities for alternating unit Euler sums. We refer the reader to [1, 2, 4] for details concerning alternating Euler sums; for our purposes here it suffices to assert that they are important instances—as are multiple zeta values—of multiple polylogarithms [2, 10].

3.2. A Lie Exponential

Let A be an alphabet, and let $X = \{X_a : a \in A\}$ be a set of $\mathrm{card}(A)$ distinct non-commuting indeterminates. Every element in $\mathbf{Q}\langle X\rangle$ can be written as a sum $F = F_0 + F_1 + \cdots$ where F_n is a homogeneous form of degree n. Those elements F for which F_n belongs to the Lie algebra generated by X for each $n > 0$ and for which $F_0 = 0$ are referred to as *Lie elements*.

Let $\mathbf{X} : \mathbf{Q}\langle A\rangle \to \mathbf{Q}\langle X\rangle$ be the canonical ring isomorphism induced by the assignments $\mathbf{X}(a) = X_a$ for all $a \in A$. If $Y = \{Y_a : a \in A\}$ is another set of non-commuting indeterminates, we similarly define $\mathbf{Y} : \mathbf{Q}\langle A\rangle \to \mathbf{Q}\langle Y\rangle$ to be the canonical ring isomorphism induced by the assignments $\mathbf{Y}(a) = Y_a$ for all $a \in A$. Let us suppose $X = \mathbf{X}(A)$ and $Y = \mathbf{Y}(A)$ are disjoint and their elements commute with each other, so that for all $a, b \in A$ we have $X_a Y_b = Y_b X_a$. If we define addition and multiplication in $\mathbf{Q}[\mathbf{X}, \mathbf{Y}]$ by $(\mathbf{X} + \mathbf{Y})(a) = X_a + Y_a$ and $(\mathbf{XY})(a) = X_a Y_a$ for all $a \in A$, then $\mathbf{Q}[\mathbf{X}, \mathbf{Y}]$ becomes a commutative $\mathbf{Q}$-algebra of ring isomorphisms $\mathbf{Z}$. For example, if $\mathbf{Z} = \mathbf{X} + \mathbf{Y}$ and $w = a_1 a_2 \cdots a_n$ where $a_1, a_2 \ldots, a_n \in A$, then

$$\mathbf{Z}(w) = (\mathbf{X} + \mathbf{Y})(a_1 a_2 \cdots a_n) = \prod_{j=1}^{n} (\mathbf{X} + \mathbf{Y})(a_j) = \prod_{j=1}^{n} \left(X_{a_j} + Y_{a_j}\right).$$

Let $G : \mathbf{Q}[\mathbf{X}, \mathbf{Y}] \to (\mathrm{Sh}_{\mathbf{Q}}[A])\langle\langle X, Y\rangle\rangle$ be defined by

$$G(\mathbf{Z}) := \sum_{w \in A^*} w\mathbf{Z}(w). \tag{10}$$

Evidently,

$$G(\mathbf{X}) = 1 + \sum_{n=1}^{\infty} \left(\sum_{a \in A} aX_a \right)^n = \frac{1}{1 - \sum_{a \in A} aX_a}. \tag{11}$$

More importantly, G is a homomorphism from the underlying $\mathbf{Q}$-vector space to the underlying multiplicative monoid $((\mathrm{Sh}_{\mathbf{Q}}[A])\langle\langle X, Y\rangle\rangle, \sqcup\!\sqcup)$.

???

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

THEOREM 3.1. *The map* $G : \mathbf{Q}[\mathbf{X}, \mathbf{Y}] \to (\mathrm{Sh}_{\mathbf{Q}}[A])\langle\langle X, Y\rangle\rangle$ *defined by (10) has the property that*

$$G(\mathbf{X} + \mathbf{Y}) = G(\mathbf{X}) \sqcup\!\sqcup G(\mathbf{Y}).$$

Proof. On the one hand, we have

$$G(\mathbf{X} + \mathbf{Y}) = \sum_{w \in A^*} w(\mathbf{X} + \mathbf{Y})(w),$$

whereas on the other hand,

$$G(\mathbf{X}) \sqcup\!\sqcup G(\mathbf{Y}) = \sum_{u \in A^*} u\mathbf{X}(u) \sqcup\!\sqcup \sum_{v \in A^*} v\mathbf{Y}(v) = \sum_{u,v \in A^*} (u \sqcup\!\sqcup v)\mathbf{X}(u)\mathbf{Y}(v).$$

Therefore, we need to show that

$$\sum_{u,v \in A^*} (u \sqcup\!\sqcup v)\mathbf{X}(u)\mathbf{Y}(v) = \sum_{w \in A^*} w(\mathbf{X} + \mathbf{Y})(w).$$

But,

$$\begin{aligned}
&\sum_{u,v \in A^*} (u \sqcup\!\sqcup v)\mathbf{X}(u)\mathbf{Y}(v) \\
&= \sum_{n \geq 0} \sum_{a_1, \ldots, a_n \in A} \sum_{k=0}^{n} \Big(\prod_{j=1}^{k} a_j \sqcup\!\sqcup \prod_{j=k+1}^{n} a_j \Big) \prod_{j=1}^{k} X_{a_j} \prod_{j=k+1}^{n} Y_{a_j} \\
&= \sum_{n \geq 0} \sum_{a_1, \ldots, a_n \in A} \sum_{k=0}^{n} \sum_{\sigma \in \mathrm{Shuff}(k, n-k)} \prod_{r=1}^{n} a_{\sigma(r)} \prod_{j=1}^{k} X_{a_j} \prod_{j=k+1}^{n} Y_{a_j},
\end{aligned}$$

using the non-recursive definition (7) of the shuffle product. For each $\sigma \in \mathrm{Shuff}(k, n-k)$, if $a_1, \ldots, a_n$ run through the elements of A, then so do $a_{\sigma(1)}, \ldots, a_{\sigma(n)}$. Hence putting $b_j = a_{\sigma(j)}$, we have that

$$\begin{aligned}
&\sum_{u,v \in A^*} (u \sqcup\!\sqcup v)\mathbf{X}(u)\mathbf{Y}(v) \\
&= \sum_{n \geq 0} \sum_{b_1, \ldots, b_n \in A} \Big(\prod_{r=1}^{n} b_r \Big) \sum_{k=0}^{n} \sum_{\sigma \in \mathrm{Shuff}(k, n-k)} \prod_{j=1}^{k} X_{b_{\sigma^{-1}(j)}} \prod_{j=k+1}^{n} Y_{b_{\sigma^{-1}(j)}} \\
&= \sum_{n \geq 0} \sum_{b_1, \ldots, b_n \in A} \Big(\prod_{r=1}^{n} b_r \Big) \prod_{j=1}^{n} (X_{b_j} + Y_{b_j}) \\
&= \sum_{w \in A^*} w(\mathbf{X} + \mathbf{Y})(w).
\end{aligned}$$

???

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

In the penultimate step, we have summed over all $\binom{n}{k}$ shuffles of the indeterminates X with the indeterminates Y, yielding all 2^n possible choices obtained by selecting an X or a Y from each factor in the product $(X_{b_1} + Y_{b_1}) \cdots (X_{b_n} + Y_{b_n})$. ∎

Remarks. Theorem 3.1 suggests that the map G defined by (10) can be viewed as a non-commutative analog of the exponential function. The analogy is clearer if we rewrite (11) in the form

$$G(\mathbf{X}) = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \Big(\sum_{a \in A} a X_a \Big)^{\sqcup\!\sqcup\, n}.$$

Just as the functional equation for the exponential function is equivalent to the binomial theorem, Theorem 3.1 is equivalent to the following shuffle analog of the binomial theorem:

PROPOSITION 3.3 (Binomial Theorem in $\mathbf{Q}\langle X\rangle\langle Y\rangle$). *Let* $X = \{X_1, X_2, \ldots, X_n\}$ *and* $Y = \{Y_1, Y_2, \ldots, Y_n\}$ *be disjoint sets of non-commuting indeterminates such that* $X_j Y_k = Y_k X_j$ *for all* $1 \le j, k \le n$. *Then*

$$\prod_{j=1}^{n} (X_j + Y_j) = \sum_{k=0}^{n} \sum_{\sigma \in \mathrm{Shuff}(k, n-k)} \prod_{j=1}^{k} X_{\sigma^{-1}(j)} \prod_{j=k+1}^{n} Y_{\sigma^{-1}(j)}.$$

Chen [6, 7] considered what is in our notation the iterated integral of (10), namely

$$G_y^x := \sum_{w \in A^*} \int_y^x w \mathbf{X}(w) \tag{12}$$

in which the alphabet A is viewed as a set of differential 1-forms. He proved [6, Theorem 6.1], [7, Theorem 2.1] the non-commutative generating function formulation

$$G_y^x = G_z^x G_y^z, \qquad y \le z \le x$$

of Proposition 2.2 and also proved [7, Theorem 4.2] that if the 1-forms are piecewise continuously differentiable, then $\log G_y^x$ is a Lie element, or equivalently, that G_y^x is a Lie exponential. However, Ree [18] showed that a formal power series

$$\log \Big(1 + \sum_{n>0} \sum_{1 \le j_1, \ldots, j_n \le m} c(j_1, \ldots, j_n) X_{j_1} \cdots X_{j_n} \Big)$$

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

in non-commuting indeterminates X_j is a Lie element if and only if the coefficients satisfy the shuffle relations

$$c(j_1,\ldots,j_n)c(j_{n+1},\ldots,j_{n+k}) = \sum_{\sigma\in\mathrm{Shuff}(n,k)} c(j_{\sigma(1)},\ldots,j_{\sigma(n+k)}),$$

for all non-negative integers n and k. Using integration by parts, Ree [18] showed that Chen's coefficients do indeed satisfy these relations, and that more generally, $G(\mathbf{X})$ as defined by (10) is a Lie exponential, a fact that can also be deduced from Theorem 3.1 and a result of Friedrichs [9, 13, 14].

Ree also proved a formula [18, Theorem 2.6] for the inverse of (10), using certain derivations and Lie bracket operations. It may be of interest to give a more direct proof, using only the shuffle operation. The result is restated below in our notation.

THEOREM 3.2 ([18, Theorem 2.6]). *Let A be an alphabet, let $X = \{X_a : a \in A\}$ be a set of non-commuting indeterminates and let $\mathbf{X} : \mathbf{Q}\langle A\rangle \to \mathbf{Q}\langle X\rangle$ be the canonical ring isomorphism induced by the assignments $\mathbf{X}(a) = X_a$ for all $a \in A$. Let $G(\mathbf{X})$ be as in (11), let R be as in Example 1, and put*

$$H(\mathbf{X}) := \sum_{w\in A^*} (-1)^{|w|} R(w)\mathbf{X}(w),$$

where $|w|$ denotes the length of the word w. Then $G(\mathbf{X}) \sqcup\!\sqcup H(\mathbf{X}) = 1$.

It is convenient to state the essential ingredient in our proof of Theorem 3.2 as an independent result.

LEMMA 3.1. *Let A be an alphabet and let R be as in Example 1. For all $w \in A^*$, we have*

$$\sum_{\substack{u,v\in A^*\\ uv=w}} (-1)^{|u|} R(u) \sqcup\!\sqcup v = \delta_{|w|,0}. \tag{13}$$

Remarks. We have used the Kronecker delta

$$\delta_{n,k} := \begin{cases} 1 & \text{if } n = k,\\ 0 & \text{otherwise.}\end{cases}$$

Since R is a $\mathbf{Q}$-algebra automorphism of $\mathrm{Sh}_{\mathbf{Q}}[A]$, applying R to both sides of (13) yields the related identity

$$\sum_{\substack{u,v\in A^*\\ uv=w}} (-1)^{|u|} u \sqcup\!\sqcup R(v) = \delta_{|w|,0}, \qquad w \in A^*.$$

???

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

Proof of Lemma 3.1. First note that if we view the elements of A as differential 1-forms and integrate the left hand side of (13) from y to x, then we obtain

$$\sum_{\substack{u,v\in A^*\\ uv=w}} (-1)^{|u|}\int_y^x R(u)\int_y^x v = \sum_{\substack{u,v\in A^*\\ uv=w}} \int_x^y u\int_y^x v = \int_y^y w = \delta_{|w|,0}$$

by Propositions 2.1 and 2.2. For an integral-free proof, we proceed as follows. Clearly (13) holds when $|w| = 0$, so assume $w = \prod_{j=1}^n a_j$ where $a_1, \ldots, a_n \in A$ and n is a positive integer. Let $\mathfrak{S}_n$ denote the group of permutations of the set of indices $\{1, 2, \ldots, n\}$, and let the additive weight-function $W : 2^{\mathfrak{S}_n} \to A^*$ map subsets of $\mathfrak{S}_n$ to words as follows:

$$W(S) := \sum_{\sigma\in S}\prod_{j=1}^n a_{\sigma(j)}, \qquad S \subseteq \mathfrak{S}_n.$$

For $k = 0, 1, \ldots, n$ let

$$\begin{aligned} c_k &:= W(\{\sigma \in \mathfrak{S}_n : \sigma^{-1}(i) < \sigma^{-1}(j) \text{ for } k \geq i > j \geq 1 \text{ and} \\ &\qquad k+1 \leq i < j \leq n\}), \\ b_k &:= W(\{\sigma \in \mathfrak{S}_n : \sigma^{-1}(i) < \sigma^{-1}(j) \text{ for } k \geq i > j \geq 1 \text{ and} \\ &\qquad k \leq i < j \leq n\}). \end{aligned}$$

Then $c_0 = b_1$, $c_n = b_n$ and $c_k = b_k + b_{k+1}$ for $1 \leq k \leq n-1$. Thus,

$$\begin{aligned} \sum_{\substack{u,v\in A^*\\ uv=w}} (-1)^{|u|} R(u) \sqcup v &= \sum_{k=0}^n (-1)^k \prod_{j=1}^k a_{k-j+1} \sqcup \prod_{j=k+1}^n a_j \\ &= \sum_{k=0}^n (-1)^k c_k \\ &= b_1 + (-1)^n b_n + \sum_{k=1}^{n-1} (-1)^k (b_k + b_{k+1}) \\ &= b_1 + (-1)^n b_n + \sum_{k=1}^{n-1} (-1)^k b_k - \sum_{k=2}^{n} (-1)^k b_k \\ &= 0, \end{aligned}$$

since the sums telescope. ∎

Remark. One can also give an integral-free proof of Lemma 3.1 by induction using the recursive definition (9) of the shuffle product.

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

Proof of Theorem 3.2. By Lemma 3.1, we have

$$\begin{aligned}
&\sum_{u\in A^*} (-1)^{|u|} R(u)\mathbf{X}(u) \sqcup\!\sqcup \sum_{v\in A^*} v\mathbf{X}(v) \\
&= \sum_{w\in A^*} \mathbf{X}(w) \sum_{\substack{u,v\in A^* \\ uv=w}} (-1)^{|u|} R(u) \sqcup\!\sqcup v \\
&= \sum_{w\in A^*} \mathbf{X}(w)\, \delta_{|w|,0} \\
&= 1.
\end{aligned}$$

Since $(\mathrm{Sh}_{\mathbf{Q}}[A])\langle\langle X\rangle\rangle$ is commutative with respect to the shuffle product, the result follows. ∎

4. COMBINATORICS OF SHUFFLE PRODUCTS

The combinatorial proof [3] of Zagier's conjecture (2) hinged on expressing the sum of the words comprising the shuffle product of $(ab)^p$ with $(ab)^q$ as a linear combination of basis subsums $T_{p+q,n}$. To gain a deeper understanding of the combinatorics of shuffles on two letters, it is necessary to introduce additional basis subsums. We do so here, and thereby find analogous expansion theorems. We conclude the section by providing generating function formulations for these results. The generating function formulation plays a key role in the proof of our main result (4), Theorem 5.1 of Section 5. The precise definitions of the basis subsums follow.

DEFINITION 4.1. ([3]) For integers $m \geq n \geq 0$ let $S_{m,n}$ denote the set of words occurring in the shuffle product $(ab)^n \sqcup\!\sqcup (ab)^{m-n}$ in which the subword a^2 appears exactly n times, and let $T_{m,n}$ be the sum of the $\binom{m}{2n}$ distinct words in $S_{m,n}$. For all other integer pairs (m,n) it is convenient to define $T_{m,n} := 0$.

DEFINITION 4.2. For integers $m \geq n+1 \geq 2$, let $U_{m,n}$ be the sum of the elements of the set of words arising in the shuffle product of $b(ab)^{n-1}$ with $b(ab)^{m-n-1}$ in which the subword b^2 occurs exactly n times. For all other integer pairs (m,n) define $U_{m,n} := 0$.

In terms of the basis subsums, we have the following decompositions:

PROPOSITION 4.1 ([3, Prop. 1]). *For all non-negative integers p and q,*

$$(ab)^p \sqcup\!\sqcup (ab)^q = \sum_{n=0}^{\min(p,q)} 4^n \binom{p+q-2n}{p-n} T_{p+q,n}. \tag{14}$$

???

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

The corresponding result for our basis (Definition 4.2) is

PROPOSITION 4.2. *For all positive integers p and q,*

$$b(ab)^{p-1} \sqcup\!\sqcup b(ab)^{q-1} = \frac{1}{2} \sum_{n=1}^{\min(p,q)} 4^n \binom{p+q-2n}{p-n} U_{p+q,n}. \tag{15}$$

Proof of Proposition 4.2. See the proof of Proposition 4.1 given in [3]. The only difference here is that a^2 occurs one less time per word than b^2 and so the multiplicity of each word must be divided by 2. The index of summation now starts at 1 because there must be at least one occurrence of b^2 in each term of the expansion. ∎

COROLLARY 4.1. *For integers $p \geq 1$ and $q \geq 0$,*

$$\begin{aligned} b(ab)^{p-1} \sqcup\!\sqcup (ab)^q = &\sum_{n=0}^{\min(p-1,q)} 4^n \binom{p+q-2n-1}{p-n-1} b\, T_{p+q-1,n} \\ &+ \frac{1}{2} \sum_{n=1}^{\min(p,q)} 4^n \binom{p+q-2n}{p-n} a\, U_{p+q,n}. \end{aligned} \tag{16}$$

Proof. From (8) it is immediate that

$$b(ab)^{p-1} \sqcup\!\sqcup (ab)^q = b[(ab)^{p-1} \sqcup\!\sqcup (ab)^q] + a[b(ab)^{p-1} \sqcup\!\sqcup b(ab)^{q-1}].$$

Now apply (14) and Proposition 4.2. ∎

PROPOSITION 4.3. *Let $x_0, x_1, \ldots$ and $y_0, y_1, \ldots$ be sequences of not necessarily commuting indeterminates, and let m be a non-negative (respectively, positive) integer. We have the shuffle convolution formulæ*

$$\begin{aligned} &\sum_{k=0}^{m} x_k\, y_{m-k} \left[(ab)^k \sqcup\!\sqcup (ab)^{m-k}\right] \\ &\qquad = \sum_{n=0}^{\lfloor m/2 \rfloor} 4^n \sum_{j=0}^{m-2n} \binom{m-2n}{j} x_{n+j}\, y_{m-n-j}\, T_{m,n}, \end{aligned} \tag{17}$$

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

and

$$\sum_{k=1}^{m-1} x_k\, y_{m-k} \left[b(ab)^{k-1} \sqcup\!\sqcup\, b(ab)^{m-k-1} \right] = \frac{1}{2} \sum_{n=1}^{\lfloor m/2 \rfloor} 4^n \sum_{j=0}^{m-2n} \binom{m-2n}{j} x_{n+j}\, y_{m-n-j}\, U_{m,n}, \quad (18)$$

respectively.

Proof. Starting with the left hand side of (17) and applying (14), we find that

$$\begin{aligned} &\sum_{k=0}^{m} x_k\, y_{m-k} \left[(ab)^k \sqcup\!\sqcup\, (ab)^{m-k} \right] \\ &= \sum_{k=0}^{m} x_k\, y_{m-k} \sum_{n=0}^{\min(k,m-k)} 4^n \binom{m-2n}{k-n} T_{m,n} \\ &= \sum_{n=0}^{\lfloor m/2 \rfloor} 4^n \sum_{k=n}^{m-n} x_k\, y_{m-k} \binom{m-2n}{k-n} T_{m,n} \\ &= \sum_{n=0}^{\lfloor m/2 \rfloor} 4^n \sum_{j=0}^{m-2n} \binom{m-2n}{j} x_{n+j}\, y_{m-n-j}\, T_{m,n}, \end{aligned}$$

which proves (17). The proof of (18) proceeds analogously from (15). ∎

As the proof shows, the products taken in (17) and (18) can be quite general; between the not necessarily commutative indeterminates and the polynomials in a, b the products need only be bilinear for the formulæ to hold. Thus, there are many possible special cases that can be examined. Here we will consider only one major application. If we confine ourselves to commuting geometric sequences, we obtain

THEOREM 4.1. *Let x and y be commuting indeterminates. In the commutative polynomial ring* $(\mathrm{Sh}_{\mathbf{Q}}[a,b])[x,y]$ *we have the shuffle convolution formulæ*

$$\sum_{k=0}^{m} x^k y^{m-k} \left[(ab)^k \sqcup\!\sqcup\, (ab)^{m-k} \right] = \sum_{n=0}^{\lfloor m/2 \rfloor} (4xy)^n (x+y)^{m-2n}\, T_{m,n} \quad (19)$$

???

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

for all non-negative integers m, and

$$\sum_{k=1}^{m-1} x^k y^{m-k} \left[b(ab)^{k-1} \sqcup\!\sqcup b(ab)^{m-k-1} \right] = \frac{1}{2} \sum_{n=1}^{\lfloor m/2 \rfloor} (4xy)^n (x+y)^{m-2n} U_{m,n} \tag{20}$$

for all integers $m \geq 2$.

Proof. In Proposition 4.3, put $x_k = x^k$ and $y_k = y^k$ for each $k \geq 0$ and apply the binomial theorem. ∎

5. CYCLIC SUMS IN $\mathbf{Sh}_{\mathbf{Q}}[A, B]$

In this final section, we establish the results (3) and (4) stated in the introduction. Let $S_{m,n}$ be as in Definition 4.1. Each word in $S_{m,n}$ has a unique representation

$$(ab)^{m_0} \prod_{k=1}^{n} (a^2b)(ab)^{m_{2k-1}} b(ab)^{m_{2k}}, \tag{21}$$

in which $m_0, m_1, \ldots, m_{2n}$ are non-negative integers with sum $m_0 + m_1 + \cdots + m_{2n} = m - 2n$. Conversely, every ordered $(2n+1)$-tuple $(m_0, m_1, \ldots, m_{2n})$ of non-negative integers with sum $m - 2n$ gives rise to a unique word in $S_{m,n}$ via (21). Thus, a bijective correspondence φ is established between the set $S_{m,n}$ and the set $C_{2n+1}(m-2n)$ of ordered non-negative integer compositions of $m-2n$ with $2n+1$ parts. In view of the relationship (5) expressing multiple zeta values as iterated integrals, it therefore makes sense to define

$$Z(\vec{s}) := \int_0^1 \varphi(\vec{s}), \qquad \vec{s} \in C_{2n+1}(m-2n), \qquad a := dt/t, \quad b := dt/(1-t).$$

Thus, if $\vec{s} = (m_0, m_1, \ldots, m_{2n})$, then

$$\begin{aligned} Z(\vec{s}) &= \int_0^1 (ab)^{m_0} \prod_{k=1}^{n} (a^2b)(ab)^{m_{2k-1}} b(ab)^{m_{2k}} \\ &= \zeta(\{2\}^{m_0}, 3, \{2\}^{m_1}, 1, \{2\}^{m_2}, 3, \{2\}^{m_3}, 1, \ldots, 3, \{2\}^{m_{2n-1}}, 1, \{2\}^{m_{2n}}), \end{aligned}$$

in which the argument string consisting of m_j consecutive twos is inserted after the jth element of the string $\{3,1\}^n$ for each $j = 0, 1, 2, \ldots, 2n$.

From [1] we recall the evaluation

$$Z(m) = \zeta(\{2\}^m) = \frac{\pi^{2m}}{(2m+1)!}, \qquad 0 \leq m \in \mathbf{Z}. \tag{22}$$

???

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

Let $\mathfrak{S}_{2n+1}$ denote the group of permutations on the set of indices $\{0, 1, 2, \ldots, 2n\}$. For $\sigma \in \mathfrak{S}_{2n+1}$ we define a group action on $C_{2n+1}(m-2n)$ by $\sigma\vec{s} = (m_{\sigma^{-1}(0)}, m_{\sigma^{-1}(1)}, \ldots, m_{\sigma^{-1}(2n)})$, where $\vec{s} = (m_0, m_1, \ldots, m_{2n})$. Let

$$\mathcal{C}(\vec{s}) := \sum_{j=0}^{2n} Z(\sigma^j \vec{s}), \qquad \sigma = (0\,1\,2\ldots 2n) \tag{23}$$

denote the sum of the $2n+1$ Z-values in which the arguments are permuted cyclically. By construction, $\mathcal{C}$ is invariant under any cyclic permutation of its argument string. The cyclic insertion conjecture [3, Conjecture 1] asserts that in fact, $\mathcal{C}$ depends only on the number and sum of its arguments. More specifically, it is conjectured that

CONJECTURE 5.1. *For any non-negative integers $m_0, m_1, \ldots, m_{2n}$, we have*

$$\mathcal{C}(m_0, m_1, \ldots, m_{2n}) = Z(m) = \frac{\pi^{2m}}{(2m+1)!},$$

where $m := 2n + \sum_{j=0}^{2n} m_j$.

An equivalent generating function formulation of Conjecture 5.1 follows.

CONJECTURE 5.2. *Let $x_0, x_1, \ldots$ be a sequence of commuting indeterminates. Then*

$$\sum_{n=0}^{\infty} y^{2n} \sum_{\substack{m_j \geq 0 \\ 0 \leq j \leq 2n}} \mathcal{C}(m_0, m_1, \ldots, m_{2n}) \coprod_{j=0}^{2n} x_j^{m_j}$$
$$= \sum_{m=0}^{\infty} Z(m) \sum_{n=0}^{\lfloor m/2 \rfloor} y^{2n} (x_0 + x_1 + \cdots + x_{2n})^{m-2n}.$$

???

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

To see the equivalence of Conjectures 5.1 and 5.2, observe that by the multinomial theorem,

$$\begin{aligned}
&\sum_{m=0}^{\infty} Z(m) \sum_{n=0}^{\lfloor m/2 \rfloor} y^{2n}(x_0 + x_1 + \cdots + x_{2n})^{m-2n} \\
&= \sum_{n=0}^{\infty} y^{2n} \sum_{m \geq 2n} Z(m)(x_0 + x_1 + \cdots + x_{2n})^{m-2n} \\
&= \sum_{n=0}^{\infty} y^{2n} \sum_{m \geq 2n} Z(m) \sum_{m_0+\cdots+m_{2n}=m-2n} \binom{m_0 + \cdots + m_{2n}}{m_0, \ldots, m_{2n}} \prod_{j=0}^{2n} x_j^{m_j} \\
&= \sum_{n=0}^{\infty} y^{2n} \sum_{m \geq 2n} Z(m) \sum_{m_0+\cdots+m_{2n}=m-2n} \coprod_{j=0}^{2n} x_j^{m_j}.
\end{aligned}$$

Now compare coefficients. Although Conjecture 5.1 remains unproved, it is nevertheless possible to reduce the problem to that of establishing the invariance of $\mathcal{C}(\vec{s})$ for $\vec{s} \in C_{2n+1}(m-2n)$. More specifically, we have the following non-trivial result.

THEOREM 5.1. *For all non-negative integers m and n with $m \geq 2n$,*

$$\sum_{\vec{s} \in C_{2n+1}(m-2n)} \mathcal{C}(\vec{s}) = Z(m) \times |C_{2n+1}(m-2n)| = Z(m) \binom{m}{2n}.$$

Example 4. If $m = 2n$, Theorem 5.1 states that

$$\mathcal{C}(\{0\}^{2n+1}) = (2n+1)\zeta(\{3,1\}^n) = Z(2n),$$

which is equivalent to the Broadhurst-Zagier formula (2) (Theorem 1 of [3]).

Example 5. If $m = 2n+1$, Theorem 5.1 states that

$$(2n+1)\mathcal{C}(1, \{0\}^{2n}) = (2n+1)Z(2n+1),$$

which is Theorem 2 of [3].

For $m > 2n+1$, Theorem 5.1 gives new results, although no additional instances of Conjecture 5.1 are settled. For the record, we note the following restatement of Theorem 5.1 in terms of Z-functions:

COROLLARY 5.1 (Equivalent to Theorem 5.1). *Let $T_{m,n}$ be as in Definition 4.1, and put $a = dt/t$, $b = dt/(1-t)$. Then, for all non-negative*

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

integers m and n, with $m \geq 2n$,

$$\sum_{\vec{s} \in C_{2n+1}(m-2n)} Z(\vec{s}) = \int_0^1 T_{m,n} = \frac{Z(m)}{2n+1}\binom{m}{2n} = \frac{2\pi^{2m}}{(2m+2)!}\binom{m+1}{2n+1}. \tag{24}$$

Proof of Theorem 5.1. In view of the equivalent reformulation (24) and the well-known evaluation (22) for $Z(m)$, it suffices to prove that with $T_{m,n}$ as in Definition 4.1 and with $a = dt/t$, $b = dt/(1-t)$, we have

$$\int_0^1 T_{m,n} = \frac{2\pi^{2m}}{(2m+2)!}\binom{m+1}{2n+1}.$$

Let

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

Then [1] $J(z) = (\sinh(\pi z))/(\pi z)$ for $z \neq 0$ and $J(0) = 1$. We have

$$\begin{aligned} J(z\cos\theta)J(z\sin\theta) &= \frac{\sinh(\pi z\cos\theta)}{\pi z\cos\theta} \cdot \frac{\sinh(\pi z\sin\theta)}{\pi z\sin\theta} \\ &= \frac{\cosh\pi z(\cos\theta+\sin\theta) - \cosh\pi z(\cos\theta-\sin\theta)}{2\pi^2 z^2 \sin\theta\cos\theta} \\ &= \frac{\cosh\pi z\sqrt{1+\sin 2\theta} - \cosh\pi z\sqrt{1-\sin 2\theta}}{\pi^2 z^2 \sin 2\theta} \\ &= \sum_{m=1}^{\infty} \frac{(\pi z)^{2m}\left\{(1+\sin 2\theta)^m - (1-\sin 2\theta)^m\right\}}{(2m)!\,\pi^2 z^2 \sin 2\theta} \\ &= \sum_{m=0}^{\infty} \frac{2(\pi z)^{2m}}{(2m+2)!} \sum_{n=0}^{\lfloor m/2 \rfloor} \binom{m+1}{2n+1} (\sin 2\theta)^{2n}. \end{aligned} \tag{25}$$

???

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

On the other hand, putting $x = z^2\cos^2\theta$ and $y = z^2\sin^2\theta$ in Theorem 4.1 yields

$$\begin{aligned}
& J(z\cos\theta)J(z\sin\theta) \\
= & \left(\sum_{k=0}^{\infty}(z\cos\theta)^{2k}\int_0^1 (ab)^k\right)\left(\sum_{j=0}^{\infty}(z\sin\theta)^{2j}\int_0^1 (ab)^j\right) \\
= & \sum_{m=0}^{\infty}\sum_{n=0}^{m}(z\cos\theta)^{2n}(z\sin\theta)^{2m-2n}\int_0^1 (ab)^n \sqcup\!\sqcup (ab)^{m-n} \\
= & \sum_{m=0}^{\infty}\sum_{n=0}^{\lfloor m/2\rfloor}(4z^4\sin^2\theta\cos^2\theta)^n(z^2\cos^2\theta + z^2\sin^2\theta)^{m-2n}\int_0^1 T_{m,n} \\
= & \sum_{m=0}^{\infty} z^{2m}\sum_{n=0}^{\lfloor m/2\rfloor}(\sin 2\theta)^{2n}\int_0^1 T_{m,n}. \qquad (26)
\end{aligned}$$

Equating coefficients of $z^{2m}(\sin 2\theta)^{2n}$ in (25) and (26) completes the proof. ∎

ACKNOWLEDGMENT

Thanks are due to the referee whose comments helped improve the exposition.

REFERENCES

1. Jonathan M. Borwein, David M. Bradley and David J. Broadhurst, "Evaluations of k-fold Euler/Zagier Sums: A Compendium of Results for Arbitrary k," *Elec. J. Comb.*, **4** (1997), No. 2, #R5.
2. Jonathan M. Borwein, David M. Bradley, David J. Broadhurst and Petr Lisoněk, "Special Values of Multiple Polylogarithms," *Trans. Amer. Math. Soc.* (to appear).
3. Jonathan M. Borwein, David M. Bradley, David J. Broadhurst and Petr Lisoněk, "Combinatorial Aspects of Multiple Zeta Values," *Elec. J. Comb.*, **5** (1998), No. 1, #R38.
4. Doug Bowman and David M. Bradley, "Resolution of Some Open Problems Concerning Multiple Zeta Evaluations of Arbitrary Depth," submitted October, 1999.
5. David J. Broadhurst, private e-mail, 1997.
6. Kuo-Tsai Chen, "Iterated Integrals and Exponential Homomorphisms," *Proc. London Math. Soc.*, (3) **4** (1954), 502–512.
7. Kuo-Tsai Chen, "Integration of Paths, Geometric Invariants and a Generalized Baker-Hausdorff Formula," *Ann. of Math.*, **65** (1957), No. 1, 163–178.
8. Kuo-Tsai Chen, "Algebras of Iterated Path Integrals and Fundamental Groups," *Trans. Amer. Math. Soc.*, **156** (1971), 359–379.
9. K. O. Friedrichs, "Mathematical Aspects of the Quantum Theory of Fields, V," *Comm. Pure Appl. Math.*, **6** (1953), 1–72.

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.

10. Alexander B. Goncharov, "Multiple Polylogarithms, Cyclotomy and Modular Complexes," *Math. Res. Lett.*, **5** (1998), No. 4, 497–516.

11. Michael E. Hoffman, "Algebraic Structures on the Set of Multiple Zeta Values," preprint.

12. Michael E. Hoffman and Yasuo Ohno, "Relations of Multiple Zeta Values and their Algebraic Expression," preprint.

13. R. C. Lyndon, "A Theorem of Friedrichs," *Mich. Math. J.*, **3** (1955-1956), 27–29.

14. Wilhelm Magnus, "On the Exponential Solution of Differential Equations for a Linear Operation," *Comm. Pure Appl. Math.*, **7** (1954), 649–673.

15. Hoang Ngoc Minh and Michel Petitot, "Lyndon words, polylogarithms and the Riemann ζ function," *Discrete Mathematics*, **217**(1-3) (2000), 273–292.

16. Yasuo Ohno, "A Generalization of the Duality and Sum Formulas on the Multiple Zeta Values," *J. Number Theory*, **74** (1999), 39–43.

17. David E. Radford, "A Natural Ring Basis for the Shuffle Algebra and an Application to Group Schemes," *J. Algebra*, **58** (1979), 432–454.

18. Rimhak Ree, "Lie Elements and an Algebra Associated with Shuffles," *Ann. of Math.*, **62** (1958), No. 2, 210–220.

19. Don Zagier, "Values of Zeta Functions and their Applications," *First European Congress of Mathematics*, Vol. II, Birkhäuser, Boston, 1994, pp. 497–512.

???

Copyright © ??? by Academic Press
All rights of reproduction in any form reserved.