The Hopf algebra structure of multiple harmonic sums

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Multiple harmonic sums appear in the perturbative computation of various quantities of interest in quantum field theory. In this article we introduce a class of Hopf algebras that describe the structure of such sums, and develop some of their properties that can be exploited in calculations.

1. MULTIPLE HARMONIC SUMS

As discussed in the introduction of [1], multiple harmonic sums occur in perturbative higher-order calculations of quantum field theory. Let \( I = (i_1, i_2, \ldots, i_k) \) be a sequence of positive integers. For positive integers \( n \), we define the multiple harmonic sums

\[
A_I(n; x_1, x_2, \ldots, x_k) = \sum_{n \geq n_1 > n_2 > \cdots > n_k \geq 1} \frac{x_1^{n_1} x_2^{n_2} \cdots x_k^{n_k}}{n_1^{i_1} n_2^{i_2} \cdots n_k^{i_k}} \tag{1}
\]

and

\[
S_I(n; x_1, x_2, \ldots, x_k) = \sum_{n \geq n_1 \geq n_2 \cdots \geq n_k \geq 1} \frac{x_1^{n_1} x_2^{n_2} \cdots x_k^{n_k}}{n_1^{i_1} n_2^{i_2} \cdots n_k^{i_k}} \tag{2}
\]

associated with \( I \) (Note that the only difference between (1) and (2) is in the inequalities in the summation variables). Both types of sums appear in [11] and [13], with a slightly different notation (\( Z \) is used in place of our \( A \)).

If \( i_1 > 1 \) and \( x_1 = x_2 = \cdots = x_k = 1 \), the sums (1) and (2) converge as \( n \rightarrow \infty \), giving the well-known multiple zeta values [6,14,7,15].

\[
\zeta(i_1, \ldots, i_k) = A_{(i_1, \ldots, i_k)}(\infty; 1, \ldots, 1),
\]

which also occur in some perturbative QFT calculations [11]. More generally, (1) and (2) converge as \( n \rightarrow \infty \) when \( |x_i| = 1 \) for all \( i \) and \( i_1 x_1 \neq 1 \). The quantities

\[
\text{Li}_I(x_1, \ldots, x_n) = A_I(\infty; x_1, \ldots, x_k)
\]

are called multiple polylogarithms [2], they generalize the classical polylogarithm \( \text{Li}_n(x_1) = A_n(\infty; x_1) \).

It is immediate from the defining equations (1) and (2) that the sums \( S_I \) can be written in terms of the \( A_I \). To state the relation precisely, let \( C(n) \) be the set of compositions of \( n \), i.e., ordered sequences \( (i_1, \ldots, i_k) \) of positive integers with \( i_1 + \cdots + i_k = n \). If \( I = (i_1, \ldots, i_k) \) is a composition of \( n \) and \( J = (j_1, \ldots, j_p) \) is a composition of \( k \), then there is a composition \( J \circ I \) of \( n \) given by

\[
(i_1 + \cdots + i_{j_1}, i_{j_1+1} + \cdots + i_{j_1+j_2}, \ldots, i_{k-j_p+1} + \cdots + i_k)
\]

(cf. [5] p. 52]). Also, compositions act on argument strings: given \( J = (j_1, \ldots, j_p) \in C(k) \) and a string \( X = (x_1, \ldots, x_k) \) of length \( k \), we have

\[
J(X) = (x_1 \cdots x_{j_1}, x_{j_1+1} \cdots x_{j_1+j_2}, \ldots, x_{k-j_p+1} \cdots x_k).
\]

Then the relation between sums of types (1) and (2) is given by

\[
S_I(n; X) = \sum_{J \in C(k)} A_{J \circ I}(n; J(X)) \tag{3}
\]

for any \( I = (i_1, \ldots, i_k) \) and \( X = (x_1, \ldots, x_k) \). Möbius inversion can be applied to (3) to obtain

\[
A_I(n; X) = \sum_{J \in C(k)} (-1)^{\ell(J)-k} S_{J \circ I}(n; J(X)), \tag{4}
\]

where \( \ell(J) \) is the number of parts of \( J \). In fact, there is a deeper relation between the \( S_I \) and the

\[\text{...}\]
2. THE EULER ALGEBRA

We recall from \[9\] the construction of the Euler algebra of index \(r\), where \(r\) is a positive integer. We start with noncommuting symbols (or “letters”) \(z_{i,j}\), where \(i, j\) are integers with \(i\) positive and \(0 \leq j \leq r - 1\). Let \(\mathcal{E}_r\) be the complex vector space generated by words in the \(z_{i,j}\) (including the empty word, denoted by \(1\)). For such a word \(w = z_{i_1,j_1} z_{i_2,j_2} \cdots z_{i_k,j_k}\), we define the degree of \(w\) to be \(|w| = i_1 + \cdots + i_k\) (and call \(\ell(w) = k\) the length of \(w\)). Now we define a multiplication \(*\) on \(\mathcal{E}_r\) as follows. We require \(1 * w = w * 1 = w\) for all words \(w\), and

\[
z_{i,j} w_1 * z_{m,n} w_2 = z_{i,j} (w_1 * z_{m,n} w_2) + z_{m,n} (z_{i,j} w_1 * w_2) + z_{i+m,j+n} (w_1 * w_2) \tag{5}
\]

for any words \(w_1, w_2\): here the addition in the second subscript is to be understood mod \(r\). For example, when \(r = 3\)

\[
z_{1,1} z_{1,2} z_{2,1} = z_{1,1} z_{1,2} z_{2,1} + z_{1,2} z_{1,1} z_{2,1} + z_{1,2} z_{2,1} z_{1,1} + z_{2,1} z_{2,2} + z_{2,2} z_{2,1}.
\]

Since each of the parenthesized products on the right-hand side of \[5\] has total length less than the left-hand side, equation \[5\] gives an inductive definition of \(*\) on \(\mathcal{E}_r\). As shown in \[9\], \((\mathcal{E}_r, *)\) is a commutative, associative graded algebra over \(\mathbb{C}\). In fact, \((\mathcal{E}_r, *)\) is a polynomial algebra. To describe the generators, we first assume that the letters \(z_{i,j}\) are totally ordered, and extend this order lexicographically to words. A word \(w\) is called Lyndon if it is smaller than any of its proper right factors \((v \neq 1\) is a proper right factor of \(w\) if \(w = uv\) for \(u \neq 1\)). Then we have the following result \[9\] Theorem 2.6.

Theorem 2.1. For positive integer \(r\), \((\mathcal{E}_r, *)\) is the polynomial algebra on the Lyndon words.

Remark. From the discussion in \[8\] Example 2, the number of Lyndon words of degree \(n\) in \(\mathcal{E}_r\) is

\[
\frac{1}{n} \sum_{d|n} \mu \left(\frac{n}{d}\right) (r + 1)^d,
\]

where the sum is over divisors of \(n\) and \(\mu\) is the Möbius function on the integers.

In the case \(r = 1\), \((\mathcal{E}_r, *)\) is the algebra \(\operatorname{QSym}\) of quasi-symmetric functions as defined by Gessel \[5\]. For a description of \(\operatorname{QSym}\) and its relation to multiple harmonic sums with unit arguments, see \[10\]. Note that \(\operatorname{QSym}\) contains the well-known algebra \(\operatorname{Sym}\) of symmetric functions: in fact, \(\operatorname{Sym}\) can be imbedded in any \(\mathcal{E}_r\) by sending the elementary symmetric function \(e_i\) to \(z_{i,0}\).

We can also define a coalgebra structure on \(\mathcal{E}_r\) as follows. The counit \(\epsilon : \mathcal{E}_r \to \mathbb{C}\) is given by

\[
\epsilon(1) = 1, \quad \epsilon(w) = 0 \quad \text{for} \quad |w| > 0
\]

and the coproduct \(\Delta : \mathcal{E}_r \to \mathcal{E}_r \otimes \mathcal{E}_r\) by

\[
\Delta(z_{i_1,j_1} z_{i_2,j_2} \cdots z_{i_k,j_k}) = \sum_{p=0}^{k} z_{i_1,j_1} \cdots z_{i_p,j_p} \otimes z_{i_{p+1},j_{p+1}} \cdots z_{i_k,j_k}.
\]

Then Theorem 3.1 of \[9\] says that \((\mathcal{E}_r, *, \Delta)\) is a graded connected Hopf algebra.

Since the \(*\)-product is commutative, the antipode \(S:\) \((\mathcal{E}_r, *, \Delta)\) is an involution, i.e., an algebra automorphism with \(S^2 = \text{id}\) (see, e.g., \[10\] Theorem III.3.4). As shown in \[8\] Theorem 3.2, there are two (not obviously identical) formulas for \(S\). Our first formula for \(S\) involves iterated products:

\[
S(w) = \sum_{w_1 w_2 \cdots w_k = w} (-1)^k w_1 * w_2 * \cdots * w_k, \tag{6}
\]

where the sum is over all decompositions of \(w\) into (nonempty) subwords \(w_1, \ldots, w_k\).

For the second formula, we shall introduce some more notation. Given a string \(a_1, \ldots, a_n\) of letters, let \([a_1, \ldots, a_n]\) be the letter obtained...
by adding all the subscripts (where of course the addition in the second subscript is mod $r$). Then
the multiplication rule (5) can be written
\[ aw * bv = a(w * bv) + b(aw * v) + [a, b](w * v) \quad (7) \]
for letters $a, b$ and words $w, v$. As above, let $C(n)$ be the set of compositions of $n$. Then
$(i_1, \ldots, i_k) \in C(n)$ acts on a word $w = a_1 \cdots a_n$ of length $n$ as follows:
\[(i_1, \ldots, i_k)[w] = \left[a_1, \ldots, a_{i_1}, [a_{i_1}+1, \ldots, a_{i_1+i_2}] \cdots [a_{n-i_k+1}, \ldots, a_n]\right].\]
Our second formula for the antipode can be written in terms of this action:
\[ S(w) = (-1)^n \sum_{I \in C(n)} J[a_n a_{n-1} \cdots a_1] \quad (8) \]
for words $w = a_1 \cdots a_n$ of length $n$.
Now let $R : \mathcal{E}_r \to \mathcal{E}_r$ be the linear function that reverses words, i.e.,
\[ R(a_1 a_2 \cdots a_n) = a_n \cdots a_1. \]
The following result can be proved by induction on word length (see [13, Theorem 9]).

**Theorem 2.2.** The function $R : \mathcal{E}_r \to \mathcal{E}_r$ is a $*$-automorphism.

Since clearly $\Delta \circ R = (R \otimes R) \circ \Delta$, $R$ is evidently an automorphism of the Hopf algebra $(\mathcal{E}_r, *, \Delta)$.

The action of compositions on words of $\mathcal{E}_r$ can be used to put a partial order $\preceq$ on words as follows. For a word $w = a_1 \cdots a_n$ of length $n$, set $v \preceq w$ if $v = I[w]$ for some $I \in C(n)$ (Note that in this case $\ell(v) \leq \ell(w)$ and $|v| = |w|$). Define
\[ \overline{w} = \sum_{v \preceq w} v = \sum_{J \in C(\ell(w))} J[w] \quad (9) \]
for words $w$ of $\mathcal{E}_r$.

Our second formula for the antipode can now be written
\[ RS(w) = SR(w) = (-1)^{\ell(w)} \overline{w} \]
for any word $w$ of $\mathcal{E}_r$. Equating the two formulas for the antipode, we have
\[ \sum_{w_1 w_2 \cdots w_k = w} (-1)^k w_1 * w_2 * \cdots * w_k = (-1)^{\ell(w)} \sum_{v \subseteq w} R(v), \]
or, after applying $R$ to both sides,
\[ \overline{w} = \sum_{w_1 \cdots w_k = R(w)} (-1)^{\ell(w)-k} w_1 * \cdots * w_k. \quad (10) \]
Now apply $RS$ to both sides of equation (10):
\[ w = \sum_{w_1 \cdots w_k = R(w)} (-1)^{\ell(w)-k} \overline{w}_1 * \cdots * \overline{w}_k. \quad (11) \]
Also, since $\overline{w} = (-1)^{\ell(w)} SR(w)$ and $SR$ is an automorphism of the Hopf algebra $(\mathcal{E}_r, *, \Delta)$, we can work with the vector space basis $\overline{w}$ just as well as with the basis consisting of the words $w$: the only difference is that the inductive rule (7) for the $*$-product is replaced by
\[ aw * bv = a(w * bv) + b(aw * v) - [a, b](w * v). \]

**3. RELATION TO MULTIPLE HARMONIC SUMS**

Now we relate the Hopf algebras $\mathcal{E}_r$ to the multiple harmonic sums. For fixed $n$, define a linear map $\rho_n : \mathcal{E}_r \to \mathbb{C}$ by
\[ \rho_n(z_{i_1,j_1} \cdots z_{i_k,j_k}) = A(i_1, \ldots, i_k)(n; \epsilon j_1, \ldots, \epsilon j_k) \]
where $\epsilon = e^{2\pi i}$. We have the following result.

**Theorem 3.1.** The function $\rho_n$ is a homomorphism of $(\mathcal{E}_r, *)$ into $\mathbb{C}$.

**Proof.** $\rho_n$ is the composition of the homomorphism $\phi_n : \mathcal{E}_r \to \mathbb{C}[t_1, \ldots, t_n]$ of [9, Theorem 7.1] with the homomorphism $\mathbb{C}[t_1, \ldots, t_n] \to \mathbb{C}$ sending $t_i$ to $1/i$, $1 \leq i \leq n$. 

Comparing the definition \([\overline{w}]\) of $\overline{w}$ with equation (3), it is evident that
\[ \rho_n(z_{i_1,j_1} \cdots z_{i_k,j_k}) = S(i_1, \ldots, i_k)(n; \epsilon j_1, \ldots, \epsilon j_k). \]
Henceforth we shall write $A_w(n)$ for $\rho_n(w)$ and $S_w(n)$ for $\rho_n(\overline{w})$ for words $w$ of $\mathcal{E}_r$, using the word to code for both the exponents and roots-of-unity arguments. In this notation, equation 8 is

\[ S_w(n) = \sum_{u \preceq w} A_u(n). \]  

(12)

Now applying $\rho_n$ to equations 10 and 11 gives respectively

\[ S_w(n) = \sum_{w_1 \cdots w_k = R(w)} (-1)^{\ell(w)-k} A_{w_1} \cdots A_{w_k}(n) \]  

(13)

and

\[ A_w(n) = \sum_{w_1 \cdots w_k = R(w)} (-1)^{\ell(w)-k} S_{w_1}(n) \cdots S_{w_k}(n). \]  

(14)

By equating the right-hand sides of equations 12 and 13, one obtains

\[ A_w(n) + (-1)^{\ell(w)} A_{R(w)}(n) = \sum_{w_1 \cdots w_k = R(w)} (-1)^{\ell(w)-k} A_{w_1}(n) \cdots A_{w_k}(n) \]

\[ - \sum_{u < w} A_u(n), \]

which shows that $A_w(n) + (-1)^{\ell(w)} A_{R(w)}(n)$ can always be written in terms of sums of length less than $\ell(w)$. Cf. the discussion in [13] §6.

4. EXAMPLE: SYMMETRIC SUMS

To illustrate the use of the techniques introduced above, we show how symmetric linear combinations of the $A_w$ and $S_w$ can be written in terms of ordinary (length 1) harmonic sums. We start in $\mathcal{E}_r$. Note that the symmetric group $\Sigma_k$ acts on words of $k$ letters by permutation, i.e.,

\[ \sigma \cdot a_1 \cdots a_k = a_{\sigma^{-1}(1)} \cdots a_{\sigma^{-1}(k)}. \]

Fix a word $w = a_1 a_2 \cdots a_k$ of $\mathcal{E}_r$, and for a set partition $\mathcal{C} = \{C_1, \ldots, C_p\}$ of $\{1, 2, \ldots, k\}$ let

\[ \mathcal{C}(w) = [a_i, i \in C_1] \ast [a_i, i \in C_2] \ast \cdots \ast [a_i, i \in C_p]. \]

Then repeated use of the multiplication rule 17 allows $\mathcal{C}(w)$ to be written as

\[ \sum_{\mathcal{B} = \{B_1, \ldots, B_q\} \subseteq \mathcal{C}} \mu(\mathcal{B}, \mathcal{C}) \mathcal{B}(w) \]  

(15)

where $\mu$ is the Möbius function for the partially ordered set of partitions of $\{1, 2, \ldots, k\}$. When $\mathcal{C} = \{\{1\}, \{2\}, \ldots, \{k\}\}$, then $\mu(\mathcal{B}, \mathcal{C}) = c(\mathcal{B})$, where

\[ c(\mathcal{B}) = (-1)^{k-\ell(\text{card } B_1 - 1) \cdots (\text{card } B_q - 1)!} \]  

(see Example 3.10.4 of [12]). In this case equation 15 is

\[ \sum_{\sigma \in \Sigma_k} \sigma \cdot w = \sum_{\mathcal{B} = \{B_1, \ldots, B_q\} \subseteq \mathcal{C}} c(\mathcal{B}) [a_i, i \in B_1] \ast \cdots \ast [a_i, i \in B_q], \]  

(16)

where the sum on the right-hand side is over all partitions $\mathcal{B}$ of $\{1, \ldots, k\}$. Now apply RS to both sides of equation 10 (and cancel signs) to get

\[ \sum_{\sigma \in \Sigma_k} \sigma \cdot \overline{w} = \sum_{\mathcal{B} = \{B_1, \ldots, B_q\} \subseteq \mathcal{C}} |c(\mathcal{B})| [a_i, i \in B_1] \ast \cdots \ast [a_i, i \in B_q], \]  

(17)

Finally, we can apply the homomorphism $\rho_n$ to equations 10 and 17 to get formulas for symmetric combinations of multiple harmonic sums in terms of ordinary harmonic sums:

\[ \sum_{\mathcal{C} \in \Sigma_k} A_{\mathcal{C}}(n) = \sum_{\mathcal{B} = \{B_1, \ldots, B_q\}} c(\mathcal{B}) A_{[a_i, i \in B_1]}(n) \ast \cdots \ast A_{[a_i, i \in B_q]}(n) \]  

(18)
\[ \sum_{\sigma \in \Sigma_k} S_{\sigma,w}(n) = \sum_{\mathcal{B} = \{B_1, \ldots, B_k\}} |c(\mathcal{B})| A_{[a_1, i \in B_1]}(n) \cdots A_{[a_i, i \in B_i]}(n). \]

Equations (19) and (20) generalize Theorem 4.1 of [1] (which is the case \( r = 1 \)). They may be compared to the corresponding formulas for multiple zeta values, which appear as Theorems 2.2 and 2.1, respectively, of [2]. Equation (19) should also be compared to equations (2.37-2.41) of [1], which exhibit the cases \( k = 2, \ldots, 6 \) for \( r = 2 \).

In the special case \( w = a^k \) (i.e., \( w \) is a power of a single letter), equation (19) reduces to

\[ S_{a^k}(n) = \frac{1}{k!} \sum_{\mathcal{B} = \{B_1, \ldots, B_k\}} |c(\mathcal{B})| A_{[b_1, a]}(n) \cdots A_{[b_q, a]}(n), \]

where \( b_i = \text{card} B_i \) and \( [ka] \) means \( \{a, a, \ldots, a\} \) with \( k \) repetitions of \( a \). Now for a given (unordered) sequence of positive integers \( b_1, \ldots, b_q \) adding up to \( k \), there are

\[ \frac{1}{m_1! \cdots m_k! b_1! \cdots b_q!} \]

partitions of the set \( \{1, 2, \ldots, k\} \) having the \( b_i \) as block sizes, where \( m_n = \text{card}\{b_i | b_i = n\} \). Thus, equation (20) can be written as

\[ S_{a^k}(n) = \sum_{b_1 + \cdots + b_q = k} \frac{1}{m_1! \cdots m_k! b_1! \cdots b_q!} A_{[b_1, a]}(n) \cdots A_{[b_q, a]}(n), \]

where the sum is over all integer partitions of \( k \) (cf. equations (2.42-2.46) of [1]). There is an analogous formula for \( A_{a^k}(n) \) differing from (21) only in the presence of signs.

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