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NEW HARMONIC NUMBER IDENTITIES WITH APPLICATIONS

Roberto Tauraso

Dipartimento di Matematica
Università di Roma "Tor Vergata", Italy
e-mail: `tauraso@mat.uniroma2.it`
WWW: `http://www.mat.uniroma2.it/~tauraso`

Abstract. We determine the explicit formulas for the sum of products of homogeneous multiple harmonic sums $\sum_{k=1}^{n}\prod_{j=1}^{r} H_k(\{1\}^{\lambda_j})$ when $\sum_{j=1}^{r}\lambda_j \le 5$. We apply these identities to the study of two congruences modulo a power of a prime.

1. Introduction

Let $\mathbf{s}=(s_1,s_2,\ldots,s_d)$ be a vector whose entries are positive integers, and define the *multiple harmonic sum* (MHS for short) for $n\ge 0$ by

$$H_n(\mathbf{s})=\sum_{1\le k_1<k_2<\cdots<k_d\le n}\frac{1}{k_1^{s_1}k_2^{s_2}\cdots k_d^{s_d}}.$$

We call d and $|\mathbf{s}|=\sum_{i=1}^{d}s_i$ its depth and its weight, respectively. This kind of sums have a long history, see for example [4], [12], and the references therein.

In this note we present an algorithmic procedure to determine a closed formula for

$$\sum_{k=1}^{n}\prod_{j=1}^{m}H_k(\mathbf{s}_j)$$

involving products of MHS evaluated at n and of total weight less or equal to $\sum_{j=1}^{n}|\mathbf{s}_j|$.

(**i**) The first step is to expand recursively any product $H_n(\mathbf{s})H_n(\mathbf{t})$ as a non-negative integral combination of MHS of weight $|\mathbf{s}|+|\mathbf{t}|$:

$$H_n(\mathbf{s})H_n(\mathbf{t})=\sum_{\mathbf{r}\in\mathbf{s}\,\uplus\,\mathbf{t}}H_n(\mathbf{r}),$$

where $\mathbf{s}\uplus\mathbf{t}$ is the so-called *stuffle product* (or *quasi-shuffle product*). If we consider the vectors $\mathbf{s}=(s_1,\mathbf{s}')$ and $\mathbf{t}=(t_1,\mathbf{t}')$ as words formed by concatenating their components then the stuffle product is recursively defined by

$$\mathbf{s}\uplus\emptyset=\emptyset\uplus\mathbf{s}=\mathbf{s},\quad \mathbf{s}\uplus\mathbf{t}=s_1(\mathbf{s}'\uplus\mathbf{t})+t_1(\mathbf{s}\uplus\mathbf{t}')+(s_1+t_1)(\mathbf{s}'\uplus\mathbf{t}').$$

So, for example,

$$H_n(1)H_n(2,3)=H_n(1,2,3)+H_n(2,1,3)+H_n(2,3,1)+H_n(2,1+3)+H_n(1+2,3).$$

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(ii) The second step is to sum over k any MHS by using recursively the following rule:

$$\sum_{k=1}^{n} H_k(\mathbf{s}) = \sum_{k=1}^{n}\sum_{j=1}^{k} \frac{H_{j-1}(\mathbf{s}')}{j^{s_d}} = \sum_{j=1}^{n} \frac{H_{j-1}(\mathbf{s}')}{j^{s_d}} \sum_{k=j}^{n} 1 = \sum_{j=1}^{n} \frac{H_{j-1}(\mathbf{s}')}{j^{s_d}}(n+1-j)$$
$$= (n+1)H_n(\mathbf{s}) - \begin{cases} H_n(\mathbf{s}', s_d-1) & \text{if } s_d > 1 \\ \displaystyle\sum_{k=1}^{n} H_k(\mathbf{s}') - H_n(\mathbf{s}') & \text{if } s_d = 1 \end{cases}$$

where $\mathbf{s} = (\mathbf{s}', s_d)$. It is easy to see that the MHS involved in the final formula have weight less than or equal to $|\mathbf{s}|$.

(iii) The last step is to simplify the formula by collecting terms by using the stuffle product relations. This can be done in various ways and the choices depend on the application of the identity.

This procedure will be employed in the next section, and it will generate a number of identities. We give two applications of these identities (we hope that many more will come out in the future). The first is about the sum

$$\sum_{k=0}^{n} (-1)^{ak} \binom{n}{k}^{a},$$

which seems to have a closed form only for very few values of the parameter $a \in \mathbb{Z}$, namely for $-1 \le a \le 3$. In [2], Cai studied a related congruence by showing that for any $a \in \mathbb{Z}$ and any prime $p \ge 5$

$$\sum_{k=0}^{p-1} (-1)^{ak} \binom{p-1}{k}^{a} \equiv \binom{ap-2}{p-1} \pmod{p^4}.$$

Here we present the following extension (see also [5] and [3] for similar results):

Theorem 1.1. *Let $p > 5$ be a prime. For any $a \in \mathbb{Z}$, we have*

$$\sum_{k=0}^{p-1} (-1)^{ak} \binom{p-1}{k}^{a} \equiv \frac{(a-1)p}{ap-1} \left(1 + \frac{a(a+1)(3a-2)}{6} p^3 X_p\right) \pmod{p^6},$$

where $X_p = \frac{B_{p-3}}{p-3} - \frac{B_{2p-4}}{4p-8}$ and B_n denotes the n-th Bernoulli number.

Moreover, by using the previous theorem for $a = -2$ we get the following corollary.

Corollary 1.2. *For any prime $p > 5$, we have*

$$\sum_{k=1}^{p-1} \frac{1}{k}\binom{2k}{k} \equiv -\frac{16}{3} p^2 X_p \pmod{p^4}.$$

This improves the congruence modulo p^3 contained in [9].

2. MHS: identities

By following the procedure introduced in the previous section, we find an explicit formula for any sum of products of homogeneous MHS like $H_k(\{1\}^d)$ up to total weight 5 ($\{1\}^d$ means that the number 1 is repeated d times):

$$\sum_{k=1}^{n} H_k(1) = (n+1)H_n(1) - n\,, \tag{1}$$

$$\sum_{k=1}^{n} H_k(\{1\}^2) = (n+1)H_n(\{1\}^2) - nH_n(1) + n\,, \tag{2}$$

$$\sum_{k=1}^{n} H_k^2(1) = (n+1)H_n^2(1) - (2n+1)H_n(1) + 2n\,, \tag{3}$$

$$\sum_{k=1}^{n} H_k(\{1\}^3) = (n+1)H_n(\{1\}^3) + n\left(H_n(1) - \frac{1}{2}H_n^2(1)\right) + \frac{n}{2}H_n(2) - n\,, \tag{4}$$

$$\begin{aligned}\sum_{k=1}^{n} H_k(1)H_k(\{1\}^2) = (n+1)H_n(1)H_n(\{1\}^2) + (3n+1)\left(H_n(1) - \frac{1}{2}H_n^2(1)\right)\\ + \frac{n+1}{2}H_n(2) - 3n\,,\end{aligned} \tag{5}$$

$$\sum_{k=1}^{n} H_k^3(1) = (n+1)H_n^3(1) + (6n+3)\left(H_n(1) - \frac{1}{2}H_n^2(1)\right) + \frac{1}{2}H_n(2) - 6n. \tag{6}$$

It is interesting to note that the formulas for $\sum_{k=1}^{n} H_k^r(1)$ when $r = 1, 2, 3$ appear as Entry 8 on page 94 in [1]. To illustrate the procedure, we show how to obtain (5).

By (i), we have

$$H_k(1)H_k(\{1\}^2) = 3H_k(\{1\}^3) + H_k(2,1) + H_k(1,2).$$

Moreover, by (ii), we obtain

$$\sum_{k=1}^{n} H_k(\{1\}^3) = (n+1)H_n(\{1\}^3) - nH_n(\{1\}^2) + nH_n(1) - n\,,$$

$$\sum_{k=1}^{n} H_k(2,1) = (n+1)H_n(2,1) - nH_n(2) + H_n(1)\,,$$

$$\sum_{k=1}^{n} H_k(1,2) = (n+1)H_n(1,2) - H_n(\{1\}^2).$$

Finally, since by (i), we have

$$H_n(1)H_n(\{1\}^2) = 3H_n(\{1\}^3) + H_n(2,1) + H_n(1,2) \quad \text{and} \quad 2H_n(\{1\}^2) = H_n^2(1) - H_n(2),$$

by applying (iii), we easily get (5).

The formulas for the total weight being 4 and 5 are contained in Tables 1 and 2, respectively: the sum $\sum_{k=1}^{n} f_k - (n+1)f_n$, where f_n is an entry in the first row, is equal to the sum of the entries of the first column, each multiplied by the linear polynomial $an+b$ contained in the intersection of the chosen row and column.

Table 1

$\sum_{k=1}^{n} f_k - (n+1)f_n$	$H_n(\{1\}^4)$	$H_n^2(\{1\}^2)$	$H_n(1)H_n(\{1\}^3)$	$H_n^2(1)H_n(\{1\}^2)$	$H_n^4(1)$
$\sum_{k=1}^{3} \frac{(-1)^{k-1}}{k!} H_n^k(1)$	$-n$	$-6n-2$	$-4n-1$	$-12n-5$	$-24n-12$
$\frac{1}{2}H_n(2)$	$-n$	$-2n-2$	$-2n-1$	$-2n-3$	-4
$\frac{1}{3}H_n(3)$	$-n$	1	$-n-1$	1	3
$\frac{1}{2}H_n(1)H_n(2)$	n	$2n$	$2n+1$	$2n+1$	0
$H_n(1,2)$	0	1	0	1	2
n	1	6	4	12	24

Table 2

$\sum_{k=1}^{n} f_k - (n+1)f_n$	$H_n(\{1\}^5)$	$H_n(1)H_n(\{1\}^4)$	$H_n(1,1)H_n(\{1\}^3)$	$H_n^2(1)H_n(\{1\}^3)$
$\sum_{k=1}^{4} \frac{(-1)^{k-1}}{k!} H_n^k(1)$	n	$5n+1$	$10n+3$	$20n+7$
$\frac{1}{2}H_n(2)$	n	$3n+1$	$4n+3$	$6n+5$
$\frac{1}{3}H_n(3)$	n	$2n+1$	n	$2n+1$
$\frac{1}{2}H_n(1)H_n(2)$	$-n$	$-3n-1$	$-4n-1$	$-6n-3$
$H_n(1,2)$	0	0	-1	-1
$\frac{1}{4}H_n(4)$	n	$n+1$	-1	-1
$\frac{1}{8}H_n^2(2)$	$-n$	$-(n+1)$	$-(2n-1)$	1
$\frac{1}{4}H_n^2(1)H_n(2)$	n	$3n+1$	$4n+1$	$6n+3$
$\frac{1}{3}H_n(1)H_n(3)$	$-n$	$-2n-1$	$-n$	$-2n-1$
$H_n(1,3)$	0	0	0	0
$H_n(1,1,2)$	0	0	1	1
n	-1	-5	-10	-20

$\sum_{k=1}^{n} f_k - (n+1)f_n$	$H_n(1)H_n^2(\{1\}^2)$	$H_n^3(1)H_n(\{1\}^2)$	$H_n^5(1)$
$\sum_{k=1}^{4} \frac{(-1)^{k-1}}{k!} H_n^k(1)$	$30n+12$	$60n+27$	$120n+60$
$\frac{1}{2}H_n(2)$	$6n+8$	$6n+13$	20
$\frac{1}{3}H_n(3)$	-3	-6	-15
$\frac{1}{2}H_n(1)H_n(2)$	$-6n-2$	$-6n-3$	0
$H_n(1,2)$	-3	-5	-10
$\frac{1}{4}H_n(4)$	-2	-3	-4
$\frac{1}{8}H_n^2(2)$	$-2n+4$	9	20
$\frac{1}{4}H_n^2(1)H_n(2)$	$6n+2$	$6n+3$	0
$\frac{1}{3}H_n(1)H_n(3)$	0	0	0
$H_n(1,3)$	1	2	5
$H_n(\{1\}^2,2)$	3	5	10
n	-30	-60	-120

3. MHS: congruences

Among the various known results about MHS modulo powers of a prime, the following ones will be crucial for us: for any prime $p > 5$, we have

$$\begin{aligned}
&H_{p-1}(1) \equiv 2p^2 X_p && \pmod{p^4},\\
&H_{p-1}(2) \equiv -4pX_p && \pmod{p^3},\\
&H_{p-1}(3) \equiv 0 && \pmod{p^2},\\
&H_{p-1}(1,2) \equiv -6X_p && \pmod{p^2},\\
&H_{p-1}(4) \equiv H_{p-1}(\{1\}^2,2) \equiv H_{p-1}(1,3) \equiv 0 && \pmod{p},
\end{aligned}$$

where $X_p = \frac{B_{p-3}}{p-3} - \frac{B_{2p-4}}{4p-8}$ (see [7] for the MHS of depth 1, see [12] and [4] for all the MHS of depth > 1 with the exception of $H_{p-1}(1,2)$ modulo p^2 which has been established in [10]).

Note that every homogeneous MHS can be expressed in terms of MHS of depth 1. More precisely (see Theorem 2.3 in [4]): given a positive integer d, then for any unordered partition $\lambda = \{\lambda_1, \lambda_2, \ldots, \lambda_r\}$ of d there is some integer c_λ such that

$$d!H_n(\{1\}^d) = \sum_{\lambda \in P(d)} c_\lambda \prod_{i=1}^{r} H_n(\lambda_i).$$

For example:

$$\begin{aligned}
2H_n(\{1\}^2) &= H_n^2(1) - H_n(2),\\
6H_n(\{1\}^3) &= H_n^3(1) - 3H_n(1)H_n(2) + 2H_n(3),\\
24H_n(\{1\}^4) &= H_n^4(1) - 6H_n^2(1)H_n(2) + 8H_n(1)H_n(3) + 3H_n^2(2) - 6H_n(4).
\end{aligned}$$

Hence, for any prime $p > 5$, we have

$$\begin{aligned} H_{p-1}(\{1\}^2) &\equiv 2pX_p && \pmod{p^3}, \\ H_{p-1}(\{1\}^3) &\equiv 0 && \pmod{p^2}, \\ H_{p-1}(\{1\}^4) &\equiv 0 && \pmod{p}. \end{aligned}$$

Therefore, by Equations (1)–(6), Tables 1 and 2, it follows that, for any prime $p > 5$, we have:

Table 3

$\sum_{k=1}^{p-1} H_k(1) \equiv -(p-1) + 2p^3 X_p$	$\pmod{p^5}$
$\sum_{k=1}^{p-1} H_k(\{1\}^2) \equiv (p-1) + (4-2p)p^2 X_p$	$\pmod{p^4}$
$\sum_{k=1}^{p-1} H_k^2(1) \equiv 2(p-1) + (2-4p)p^2 X_p$	$\pmod{p^4}$
$\sum_{k=1}^{p-1} H_k(\{1\}^3) \equiv -(p-1) + (2-4p)pX_p$	$\pmod{p^3}$
$\sum_{k=1}^{p-1} H_k(1)H_k(\{1\}^2) \equiv -3(p-1) + (-6p)pX_p$	$\pmod{p^3}$
$\sum_{k=1}^{p-1} H_k^3(1) \equiv -6(p-1) + (-2-6p)pX_p$	$\pmod{p^3}$
$\sum_{k=1}^{p-1} H_k(\{1\}^4) \equiv (p-1) + (-2p)X_p$	$\pmod{p^2}$
$\sum_{k=1}^{p-1} H_k^2(\{1\}^2) \equiv 6(p-1) + (-6)X_p$	$\pmod{p^2}$
$\sum_{k=1}^{p-1} H_k(1)H_k(\{1\}^3) \equiv 4(p-1) + (-2p)X_p$	$\pmod{p^2}$
$\sum_{k=1}^{p-1} H_k^2(1)H_k(\{1\}^2) \equiv 12(p-1) + (-6+2p)X_p$	$\pmod{p^2}$
$\sum_{k=1}^{p-1} H_k^4(1) \equiv 24(p-1) + (-12+8p)X_p$	$\pmod{p^2}$
$\sum_{k=1}^{p-1} H_k(\{1\}^5) \equiv 1$	$\pmod{p}$
$\sum_{k=1}^{p-1} H_k(1)H_k(\{1\}^4) \equiv 5$	$\pmod{p}$
$\sum_{k=1}^{p-1} H_k(\{1\}^2)H_k(\{1\}^3) \equiv 10 + 6X_p$	$\pmod{p}$
$\sum_{k=1}^{p-1} H_k^2(1)H_k(\{1\}^3) \equiv 20 + 6X_p$	$\pmod{p}$
$\sum_{k=1}^{p-1} H_k(1)H_k^2(\{1\}^2) \equiv 30 + 18X_p$	$\pmod{p}$
$\sum_{k=1}^{p-1} H_k^3(1)H_k(\{1\}^2) \equiv 60 + 30X_p$	$\pmod{p}$
$\sum_{k=1}^{p-1} H_k^5(1) \equiv 120 + 60X_p$	$\pmod{p}$

Note that $\sum_{k=1}^{p-1} H_k^r(1) \pmod{p^{4-r}}$ for $r = 1, 2, 3$ have been established by Z. W. Sun in [8].

4. Proof of Theorem 1.1 and Corollary 1.2

Proof of Theorem 1.1. Assume that $p > 5$ is a prime, then for $k = 1, \ldots, p-1$ we have that

$$(-1)^k \binom{p-1}{k} = \prod_{j=1}^{k} \left(1 - \frac{p}{j}\right) \equiv 1 + \sum_{j=1}^{5} (-p)^j H_k(\{1\}^j) \pmod{p^6}.$$

Hence we have

$$(-1)^{ak}\binom{p-1}{k}^a \equiv 1+\sum_{j=1}^{5}(-p)^j\sum_{r=1}^{j}\binom{a}{r}\sum_{\lambda\in\mathcal{P}(j,r)}\binom{j}{\lambda_1,\dots,\lambda_r}\prod_{i=1}^{r}H_k(\{1\}^{\lambda_i}) \pmod{p^6},$$

where $\mathcal{P}(j,r)$ is the set of the integer partitions λ of j into r parts.

By summing over k, we find

$$\sum_{k=0}^{p-1}(-1)^{ak}\binom{p-1}{k}^a = p+\sum_{j=1}^{5}(-p)^j\sum_{r=1}^{j}\binom{a}{r}\sum_{\lambda\in\mathcal{P}(j,r)}\binom{j}{\lambda_1,\dots,\lambda_r}\sum_{k=1}^{p-1}\prod_{i=1}^{r}H_k(\{1\}^{\lambda_i}) \pmod{p^6}.$$

Finally, by Table 3, we can compute

$$(-p)^j\sum_{k=1}^{p-1}\prod_{i=1}^{r}H_k(\{1\}^{\lambda_i}) \pmod{p^6}$$

for any partition $\lambda\in\mathcal{P}(j,r)$, and we get easily the result. □

Proof of Corollary 1.2. In [6] Staver proved that for any integer $n\geq 1$

$$\sum_{k=1}^{n}\frac{1}{k}\binom{2k}{k}=\binom{2n}{n}\frac{2n+1}{3n^2}\sum_{k=0}^{n-1}\binom{n-1}{k}^{-2}.$$

Letting $n=p$, by Theorem 1.1 for $a=-2$ we have

$$\begin{aligned}\sum_{k=1}^{p-1}\frac{1}{k}\binom{2k}{k} &= \frac{1}{p}\binom{2p}{p}\left(\frac{2p+1}{3p}\sum_{k=0}^{p-1}\binom{p-1}{k}^{-2}-1\right)\\ &\equiv \frac{2}{p}\binom{2p-1}{p-1}\left(\left(1-\frac{8}{3}p^3X_p\right)-1\right)\equiv -\frac{16}{3}p^2X_p \pmod{p^4},\end{aligned}$$

where in the last step we used the fact that $\binom{2p-1}{p-1}\equiv 1 \pmod{p^3}$ by Wolstenholme's theorem. □

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