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Mod p structure of alternating and non-alternating multiple harmonic sums

par Jianqiang ZHAO

Dedicated to the memory of Prof. Shiing-Shen Chern on his birth centennial

Résumé. Le théorème bien connu de Wolstenholme affirme que, pour tout premier $p > 3$, la $(p-1)$-ième somme partielle de la série harmonique est congrue à 0 modulo p^2. Si on remplace la série harmonique par $\sum_{k\geq 1} 1/n^k$ pour k pair alors la congruence est vraie seulement modulo p au lieu de modulo p^2. On peut considérer des généralisations aux sommes harmoniques multiples (SHM) et aux aux sommes harmoniques multiples alternées (SHMA) qui sont des sommes partielles de séries zêta multiples et, respectivement, de sommes d'Euler alternées. Beaucoup de résultats dans cette direction ont été obtenus dans les articles récents [6, 7, 8, 10, 11, 12], que nous récapitulerons dans ce papier. Il apparait que, pour un premier p, la $(p-1)$-ième somme partielle d'une SHM ou SHMA générale n'est plus congrue à 0 modulo p ; cependant elle peut souvent être exprimée en terme de nombres de Bernoulli. Donc c'est un problème assez intéressant de trouver qui ils sont. Dans cet article, nous fournirons un cadre théorique dans lequel ce genre de résulats peut s'exprimer et être étudié plus longuement. Nous calculerons aussi quelques SHM supplémentaires modulo un premier p quand le poids est inférieur à 13.

Abstract. The well-known Wolstenholme's Theorem says that for every prime $p > 3$ the $(p-1)$-st partial sum of the harmonic series is congruent to 0 modulo p^2. If one replaces the harmonic series by $\sum_{k\geq 1} 1/n^k$ for k even, then the modulus has to be changed from p^2 to just p. One may consider generalizations of this to multiple harmonic sums (MHS) and alternating multiple harmonic sums (AMHS) which are partial sums of multiple zeta value series and the alternating Euler sums, respectively. A lot of results along this direction have been obtained in the recent articles [6, 7, 8, 10, 11, 12], which we shall summarize in this paper. It turns out that for a prime p the $(p-1)$-st sum of the general MHS and AMHS modulo p is not congruent to 0 anymore; however, it

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often can be expressed by Bernoulli numbers. So it is a quite interesting problem to find out exactly what they are. In this paper we will provide a theoretical framework in which this kind of results can be organized and further investigated. We shall also compute some more MHS modulo a prime p when the weight is less than 13.

1. Introduction

The multiple zeta values (MZVs) are defined by the infinite series:

$$\zeta(\vec{s}) = \zeta(s_1, \ldots, s_l) := \sum_{1 \le k_1 < \cdots < k_l} k_1^{-s_1} \cdots k_l^{-s_l}. \tag{1.1}$$

Historically Euler was the first to study sums of this type. In recent years many interesting and important applications of these values have been found in diverse areas such as algebraic geometry and physics. To study the algebraic structure of these values, Hoffman introduces in [4] the quasi-shuffle algebra which reflects the two different kinds of shuffle relations among MZVs.

In [10] we study the partial sums of these series which are called the multiple harmonic sums (MHS for short) by the physicists [1, 2, 9]. Tautaro [7] defines its alternating analog (AMHS for short) as follows. Let $d > 0$ and let $\vec{s} := (s_1, \ldots, s_d) \in (\mathbb{Z}^*)^d$. We define the *alternating multiple harmonic sum* as

$$H(\vec{s}; n) := \sum_{1 \le k_1 < k_2 < \cdots < k_d \le n} \prod_{i=1}^{d} \frac{\operatorname{sgn}(s_i)^{k_i}}{k_i^{|s_i|}}. \tag{1.2}$$

By convention we set $H(\vec{s}; n) = 0$ any $n < d$, and $H(\emptyset; 0) = 1$. We call $\ell(\vec{s}) := d$ and $|\vec{s}| := \sum_{i=1}^{d} |s_i|$ its *depth* and *weight*, respectively. Notice that the depth $\ell(\vec{s})$ is sometimes called the length in the literature. When every s_i is positive we recover MHS exactly. To facilitate our study we also need to consider (cf. [5, 6])

$$S(s_1, \ldots, s_l; n) := \sum_{1 \le k_1 \le \cdots \le k_l \le n} \prod_{i=1}^{d} \frac{\operatorname{sgn}(s_i)^{k_i}}{k_i^{|s_i|}}. \tag{1.3}$$

The main purpose of [10] is to generalize the well-known Wolstenholme's Theorem to other MHS. At about the same time, in [5] Hoffman extended his earlier results of [4] concerning multiple zeta values to MHS and begins the study of their mod p structures. In [6] Hoffman further computed these sums modulo a prime p when the weights are less than 10. In another direction, Tautaro and the author [7, 8] recently started to consider the congruence properties of AMHS. We found that similar to MHS the congruences often involves Bernoulli numbers. However, Euler polynomials and

Euler numbers also play significant roles. For example, Fermat's quotient $q_p = (2^p - 1)/p$ naturally appears in many congruence relations of AMHS.

In this paper we will first provide a theoretical framework in which the above mentioned congruence relations can be organized and further investigated. Then we sketch an idea of carrying out the computation on computers. At the end we provide as examples some more computations of MHS and AMHS with weights less than 13. We want to point out that because the S-sums enjoy a nicer duality relation (see section 3) we will concentrate on them in this paper for the MHS.

2. The setup

Let $\mathbf{P}$ denote the set of primes. For every prime p we denote by $\mathbb{F}_p = \mathbb{Z}/p\mathbb{Z}$ the set of equivalent classes of integers modulo p. Define an additive group

$$\mathbb{A}(n) := \prod_{p\in\mathbf{P},\ p>n} \mathbb{F}_p$$

with the addition carried out componentwise. For any positive integer n we define

$$\mathbb{Q}(n) = \{a/b \in \mathbb{Q} : a/b \text{ is reduced and if a prime } p|b \text{ then } p \leq n\}$$

regarded as a commutative ring with identity. For example, because no primes greater than $p-1$ can appear in the denominator of $H(\vec{s}; p-1)$ and $S(\vec{s}; p-1)$ by their definitions we must have

$$H_{\vec{s}} := (H(\vec{s}; p-1))_{p\in\mathbf{P}} \in \mathbb{A}(1), \text{ and } S_{\vec{s}} := (S(\vec{s}; p-1))_{p\in\mathbf{P}} \in \mathbb{A}(1).$$

Throughout this paper, by abuse of notation we will denote by the same $S_{\vec{s}}$ its projections to $\mathbb{A}(|\vec{s}| + 2)$. This should cause no confusion.

Lemma 2.1. *The subset of rational numbers $\mathbb{Q}(n)$ can be embedded in $\mathbb{A}(n)$ diagonally. Namely, the map $\mathbb{Q}(n) \longrightarrow \mathbb{A}(n)$, $r \longmapsto (r)_{p\in\mathbf{P},p>n}$ is a group monomorphism.*

Proof. Suppose $(x_p)_p, (y_p)_p \in \mathbb{A}(n)$ are the images of two rational numbers x and y in $\mathbb{Q}(n)$ respectively. If $x_p = y_p$ for all $p > n$ then we have

$$x - y \equiv 0 \pmod{p}$$

for all but finitely many primes p. Let $x = a/b$ and $y = c/d$ be their reduced fraction representations. Then we must have $ad - bc$ is divisible by infinitely many primes. Hence $ad = bc$ which implies $x = y$. $\square$

Letting $\mathbb{Q}(n)$ act on $\mathbb{A}(n)$ diagonally through multiplication we see that $\mathbb{A}(n)$ becomes a faithful $\mathbb{Q}(n)$-module by the lemma. Now we can define the sub-$\mathbb{Q}(n+2)$-module of $\mathbb{A}(n+2)$ generated by the weight n MHS and AMHS by

$$\mathbb{M}(n) = \Big\langle S_{\vec{s}} \in \mathbb{A}(n+2) : |\vec{s}| = n, \text{all components of } \vec{s} \text{ are positive} \Big\rangle,$$
$$\mathbb{AM}(n) = \Big\langle H_{\vec{s}} \in \mathbb{A}(n+2) : |\vec{s}| = n, \text{all components of } \vec{s} \text{ are in } \mathbb{Z} \Big\rangle,$$

respectively. Both of these two modules are free since $\mathbb{A}(n)$ is clearly free. For example, in weight 3 we have by [10, Thm. 2.13,Thm. 3.1]

$$\begin{aligned} S_{1,1,1} &= (S(1,1,1;p-1))_{p>5} & S_{2,1} &= (S(2,1;p-1))_{p>5} \\ &= 0 \in \mathbb{A}(5), & &= (-B_{p-3})_{p>5} \in \mathbb{A}(5), \\ S_3 &= (S(3;p-1))_{p>5} & S_{1,2} &= (S(1,2;p-1))_{p>5} \\ &= 0 \in \mathbb{A}(5), & &= (B_{p-3})_{p>3} \in \mathbb{A}(5). \end{aligned}$$

So as a sub-$\mathbb{Q}(5)$-module, $\mathbb{M}(3) = \langle S_{1,1,1}, S_3, S_{2,1}, S_{1,2} \rangle$ is generated by $(-B_{p-3})_{p>5}$ in $\mathbb{A}(5)$. By the same reason we can summarize the results in [6] and [10] in the following

Theorem 2.1. *We have*

$$\begin{aligned} &\mathbb{M}(1) = \langle 0 \rangle, \quad \mathbb{M}(2) = \langle 0 \rangle, \quad \mathbb{M}(4) = \langle 0 \rangle, \\ &\mathbb{M}(3) = \big\langle (B_{p-3})_{p>5} \big\rangle, \quad \mathbb{M}(5) = \big\langle (B_{p-5})_{p>7} \big\rangle, \quad \mathbb{M}(6) = \big\langle (B^2_{p-3})_{p>8} \big\rangle, \\ &\mathbb{M}(7) = \big\langle (B_{p-7})_{p>9}, S_{4111} \big\rangle, \quad \mathbb{M}(8) = \big\langle (B_{p-3}B_{p-5})_{p>10}, S_{611} \big\rangle, \\ &\mathbb{M}(9) = \big\langle (B_{p-9})_{p>10}, (B^3_{p-3})_{p>10}, S_{6111} \big\rangle, \end{aligned}$$

where we have used shorthand $S_{4111} = S_{4,1,1,1}$ and so on.

Remark 2.2. Numerical evidence shows that $(B_{p-7})_{p>9}$ and $S_{4111} \in \mathbb{A}(9)$ are $\mathbb{Q}(9)$-linearly independent and $(B_{p-3}B_{p-5})_{p>10}$ and $S_{611} \in \mathbb{A}(10)$ are $\mathbb{Q}(10)$-linearly independent. Note that even though for $p = 37$ we have $S(6,1,1;p-1) \not\equiv 0 \pmod p$ while $B_{p-5} \equiv 0 \pmod p$ this is not enough to show the linear independence. What we need is to show that there do NOT exist two rational numbers $a, b \in \mathbb{Q}(10)$ such that

$$aS(6,1,1;p-1) + bB_{p-3}B_{p-5} \equiv 0 \pmod p \quad \forall p > 10.$$

At the moment we cannot exclude the possibility that a is a multiple of 37 and therefore the the above congruence holds for $p = 37$.

Remark 2.3. Numerical evidence shows that S_{6111} can be removed from $\mathbb{M}(9)$. In fact, for all primes p between 11 and 2000 we have

$$S(6,1,1,1;p-1) \equiv -\frac{1}{54}B^3_{p-3} - \frac{1889}{648}B_{p-9} \pmod p.$$

See [10, Conj. 3.12].

Definition 2.4. An l-tuple of indices $I = (i_1, \dots, i_l)$ is called *admissible* if $i_j \geq 3$ and i_j is odd for every $j = 1, \dots, l$. We call $|I| = i_1 + \cdots + i_l$ its weight. For an admissible index I we abuse the notation by putting

$$p - I := (p - i_1, \dots, p - i_l), \quad B_I := \prod_{j=1}^{l} B_{i_j}.$$

The following conjecture is the first obstacle to understanding the mod p structure of the MHS.

Conjecture 2.1. *For any positive integer n, if $I_1, \dots, I_k$ are pairwise distinct, admissible and have the same weight n then $(B_{p-I_1})_p, \dots, (B_{p-I_k})_p \in \mathbb{A}(n)$ are $\mathbb{Q}(n+2)$-linearly independent.*

Assuming Conjecture 2.1 we can obtain a lower bound for the size of $\mathbb{M}(n)$.

Proposition 2.1. *If Conjecture* 2.1 *is true then*

$$\operatorname{rank}_{\mathbb{Q}(n+2)} \mathbb{M}(n) \geq \sum_{\substack{1 \leq k \leq \lfloor n/3 \rfloor \\ 2 | (n-k)}} \binom{(n-k)/2 - 1}{k - 1} \tag{2.1}$$

where when $n = 3$, $k = 1$ we set $\binom{0}{0} = 1$.

Proof. For all positive integers $k \leq n$ we define

$$\mathcal{I}_{k,n} := \Big\{ I = (i_1, \dots, i_k) : |I| = n, 3 \leq i_j \text{ is odd for all } j = 1, \dots, k \Big\},$$
$$\mathcal{J}_{k,n} := \Big\{ I = (i_1, \dots, i_k) : |I| = n, 1 \leq i_j \text{ is odd for all } j = 1, \dots, k \Big\}.$$

Then we only need to show that the right hand side of (2.1) is the cardinality $\sharp \mathcal{I}_n$ of the set $\mathcal{I}_n := \bigcup_{k=1}^{n} \mathcal{I}_{k,n}$. But we have an obvious one-to-one correspondence for all $k \leq n/3$:

$$\begin{aligned} f : \mathcal{J}_{k,n-2k} &\longrightarrow \mathcal{I}_{k,n} \\ I = (i_1, \dots, i_k) &\longmapsto (i_1 + 2, \dots, i_k + 2) \end{aligned}$$

with the inverse map $f^{-1}(i_1, \dots, i_k) = (i_1 - 2, \dots, i_k - 2)$. This implies that

$$\sharp \mathcal{I}_n = \sum_{k=1}^{\lfloor n/3 \rfloor} \sharp \mathcal{J}_{k,n-2k}.$$

But clearly for any $k \leq n/3$ there is another one-to-one correspondence

$$\begin{aligned} g : \mathcal{J}_{k,n-2k} &\longrightarrow \left\{ (y_1, \dots, y_k) : \begin{array}{l} y_1 + \cdots + y_k = (n-k)/2, \\ y_1, \dots, y_k \in \mathbb{N} \end{array} \right\} \\ I = (i_1, \dots, i_k) &\longmapsto \left(\frac{i_1 + 1}{2}, \dots, \frac{i_k + 1}{2} \right) \end{aligned}$$

whose inverse is $g^{-1}(y_1,\dots,y_k)=(2y_1-1,\dots,2y_k-1)$. In particular, if n and k have different parity then $\mathcal{J}_{k,n-2k}=\emptyset$; otherwise, $\sharp\mathcal{J}_{k,n-2k}=\binom{(n-k)/2-1}{k-1}$. The proposition follows immediately. $\square$

Let us turn to AMHS now. By the main result of [7, 10] we get

$$\mathbb{AM}(1)=\big\langle (q_p)_{p>3}\big\rangle,\quad \mathbb{AM}(2)=\big\langle (q_p^2)_{p>4}\big\rangle,\quad \mathbb{AM}(3)=\big\langle (q_p^3)_{p>5},(B_{p-3})_{p>5}\big\rangle.$$

By the computation in the last section of [8] we find that

$$\begin{aligned}\mathbb{AM}(4)=\big\langle (q_p^4)_{p>6},(qB_{p-3})_{p>6},H(1,-3),H(1,-1,-2),\\ H(-1,1,1,1),H(1,-1,-1,-1)\big\rangle,\end{aligned}$$

where we have used $H(\vec{s})$ to denote $(H(\vec{s};p-1))_{p>|\vec{s}|+2}$. Similar to the situation for MHS where Conjecture 2.1 is the main obstacle we need to resolve the following conjecture first in order to understand the mod p structure of AMHS.

Conjecture 2.2. *Let n be a positive integer. Assume $I_1,\dots,I_k$ are pairwise distinct, admissible and of weight $w_1,\dots,w_k\le n$, respectively. Then $(q_p^n)_p,(q_p^{n-w_1}B_{p-I_1})_p,\dots,(q_p^{n-w_k}B_{p-I_k})_p\in\mathbb{A}(n)$ are $\mathbb{Q}(n+2)$-linearly independent.*

By the proof of Prop. 2.1 we can easily find the following result..

Proposition 2.2. *If Conjecture 2.2 is true then*

$$\operatorname{rank}_{\mathbb{Q}(n+2)}\mathbb{AM}(n)\ge 1+\sum_{m=3}^{n}\sum_{\substack{1\le k\le\lfloor m/3\rfloor\\ 2|(m-k)}}\binom{(m-k)/2-1}{k-1}, \tag{2.2}$$

where when $m=3$, $k=1$ we set $\binom{0}{0}=1$.

3. A brief review of duality and other relations

We treat only MHS in this section. Let's first recall the definition of the duality operation on MHS. Let k be a positive integer and $\vec{s}=(i_1,\dots,i_k)$ of weight $n=|\vec{s}|$. We define the power set to be the partial sum sequence of $\vec{s}$: $P(\vec{s})=(i_1,i_1+i_2,\dots,i_1+\dots+i_{k-1})$ as a subset of $(1,2,\dots,n-1)$. Clearly P provides a one-to-one correspondence between the compositisons of weight n and the subsets of $(1,2,\dots,n-1)$. Then $\vec{s}^*$ is the compositison of weight n corresponding to the complimentary subset of $P(\vec{s})$ in $(1,2,\dots,n-1)$. Namely,

$$\vec{s}^*=P^{-1}\big((1,2,\dots,n-1)-P(\vec{s})\big).$$

It's easy to see that $\vec{s}^{**}=\vec{s}$ so $*$ is a convolution. For example, if $i_1,i_k\ge 1,i_2,\dots,i_{k-1}\ge 2$ then we have the dual

$$(i_1,\dots,i_k)^*=(1^{i_1-1},2,1^{i_2-2},2,1^{i_3-2},\dots,2,1^{i_{k-1}-2},2,1^{i_k-1}).$$

Here, we set $1^n = \{1\}^n$ where for an ordered set $(s_1, \dots, s_t)$ we denote by $\{s_1, \dots, s_t\}^n$ the set formed by repeating $(s_1, \dots, s_t)$ n times. An important relation between $\vec{s}$ and its dual is the following:

$$\ell(\vec{s}) + \ell(\vec{s}^*) = |\vec{s}| + 1. \tag{3.1}$$

Next we define the *reversal* of $\vec{s}$ by $\overleftarrow{s} = (s_l, \dots, s_1)$. By substitution of indices $k \to p - k$ it's easy to show that

$$H_{\overleftarrow{s}} = (-1)^{|\vec{s}|} H_{\vec{s}}, \quad S_{\overleftarrow{s}} = (-1)^{|\vec{s}|} S_{\vec{s}}. \tag{3.2}$$

The following important result is due to Hoffman:

Theorem 3.1. ([5, Thm. 6.7]) *For all $\vec{s} = (s_1, \dots, s_l)$ we have in $\mathbb{A}(1)$*

$$S_{\vec{s}^*} = -S_{\vec{s}}. \tag{3.3}$$

We also have the following equalities:

$$S_{\vec{s}} = \sum_{\vec{r} \preceq \vec{s}} H_{\vec{r}}, \tag{3.4}$$

$$H_{\vec{s}} = \sum_{\vec{r} \preceq \vec{s}} (-1)^{\ell(\vec{s}) - \ell(\vec{r})} S_{\vec{r}} \tag{3.5}$$

where $\vec{r} \prec \vec{s}$ means $\vec{r}$ can be obtained from $\vec{s}$ by combining some of its parts, and for prime p

$$S(\overleftarrow{s}; p-1) \equiv \sum_{\bigsqcup_{j=1}^{l} \vec{s}_i = \vec{s}} (-1)^{\ell(\vec{s}) - l} \prod_{j=1}^{l} H(\vec{s}_j; p-1) \pmod{p} \tag{3.6}$$

$$H(\overleftarrow{s}; p-1) \equiv \sum_{\bigsqcup_{j=1}^{l} \vec{s}_i = \vec{s}} (-1)^{\ell(\vec{s}) - l} \prod_{j=1}^{l} S(\vec{s}_j; p-1) \pmod{p} \tag{3.7}$$

where $\bigsqcup_{j=1}^{l} \vec{s}_i$ is the catenation of $\vec{s}_1$ to $\vec{s}_l$.

To put congruences (3.6) and (3.7) inside our theoretical framework, we define multiplication componentwise on $\mathbb{A}(n)$ so that $\mathbb{A}(n)$ now becomes a $\mathbb{Q}(n)$-algebra. As a convention, if an element $e \in A(n)$ appears in an expression which makes sense in $\mathbb{A}(m)$ for some $m > n$ we take e as its image of projection from $\mathbb{A}(n) \to \mathbb{A}(m)$. By this extension of definition we can now write down the following equations in $\mathbb{A}(1)$:

$$S_{\overleftarrow{s}} = \sum_{\bigsqcup_{j=1}^{l} \vec{s}_i = \vec{s}} (-1)^{\ell(\vec{s})-l} \prod_{j=1}^{l} H_{\vec{s}_j} \tag{3.8}$$

$$H_{\overleftarrow{s}} = \sum_{\bigsqcup_{j=1}^{l} \vec{s}_i = \vec{s}} (-1)^{\ell(\vec{s})-l} \prod_{j=1}^{l} S_{\vec{s}_j}. \tag{3.9}$$

In [6] Hoffman extended his theory of the Hopf algebra of the quasi-symmetric functions to MHS in a very insightful way.

4. Some useful reduction results

In [6] Hoffman studied the mod p structure of the MHS of weight up to 9. In order to consider the general case we first need to provide some reduction relations among the sums because according to the next result there are too many sums of a fixed weight.

Lemma 4.1. *The number of different MHS of weight w is 2^{w-1}. The number of different AMHS of weight w is $2 \cdot 3^{w-1}$.*

Proof. The number of MHS of weight w and depth d is obviously equal to $\binom{w-d}{d-1}$. So the number of MHS of weight w is

$$\sum_{d=1}^{w} \binom{w-1}{d-1} = \sum_{j=0}^{w-1} \binom{w-1}{j} = 2^{w-1}.$$

Similarly, The number of AMHS of weight w and depth d is obviously equal to $\binom{w-d}{d-1} \cdot 2^d$. Then the number of AMHS of weight w is

$$\sum_{d=1}^{w} \binom{w-1}{d-1} 2^d = \sum_{j=0}^{w-1} \binom{w-1}{j} 2^{j+1} = 2 \cdot 3^{w-1}.$$

□

Lemma 4.2. *Suppose $\vec{s}$ has weight n, depth l and positive components. If w and l have the same parity then $S_{\vec{s}}$ can be written as a sum of products of the form $S_{\vec{s}_1} \cdots S_{\vec{s}_k}$ where either $k > 1$ and all the weights $|\vec{s}_j| < n$ or, $k = 1$ and $\ell(\vec{s}_1) < l$.*

Proof. This follows easily from (3.2), (3.5) and (3.9):

$$S_{\vec{s}} + \sum_{\vec{r} \prec \vec{s}} (-1)^{\ell(\vec{s})-\ell(\vec{r})} S_{\vec{r}} = H_{\vec{s}} = -S_{\vec{s}} + \sum_{\bigsqcup_{j=1}^{l} \vec{s}_i = \vec{s}, l \geq 2} (-1)^{l} \prod_{j=1}^{l} S_{\vec{s}_j}.$$

So we have

$$S_{\vec{s}} = \frac{1}{2}\left(\sum_{\bigsqcup_{j=1}^{l} \vec{s}_i=\vec{s}, l\geq 2} (-1)^l \prod_{j=1}^{l} S_{\vec{s}_j} - \sum_{\vec{r}\prec \vec{s}} (-1)^{\ell(\vec{s})-\ell(\vec{r})} S_{\vec{r}} \right).$$

□

Thanks to [10, Thm. 3.1 and Thm. 3.5] we know that to determine $\mathbb{M}(n)$ we only need to solve $S(\vec{s})$, $|\vec{s}|=n$, where

$$\ell(\vec{s}) \text{ is odd and } 3 \leq \ell(\vec{s}) \leq n/2 \text{ if } n \text{ is even,}$$

and

$$\ell(\vec{s}) \text{ is even and } 4 \leq \ell(\vec{s}) \leq (n+1)/2 \text{ if } n \text{ is odd.}$$

So we have the following table:

$\lvert\vec{s}\rvert$	9	10	11	12	13	14	15
$\ell(\vec{s})$	4	3,5	4,6	3,5	4,6	3,5,7	4,6,8

TABLE 4.1. The key depths according to the weight.

5. Computations of $\mathbb{M}(n)$ for $n < 13$

We now summarize the idea of our computer aided computation. For any fixed weight, first we will use the reduction relations given above among the MHS to reduce the number of sums that we really need to compute and think them as unknowns, then by using Maple or any other algebra system we can solve these unknowns by regarding the shuffle relations and dualities as equations.

We illustrate this by carrying out the computation for $\mathbb{M}(9)$ in detail. By Table 4.1 we only need to solve the 28 depth four sums. By Maple, the shuffle relations produced by multiplying S_1 with the following 27 weight 8 sums are enough to produce virtually the same solution of Hoffman in [6]:

$$S_{4112}, S_{3221}, S_{3212}, S_{3122}, S_{2411}, S_{2321}, S_{2312}, S_{2231}, S_{2141},$$
$$S_{41111}, S_{32111}, S_{31211}, S_{31121}, S_{31112}, S_{23111}, S_{21311}, S_{21131}, S_{22211},$$
$$S_{22121}, S_{22112}, S_{14111}, S_{13211}, S_{13121}, S_{311111}, S_{131111}, S_{113111}, S_{221111}.$$

Similarly, we found the following:

$$\mathbb{M}(10) = \left\langle B_{p-3}B_{p-7}, B_{p-5}^2, S_{22141}, S_{811}, S_{61111} \right\rangle,$$

$$\mathbb{M}(11) = \left\langle B_{p-11}, B_{p-3}^2 B_{p-5}, B_{p-3}S_{611}, S_{7211}, S_{7121}, S_{611111}, S_{2261}, S_{3431} \right\rangle,$$

$$\mathbb{M}(12) = \Big\langle B_{p-3}^4, B_{p-3}B_{p-9}, B_{p-5}B_{p-7}, B_{p-3}S_{6111}, B_{p-5}S_{4111}, S_{22512}, S_{291}, S_{33132}, S_{42213} \Big\rangle.$$

Note that in weight 10 if we indeed need S_{22141} then $\mathbb{M}(10)$ can NOT be generated by height one sums $S_{h1\dots1}$ in Hoffman's terms, because $S^*_{511111} = S_{61111}$, $S^*_{4,1^6} = S_{7111} = \frac{1}{4}B_{p-3}B_{p-7} + \frac{1}{8}B^2_{p-5} - \frac{5}{4}S_{811}$, $S^*_{3,1^7} = S_{811}$, $S^*_{2,1^8} = S_{91} = 0$, and $S_{1^{10}} = 0$.

Also in weight 10, we find $S_{2332} = 0$. In weight 12 we find $S_{534} = S_{435} = S_{23232} = S_{23322} = 0$.

References

[1] J. Blümlein, *Algebraic relations between harmonic sums and associated quantities.* Comput. Phys. Commun. **159** (2004), 19–54. arXiv: hep-ph/0311046.

[2] J. Blümlein and S. Kurth, *Harmonic sums and Mellin transforms up to two-loop order.* Phys. Rev. D **60** (1999), art. 01418. arXiv: hep-ph/9810241.

[3] M.E. Hoffman, *The Hopf algebra structure of multiple harmonic sums.* Nuclear Phys. B (Proc. Suppl.) **135** (2004), 214–219. arXiv: math.QA/0406589.

[4] M.E. Hoffman, *Quasi-Shuffle Products.* J. Algebraic Combin. **11** (2000), 49–68.

[5] M.E. Hoffman, *Algebraic aspects of multiple zeta values.* In: Zeta Functions, Topology and Quantum Physics, Developments in Mathematics 14, T. Aoki et. al. (eds.), Springer, 2005, New York, pp. 51–74. arXiv: math.QA/0309425.

[6] M.E. Hoffman, *Quasi-symmetric functions and mod p multiple harmonic sums.* arXiv: math.NT/0401319

[7] R. Tauraso, *Congruences involving alternating multiple harmonic sum.* Elec. J. Combinatorics, **17**(1) (2010), R16.

[8] R. Tauraso and J. Zhao, *Congruences of alternating multiple harmonic sums.* In press: J. Comb. and Number Theory. arXiv: math/0909.0670

[9] J.A.M. Vermaseren, *Harmonic sums, Mellin transforms and integrals.* Int. J. Modern Phys. A **14** (1999), 2037–2076. arXiv: hep-ph/9806280.

[10] J. Zhao, *Wolstenholme type Theorem for multiple harmonic sums.* Intl. J. of Number Theory, **4**(1) (2008), 73–106. arXiv: math/0301252.

[11] J. Zhao, *Finiteness of p-divisible sets of multiple harmonic sums.* In press: Annales des Sciences Mathématiques du Québec. arXiv: math/0303043.

[12] X. Zhou and T. Cai, *A generalization of a curious congruence on harmonic sums.* Proc. Amer. Math. Soc. **135** (2007), 1329-1333

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