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WOLSTENHOLME TYPE THEOREM FOR MULTIPLE HARMONIC SUMS

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In this paper, we will study the p-divisibility of multiple harmonic sums (MHS) which are partial sums of multiple zeta value series. In particular, we provide some generalizations of the classical Wolstenholme's Theorem to both homogeneous and non-homogeneous sums. We make a few conjectures at the end of the paper and provide some very convincing evidence.

Keywords: Multiple harmonic sum (MHS); multiple zeta values; Bernoulli numbers; irregular primes.

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1. Introduction

The Euler–Zagier multiple zeta functions of length one are nested generalizations of Riemann zeta function. They are defined as

$$\zeta(\mathbf{s}) = \zeta(s_1, \dots, s_l) = \sum_{0<k_1<\cdots<k_l} k_1^{-s_1} \cdots k_l^{-s_l} \tag{1.1}$$

for complex variables $s_1, \dots, s_l$ satisfying $\text{Re}(s_j) + \cdots + \text{Re}(s_l) > l - j + 1$ for all $j = 1, \dots, l$. We call $|\mathbf{s}| = s_1 + \cdots + s_l$ the weight and denote the length by $l(\mathbf{s})$. The special values of multiple zeta functions at positive integers have significant arithmetic and algebraic meanings, whose defining series (1.1) will be called *MZV series*, including the divergent ones like $\zeta(\dots, 1)$. These obviously generalize the notion of harmonic series whose weight is equal to 1.

MZV series are related to many aspects of number theory. One of the most beautiful computations carried out by Euler is the following evaluation of zeta values at even positive integers:

$$2\zeta(2m) = (-1)^{m+1}\frac{(2\pi)^{2m}}{(2m)!}B_{2m},$$

where B_k are Bernoulli numbers defined by the Maclaurin series $t/(e^t-1) = \sum_{k=0}^{\infty} B_k t^k/k!$. In this paper, we will study partial sums of MZV series which turn out to be closely related to Bernoulli numbers too. These sums have been called (non-alternating) *multiple harmonic sums* (MHS for short) and studied by theoretical physicists (see [5, 6] and their references). Their main interest is fast computation of their exact values and the algebraic relations among them. Our focus, however, is on p-divisibility of these sums for various primes p and special attention will be paid to the cases where the sums are divisible by higher powers of primes than ordinarily expected which is often related to the irregular primes, i.e. primes p which divide some Bernoulli numbers B_t for some positive even integers $t < p-2$. We say in this case (p,t) is an irregular pair.

1.1. *Wolstenholme's Theorem*

Put $\mathbf{s} := (s_1, \ldots, s_l) \in \mathbb{N}^l$ and denote the nth partial sum of MZV series by

$$H(\mathbf{s}; n) = H(s_1, \ldots, s_l; n) := \sum_{1 \le k_1 < \cdots < k_l \le n} k_1^{-s_1} \cdots k_l^{-s_l}, \quad n \in \mathbb{Z}_{\ge 0}. \tag{1.2}$$

By convention we set $H(\mathbf{s}; r) = 0$ for $r = 0, \ldots, l-1$, and $H(\emptyset; 0) = 1$. To facilitate our study we also define (cf. [26, 27])

$$S(s_1, \ldots, s_l; n) := \sum_{1 \le k_1 \le \cdots \le k_l \le n} k_1^{-s_1} \cdots k_l^{-s_l}, \quad n \in \mathbb{Z}_{\ge 0}. \tag{1.3}$$

To save space, for an ordered set $(e_1, \ldots, e_t)$ we denote by $\{e_1, \ldots, e_t\}^d$ the set formed by repeating $(e_1, \ldots, e_t)$ d times. For example $H(\{s\}^l; n)$ is just a partial sum of the nested zeta value series $\zeta(s)$ of length one which we refer to as a *homogeneous* partial sum. The partial sums of nested harmonic series are related to Stirling numbers $St(n, j)$ of the first kind which are defined by the expansion

$$x(x+1)(x+2)\cdots(x+n-1) = \sum_{j=1}^{n} St(n,j) x^j.$$

We have $St(n,n) = 1$, $St(n, n-1) = n(n-1)/2$, and $St(n,1) = (n-1)!$. It is also easy to see that

$$St(n,j) = (n-1)! \cdot H(\{1\}^{j-1}; n-1), \quad \text{for } j = 1, \ldots, n. \tag{1.4}$$

Now we restrict n to prime numbers.

Theorem 1.1 ([25, p. 89]). *For any prime number* $p \ge 5$, $St(p, 2) \equiv 0 \pmod{p^2}$.

We find on the Internet the following generalization of the above theorem by Bruck [8] although no proof is given there. Denote by $\mathfrak{p}(m)$ the parity of m which is 1 if m is odd and 2 if m is even.

Theorem 1.2. *For any prime number* $p \ge 5$ *and positive integer* $l = 1, \ldots, p-3$, *we have*

$$St(p, l+1) \equiv 0, \quad H(\{1\}^l; p-1) \equiv 0 \pmod{p^{\mathfrak{p}(l+1)}}.$$

This of course implies that $p|St(p,l)$ for $1 < l < p$ which was known to Lagrange [25, p. 87].

It is noticed that not only p^2 but also p^3 possibly divides $St(p,2)$, though rarely, and therefore p^3 possibly divides the numerator of $H(1;p-1)$ written in the reduced form. So far we know this happens only for $p = 16843$ and $p = 2124679$ among all the primes up to 12 million (see [30, 38, 16, 9, 10]). The reason, Gardiner told us in [19], is that these two primes are the only primes p in this range such that p divides the numerator of B_{p-3}. Bruck [8] further gave a heuristic argument to show that there should be infinitely many primes p such that p^3 divides $S(p,2)$, which is equivalent to say that there are infinitely many irregular pairs $(p,p-3)$.

There are other generalizations of Wolstenholme's Theorem to MHS. Bayat proved (corrected version, see Remark 2.3)

Theorem 1.3 ([4, Theorem 3]). *For any positive integer s and prime number $p \geq k+3$ we have*

$$H(s;p-1) \equiv 0 \pmod{p^{\mathfrak{p}(s+1)}}.$$

In [34] Slavutskii showed:

Theorem 1.4 ([34, Theorem 2]). *Let s and m be two positive integers such that $(m,6) = 1$. Let $t = (\phi(m)-1)s$ and $A_n(m) = \prod_{p|m}(1-p^{n-1})B_n$ be the Agoh's function, where $\phi(m)$ is the Euler's Phi function. Then*

$$H^*(s;m-1) = \sum_{\substack{1 \leq k < m \\ (k,p)=1}} \frac{1}{k^s} \equiv \begin{cases} mA_t(m) & \pmod{m^2} \quad \text{if } s \text{ is even,} \\ \left(\dfrac{t}{2}\right) m^2 A_{t-1}(m) & \pmod{m^2} \quad \text{if } s \text{ is odd.} \end{cases}$$

1.2. *Homogeneous MHS*

The classical result of Wolstenholme is the original motivation of our study. We will prove the following generalization of Theorems 1.1 and 1.2 to homogeneous MHS (see Theorem 2.13).

Theorem 1.5. *Let s and l be two positive integers. Let p be an odd prime such that $p \geq l+2$ and $p-1$ divides none of ls and $ks+1$ for $k = 1,\dots,l$. Then*

$$H(\{s\}^l;p-1) \equiv 0 \pmod{p^{\mathfrak{p}(ls-1)}}.$$

In particular, the above is always true if $p \geq ls+3$.

We also consider some cases when the congruences hold modulo higher powers of p. Recently, Zhou and Cai [42] prove that:

Theorem 1.6. *Let s and l be two positive integers. Let p be a prime such that $p \geq ls+3$*

$$H(\{s\}^l;p-1) \equiv S(\{s\}^l;p-1) \equiv \begin{cases} (-1)^l \dfrac{s(ls+1)p^2}{2(ls+2)} B_{p-ls-2} & \pmod{p^3} \quad \text{if } 2 \nmid ls, \\ (-1)^{l-1} \dfrac{sp}{ls+1} B_{p-ls-1} & \pmod{p^2} \quad \text{if } 2 \mid ls. \end{cases}$$

We will prove an analog of this in the non-homogeneous even weight length two case (see Theorem 3.2).

1.3. *Non-homogeneous MHS*

The third section of this paper deals with non-homogeneous MHS. We consider the length two case in Theorem 3.1 whose proof relies heavily on generating functions of the Bernoulli polynomials and properties of Bernoulli numbers such as Claussen–von Staudt Theorem.

Theorem 1.7. *Let s_1, s_2 be two positive integers and p be an odd prime. Let $s_1 \equiv m,\ s_2 \equiv n \pmod{p-1}$ where $0 \le m, n \le p-2$. If $m, n \ge 1$ then*

$$H(s_1, s_2; p-1) \equiv \begin{cases} \dfrac{(-1)^n}{m+n}\dbinom{m+n}{m} B_{p-m-n} & \pmod p \quad \text{if } p \ge m+n, \\ 0 & \pmod p \quad \text{if } p < m+n. \end{cases}$$

The same idea but more complicated computation enables us to deal with the length three odd weight case completely (see Theorem 3.5).

Theorem 1.8. *Let p be an odd prime. Let $(s_1, s_2, s_3) \in \mathbb{N}^3$ and $0 \le l, m, n \le p-2$ such that $s_1 \equiv l, s_2 \equiv m, s_3 \equiv n \pmod{p-1}$. If $l, m, n \ge 1$ and $w = l+m+n$ is an* odd *number then*

$$H(s_1, s_2, s_3; p-1) \equiv I(l, m, n) - I(n, m, l) \pmod p$$

where

$$I(l,m,n) = \begin{cases} 0 & \text{if } w \ge 2p, \text{ or if } l+m < p \text{ and } p < w < 2p-1, \\ \dfrac{1}{2n} & \text{if } w = p, 2p-1, \\ (-1)^{n+1}\dbinom{w'}{n}\dfrac{B_{p-w'}}{2w'} & \text{otherwise, where } w' = w-(p-1). \end{cases}$$

For the even weight cases in length three, we are only able to determine the p-divisibility for $H(4,3,5;p-1)$, $H(5,3,4;p-1)$ and the three MHS of weight 4: $H(1,1,2;p-1)$, $H(1,2,1;p-1)$, and $H(2,1,1;p-1)$, which are distinctly different from the behavior of others.

Recently, Hoffman studies the same kind of questions independently in [26, 27] from a different viewpoint. We strongly encourage the interested reader to compare his results to ours. For example, Hoffman defines the duality operation on compositison of indices (see [26, §6]). We can apply this to a few of the above results to find more Wolstenhomles type congruence in Sec. 3.7.

Theorem 1.9. *Let p be a prime and $\mathbf{s} \in \mathbb{N}^l$. Assume $p > |\mathbf{s}| + 2$. Then*

$$H(\mathbf{s}; p-1) \equiv S(\mathbf{s}; p-1) \equiv 0 \pmod p$$

provided $\mathbf{s}$ *has one of the following forms*:

(a) $\mathbf{s} = (\{1\}^m, 2, \{1\}^n)$ *for* $m, n \geq 0$ *and* $m+n$ *is even.*
(b) $\mathbf{s} = (\{1\}^n, 2, \{1\}^{n-1}, 2, \{1\}^{n+1})$ *where* $n \geq 2$ *is even.*
(c) $\mathbf{s} = (\{1\}^{n+1}, 2, \{1\}^{n-1}, 2, \{1\}^n)$ *where* $n \geq 2$ *is even.*
(d) $\mathbf{s} = (\{1\}^n, 2, \{1\}^n, 2, \{1\}^n)$ *where* $n \geq 0$.

One can also investigate the MHS $H(\mathbf{s}; n)$ with fixed $\mathbf{s}$ but varying n. We will carry this out in another paper [39]. Such a study for harmonic series was initiated systematically by Eswarathasan and Levine [18] and Boyd [7], independently.

The theory of Bernoulli numbers and irregular primes has a long history, and results in this direction are scattered throughout the mathematical literature for almost three hundred years starting with the posthumous work "Ars Conjectandi" (1713) by Jakob Bernoulli (1654–1705), see [15]. Without attempting to be complete, we only list some of the modern references at the end.

2. Generalizations of Wolstenholme's Theorem

It is known to every number theorist that for every odd prime p the sum of reciprocals of 1 to $p-1$ is congruent to 0 modulo p. However, it is a little surprising to know that the sum actually is congruent to 0 modulo p^2 if $p \geq 5$. This remarkable theorem was proved by Wolstenholme in 1862.

2.1. *Generalization to zeta-value series*

To generalize Wolstenholme's Theorem we need the classical Claussen–von Staudt Theorem on Bernoulli numbers (see, for example, [28, p. 233, Theorem 3]):

Lemma 2.1. *For* $m \in \mathbb{N}$, $B_{2m} + \sum_{p-1|2m} 1/p$ *is an integer.*

We begin with a special case of our generalization which only deals with MHS of length one. The general case will be built upon this.

Lemma 2.2. *Let p be an odd prime and s be a positive integer. Then*

$$H(s; p-1) \equiv \begin{cases} 0 & \pmod{p^{\mathfrak{p}(s+1)}} \quad \text{if } p-1 \nmid s, s+1, \\ -1 & \pmod{p} \quad \text{if } p-1 | s, \\ \dfrac{-p(n+1)}{2} & \pmod{p^2} \quad \text{if } s+1 = n(p-1). \end{cases} \tag{2.1}$$

Remark 2.3. (1) The conditions in Bayat's generalization of Wolstenholme's Theorem [4, Theorem 3] should be corrected. For example, taking $k = 2$ and $p = 5$ in [4, Theorem 3(i)] we only get $H(3;4) = 2035/1728 \not\equiv 0 \pmod{5^2}$. In general, if $2k = p-1$ in [4, Theorem 3(i)] we find that $H(2k-1; p-1) \equiv -p \pmod{p^2}$ by taking $s = 2k-1$ and $n = 1$ in our lemma.

(2) Most of the lemma follows from Slavutskii's result Theorem 1.4. However, we need a more direct proof which we will reference later.

Proof. If $p-1|s$ then $H(s; p-1) \equiv p-1 \equiv -1 \pmod{p}$ by Fermat's Little Theorem. So we assume $p-1 \nmid s$. This implies that the map $a \to a^{-s}$ is nontrivial on $(\mathbb{Z}/p\mathbb{Z})^\times$, say $b^s \not\equiv 1 \pmod{p}$ for some $1 < b < p$. Then it's not hard to see that $(1-b^{-s})H(s; p-1) \equiv 0 \pmod{p}$ and therefore $H(s; p-1) \equiv 0 \pmod{p}$. This holds for any s such that $p-1 \nmid s$, whether it is even or odd.

The last case of modulus p^2 for odd s can be handled by the same argument as in the proof of Wolstenholme's Theorem. We produce two proofs below for both completeness and future reference.

Let s be an odd positive integer. Choose n large enough so that $t := np(p-1) - s \geq 3$ is odd. Then by the general form of Fermat's Little Theorem

$$H(s; p-1) = \sum_{k=1}^{p-1} \frac{1}{k^s} \equiv \sum_{k=1}^{p-1} \frac{k^{np(p-1)}}{k^s} \equiv \sum_{k=1}^{p-1} k^t \pmod{p^2}.$$

By a classical result of sums of powers (see [28, p. 229]) we know that

$$\sum_{k=1}^{p-1} k^t = \frac{1}{t+1}(B_{t+1}(p) - B_{t+1}) \quad \text{for } t \geq 1, \tag{2.2}$$

where $B_m(x)$ are the Bernoulli polynomials. Further,

$$B_{t+1}(p) = \sum_{j=0}^{t+1} \binom{t+1}{j} B_j p^{t+1-j}.$$

Observing that pB_j is always p-integral by Lemma 2.1 we have

$$\sum_{k=1}^{p-1} k^t \equiv pB_t + \frac{t}{2} p^2 B_{t-1} \pmod{p^2}. \tag{2.3}$$

When $p-1 \nmid s+1$ the lemma follows from the facts that $B_j = 0$ if $j > 2$ is odd and that $B_{t-1} = B_{np(p-1)-s-1}$ is p-integral by Lemma 2.1. If $p-1|s+1$ and $s+1 = m(p-1)$ then we choose $n = m$ in the above argument. Then $t = np(p-1) - n(p-1) + 1$ is odd. So $B_t = 0$, $p-1|t-1$ and $pB_{t-1} \equiv -1 \pmod{p}$ by Lemma 2.1 again. From congruence (2.3) we get

$$H(s; p-1) \equiv \frac{-pt}{2} \equiv \frac{-p(n+1)}{2} \pmod{p^2}.$$

In fact, there is a shorter proof for the odd case if $p-1 \nmid s+1$ which is not as transparent as the above proof. By binomial expansion we see that

$$2\sum_{k=1}^{p-1} \frac{1}{k^s} = \sum_{k=1}^{p-1} \left(\frac{1}{k^s} + \frac{1}{(p-k)^s} \right) \equiv \sum_{k=1}^{p-1} \frac{spk^{s-1}}{k^s(p-k)^s} \pmod{p^2}.$$

Noticing that $1/(p-k)^s \equiv -1/k^s \pmod p$ we have

$$2\sum_{k=1}^{p-1}\frac{1}{k^s} \equiv \sum_{k=1}^{p-1}\frac{-sp}{k^{s+1}} \equiv 0 \pmod{p^2}$$

whenever $p-1 \nmid s+1$ because p divides $\sum_{k=1}^{p-1} 1/k^{s+1}$ by the even case. □

When $s = p^e$ we can work more carefully with binomial expansion in the shorter proof and see that p^{2+e} divides $H(s;p-1)$. When $e=1$ this explains the fact that 125 divides $H(5;4)$. We record the phenomenon in the following proposition.

Proposition 2.4. *Let s be a positive integer and $v_p(s) = v$ and $v_p(s+1) = u$ (so that either u or v is 0). If $p \geq 5$ is a regular prime then*

$$v_p(H(s;p-1)) = \begin{cases} 0 & \text{if } p-1|s, \\ v+1 & \text{if } s \text{ is even and } p-1\nmid s, \\ u+v+1 & \text{if } s \text{ is odd and } p-1|s+1, \\ u+v+2 & \text{if } s \text{ is odd and } p-1\nmid s+1. \end{cases} \tag{2.4}$$

Suppose p is irregular and let $1 \leq m < p(p-1)$ such that

$$m \equiv \begin{cases} -s & \pmod{p(p-1)} \quad \text{if } s \text{ is even,} \\ -s-1 & \pmod{p(p-1)} \quad \text{if } s \text{ is odd.} \end{cases}$$

If $p-1 \nmid s+2, s+3$ and $p^2 \nmid B_m/m$ then the nonzero valuations can increase by at most 1*.*

Proof. We only consider the case when $p-1 \nmid s$. Suppose $s = p^v a$ and $p \nmid a$. Let $e \geq v+2$ be any positive integer such that $t := p^e(p-1) - s > 1$. Then $p-1 \nmid t$. It follows from Fermat's Little Theorem that

$$H(s;p-1) \equiv \sum_{k=1}^{p-1} k^t \pmod{p^{v+3}}.$$

If s is even then t is even and

$$\begin{aligned} H(s;p-1) &\equiv pB_t + \frac{t(t-1)}{6}p^3 B_{t-2} && \pmod{p^{v+3}} \\ &\equiv -ap^{v+1}\frac{B_{t'}}{t'} + \frac{(t-1)(t-2)}{6t''}p^{v+3}B_{t''} && \pmod{p^{v+3}} \end{aligned}$$

by Kummer congruences, where $t \equiv t', t-2 \equiv t'' \pmod{p(p-1)}$ and $1 \leq t', t'' < p(p-1)$. Note that v_p-valuation of the first term is $v+1$ or higher depending on whether (p,t') is regular pair or not. The smallest v_p-valuation of the second term is $v+2$ which happens if and only if $p-1|t''$. If p is irregular then $p-1 \nmid t''$ by our assumption $p-1 \nmid s+2$ and hence the second term is always divisible by p^{v+3}. It follows that the v_p-valuation is $v+1$ if p is regular and is at most $v+2$ if p is irregular since we assumed $p^2 \nmid B_{t'}/t'$. This proves the proposition when s is even.

When s is odd, then we need to consider two cases: $u = 0$ or $v = 0$. Both proofs in these two cases are similar to the even case and hence we leave the details to the interested readers. □

Remark 2.5. One can improve the above by a case by case analysis modulo higher p-powers. For example, one should be able to prove that the nonzero valuations can increase by at most 6 if p is irregular less than 12 million.

Remark 2.6. Numerical evidence shows that if p is irregular then the nonzero valuations seem to increase by at most 1 in most cases. The first counterexample appears with $p = 37$, and $s = 1048$. Note that s is even and $p-1 \nmid s$ so that if one leaves out the conditions in the lemma then the prediction would say $v_p(H(s; p-1))$ is at most 2 because 37 is irregular. But we have $v_{37}(H(1048; 36)) = 3$ because $37^2 | B_{p(p-1)-s} = B_{284}$.

Corollary 2.7. *Let $s \geq 4$ be a positive integer. Let $p \geq 3$ be a prime. If p is irregular then we assume it satisfies the conditions in the proceeding proposition. Then $H(s; p-1) \not\equiv 0 \pmod{p^s}$.*

Proof. The case $p = 3$ can be proved directly because $1 + 2^s < 3^s$ if $s \geq 2$ and

$$1 + \frac{1}{2^s} = \frac{1 + 2^s}{2^s} \not\equiv 0 \pmod{3^s}.$$

Suppose $p \geq 5$. Let $s = p^v a$ where $p \nmid a$. If p is regular then by Proposition 2.4 the largest value of $v_p(H(s; p-1))$ is $v+2$ which is less than s because $s \geq 4$ and $p \geq 5$. If p is irregular satisfying the conditions in Proposition 2.4 then the largest value of $v_p(H(s; p-1)$ is at most $v+3$ which is still less than s because $s \geq 4$ and $p \geq 37$. □

2.2. *p-divisibility, Bernoulli numbers and irregular primes*

Numerical evidence shows that congruences in Lemma 2.2 is not always optimal. For almost every MHS of length less than four, every once in a while a higher than expected power of p divides its $(p-1)$st partial sum. A closer look of this phenomenon reveals that all such primes are irregular primes. Going through the proof of Lemma 2.2 a bit more carefully one can obtain the following improvement.

Theorem 2.8. *Suppose n is a positive integer and p is an odd prime such that $p \geq 2n+3$. Then we have the congruences*:

$$\begin{aligned} \frac{-2}{2n-1} \cdot H(2n-1; p-1) &\equiv p \cdot H(2n; p-1) \\ &\equiv p^2 \cdot \frac{2n}{2n+1} \cdot B_{p-2n-1} \pmod{p^3}. \end{aligned} \tag{2.5}$$

Therefore the following statements are equivalent:

(1) $B_{p-2n-1} \equiv 0 \pmod{p}$.

(2) $H(2n; p-1) = \sum_{k=1}^{p-1} 1/k^{2n} \equiv 0 \pmod{p^2}$.

(3) $H(2n-1; p-1) = \sum_{k=1}^{p-1} 1/k^{2n-1} \equiv 0 \pmod{p^3}$.

(4) $H(n, n; p-1) = \sum_{1 \le k_1 < k_2 < p} 1/(k_1 k_2)^n \equiv 0 \pmod{p^2}$.

Proof. The congruence relation (2.5) and the equivalence of (1) to (3) in the theorem follows from the two congruences in [31] after [18, (16)]. See also [21, p. 281]. The equivalence of (2) and (4) follows immediately from the shuffle relation

$$H(n; p-1)^2 = 2H(n, n; p-1) + H(2n; p-1). \tag{2.6}$$

Some authors call this a quasi-shuffle or stuffle relation, i.e. "shuffling" plus "stuffing". □

Remark 2.9. This theorem also follows directly from a result of [42]. See Theorem 2.14.

Gardiner [19] proves the special case of the equivalence when $n = 1$. He has one more equivalence condition which involves the combinatorial number $\binom{2p}{p}$. Other variations of the classical Wolstenholme's Theorem can be found in [1]. It would be an interesting problem to find the analog for the zeta value series. It is also worth mentioning that it is not known whether $\binom{2n}{n} \equiv 2 \pmod{n^3}$ would imply n is a prime, which is called the converse of Wolstenholm's Theorem [33].

2.3. *Hoffman's duality*

In this section we recall Hoffman's "dual" operation of the compositisons and provide new congruence modulo a prime square. These results will be extremely useful when we deal with MHS of arbitrary lengths.

Let us first recall the definitions. Let k be a positive integer and $\mathbf{s} = (i_1, \ldots, i_k)$ of weight $n = |\mathbf{s}|$. We define the power set to be the partial sum sequence of $\mathbf{s}$: $P(\mathbf{s}) = (i_1, i_1 + i_2, \ldots, i_1 + \cdots + i_{k-1})$ as a subset of $(1, 2, \ldots, n-1)$. Clearly P provides a one-to-one correspondence between the compositions of weight n and the subsets of $(1, 2, \ldots, n-1)$. Then $\mathbf{s}^*$ is the compositison of weight n corresponding to the complimentary subset of $P(\mathbf{s})$ in $(1, 2, \ldots, n-1)$. Namely,

$$\mathbf{s}^* = P^{-1}((1, 2, \ldots, n-1) - P(\mathbf{s})).$$

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

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

Further we set the reversal $\overline{\mathbf{s}}=(s_l,\dots,s_1)$. The following important result is due to Hoffman:

Theorem 2.10 ([26, Theorem 6.8]). *For* $\mathbf{s}=(s_1,\dots,s_l)$ *and any positive integer* n *define*

$$S(\mathbf{s};n)=\sum_{1\le k_1\le\cdots\le k_l\le n} k_1^{-s_1}\cdots k_l^{-s_l}. \tag{2.7}$$

Then for all prime p

$$S(\mathbf{s}^*;p-1)\equiv -S(\mathbf{s};p-1) \qquad \pmod p, \tag{2.8}$$

$$S(\overline{\mathbf{s}};p-1)\equiv (-1)^{|\mathbf{s}|}S(\mathbf{s};p-1) \pmod p. \tag{2.9}$$

We also have the following equalities:

$$S(\mathbf{s};n)=\sum_{\mathbf{i}\preceq\mathbf{s}} H(\mathbf{i};n), \tag{2.10}$$

where $\mathbf{i}\prec\mathbf{s}$ *means* $\mathbf{i}$ *can be obtained from* $\mathbf{s}$ *by combining some of its parts, and*

$$(-1)^{l(\mathbf{s})}S(\overline{\mathbf{s}};p-1)=\sum_{\bigsqcup_{j=1}^l \mathbf{s}_j=\mathbf{s}} (-1)^l\prod_{j=1}^l H(\mathbf{s}_j;p-1) \tag{2.11}$$

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

Proof. Note that in [26] the right-hand side of (2.7) is denoted by $S(\overline{\mathbf{s}};n)$ instead. But it is not difficult to verify that for any $\mathbf{s}$

$$\overline{\mathbf{s}}^*=\overline{\mathbf{s}^*}. \tag{2.12}$$

So (2.8) is equivalent to [26, Theorem 6.8]. Congruence (2.9) follows readily from the substitution of indices: $k\to p-k$.

Equations (2.11) and (2.10) relate S-version multiple harmonic series and our H-version (denoted by A by Hoffman). Equation (2.10) is [26, Eq. (7)]) and (2.11) is equivalent to the second unlabeled formula in the proof of [26, Theorem 6.8]. □

Next we want to provide a more precise version of congruence (2.8).

Theorem 2.11. *Let* $\mathbf{s}$ *be any compositison of weight* w. *Let* p *be an arbitrary odd prime. Then*

$$-S(\mathbf{s}^*;p-1)\equiv S(\mathbf{s};p-1)+p\left(\sum_{\mathbf{t}\preceq\mathbf{s}} H(\mathbf{t}\sqcup\{1\};p-1)\right) \pmod{p^2}. \tag{2.13}$$

Proof. For any sequence $\{f(n)\}_{n\geq -1}, f(-1)=0$ we know there are two operators Σ and ∇:

$$\Sigma f(n)=\sum_{i=0}^{n} f(i), \quad \nabla f(n)=f(n)-f(n-1), \quad \forall n\geq 0.$$

Recall that $\Sigma\nabla S(\mathbf{s};n)=-S(\mathbf{s}^*;n)$ for any $\mathbf{s}$ and positive number n by [27, Theorem 4.2]. Then for any odd prime p we have

$$\begin{aligned}
-S(\mathbf{s}^*;p-1) &= \Sigma\nabla S(\mathbf{s};p-1)(n)=\sum_{i=0}^{p-1}\binom{p}{i+1}(-1)^i S(\mathbf{s};i)\\
&= S(\mathbf{s};p-1)(n)+p\left(\sum_{i=0}^{p-2}\frac{1}{i+1}\binom{p-1}{i}(-1)^i S(\mathbf{s};i)\right)\\
&\equiv S(\mathbf{s};p-1)(n)+p\left(\sum_{i=0}^{p-2}\frac{1}{i+1}S(\mathbf{s};i)\right) \pmod{p^2}\\
&\equiv S(\mathbf{s};p-1)(n)+p\left(\sum_{i=0}^{p-2}\sum_{\mathbf{t}\preceq\mathbf{s}}\frac{H(\mathbf{t};i)}{i+1}\right) \pmod{p^2}\\
&\equiv S(\mathbf{s};p-1)(n)+p\left(\sum_{\mathbf{t}\preceq\mathbf{s}}H(\mathbf{t}\sqcup\{1\};p-1)\right) \pmod{p^2}.
\end{aligned}$$

This completes the proof of the theorem. □

2.4. *Wolstenholme type theorem for homogeneous MHS*

In the above we have studied the p-divisibility of $H(s;p-1)$ for positive integers s. Not much can be said when the length of $\mathbf{s}$ is large except in the case of homogeneous MHS.

First we can easily verify the following shuffle relations: for any positive integers $n,m,s_1,\ldots,s_l$,

$$\begin{aligned}
H(m;n)\cdot H(s_1,\ldots,s_l;n) &= \sum_{\mathbf{s}\in\mathrm{Shfl}(m,(s_1,\ldots,s_l))} H(\mathbf{s};n)\\
&\quad+\sum_{j=1}^{l} H\big(s_1,\ldots,s_{j-1},s_j+m,s_{j+1},\ldots,s_l;n\big)
\end{aligned}$$

where for any two ordered sets $(r_1,\ldots,r_t)$ and $(r_{t+1},\ldots,r_n)$ the shuffle operation is defined by

$$\mathrm{Shfl}\big((r_1,\ldots,r_t),(r_{t+1},\ldots,r_n)\big):=\bigcup_{\substack{\sigma \text{ permutes } \{1,\ldots,n\},\\ \sigma^{-1}(1)<\cdots<\sigma^{-1}(t),\\ \sigma^{-1}(t+1)<\cdots<\sigma^{-1}(n)}}\big(r_{\sigma(1)},\ldots,r_{\sigma(n)}\big).$$

It is not too hard to see that every homogeneous MHS can be expressed in terms of length one MHS. Indeed, by using symmetric functions we can obtain a precise relation.

Let $p_i = \sum_{j\geq 1} x_j^i$ be the power-sum symmetric functions and $e_i = \sum_{j_1<\cdots<j_i} x_{j_i}\cdots x_{j_i}$ be the elementary symmetric functions of degree i. Let $P(l)$ be the set of unordered partitions of l. For $\lambda = (\lambda_1,\dots,\lambda_r) \in P(l)$ we set $p_\lambda = \prod_{i=1}^r p_{\lambda_i}$. Recall that the expression of e_l in terms of p_i is given by the following formula (see [32, p. 28]):

$$l!e_l = \begin{vmatrix} p_1 & 1 & 0 & \cdots & 0 \\ p_2 & p_1 & 2 & \cdots & 0 \\ & & & \ddots & 0 \\ p_{l-1} & p_{l-2} & p_{l-3} & \cdots & l-1 \\ p_l & p_{l-1} & p_{l-2} & \cdots & p_1 \end{vmatrix} = \sum_{\lambda\in P(l)} c_\lambda p_\lambda. \tag{2.14}$$

Lemma 2.12 ([27, Theorem 2.3]). *Let s, l and n be positive integers. For $\lambda = (\lambda_1,\dots,\lambda_r) \in P(l)$ we put $H_\lambda(s;n) = \prod_{i=1}^r H(\lambda_i s;n)$. Then*

$$l!H\big(\{s\}^l;n\big) = \sum_{\lambda\in P(l)} c_\lambda H_\lambda(s;n) \tag{2.15}$$

where c_λ are given by (2.14).

It is obvious that $c_{(1,\cdots,1)} = 1$. When $l = 3$ we have $c_{(3)} = 2$ and $c_{(1,2)} = -3$, which implies

$$6H(\{s\}^3;n) = H(s;n)^3 - 3H(s;n)H(2s;n) + 2H(3s;n). \tag{2.16}$$

When $l = 4$ we have $c_{(4)} = c_{(1,1,2)} = -6$, $c_{(1,3)} = 8$, and $c_{(2,2)} = 3$, which implies

$$\begin{aligned} 24H(\{s\}^4;n) = {} & H(s;n)^4 - 6H(s;n)^2H(2s;n) + 8H(s;n)H(3s;n) \\ & + 3H(2s;n)^2 - 6H(4s;n). \end{aligned}$$

Theorem 2.13. *Let s and l be two positive integers. Let p be an odd prime such that $p \geq l+2$ and $p-1$ divides none of sl and $ks+1$ for $k = 1,\dots,l$. Then the homogeneous MHS*

$$H(\{s\}^l;p-1) \equiv S(\{s\}^l;p-1) \equiv 0 \pmod{p^{\mathfrak{p}(ls-1)}}.$$

In particular, if $p \geq ls+3$ then the above is always true and so $p|H(\{s\}^l;p-1)$.

Proof. Congruence for H follows from Eq. (2.15) and Lemma 2.2. Congruence for S then follows from (2.11). □

Recently, Zhou and Cai obtain the following improved version of the above result, see [42]

Theorem 2.14. *Let s and l be two positive integers. Let p be a prime such that $p \geq ls+3$*

$$(-1)^{l-1} H(\{s\}^l; p-1) \equiv S(\{s\}^l; p-1) \equiv \begin{cases} -\dfrac{s(ls+1)p^2}{2(ls+2)} B_{p-ls-2} \pmod{p^3} & \text{if } 2 \nmid ls, \\ \dfrac{sp}{ls+1} B_{p-ls-1} \pmod{p^2} & \text{if } 2 \mid ls. \end{cases}$$

Proof. Congruence for H follows from [42]. Congruence for S then follows from (2.11) and an induction on l. □

2.5. *Higher divisibility and distribution of irregular pairs*

Computations show that often a higher than expected prime powers divides $H(\mathbf{s}, p-1)$. The following result is an easy consequence of Theorem 2.14:

Proposition 2.15. *Let p be an odd prime. Let l and s be two positive integers.*

(a) *Suppose ls is odd. Then $(p, p-ls-2)$ is an irregular pair if and only if*

$$H(\{s\}^l; p-1) \equiv S(\{s\}^l; p-1) \equiv 0 \pmod{p^3}.$$

(b) *Suppose ls is even. Then $(p, p-ls-1)$ is an irregular pair if and only if*

$$H(\{s\}^l; p-1) \equiv S(\{s\}^l; p-1) \equiv 0 \pmod{p^2}.$$

One of the first instances of this proposition is when $s=1$ and $l=3$ given by the first irregular pair $(37, 32)$, which, by our proposition, implies that $H(1,1,1;36) \equiv 0 \pmod{37^3}$. The case when $s=3$ and $l=3$ appears first with the irregular pair $(9311, 9300)$. So we know $H(3,3,3;9310) \equiv 0 \pmod{9311^3}$.

We believe these are just the first two of infinitely many such pairs because evidently not only Bernoulli numbers but also the difference $p-t$ for irregular pairs (p,t) are evenly distributed modulo any prime. Precisely, we have the following

Conjecture 2.16. *For any fixed positive integer M and integer c such that $0 \leq c < M$ we have*

$$\lim_{X\to\infty} \frac{\sharp\{(p,t) : \text{prime } p|B_t, t \text{ even}, p<X, p-t \equiv c \pmod{M}\}}{\sharp\{(p,t) : \text{prime } p|B_t, \ t \text{ even}, \ p<X\}} = \begin{cases} 0 & \text{if } 2|c, \ 2|M, \\ \dfrac{1}{M} & \text{if } 2 \nmid M, \\ \dfrac{2}{M} & \text{if } 2 \nmid c, \ 2|M. \end{cases}$$

Table 1. Distribution of $p - t \pmod 3$ for irregular pairs (p, t).

m	$N(0,m)$	$P(0,m)$	$N(1,m)$	$P(1,m)$	$N(2,m)$	$P(2,m)$
1,000	322	32.20	343	34.30	335	33.50
2,000	664	33.20	666	33.30	670	33.50
3,000	996	33.20	1005	33.50	999	33.30
4,000	1318	32.95	1352	33.80	1330	33.25
5,000	1637	32.74	1676	33.52	1687	33.74
6,000	1978	32.97	1999	33.32	2023	33.72
7,000	2310	33.00	2340	33.43	2350	33.57
8,000	2628	32.85	2683	33.54	2689	33.61
9,000	2968	32.98	3017	33.52	3015	33.50
10,000	3310	33.10	3354	33.54	3336	33.36
11,000	3672	33.38	3673	33.39	3655	33.22

Further we can replace the sets by restricting p to all irregular primes with a fixed irregular index which is defined as the number of such pairs for a fixed p.

As a result we expect there are about one-third irregular pairs satisfying the conditions in Proposition 2.15 for $l = 3$ and various s. In Table 1 we count the first 11,000 irregular pairs. We denote by $N(k, m)$ the number of irregular pairs (p, t) satisfying $p - t \equiv k \pmod 3$ in the top m irregular pairs, $0 \leq k \leq 2$, and by $P(k, m)$ the percentage of such pairs. For irregular primes with fixed index we compiled some more tables in the Appendix A at the end of this paper.

Buhler *et al.* [10] computed all the irregular primes less than 12 million and associated cyclotomic invariants by using multisectioning/convolution methods and an improvement of an idea of Shokrollahi [35]. The details can be found also in [14, p. 493]. It is possible to use the new congruences found in this paper to compute these irregular primes, for example, by Theorem 3.1 in the next section. However, it takes a much longer time than the method of Buhler et al. because we need to take a double sum even though the modulus is reduced to p instead of p^2.

3. Non-Homogeneous MHS

Having dealt with homogeneous MHS we would like to do some initial experiments on the non-homogeneous ones.

3.1. *Non-homogeneous sums of length 2*

We begin with $H(1, 2)$ and $H(2, 1)$. For any positive integer n from the shuffle relation we have

$$H(1, 2; n) + H(2, 1; n) = H(1; n) \cdot H(2; n) - H(3; n). \tag{3.1}$$

However, it seems to be quite difficult to disentangle $H(1,2;n)$ from $H(2,1;n)$. Maple Computation for primes up to 20,000 confirms the following

Theorem 3.1. *Let s_1, s_2 be two positive integers and p be an odd prime. Let $s_1 \equiv m, s_2 \equiv n \pmod{p-1}$ where $0 \le m, n \le p-2$. Then*

$$H(s_1, s_2; p-1) \equiv \begin{cases} 1 & \pmod p \quad \text{if } (m,n) = (0,0), (1,0), \\ -1 & \pmod p \quad \text{if } (m,n) = (0,1), \\ \dfrac{(-1)^n}{m+n}\dbinom{m+n}{m} B_{p-m-n} & \pmod p \quad \text{if } p \ge m+n \text{ and } m,n \ge 1, \\ 0 & \pmod p \quad \text{otherwise.} \end{cases}$$

In particular, if $p \ge s+t$ for two positive integers s_1 and s_2 then we always have

$$S(s_1, s_2; p-1) \equiv H(s_1, s_2; p-1) \equiv \frac{(-1)^{s_2}}{s_1+s_2}\binom{s_1+s_2}{s_1} B_{p-s_1-s_2} \pmod p. \tag{3.2}$$

Proof. We leave the trivial cases to the interested readers and assume in the rest of the proof that $m, n \ge 1$.

Let $M = p-1-m$ and $N = p-1-n$. Then $1 \le M, N \le p-2$. By Fermat's Little Theorem

$$H(m,n;p-1) \equiv \sum_{1 \le k_1 < k_2 \le p-1} k_1^M k_2^N \pmod p.$$

Define the formal power series in two variables

$$f(x,y) = \sum_{r,s=0}^{\infty} \left(\sum_{1 \le k_1 < k_2 \le p-1} k_1^r k_2^s \right) \frac{x^r y^s}{r! s!}. \tag{3.3}$$

Exchanging summation we get

$$\begin{aligned} f(x,y) = \sum_{1 \le k_1 < k_2 \le p-1} e^{k_1 x + k_2 y} &= \frac{e^{p(x+y)} - e^{x+y}}{(e^{x+y}-1)(e^x-1)} - \frac{(e^{py}-e^y)e^x}{(e^y-1)(e^x-1)} \\ &= \sum_{i=-1}^{\infty} \sum_{j=-1}^{\infty} \frac{B_{j+1}(p) - B_{j+1}(1)}{(i+1)!(j+1)!} (B_{i+1} x^i (x+y)^j - B_{i+1}(1) x^i y^j) \end{aligned}$$

where $B_m(1) = B_m$ if $m \ne 1$ and $B_1(1) = -B_1 = \frac{1}{2}$. We only care about the above sum when $1 \le i, j \le p-2$ since $1 \le M, N \le p-2$. So we may as well replace $B_m(1)$ by B_m everywhere in the last display and throw away the terms with $j = 0, \pm 1$.

The resulting power series is

$$g(x,y) \equiv \sum_{i=-1}^{\infty}\sum_{j=2}^{\infty}\sum_{l=1}^{j} \frac{pB_{i+1}B_j}{(i+1)!j!}\binom{j}{l} x^{l+i}y^{j-l} \pmod p. \tag{3.4}$$

Let $l+i=M$ and $j-l=N$. Then we see that the coefficient of x^My^N is

$$\sum_{l=1}^{M} \frac{pB_{M-l+1}B_{N+l}}{(M-l+1)!(N+l)!}\binom{N+l}{l} = \sum_{l=1}^{M} \frac{pB_{M-l+1}B_{N+l}}{(M-l+1)!N!l!}. \tag{3.5}$$

Note that $0 \le M-l+1 \le M \le p-2$ and $2 \le N+1 \le N+l \le M+N \le 2p-4$. If $M+N < p-2$ (i.e. $m+n > p$) then (3.5) is always congruent to 0 mod p. Otherwise, if $M+N \ge p-2$ then all the terms are in $p\mathbb{Z}_p$ except when $N+l = p-1$. Hence

$$\frac{1}{M!N!} \sum_{1\le k_1<k_2\le p-1} k_1^M k_2^N \equiv \frac{pB_{M+N+2-p}B_{p-1}}{(M+N+2-p)!N!(p-1-N)!} \pmod p.$$

So finally we arrive at

$$H(m,n;p-1) = \sum_{1\le k_1<k_2\le p-1} \frac{1}{k_1^m k_2^n} \equiv \frac{-(p-m-1)!B_{p-m-n}}{n!(p-m-n)!} \pmod p.$$

One can now use Wilson's Theorem to get the final congruence for H in our theorem without too much difficulty. For S we now use $S(s_1,s_2) = H(s_1,s_2) + H(s_1+s_2)$ and Theorem 1.3. □

Taking $s_1 = 1, s_2 = 2$ in the theorem we obtain $H(1,2;p-1) \equiv B_{p-3} \pmod p$ for $p \ge 3$. We verified this on Maple for the only two known irregular pairs of the form $(p, p-3)$, namely, $p = 16843$ and $p = 2124679$. If we take $s_1 = 2, s_2 = 3$ we find that $H(2,3;p-1) \equiv B_{p-5} \pmod p$ if $p \ge 5$. There is only one irregular pair of the form $(p, p-5)$ among all primes less than 12 million, namely, $(37, 32)$. Indeed, for $p = 37$ computation shows that $H(2,3;36) \equiv 0 \pmod{37}$. As a matter of fact, we formulated Theorem 3.1 only after we had found these intriguing examples.

We now can provide an analog of Theorem 2.14 in the non-homogeneous case of length two.

Theorem 3.2. *Let p be an odd prime. Suppose s and t are two positive integers of same parity such that $p > s+t+1$. Then*

$$H(s,t;p-1) \equiv p\left[(-1)^s t\binom{s+t+1}{s} - (-1)^s s\binom{s+t+1}{t} - s - t\right]\frac{B_{p-s-t-1}}{2(s+t+1)} \pmod{p^2}$$

$$S(s,t;p-1) \equiv p\left[(-1)^s t\binom{s+t+1}{s} - (-1)^s s\binom{s+t+1}{t} + s + t\right]\frac{B_{p-s-t-1}}{2(s+t+1)} \pmod{p^2}.$$

Proof. By the shuffle relation (dropping $p-1$ again) we see that

$$H(s)\cdot H(t) = H(s,t) + H(t,s) + H(s+t). \tag{3.6}$$

By the conditions on s_1 and s_2 we know from (2.5)

$$H(s)\cdot H(t) \equiv 0, H(s+t) \equiv \frac{p(s+t)}{s+t+1} B_{p-s-t-1} \pmod{p^2}. \tag{3.7}$$

Therefore

$$H(s,t) + H(t,s) \equiv \frac{-p(s+t)}{s+t+1} B_{p-s-t-1} \pmod{p^2}. \tag{3.8}$$

Moreover, by the old substitution trick $i, j \to p-i, p-j$

$$\begin{aligned} H(s,t) &= \sum_{1\le j<i<p} \frac{1}{(p-i)^s (p-j)^t} \\ &\equiv \sum_{1\le j<i<p} \frac{1}{i^s j^t}\left(1+\frac{p}{i}\right)^s \left(1+\frac{p}{j}\right)^t \qquad \pmod{p^2} \quad (s+t \text{ is even}) \\ &\equiv \sum_{1\le j<i<p} \frac{1}{i^s j^t}\left(1+\frac{ps}{i}+\frac{pt}{j}\right) \qquad \pmod{p^2} \\ &\equiv H(t,s) + psH(t,s+1) + ptH(t+1,s) \pmod{p^2} \\ &\equiv H(t,s) + p\left[(-1)^{s+1} s \binom{s+t+1}{t} + (-1)^s t \binom{s+t+1}{t+1}\right] \\ &\quad \times \frac{B_{p-s-t-1}}{s+t+1} \pmod{p^2}. \end{aligned}$$

Combined with (3.8) this completes the proof of the congruence for H. Then the S part follows from the identity $S(s,t) = H(s,t) + H(s+t)$. □

3.2. *The case of palindrome* $\mathbf{s}$

Recall that for $\mathbf{s} = (s_1, \ldots, s_l)$ we have set its reversal $\overline{\mathbf{s}} = (s_l, \ldots, s_1)$.

Lemma 3.3. *Let p be an odd prime. Let l be a positive integer and $\mathbf{s} \in \mathbb{N}^l$. Let $|\mathbf{s}| = \sum_{i=1}^{l} s_i$ be the weight of* $\mathbf{s}$. *Then*

$$\begin{aligned} H(\mathbf{s}; p-1) &\equiv (-1)^{|\mathbf{s}|} H(\overline{\mathbf{s}}; p-1) \pmod{p}, \\ S(\mathbf{s}; p-1) &\equiv (-1)^{|\mathbf{s}|} S(\overline{\mathbf{s}}; p-1) \pmod{p}. \end{aligned} \tag{3.9}$$

Proof. Use the old substitution trick $k_i \to p - k_i$ for all i in the definitions (1.2) and (1.3). □

An immediate consequence of this lemma is

Corollary 3.4. *Let p be an odd prime. If $\mathbf{s} = \overline{\mathbf{s}}$ and $|\mathbf{s}|$ is odd then*

$$H(\mathbf{s}; p-1) \equiv S(\mathbf{s}; p-1) \equiv 0 \pmod{p}. \tag{3.10}$$

On the contrary, a lot of examples show that if the weight $|\mathbf{s}| \geq 6$ is even and if the length is bigger than two, then we often have $H(\mathbf{s}; p-1) \not\equiv 0 \pmod p$ when p is large (say, $p \geq 2|\mathbf{s}|$), even in the case that $\mathbf{s}$ is a palindrome. For example, in length three if $\mathbf{s} \neq (4,3,5), (5,3,4)$ then this seems to be always the case (see Problem 3.9). A remarkable different pattern occurs for length three weight four case which we will consider in Sec. 3.4. Clarifying this completely might be a crucial step to understand the structure of $H(\mathbf{s}; p-1)$ in general.

3.3. *Multiple harmonic sums of length three with odd weight*

One may want to generalize Theorem 3.1 to MHS of longer lengths. However, the proofs become much more involved. Extensive computation confirms the following

Theorem 3.5. *Let p be an odd prime. Let $(s_1, s_2, s_3) \in \mathbb{N}^3$ and $0 \leq l, m, n \leq p-2$ such that $s_1 \equiv l, s_2 \equiv m, s_3 \equiv n \pmod{p-1}$. Then*

$$\begin{aligned}
&H(0,m,n;p-1)\\
&\quad \equiv H(m-1,n;p-1) - H(m,n;p-1), && \pmod p,\\
&H(l,0,n;p-1)\\
&\quad \equiv H(l,n-1;p-1) - H(l,n;p-1) - H(l-1,n;p-1) && \pmod p,\\
&H(l,m,0;p-1)\\
&\quad \equiv -H(l,m-1;p-1) - H(l,m;p-1) && \pmod p.
\end{aligned}$$

If $l, m, n \geq 1$ then we assume further that $w = l+m+n$ is an odd *number. Then*

$$H(s_1, s_2, s_3; p-1) \equiv I(l,m,n) - I(n,m,l) \pmod p$$

where I

$$I(l,m,n) = \begin{cases} 0 & \textit{if } w \geq 2p, \textit{ or if } l+m<p \textit{ and } p<w<2p-1,\\ \dfrac{1}{2n} & \textit{if } w = p, 2p-1,\\ (-1)^{n+1}\dbinom{w'}{n}\dfrac{B_{p-w'}}{2w'} & \textit{otherwise, where } w' = w-(p-1). \end{cases}$$

In particular, if a prime $p > l+m+n$ for positive integers l, m, n such that $w = l+m+n$ is odd then

$$H(l,m,n;p-1) \equiv -S(l,m,n;p-1) \equiv (-1)^n \left[\binom{w}{l} - \binom{w}{n}\right] \frac{B_{p-w}}{2w} \pmod p. \tag{3.11}$$

Proof. One we mimic the proof of the length two case but it will be tedious. In [27, Theorem 6.2] Hoffman presents an easier one by using shuffle relations and S-version of the MHS. In what follows we provide yet another proof with the condition that $p > w+1$. This is similar to the proof in [27, Theorem 6.1].

First we put no restriction on the parity of w. Recall that by Bernoulli polynomials we have

$$\sum_{i=1}^{n} i^d = \sum_{a=0}^{d} \binom{d+1}{a} \frac{B_a}{d+1} n^{d+1-a}. \tag{3.12}$$

So modulo p we have by Fermat's Little Theorem

$$\begin{aligned}
&H(r,s,t;p-1)\\
&\quad\equiv \sum_{i=1}^{p-1} \frac{1}{i^t} \sum_{j=1}^{i-1} j^{p-1-s} \sum_{k=1}^{j-1} k^{p-1-r}\\
&\quad\equiv \sum_{i=1}^{p-1} \frac{1}{i^t} \sum_{j=1}^{i-1} \sum_{a=0}^{p-1-r} \binom{p-r}{a} \frac{B_a}{p-r} j^{\kappa(a)+p-r-s-a}\\
&\quad\equiv \sum_{i=1}^{p-1} \frac{1}{i^t} \sum_{a=0}^{p-1-r} \binom{p-r}{a} \frac{B_a}{p-r} \sum_{j=1}^{i-1} j^{\kappa(a)+p-r-s-a}\\
&\quad\equiv \sum_{i=1}^{p-1} \sum_{a=0}^{p-1-r} \binom{p-r}{a} \frac{B_a}{p-r} \cdot\\
&\qquad \sum_{b=0}^{\kappa(a)+p+1-r-s-a} \binom{\kappa(a)+p+1-r-s-a}{b} \frac{B_b \cdot i^{\kappa(a)+p+1-w-a-b}}{\kappa(a)+p+1-r-s-a},
\end{aligned}$$

where $\kappa(a) = 0$ if $a \le p-r-s$ and $\kappa(a) = p-1$ if $a > p-r-s$. Now take the sum of powers of i first and observe that $\sum_{i=1}^{p-1} i^l \equiv 0 \pmod p$ unless $l \equiv 0 \pmod{p-1}$. Note that it is impossible to have $\kappa(a)+p+1-w-a-b \equiv 0 \pmod{p-1}$ if $a > p+1-w$, unless $a > p-r-s$. Hence we get:

$$\begin{aligned}
&H(r,s,t;p-1)\\
&\quad\equiv -\sum_{a=0}^{p+1-w} \binom{p-r}{a} \frac{B_a}{p-r} \binom{p+1-r-s-a}{t} \frac{B_{p+1-w-a}}{p+1-r-s-a}\\
&\qquad - \sum_{a=\max\{p+1-r-s,p+2-w\}}^{p-1-r} \binom{p-r}{a} \frac{B_a}{p-r} \binom{2p-r-s-a}{t} \frac{B_{2p-w-a}}{2p-r-s-a}\\
&\quad\equiv -\sum_{a=0}^{p+1-w} (-1)^{a+t} \binom{r+a}{a} \frac{B_a}{r+a} \binom{w+a-1}{t} \frac{B_{p+1-w-a}}{w+a-1}\\
&\qquad - \sum_{a=\max\{p+1-r-s,p+2-w\}}^{p-1-r} (-1)^{a+t} \binom{r+a}{a} \frac{B_a}{r+a} \binom{w+a}{t} \frac{B_{2p-w-a}}{w+a}.
\end{aligned} \tag{3.13}$$

When w is odd we obtain Theorem 3.5 when $p > w+1$ by noticing that there are only two nontrivial terms in (3.13) corresponding to $a = 1$ and $a = p - w$. □

3.4. *Some remarkable cases of length three with even weight*

Applying (3.8) to $(s_1, s_2) = (1, 3)$ together with shuffle product $H(1, 1; p-1) \cdot H(2; p-1)$ we get

$$H(2,1,1;p-1) + H(1,2,1;p-1) + H(1,1,2;p-1) \equiv \frac{4p}{5} B_{p-5} \pmod{p^2}. \tag{3.14}$$

By Lemma 3.3 we can even see that

$$H(2,1,1;p-1) \equiv H(1,1,2;p-1) \pmod{p}. \tag{3.15}$$

However, is it true that in fact all of these sums are congruent to 0 mod p? Now from (3.13) we can compute easily that modulo p

$$H(1,2,1;p-1) \equiv \sum_{a=0}^{p-3} B_a B_{p-3-a}, \tag{3.16}$$

$$H(1,1,2;p-1) \equiv -\sum_{a=0}^{p-3} \frac{2+a}{2} B_a B_{p-3-a}, \tag{3.17}$$

$$H(2,1,1;p-1) \equiv \sum_{a=0}^{p-3} \frac{1+a}{2} B_a B_{p-3-a}. \tag{3.18}$$

Set

$$A := \sum_{a=0}^{p-3} B_a B_{p-3-a}, \quad B := \sum_{a=0}^{p-3} a B_a B_{p-3-a}.$$

Then from (3.14), (3.16) to (3.18)

$$\frac{A}{2} \equiv 0 \pmod{p}.$$

Moreover, from (3.15), (3.17) and (3.18)

$$-\left(A + \frac{B}{2}\right) \equiv \frac{A}{2} + \frac{B}{2} \pmod{p}.$$

Consequently we have

Corollary 3.6. *For every prime $p \geq 7$ we get*

$$\sum_{a=0}^{p-3} B_a B_{p-3-a} \equiv \sum_{a=0}^{p-3} a B_a B_{p-3-a} \equiv 0 \pmod{p}. \tag{3.19}$$

Therefore we have

$$H(1,2,1;p-1) \equiv H(1,1,2;p-1) \equiv H(2,1,1;p-1) \equiv 0 \pmod{p}. \tag{3.20}$$

Using Maple we further find the following very stimulating example

$$H(1,2,1;36) = \frac{2234416196881673576349577192603}{1151149136943530805554073600000} \equiv 0 \pmod{37^2}.$$

Proposition 3.7. *For all prime $p \geq 7$ we have*

$$S(1,2,1;p-1) \equiv H(1,2,1;p-1) \equiv -\frac{9}{10} pB_{p-5} \pmod{p^2}, \tag{3.21}$$

$$S(1,1,2;p-1) \equiv H(2,1,1;p-1) \equiv \frac{3}{5} pB_{p-5} \pmod{p^2}, \tag{3.22}$$

$$S(2,1,1;p-1) \equiv H(1,1,2;p-1) \equiv \frac{11}{10} pB_{p-5} \pmod{p^2}. \tag{3.23}$$

Proof. Omitting $H(\cdots;p-1)$ we let $A = H(1,2,1), B = H(2,1,1)$ and $C = H(1,2,2)$. Equation (3.14) says that

$$A + B + C \equiv \frac{4}{5} pB_{p-5} \pmod{p^2}. \tag{3.24}$$

Now by the shuffle relations

$$H(1)H(2,1) = A + 2B + H(3,1) + H(2,2), \tag{3.25}$$

From Theorem 3.2 we get

$$A + 2B \equiv \frac{3}{10} pB_{p-5} \pmod{p^2} \tag{3.26}$$

Hence it suffice to show (3.21). From (2.10) we see that

$$\begin{aligned} S(1,2,1) &= H(1,2,1) + H(3,1) + H(1,3) + H(4) \\ &= H(1,2,1) + H(1) \cdot H(3) \equiv H(1,2,1) \pmod{p^2} \end{aligned} \tag{3.27}$$

$$S(2,2) = H(2,2) + H(4) = -H(2,2) + H(2)^2 \equiv -H(2,2) \pmod{p^2}. \tag{3.28}$$

Now because $(1,2,1)^* = (2,2)$ by Theorem 2.11 we have

$$\begin{aligned} -S(2,2) \equiv\ & S(1,2,1) \\ & + p(H(1,2,1,1) + H(3,1,1) + H(1,3,1) + H(4,1)) \pmod{p^2}. \end{aligned} \tag{3.29}$$

By Corollary 3.4 $H(1,3,1) \equiv 0 \pmod{p}$. So using expressions (3.27) and (3.28) we can simplify the preceding congruence to

$$H(2,2) \equiv H(1,2,1) + p(H(1,2,1,1) + H(3,1,1) + H(4,1)) \pmod{p^2}. \tag{3.30}$$

Now that $(1,2,1,1)^* = (2,3)$ we find from congruence (2.8) that modulo p

$$\begin{aligned} -S(2,3) &\equiv S(1,2,1,1) \\ &\equiv H(1,2,1,1) + H(3,1,1) + H(1,3,1) \\ &\quad + H(1,2,2) + H(4,1) + H(3,2) + H(1,4) + H(5) \pmod{p}. \end{aligned}$$

Note that

$$H(1,3,1) \equiv 0, H(4,1) + H(1,4) = H(1) \cdot H(4) - H(5) \equiv 0 \pmod p.$$

So (2.10) implies that

$$-H(2,3) \equiv -S(2,3) \equiv H(1,2,1,1) + H(3,1,1) + H(1,2,2) + H(3,2) \pmod p.$$

Namely

$$\begin{aligned} H(1,2,1,1) &\equiv -H(2,3) - H(3,2) - H(3,1,1) - H(1,2,2) && \pmod p \\ &\equiv H(5) - H(3,1,1) - H(1,2,2) && \pmod p \\ &\equiv -H(3,1,1) - H(1,2,2) && \pmod p. \end{aligned}$$

Plugging this into (3.30) we see that

$$H(2,2) \equiv H(1,2,1) + p(H(4,1) - H(1,2,2)) \pmod{p^2}.$$

Using Theorems 2.14 and 3.2 we can now compute easily that

$$\begin{aligned} H(2,2) &\equiv -\frac{2}{5} p B_{p-5} \pmod{p^2}, \\ H(4,1) &\equiv -B_{p-5}, \\ H(1,2,2) &\equiv -\frac{3}{2} B_{p-5} \pmod p. \end{aligned}$$

These together with (3.27) lead to congruence (3.21).

We now can solve (3.24) and (3.26) to get congruences for H in (3.22) and (3.23). For the S version of the MHS (2.11) yields

$$\begin{aligned} S(2,1,1) &= H(1,1,2) - H(1)H(1,2) - H(1,1)H(2) + H(1)^2 H(2) \\ &\equiv H(1,1,2) \pmod{p^2}, \\ S(1,1,2) &= H(2,1,1) - H(2)H(1,1) - H(2,1)H(1) + H(2)H(1)^2 \\ &\equiv H(2,1,1) \pmod{p^2}. \end{aligned}$$

We have completed the proof of the proposition. □

In [41], by using the shuffle relations and Hoffman's duality we will study the mod p structure of the MHS for lower weights. In particular, we will prove

Proposition 3.8. *For all prime $p \geq 17$ we have*

$$\begin{aligned} H(4,3,5;p-1) &\equiv H(5,3,4;p-1) \\ &\equiv S(2,3,2,3,2;p-1) \equiv S(2,3,3,2,2;p-1) \equiv 0 \pmod p. \end{aligned} \quad (3.31)$$

Problem 3.9. Numerical evidence shows that if $(r,s,t) \neq (5,3,4),(4,3,5)$ and $r+s+t \geq 6$ is even then the density of primes p such that $p \nmid H(r,s,t;p-1)$ among all primes is always 1; however, there is always p such that $p | H(r,s,t;p-1)$. Can one generalize the formula in Theorem 3.5 to prove this?

3.5. *Some congruences modulo prime squares*

We know from Theorem 3.5 that $H(r,s,r;p-1)\equiv 0 \pmod p$ if s is an odd number and $p>2r+s$. Modulo p^2 we have (using substitution of indices $k\to p-k$)

$$\begin{aligned}H(r,s,r;p-1)\equiv&-H(r,s,r;p-1)\\&-p\big[2rH(r+1,s,r;p-1)+sH(r,s+1,r;p-1)\big].\end{aligned}\tag{3.32}$$

Hence

$$H(r,s,r;p-1)\equiv -p\left[rH(r+1,s,r;p-1)+\frac{s}{2}H(r,s+1,r;p-1)\right]\pmod{p^2}.\tag{3.33}$$

Proposition 3.10. *For all prime $p>5$ we have*

$$H(1,3,1;p-1)\equiv S(1,3,1;p-1)\equiv 0 \pmod{p^2}\tag{3.34}$$

$$-H(2,1,2;p-1)\equiv S(2,1,2;p-1)\equiv \frac{1}{3}B_{p-3}^2 p \pmod{p^2}.\tag{3.35}$$

For all prime $p>7$ set $b_8(p)=(5S(6,1,1;p-1)+B_{p-5}B_{p-3})/2$ then we have

$$-H(1,5,1;p-1)\equiv S(1,5,1;p-1)\equiv b_8(p)p \pmod{p^2}\tag{3.36}$$

$$-H(2,3,2;p-1)\equiv S(2,3,2;p-1)\equiv 4b_8(p)p \pmod{p^2},\tag{3.37}$$

$$-H(3,1,3;p-1)\equiv S(3,1,3;p-1)\equiv b_8(p)p \pmod{p^2}.\tag{3.38}$$

Proof. We drop $p-1$ throughout the proof. Notice that by (2.11)

$$S(a,b,c)\equiv(-1)^{a+b+c}H(a,b,c) \pmod p.\tag{3.39}$$

From (3.33) we have

$$\begin{aligned}2H(1,3,1)&\equiv -p[2H(2,3,1)+3H(1,4,1)] &\pmod{p^2},\\ 2H(2,1,2)&\equiv -p[4H(3,1,2)+H(2,2,2)] &\pmod{p^2},\\ 2H(1,5,1)&\equiv -p[2H(2,5,1)+5H(1,6,1)] &\pmod{p^2},\\ 2H(2,3,2)&\equiv -p[4H(3,3,2)+3H(2,4,2)] &\pmod{p^2},\\ 2H(3,1,3)&\equiv -p[6H(4,1,3)+H(3,2,3)] &\pmod{p^2}.\end{aligned}$$

By [27, Theorem 7.2] we know that

$$\begin{aligned}H(2,3,1)&\equiv S(2,3,1)\equiv 3S(4,1,1) &\pmod p,\\ H(1,4,1)&\equiv S(1,4,1)\equiv -2S(4,1,1) &\pmod p,\\ H(3,1,2)&\equiv S(3,1,2)\equiv -S(4,1,1)\equiv \tfrac{1}{6}B_{p-3}^2 &\pmod p\end{aligned}$$

which yield (3.34) and (3.35). Similarly, (3.36) follows from [27, Theorem 7.4] because

$$\begin{aligned}2S(2,5,1)&\equiv -2S(5,2,1)-2S(5,1,2) &\pmod p,\\ &\equiv 5S(6,1,1)-B_{p-5}B_{p-3} &\pmod p,\\ S(1,6,1)&\equiv -2S(6,1,1) &\pmod p.\end{aligned}$$

Also from [27, Theorem 7.4]

$$\begin{aligned} S(3,3,2) &\equiv 4b_8(p) && \pmod p, \\ S(2,4,2) &\equiv -2S(4,2,2) \equiv -2S(3,3,2) && \pmod p, \\ S(3,2,3) &\equiv -2S(3,3,2) && \pmod p, \\ S(4,1,3) &\equiv b_8(p) && \pmod p. \end{aligned}$$

These lead to the last two congruence of the proposition immmediately. □

By similar argument we can compute $H(r,s,r;p-1) \pmod{p^2}$ for odd s if we know the values $S(\mathbf{s};p-1) \pmod p$ for all $\mathbf{s}$ of length three and weight $2r+s+1$. When we apply a similar argument to $\mathbf{s}=(1,3,1,3)$ we find

Proposition 3.11. *For all primes $p>8$ the following three congruences are equivalent*:

$$H(1,3,1,3;p-1) \equiv -\frac{31}{72}pB_{p-9} \pmod{p^2}, \tag{3.40}$$

$$H(3,1,3,1;p-1) \equiv -\frac{1}{72}pB_{p-9} \pmod{p^2}, \tag{3.41}$$

$$S(6,1,1,1;p-1) \equiv -\frac{1}{54}B_{p-3}^3 - \frac{1889}{648}B_{p-9} \pmod{p}. \tag{3.42}$$

Proof. (i) ⇔ (ii). To save space we write H_{1313} for $H(1,3,1,3;p-1)$ and similarly for other sums. By (2.11) we have

$$-S_{1331} = H_{1331} - H_1H_{331} - H_{13}H_{31} - H_{133}H_1 + \cdots \equiv H_{1331} \pmod{p^2}. \tag{3.43}$$

By (2.10) we get

$$S_{1331} = H_{1331} + H_{431} + H_{134} + H_{161} + H_{44} + H_1H_7. \tag{3.44}$$

Now by the shuffle relations we see that

$$H_3H_{131} = H_{3131} + H_{1313} + 2H_{1331} + H_{431} + H_{134} + H_{161} \equiv 0 \pmod{p^2}. \tag{3.45}$$

Adding (3.43), (3.44) and (3.45) we find that

$$H_{3131} + H_{1313} \equiv H_{44} \equiv -\frac{4}{9}pB_{p-9} \pmod{p^2}. \tag{3.46}$$

(i) ⇔ (iii). When prime $p>9$ by Hoffman's computation we can express all harmonic sums $S(\mathbf{s};p-1)$ and $H(\mathbf{s};p-1)$ of weight 9 by linear combinations of B_{p-9}, B_{p-3}^3, and S_{6111}. By Maple computation (see [41]) we find that

$$H_{1313} \equiv -S_{3131} \equiv \frac{449p}{54}B_{p-9} + \frac{p}{18}B_{p-3}^3 + 3pS_{6111} \pmod{p^2}.$$ □

However, at present we cannot prove any of the congruences in Proposition 3.11.

Conjecture 3.12. *The three congruence* (3.40) *to* (3.42) *are always true for all primes $p>8$.*

We have verified the congruences in (3.40) to (3.42) for all primes p such that $10 < p < 2000$.

3.6. *Some congruences of Bernoulli numbers*

From Corollary 3.6 we see that for every prime $p \geq 7$ we have

$$\sum_{a=0}^{p-3} B_a B_{p-3-a} \equiv \sum_{a=0}^{p-3} a B_a B_{p-3-a} \equiv 0 \pmod{p}.$$

Can we generalize this? The answer turns out to be affirmative.

Proposition 3.13. *For every prime $p \geq 9$ we have*

$$\sum_{a=0}^{p-5} B_a B_{p-5-a} \equiv -\frac{2}{3} B_{p-3}^2 \pmod{p}.$$

Proof. By (3.13) we have for any even number n

$$H(1, n, 1; p-1) \equiv \sum_{a=0}^{p-n-1} (-1)^a B_a B_{p-n-1-a} + \sum_{a=p-n}^{p-2} (-1)^a B_a B_{2p-n-2-a}. \tag{3.47}$$

Taking $n = 4$ and comparing with [27, Theorem 7.2] we get

$$\sum_{a=0}^{p-5} B_a B_{p-5-a} + B_{p-3}^2 \equiv H(1, 4, 1) \equiv S(1, 4, 1) \equiv \frac{1}{3} B_{p-3}^2 \pmod{p}.$$

This proves the proposition. □

The following result is straightforward.

Proposition 3.14. *For all positive number n and prime $p > n + 3$ we have*

$$\begin{aligned} H(1, 1, 1, n; p-1) &\equiv -(-1)^n H(n, 1, 1, 1; p-1) \equiv (-1)^n S(1, 1, 1, n; p-1) \\ &\equiv -S(n, 1, 1, 1; p-1) \equiv \sum_{a=0}^{p-2} \sum_{b=0}^{p-n-1} (-1)^{b+n} \binom{a+b}{b} \binom{a+b+n}{n} \\ &\quad \times \frac{B_a B_b B_{p-n-1-a-b}}{(a+1)(a+b+1)} \pmod{p}. \end{aligned}$$

3.7. *Multiple harmonic sums of arbitrary length*

To prove the main result in this section let us recall the Bernoulli polynomial $B_m(x)$ which is defined by the following generating function

$$\frac{te^{xt}}{e^t - 1} = \sum_{m=0}^{\infty} B_m(x) \frac{t^m}{m!}.$$

These polynomials satisfy (see [28, p. 248]):

$$B_m(x) = \sum_{k=0}^{m} \binom{m}{k} B_k x^{m-k} \tag{3.48}$$

$$B'_m(x) = mB_{m-1}(x) \quad \forall m \geq 1. \tag{3.49}$$

Lemma 3.15. *For any even integer $n \geq 0$ and prime $p \geq 3n+7$ we have*

$$\sum_{a,b\geq 0,\, a+b=p-3n-3} \frac{B_b}{p-b}\binom{p-b}{n+1}\frac{B_a}{p-a}\binom{p-a}{n+2} \equiv 0 \pmod p, \tag{3.50}$$

$$\sum_{a,b\geq 0,\, a+b=p-3n-3} \frac{B_b}{p-b}\binom{p-b}{n+1}\frac{B_a}{p-a}\binom{p-a}{n+1} \equiv 0 \pmod p. \tag{3.51}$$

Proof. Throughout the proof all congruences are modulo p. First we set

$$A = \sum_{a,b\geq 0,\, a+b=p-3n-3} \frac{B_b}{p-b}\binom{p-b}{n+1}\frac{B_a}{p-a}\binom{p-a}{n+2},$$

$$B = \sum_{a,b\geq 0,\, a+b=p-3n-3} \frac{B_b}{p-b}\binom{p-b}{n+1}\frac{B_a}{p-a}\binom{p-a}{n+1}.$$

We have

$$A \equiv -\sum_{a,b\geq 0,\, a+b=p-3n-3} \frac{n+1+a}{n+2}\cdot\frac{B_b}{p-b}\binom{p-b}{n+1}\frac{B_a}{p-a}\binom{p-a}{n+1}. \tag{3.52}$$

Now exchange the index a and b in A we get

$$\begin{aligned} A &= \sum_{a,b\geq 0,\, a+b=p-3n-3} \frac{B_b}{p-b}\binom{p-b}{n+2}\frac{B_a}{p-a}\binom{p-a}{n+1} \\ &\equiv \sum_{a,b\geq 0,\, a+b=p-3n-3} \frac{2n+2+a}{n+2}\cdot\frac{B_b}{p-b}\binom{p-b}{n+1}\frac{B_a}{p-a}\binom{p-a}{n+1}. \end{aligned} \tag{3.53}$$

Adding (3.52) to (3.53) we find

$$2A \equiv \sum_{a,b\geq 0,\, a+b=p-3n-3} \frac{n+1}{n+2}\cdot\frac{B_b}{p-b}\binom{p-b}{n+1}\frac{B_a}{p-a}\binom{p-a}{n+1} \equiv \frac{n+1}{n+2}B. \tag{3.54}$$

Now for any non negative integer m and b such that $b+m+1<p$ we have

$$\frac{(-1)^m}{p-b}\binom{p-b}{m+1} \equiv (-1)^b m\binom{p-m-1}{b}. \tag{3.55}$$

We get

$$B \equiv n^2 \sum_{a,b\geq 0,\, a+b=p-3n-3} B_b\binom{p-n-1}{b}B_a\binom{p-n-1}{a} \tag{3.56}$$

because all the terms with odd index a are zero. Let us denote by Coeff$[i, f(x)]$ the coefficient of x^i in the polynomial $f(x)$. Then (3.56) means that

$$\begin{aligned} B &\equiv n^2\text{Coeff}[p+n+1, B^2_{p-n-1}(x)] \\ &\equiv \frac{n^2}{p+n+1}\text{Coeff}[p+n, (B^2_{p-n-1}(x))'] \\ &\equiv \frac{n^2}{n+1}\text{Coeff}[p+n, 2(p-n-1)B_{p-n-1}(x)B_{p-n-2}(x)] \end{aligned}$$

by (3.49). From (3.48) this yields

$$\begin{aligned} B &\equiv -2n^2 \sum_{a,b\geq 0,\, a+b=p-3n-3} B_b\binom{p-n-1}{b}B_a\binom{p-n-2}{a} \\ &\equiv \frac{2n}{n+1}\sum_{a,b\geq 0,\, a+b=p-3n-3} \frac{B_b}{p-b}\binom{p-b}{n+1}\frac{B_a}{p-a}\binom{p-a}{n+2} \end{aligned}$$

by (3.55). Therefore

$$B \equiv \frac{2n}{n+1}A. \tag{3.57}$$

Now the lemma follows easily by (3.54) and (3.57). □

Theorem 3.16. *Let p be a prime and $\mathbf{s} \in \mathbb{N}^l$. Assume $p > |\mathbf{s}| + 2$. Then*

$$H(\mathbf{s}; p-1) \equiv 0 \pmod p$$

if $\mathbf{s}$ *has the following forms:*

(a) $\mathbf{s} = \big(\{1\}^m, 2, \{1\}^n\big)$ *for* $m, n \geq 0$ *and* $m+n$ *is even.*
(b) $\mathbf{s} = (\{1\}^n, 2, \{1\}^{n-1}, 2, \{1\}^{n+1})$ *where* $n \geq 2$ *is even.*
(c) $\mathbf{s} = (\{1\}^{n+1}, 2, \{1\}^{n-1}, 2, \{1\}^n)$ *where* $n \geq 2$ *is even.*
(d) $\mathbf{s} = (\{1\}^n, 2, \{1\}^n, 2, \{1\}^n)$ *where* $n \geq 0$.

Furthermore, in the first and last cases we also have $S(\mathbf{s}; p-1) \equiv 0 \pmod p$. *Moreover, when* $m+n$ *is even we have*

$$\begin{aligned} H(\{1\}^{m-1}, 2, \{1\}^{n-1}; p-1) &\equiv S(\{1\}^{n-1}, 2, \{1\}^{m-1}; p-1) \\ &\equiv \left\{(-1)^n\left[n\binom{m+n+1}{m} - m\binom{m+n+1}{n}\right]\right. \\ &\quad \left. + \binom{m+n+1}{n} + 1\right\}\frac{pB_{p-m-n-1}}{m+n+1} \pmod{p^2}. \end{aligned} \tag{3.58}$$

Proof. We omit $p-1$ in $S(-; p-1)$ and $H(-; p-1)$.

(a) Let $\mathbf{s} = (n, m)$ then we have $\mathbf{s}^* = (\{1\}^{n-1}, 2, \{1\}^{m-1})$. Note that $w := |\mathbf{s}| = |\mathbf{s}^*| = m+n$, $l(\mathbf{s}^*) = m+n-1$, and $l(\mathbf{s}) = 2$. By our refined version (2.13) of [26, Theorem 6.7]

$$-S(\mathbf{s}^*) \equiv S(\mathbf{s}) + p(H(n,m,1) + H(m+n,1)) \tag{3.59}$$

$$\equiv \left\{(-1)^n\left[m\binom{w+1}{n} - n\binom{w+1}{m}\right] - \binom{w+1}{n} - 1\right\}\frac{pB_{p-w-1}}{w+1} \pmod{p^2}, \tag{3.60}$$

by Theorems 3.2, 3.1 and 3.5. Applying (2.11) to $\mathbf{s}^*$ we get

$$-(-1)^w S(\mathbf{s}^*) = \sum_{\bigsqcup_{j=1}^{l} \mathbf{s}_j = \overline{\mathbf{s}^*}} (-1)^l \prod_{j=1}^{l} H(\mathbf{s}_j). \tag{3.61}$$

If w is even then for each $l > 1$ either one of $\mathbf{s}_j = \{1\}^d$ with odd d, or else all $\mathbf{s}_j = \{1\}^{d_j}$ for even d_j except one term $\mathbf{s}_j = (\{1\}^{m'}, 2, \{1\}^{n'})$ where $m' + n' < m + n - 2$ is even. By induction on the length of $\mathbf{s}^*$ (note that $H(2) \equiv 0 \pmod p$) we get

$$S(\mathbf{s}^*) \equiv H(\overline{\mathbf{s}^*}) \pmod{p^2}.$$

With (3.60) this proves case (a).

For future reference we prove some congruences for arbitrary m and n in this case. Since $|\mathbf{s}| - l(\mathbf{s}) = w - 2$ we have by (2.11)

$$\begin{aligned}(-1)^w S(\mathbf{s}) &= (-1)^{|\mathbf{s}|-l(\mathbf{s})} S(\mathbf{s}) \\ &= -H(\mathbf{s}) + H(m+1)\cdot H(n+1) \equiv -H(\mathbf{s}) \pmod p \end{aligned} \tag{3.62}$$

by Theorem 1.3. Now if $l \geq 2$ then in (3.61) one of $\mathbf{s}_j = \{1\}^d$ for some positive d so that $H(\mathbf{s}_j) \equiv 0 \pmod p$. Thus

$$(-1)^w S(\mathbf{s}^*) \equiv H(\overline{\mathbf{s}^*}) \equiv (-1)^w H(\mathbf{s}^*) \pmod p. \tag{3.63}$$

Combining this with (2.8) and (3.62) we see that whether w is even or odd it is always true that

$$H(\mathbf{s}) \equiv (-1)^w H(\mathbf{s}^*) \pmod p. \tag{3.64}$$

In the rest of the proof we assume all congruences are modulo p.

(b) Let $\mathbf{s} = (\{1\}^n, 2, \{1\}^{n-1}, 2, \{1\}^{n+1})$ where $n \geq 2$ is even. Then $\mathbf{s}^* = (n+1, n+1, n+2)$. So $|\mathbf{s}| = |\mathbf{s}^*| = 3n+4$, $l(\mathbf{s}) = 3n+2$, and $l(\mathbf{s}^*) = 3$. Since n is even we have by applying (2.11) to $\mathbf{s}^*$

$$S(\mathbf{s}^*) \equiv H(\mathbf{s}^*) - H(2n+2, n+2) - H(n+1, 2n+3) + H(3n+4) \equiv H(\mathbf{s}^*) \tag{3.65}$$

by Theorems 3.2 and 1.3. Applying (2.11) to $\mathbf{s}$ and using the fact that $H(\{1\}^d) \equiv 0$ for any d we have

$$\begin{aligned} S(\mathbf{s}) \equiv (-1)^{|\mathbf{s}|-l(\mathbf{s})} S(\mathbf{s}) &\equiv -H(\mathbf{s}) + \sum_{a=0}^{n-1} H(\{1\}^n, 2, \{1\}^a)\cdot H(\{1\}^{n-1-a}, 2, \{1\}^{n+1}) \\ &\equiv -H(\mathbf{s}) + \sum_{a=0}^{n-1} H(n+1, a+1)\cdot H(n-a, n+2) \end{aligned}$$

by (3.64). Hence by (2.8) and (3.65)

$$H(\mathbf{s}) \equiv H(n+1,n+1,n+2) + \sum_{a=0}^{n-1} H(n+1,a+1)\cdot H(n-a,n+2). \tag{3.66}$$

We know that for all $j,k<p$ we have

$$\sum_{a=0}^{p-2}(k/j)^a \equiv \begin{cases} 0 & \pmod p \quad \text{if } j\neq k,\\ -1 & \pmod p \quad \text{if } j=k. \end{cases}$$

It follows that

$$\begin{aligned}\sum_{a=0}^{p-2} H(n+1,a+1)\cdot H(n-a,n+2) &= \sum_{a=0}^{p-2}\sum_{1\le i<j<p}\sum_{1\le k<l<p}\frac{1}{i^{n+1}j^{a+1}}\frac{1}{k^{n-a}l^{n+2}}\\ &\equiv -\sum_{1\le i<j=k<l<p}\frac{1}{i^{n+1}j^{n+1}l^{n+2}}\\ &= -H(n+1,n+1,n+2).\end{aligned}$$

Together with (3.66) we see that

$$\begin{aligned}H(\mathbf{s}) &\equiv -\sum_{a=n}^{p-2} H(n+1,a+1)\cdot H(n-a,n+2)\\ &\equiv -\sum_{a=2n+1}^{p-n-2}\frac{(-1)^a B_{p-n-2-a}}{n+2+a}\binom{n+2+a}{n+1}\frac{B_{a-2n-1}}{p+2n+1-a}\binom{p+2n+1-a}{n+2}\end{aligned}$$

by Theorem 3.1. Under substitution $a\to 2n+1+a$ we get:

$$H(\mathbf{s}) \equiv \sum_{a=0}^{p+1-w}(-1)^a\binom{w-1+a}{n+1}\frac{B_{p+1-w-a}}{w-1+a}\binom{p-a}{n+2}\frac{B_a}{p-a} \equiv 0 \pmod p \tag{3.67}$$

by (3.50). This combined with (3.65) completes the proof of case (b).

(c) It follows from (b) by taking $\bar{\mathbf{s}}$.

(d) When $n=0$ or n is odd this follows from Theorem 2.13 and Lemma 3.3, respectively. When $n\geq 2$ is even the proof is almost the same as that of case (b) except at the end one need resort to (3.51). The congruence for S follows from the fact that $(\{1\}^n,2,\{1\}^n,2,\{1\}^n)^* = (n+1,n+2,n+1)$ and therefore

$$-S(\mathbf{s}) \equiv S(\mathbf{s}^*) = H(\mathbf{s}^*) + H(n+2)H(2n+3) \equiv 0$$

by (2.8), (2.10) and the shuffle relations. □

Remark 3.17. Note that in cases (b) and (c) we usually have $S(\mathbf{s})\not\equiv 0 \pmod p$. For example, in case (b) we have $S(\mathbf{s}) \equiv -S(\mathbf{s}^*) \equiv -H(\mathbf{s}^*) \equiv H(n+1,n+1,n+2) \pmod p$ by (3.65). We know that $H(3,3,4;12)\equiv 8 \pmod{13}$, $H(5,5,6;18)\equiv 15 \pmod{19}$ and $H(7,7,8;28)\equiv 26 \pmod{29}$.

Theorem 3.18. *Let* $\mathbf{s} = \{r,s\}^n$ *for some* $r,s \geq 1$ *and* $p \geq |\mathbf{s}|+2$ *be a prime. Then*

$$H(\mathbf{s};p-1) \equiv S(\mathbf{s};p-1) \equiv 0 \pmod p$$

provided n, r *and* s *satisfy either of the following two conditions*:

(i) $n = 1,2$, *both* r *and* s *are even*, *or*
(ii) n *is any positive integer*, *both* r *and* s *are odd.*

Remark 3.19. When $n = 1$ this is Theorem 3.1. When $n = 2$, this has been confirmed by Hoffman (see the remarks after [27, Theorem 6.3]).

Proof. By the above remark we may assume r and s are odd and proceed by induction on n. In the following we will drop $p-1$ again. By the shuffle relations and equation (2.10) it is straightforward to verify that

$$\begin{aligned} S(\{r,s\}^n) &= \sum_{\mathbf{t}\preceq\{r,s\}^n} H(\mathbf{t}) \\ &= H(\{r,s\}^n) + H(r+s)\cdot \sum_{\mathbf{t}\preceq\{r,s\}^{n-1}} H(\mathbf{t}) \\ &= H(\{r,s\}^n) + H(r+s)\cdot S(\{r,s\}^{n-1}) \equiv H(\{r,s\}^n) \pmod p \qquad (3.68) \end{aligned}$$

by Theorem 1.3. On the other hand, from (2.11) we find that

$$S(\{r,s\}^n) \equiv \sum_{\bigsqcup_{i=1}^l \mathbf{s}_i=\{r,s\}^n} (-1)^l H(\mathbf{s}_1)\cdots H(\mathbf{s}_l) \pmod p.$$

Now if $l>1$ then either $\mathbf{s}_1 = \{r,s\}^d$ for some $d<n$ in which case $H(\mathbf{s}_1)\equiv 0 \pmod p$ by induction assumption, or else $\mathbf{s}_1 = \{r,s\}^d \sqcup \{r\}$, in which case $\mathbf{s}_1$ is a palindrome of odd weight and hence $H(\mathbf{s}_1)\equiv 0 \pmod p$ by Corollary 3.4. Consequently

$$S(\{r,s\}^n) \equiv -H(\{r,s\}^n) \pmod p.$$

Together with (3.68) it shows that $H(\{r,s\}^n) \equiv S(\mathbf{s};p-1) \equiv 0 \pmod p$ and the theorem is proved. □

When both r and s are even but $n>2$ the theorem does not hold in general. For examples,

$$H(\{2,4\}^3;22) \equiv 21 \pmod{23}, \quad H(\{2,4\}^4;28) \equiv 20 \pmod{29}.$$

3.8. *Some conjectures in the general cases*

When the length $l \geq 4$ numerical evidence up to length 40 shows the following conjecture is true.

Conjecture 3.20. *Let* $\mathbf{s}\in\mathbb{N}^l$ *and* $p \geq |\mathbf{s}|$ *be a prime. Then*

$$H(\mathbf{s};p-1) \equiv 0 \pmod p$$

if **s** *has one of the following forms*:

(1) $\mathbf{s} = (\{\{1\}^m, 2, \{1\}^n, 2\}^q, \{1\}^m, 2, \{1\}^n)$ *for* $q, m, n \geq 0$, *where either* (i) q *is odd, or* (ii) q *is even and* $m + n$ *is even.*
(2) $\mathbf{s} = (\{2\}^m, \{3, \{2\}^m\}^n)$ *for* $m, n \geq 0$.
(3) $\mathbf{s} = (1, \{2\}^m, \{1, \{2\}^{m+1}\}^n, 1, \{2\}^m, 1)$ *for* $m, n \geq 0$ *and* n *is even.*

Note that the congruences in Conjecture 3.20 usually are not satisfied by the S-version of MHS. We conclude our paper by

Problem 3.21. Are there any other **s** satisfying Wolstenholme type theorem besides those listed in the paper? More generally, is there a formula similar to Theorem 3.5 for arbitrary **s**?

Appendix A. Distribution of Irregular Primes

Table 1 in the paper and the following Table 2 give us some evidence to Conjecture 2.16.

In Table 2 we count the first 30,000 irregular primes with irregular index $i_p = 1$, first 15,000 irregular primes with index 2 (producing 30,000 irregular pairs), and all the irregular primes $< 12,000,000$ with index 3 (producing $3 \times 9824 = 29472$ irregular pairs). We denote by $N(k, m)$ the number of irregular pairs (p, t) satisfying

Table 2. Distribution of $p - t \pmod 3$ for irregular pairs (p, t) with $i_p = 1, 2, 3$.

$m(i_p = 1)$	$N_1(0, m)$	$P_1(0, m)$	$N_1(1, m)$	$P_1(1, m)$	$N_1(2, m)$	$P_1(2, m)$
3,000	979	32.63	1016	33.87	1005	33.50
6,000	1968	32.80	2026	33.77	2006	33.43
9,000	2954	32.82	3049	33.88	2997	33.30
12,000	4018	33.48	4042	33.68	3940	32.83
15,000	5001	33.34	5039	33.59	4960	33.07
18,000	5993	33.29	6075	33.75	5932	32.96
21,000	6972	33.20	7095	33.79	6933	33.01
24,000	7973	33.22	8118	33.82	7909	32.95
27,000	8968	33.22	9090	33.67	8942	33.12
30,000	9993	33.30	10055	33.52	9952	33.17
$m(i_p = 2)$	$N_2(0, m)$	$P_2(0, m)$	$N_2(1, m)$	$P_2(1, m)$	$N_2(2, m)$	$P_2(2, m)$
3,000	981	32.70	993	33.10	1026	34.20
6,000	2029	33.82	1977	32.95	1994	33.23
9,000	3033	33.70	3033	33.70	2934	32.60
12,000	4049	33.74	4005	33.38	3946	32.88
15,000	5013	33.42	5001	33.34	4986	33.24
18,000	6024	33.47	6012	33.40	5964	33.13
21,000	7064	33.64	6981	33.24	6955	33.12
24,000	8062	33.59	7962	33.18	7976	33.23
27,000	9085	33.65	8927	33.06	8988	33.29
30,000	10096	33.65	9910	33.03	9994	33.31

Table 2. (*Continued*)

$m(i_p = 3)$	$N_3(0, m)$	$P_3(0, m)$	$N_3(1, m)$	$P_3(1, m)$	$N_3(2, m)$	$P_3(2, m)$
3,000	997	33.23	1001	33.36	1002	33.40
6,000	2027	33.78	1994	33.23	1979	32.98
9,000	3065	34.05	2968	32.97	2967	32.96
12,000	4102	34.18	3955	32.96	3943	32.86
15,000	5124	34.16	4944	32.96	4932	32.88
18,000	6091	33.84	5956	33.09	5953	33.07
21,000	7087	33.74	6921	32.95	6992	33.29
24,000	8067	33.61	7943	33.09	7990	33.29
27,000	9046	33.50	8974	33.23	8980	33.26
29,472	9889	33.55	9812	33.29	9771	33.15

$p - t \equiv k \pmod 3$ in the top m irregular pairs, $0 \le k \le 2$, and by $P(k, m)$ the percentage of such pairs. We put a subscript i for irregular primes of index i.

Between 3 and 12 million there are only 1282 irregular primes with irregular index 4 (producing 5128 irregular pairs), and 127 irregular primes with irregular index 5 (producing 635 irregular pairs). We provide the data for them in Tables 3 and 4. There are 13 irregular primes $< 12,000,000$ with irregular index 6, producing 78 pairs. For them we have $N_6(0, 78) = 25$, $N_6(1, 78) = 27$, and $N_6(2, 78) = 26$. There are merely 4 irregular primes in the same range with irregular index 7, producing 28 pairs. For these pairs: $N_7(0, 28) = 10$, $N_7(1, 28) = 9$, and $N_7(2, 28) = 9$, which is the best we can hope.

Table 3. Distribution of $p - t \pmod 3$ for irregular pairs (p, t) with $i_p = 4$.

$m(i_p = 4)$	$N_4(0, m)$	$P_4(0, m)$	$N_4(1, m)$	$P_4(1, m)$	$N_4(2, m)$	$P_4(2, m)$
600	196	32.67	202	33.67	202	33.67
1,200	388	32.33	390	32.50	422	35.17
1,800	569	31.61	615	34.17	616	34.22
2,400	769	32.04	818	34.08	813	33.88
3,000	948	31.60	1032	34.40	1020	34.00
3,600	1161	32.25	1217	33.81	1222	33.94
4,200	1341	31.93	1428	34.00	1431	34.07
4,800	1537	32.02	1624	33.83	1639	34.15
5,128	1645	32.05	1734	33.79	1749	34.08

Table 4. Distribution of $p - t \pmod 3$ for irregular pairs (p, t) with $i_p = 5$.

$m(i_p = 5)$	$N_5(0, m)$	$P_5(0, m)$	$N_5(1, m)$	$P_5(1, m)$	$N_5(2, m)$	$P_5(2, m)$
100	31	31.00	33	33.00	36	36.00
200	71	35.50	58	29.00	71	35.50
300	111	37.00	87	29.00	102	34.00
400	145	36.25	115	28.75	140	35.00
500	179	35.80	154	30.80	167	33.40
600	218	36.33	190	31.67	192	32.00
635	230	35.94	200	31.25	205	32.03

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