Multiple Harmonic Sums I:
Generalizations of Wolstenholme’s Theorem*

Jianqiang Zhao†

Department of Mathematics, Eckerd College, St. Petersburg, Florida 33711, USA

Abstract. In this note we will study the \( p \)-divisibility of multiple harmonic sums. 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, multiple zeta values, Bernoulli numbers, irregular primes

1 Introduction

The Euler-Zagier multiple zeta functions of length \( l \) are nested generalizations of Riemann zeta function. They are defined as

\[
\zeta(s) = \zeta(s_1, \ldots, s_l) = \sum_{0 < k_1 < \cdots < k_l} k_1^{-s_1} \cdots k_l^{-s_l}
\]

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

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

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 and studied by theoretical physicists (see [4] 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 \( s := (s_1, \ldots, s_l) \in \mathbb{N}^l \) and denote the \( n \)th partial sum of MZV series by

\[
H(s; n) = H(s_1, \ldots, s_l; n) := \sum_{1 \leq k_1 < \cdots < k_l \leq n} k_1^{-s_1} \cdots k_l^{-s_l}, \quad n \in \mathbb{Z}_{\geq 0}.
\]
By convention we set \( H(s;r) = 0 \) for \( r = 0, \ldots, l - 1 \), and \( H(0;0) = 1 \). To facilitate our study we also define (cf. \cite{25, 26})

\[
S(s_1, \ldots, s_l; n) := \sum_{1 \leq k_1 \leq \cdots \leq k_l \leq n} k_1^{−s_1} \cdots k_l^{−s_l}, \quad n \in \mathbb{Z}_{\geq 0}.
\] (3)

To save space, for an ordered set \( \{e_1, \ldots, e_l\} \) we denote by \( \{e_1, \ldots, e_l\}^d \) the set formed by repeating \( \{e_1, \ldots, e_l\} \) \( d \) times and \( 1^d = \{1\}^d \). For example \( H(\{s\}^1; n) \) is just a partial sum of the nested zeta value series \( \zeta(s) \) of length \( l \) which we refer to as a homogenous 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’s also easy to see that

\[
St(n, j) = (n-1)! \cdot H(1^{j-1}; n-1), \quad \text{for} \ j = 1, \ldots, n.
\] (4)

Now we restrict \( n \) to prime numbers.

**Theorem 1.1.** (Wolstenholme 1862 \cite[p.89]{21}) For any prime number \( p \geq 5 \), \( St(p, 2) \equiv 0 \pmod{p^2} \).

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

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

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

This of course implies that \( p|St(p, l) \) for \( 1 < l < p \) which was known to Lagrange \cite[p.87]{21].

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 \cite{29, 33, 35, 39, 40}). The reason, Gardiner told us in \cite{13}, is that these two primes are the only primes \( p \) in this range such that \( p \) divides the numerator of \( B_{p-3} \). Bruck \cite[although there is no proof is given there. Denote by \( p(m) \) the parity of \( m \) which is \( 1 \) if \( m \) is odd and \( 2 \) if \( m \) is even.

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

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

In \cite{32} Slavutskii showed

**Theorem 1.4.** (\cite[Thm. 2]{32}) Let \( s \) and \( m \) be two positive integers such that \( (m, 6) = 1 \). Let \( t = (\phi(m) - 1)s \) and \( A_n(m) = \prod_{p|m}(1 - p^{-1})B_n \) be the Agoh’s function, where \( \phi(m) \) is the Euler’s Phi function. Then

\[
H^*(s; m-1) = \sum_{1 \leq k < m \atop (k, p) = 1} \frac{1}{k^s} \equiv \begin{cases} mA_s(m) & \text{mod } m^2 \\ (t/2)m^2A_{s-1}(m) & \text{mod } m^2 \end{cases} \quad \text{if } s \text{ is even,} \\
\end{cases}
\]

\[
H^*(s; m-1) = \sum_{1 \leq k < m \atop (k, p) = 1} \frac{1}{k^s} \equiv \begin{cases} mA_s(m) & \text{mod } m^2 \\ (t/2)m^2A_{s-1}(m) & \text{mod } m^2 \end{cases} \quad \text{if } s \text{ is odd.}
\]
1.2 Homogeneous multiple harmonic sums

The classical result of Wolstenholme is the original motivation of our study. We will prove the following generalization of Thm. 3.1 and Thm. 1.2 to homogeneous multiple harmonic sums (see Thm. 2.14).

**Theorem 1.6.** 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 $kls + 1$ for $k = 1, \ldots, l$. Then

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

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

We also look at some cases when the congruences hold modulo higher powers of $p$. Recently, Zhou and Cai [39] prove that

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

$$H(\{s\}^l; p - 1) \equiv S(\{s\}^l; p - 1) \equiv \begin{cases} \frac{(-1)^ls(is + 1)p^2}{2(is + 2)} B_{p-ls-2} \pmod{p^3} \text{ if } 2 \mid l, \\ \frac{(-1)^l1}{ls + 1} B_{p-ls-1} \pmod{p^2} \text{ if } 2 \mid l. \end{cases}$$

We will prove an analog of this in the non-homogeneous even weight length two case (see Thm. 2.14).

1.3 Non-homogeneous multiple harmonic sums

The third section of this paper deals with non-homogeneous multiple harmonic sums. We consider the length 2 case in Thm. 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 $0 \leq m, n \leq p - 2$. If $m, n \geq 1$ then

$$H(s_1, s_2; p - 1) \equiv \begin{cases} \frac{(-1)^n}{m + n} \binom{m + n}{m} B_{p-m-n} \pmod{p} \text{ if } p \geq m + n, \\ 0 \pmod{p} \text{ if } p < m + n. \end{cases}$$

The same idea but more complicated computation enables us to deal with the length 3 odd weight case completely (see Thm. 3.4).

**Theorem 1.8.** 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 $s_1 \equiv l, s_2 \equiv m, s_3 \equiv n \pmod{p - 1}$. If $l, m, n \geq 1$ and $w = l + m + n$ is an odd number then

$$H(l, m, n; p - 1) \equiv I(l, m, n) - I(n, m, l) \pmod{p}$$

where $I$ is defined as follows. Let $w' = w - (p - 1)$ if $p < w < 2p$ and $w' = w$ otherwise. Then

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

However, it seems to be extremely difficult to adopt the same machinery for general larger length cases. For the even weight cases in length 3, 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 multiple harmonic sums 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, M. Hoffman studies the same kind of questions independently in [25] from a different viewpoint. We strongly encourage the interested reader to compare his results to ours. For example, Hoffman defines the convolution operation on composite of indices (see [25] §6). We can apply this to a few of the above results to find more Wolstenholme’s type congruence in section 3.7.
Theorem 1.9. Let \( p \) be a prime and \( s \in \mathbb{N}^+ \). Assume \( p > |s| + 2 \). Then

\[
H(s; p - 1) \equiv S(s; p - 1) \equiv 0 \pmod{p}
\]

provided \( s \) has one of the following forms:

1. \( s = (1^m, 2, 1^n) \) for \( m, n \geq 0 \) and \( m + n \) is even.
2. \( s = (1^n, 2, 1^{n-1}, 2, 1^{n+1}) \) where \( n \geq 2 \) is even.
3. \( s = (1^{n+1}, 2, 1^{n-1}, 2, 1^n) \) where \( n \geq 2 \) is even.
4. \( s = (1^n, 2, 1^n, 2, 1^n) \) where \( n \geq 0 \).

In [38] we will look at the mod \( p \) structure of the multiple harmonic sums for lower weights.

One can also investigate the multiple harmonic sum \( H(s; n) \) with fixed \( s \) but varying \( n \). We will carry this out in the second part of this series [36]. Such a study for harmonic series was initiated systematically by Eswarathasan and Levine [17] 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 [14]. Without attempting to be complete, we only list some of the modern references at the end. In particular, I learned a lot from the work by Buhler, Crandall, Ernvall, Johnson, Metsänkylä, Sompośki, Shokrollahi, Levine [17], Gardiner [18] on the nice and surprising relations between partial sums of harmonic series and irregular primes. For earlier history, one can consult [35] and its references. Often in my computation I use the table for irregular primes less than 12 million available online at ftp://ftp.reed.edu/users/jpb maintained by Buhler. My interest on multiple harmonic sums was aroused by the work of Boyd [7], Eswarathasan and Levine [17], and Gardiner [18] on the nice and surprising relations between partial sums of harmonic series and irregular primes. I’m indebted to all of them for their efforts on improving our knowledge of this beautiful part of number theory.

2 Generalizations of Wolstenholme’s Theorem

It’s 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’s a little surprising (at least for me) 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 Clausen-von Staudt Theorem on Bernoulli numbers (see, for example, [27] p. 233, Thm. 3):

Lemma 2.1. For \( m \in \mathbb{N} \), \( B_{2m} + \sum_{p\mid 2m} 1/p \) is an integer.

We begin with a special case of our generalization which only deals with zeta-value series, i.e., MZV series of length 1. The general case will be built upon this.

Lemma 2.2. Let \( p \) be an odd prime and \( s \) be a positive integer. Then

\[
H(s; p - 1) \equiv \begin{cases} 
0 & \text{mod } p^{s+1} \text{ if } p - 1 \nmid s, s + 1, \\
-1 & \text{mod } p \text{ if } p - 1 \mid s, \\
-p(n + 1)/2 & \text{mod } p^2 \text{ if } s + 1 = n(p - 1).
\end{cases}
\]

Remarks 2.3. (1) The conditions in Bayat’s generalization of Wolstenholme’s Theorem [4] Thm. 3] should be corrected. For example, taking \( k = 2 \) and \( p = 5 \) in [4] Thm. 3(i)] we only get \( H(3; 4) = 2035/1728 \neq 0 \pmod{5^2} \). In general, if \( 2k = p - 1 \) in [4] Thm. 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 Thm. [14] However, we need a more direct proof which we will reference later.
Proof. If \( p - 1 | s \) then \( H(s; p - 1) \equiv p - 1 \equiv -1 \) (mod \( p \)) by Fermat’s Little Theorem. So we assume \( p - 1 \nmid s \). This implies that the map \( a \to a^{s-1} \) is nontrivial on \((\mathbb{Z}/p\mathbb{Z})^\times\), say \( b^s \neq 1 \) (mod \( p \)) for some \( 1 < b < p \). Then it’s not hard to see that \( (1 - b^{-s})H(s; p - 1) \equiv 0 \) (mod \( p \)) and therefore \( H(s; p - 1) \equiv 0 \) (mod \( p \)). 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 later 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

\[
H(s; p - 1) = \sum_{k=1}^{p-1} \frac{1}{k^s} = \sum_{k=1}^{p-1} \frac{knp(p-1)}{k^s} = \sum_{k=1}^{p-1} k^t. \quad \text{(mod } p^2\text{)}
\]

By a classical result of sums of powers (see [27, p. 229]) we know that

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

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

\[
\sum_{k=1}^{p-1} k^t \equiv pB_t + \frac{t}{2} p^2 B_{t-1} \quad \text{(mod } p^2\text{)}. \quad \text{(6)}
\]

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 \( t = np(p - 1) - m(p - 1) + 1 \) is odd. So \( B_t = 0, p - 1 | t - 1 \) and \( pB_{t-1} \equiv -1 \) (mod \( p \)) by Lemma 2.1 again. From congruence (6) we get

\[
H(s; p - 1) \equiv -pt/2 \equiv -p(n + 1)/2 \quad \text{(mod } p^2\text{)}.
\]

In fact, there’s a shorter proof for the odd case which is not as transparent as the above proof. By binomial expansion we see that

\[
2 \sum_{k=1}^{p-1} \frac{1}{k^s} = \sum_{k=1}^{p-1} \left( \frac{1}{k^s} + \frac{1}{(p-k)^s} \right) \equiv \sum_{k=1}^{p-1} \frac{spk^{s-1}}{k^s(p-k)^s} \quad \text{(mod } p^2\text{)}.
\]

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

\[
2 \sum_{k=1}^{p-1} \frac{1}{k^s} \equiv \sum_{k=1}^{p-1} \frac{-sp}{k^s+1} \equiv 0 \quad \text{(mod } p^2\text{)}
\]

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

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 \( p^e \) is a regular prime then

\[
v_p(H(s; p - 1)) = \begin{cases} 
0 & \text{if } p - 1 | s, \\
\frac{v+1}{u+1} & \text{if } s \text{ is even and } p - 1 \nmid s, \\
\frac{u+2}{u+v+1} & \text{if } s \text{ is odd and } p - 1 | s + 1.
\end{cases}
\]
Suppose $p$ is irregular and let $1 \leq m < p(p-1)$ such that

\[
m \equiv \begin{cases} 
-s & \text{(mod } p(p-1)\text{) if } s \text{ is even}, \\
-s-1 & \text{(mod } p(p-1)\text{) if } s \text{ is odd}.
\end{cases}
\]

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.

\textbf{Proof.} We only consider the case when $p-1 \nmid s$. Suppose $s = p^u a$ and $p \nmid a$. Let $e \geq v+2$ be any positive integer such that $t \equiv p^e(p-1)-s > 1$. 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

\[
H(s; p-1) \equiv pB_1 + \frac{t(t-1)}{6}p^3B_{t-2} \pmod{p^{v+3}}
\]

\[
\equiv -ap^{v+1}B_{t'} + \frac{(t-1)(t-2)}{6t''}p^{v+3}B_{t''} \pmod{p^{v+3}}
\]

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 or not. The smallest $v_p$-valuation of the second term is $v+2$ which happens if and only if $p \nmid t''$. 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.

\textbf{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.

\textbf{Remark 2.6.} Numerical evidence shows that if $p$ is irregular then the nonzero valuations seems 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 $37^2|B_{p(p-1)-s} = B_{284}$.

\textbf{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 preceding proposition. Then $H(s; p-1) \not\equiv 0 \pmod{p^s}$.

\textbf{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 $s = p^u a$ where $p \nmid a$. If $p$ is regular then by Prop. 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 Prop. 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 $p \geq 37$. \hfill \Box

\subsection*{2.2 $p$-divisibility, Bernoulli numbers, and irregular primes}

Numerical evidence shows that congruences in Lemma 2.2 is not always optimal. For any zeta value series, 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:

$$\frac{-2}{2n-1} \cdot H(2n-1; p-1) \equiv p \cdot H(2n;p-1) \equiv p^2 \cdot \frac{2n}{2n+1} \cdot B_{p-2n-1} \pmod{p^3}. \quad (7)$$

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

Proof. The congruence relation (4) and the equivalence of (1) to (3) in the theorem follows from the two congruences in [30] after [17, (16)]. See also [20, p. 281]. The equivalence of (2) and (4) follows immediately from the shuffle relation*:

$$H(n;p-1)^2 = 2H(n,n;p-1) + H(2n;p-1). \quad (8)$$

Remark 2.9. This theorem also follows directly from a result of [30]. See Thm. [20, 16]

Gardiner [18] proves the special case of the equivalence when $n = 1$. He has one more equivalence condition which involves the combinatorial number $\binom{2n}{p}$. Other variations of the classical Wolstenholme’s Theorem can be found in [11]. 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 $\binom{2n}{p} \equiv 2 \pmod{n^3}$ would imply $n$ is a prime, which is called the converse of Wolstenholme’s Theorem [31].

2.3 Hoffman’s convolution

In this section we recall Hoffman’s convolution operation of the composites and provide new congruence modulo a prime square. These results will be extremely useful when we deal with multiple harmonic sums of arbitrary lengths.

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

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

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

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

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

Theorem 2.10. ([25, Thm. 6.8]) For $s = (s_1, \ldots, s_l)$ and any positive integer $n$ define

$$S(s;n) = \sum_{1 \leq k_1 \leq \cdots \leq k_l \leq n} k_1^{-s_1} \cdots k_l^{-s_l}. \quad (9)$$

*Some authors call this a stuffle relation, i.e., “shuffling” plus “stuffing”.
Then for all prime $p$

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

(10)

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

(11)

We also have the following equalities:

$$S(s; n) = \sum_{i \leq s} H(i; n),$$

(12)

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

$$( -1)^{|i|} S(\overline{s}; p - 1) = \sum_{\bigcup_{j=1}^{l} s_j = s} (-1)^{|l|} \prod_{j=1}^{l} H(s_j; p - 1) \pmod{p}$$

(13)

where $\bigcup_{j=1}^{l} s_j$ is the catenation of $s_1$ to $s_l$.

**Proof.** Note that in [25] the right hand side of (9) is denoted by $S(\overline{s}; n)$ instead. But it’s not difficult to verify that for any $s$

$$s^* = \overline{s^t}.$$  

(14)

So (10) is equivalent to [26] Thm. 6.8. Congruence (11) follows readily from the substitution of indices: $k \rightarrow p - k$.

Equations (13) and (12) relate $S$-version multiple harmonic series and our $H$-version (denoted by $A$ by Hoffman). Equation [25] Eq. (7)) and (13) is equivalent to the second unlabelled formula in the proof of [25] Thm. 6.8. \qed

Next we want to provide a more precise version of congruence (10).

**Theorem 2.11.** Let $s$ be any composite of weight $w$. Let $p$ be an arbitrary odd prime. Then

$$- S(s^*; p - 1) \equiv S(s; p - 1) + p \left( \sum_{t \leq s} H(t \cup \{1\}; p - 1) \right) \pmod{p^2}.$$  

(15)

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

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

Recall that $\Sigma \nabla S(s; n) = -S(s^*; n)$ for any $s$ and positive number $n$ by [25] Thm. 4.2]. Then for any odd prime $p$ we have

$$- S(s^*; p - 1) = \Sigma \nabla S(s; p - 1)(n) = \sum_{i=0}^{p-1} \begin{pmatrix} p \cr i + 1 \end{pmatrix} (-1)^i S(s; i)$$

$$= \sum_{i=0}^{p-2} \begin{pmatrix} 1 \cr i + 1 \end{pmatrix} \left( \begin{pmatrix} p - 1 \cr i \end{pmatrix} (-1)^i S(s; i) \right)$$

$$\equiv S(s; p - 1)(n) + \sum_{i=0}^{p-2} \begin{pmatrix} 1 \cr i + 1 \end{pmatrix} S(s; i) \pmod{p^2}$$

$$\equiv S(s; p - 1)(n) + p \left( \sum_{i=0}^{p-2} S(s; i) \right) \pmod{p^2}$$

$$\equiv S(s; p - 1)(n) + p \left( \sum_{t \leq s} \sum_{i=1}^{t} H(t; i) \right) \pmod{p^2}$$

$$\equiv S(s; p - 1)(n) + p \left( \sum_{t \leq s} H(t \cup \{1\}; p - 1) \right) \pmod{p^2}.$$  

\qed
2.4 Wolstenholme type theorem for homogeneous sums

In the above we have studied the $p$-divisibility of $H(s; p - 1)$ for positive integers $s$. It is difficult to start with arbitrary $s$ so we only consider the homogeneous multiple harmonic sums at the moment.

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

$$H(m; n) \cdot H(s_1, \ldots, s_t; n) = \sum_{s \in \text{Shfl}(m, (s_1, \ldots, s_t))} H(s; n) + \sum_{j=1}^{t} H(s_1, \ldots, s_{j-1}, s_j + m, s_{j+1}, \ldots, s_t; n)$$

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

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

Hence for any $k = 1, \ldots, l - 1$, we have

$$H(ks; n) \cdot H(\{s\}^{l-k}; n) = \sum_{s \in \text{Shfl}(\{ks\}, \{s\}^{l-k})} H(s; n) + \sum_{s \in \text{Shfl}(\{(k+1)s\}, \{s\}^{l-k-1})} H(s; n).$$

Applying $\sum_{k=1}^{l-1} (-1)^{k-1}$ on both sides we get

**Lemma 2.12.** Let $s, l$ and $n$ be three positive integers. Then

$$l! H(\{s\}^l; n) = \sum_{k=1}^{l} (-1)^{k-1} H(ks; n) \cdot H(\{s\}^{l-k}; n). \quad (16)$$

We now need a formula of the homogeneous multiple harmonic sum $H(\{s\}^l; n)$ in terms of partial sums of ordinary zeta value series. Let $P(l)$ be the set of unordered partitions of $l$. For example, $P(2) = \{(1, 1), (2)\}, P(3) = \{(1, 1, 1), (1, 2), (3)\}$ and so on.

**Lemma 2.13.** Let $s, l$ and $n$ be positive integers. For $\lambda = (\lambda_1, \ldots, \lambda_l) \in P(l)$ we put $H_\lambda(s; n) = \prod_{i=1}^{l} H(\lambda_is; n)$ and define $c_\lambda = (-1)^l \cdot \prod_{i=1}^{l} (\lambda_i - 1)!$. Then

$$l! H(\{s\}^l; n) = \sum_{\lambda \in P(l)} c_\lambda H_\lambda(s; n). \quad (17)$$

**Proof.** It follows easily from [26 Thm. 2.3].

It is obvious that $c_{(1, \ldots, 1)} = 1$. When $l = 3$ we have $c_{(1, 2)} = -2c_1 + c_2 = -3$, which implies

$$6H(\{s\}^3; n) = H(s; n)^3 - 3H(s; n)H(2s; n) + 2H(3s; n). \quad (18)$$

When $l = 4$ we have $c_{(1, 1, 2)} = c_{(1, 2)} - 3c_{(1, 1)} = -6, c_{(1, 3)} = c_3 = 6c_1 = 8,$ and $c_{(2, 2)} = 3c_2 = -3$, which implies

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

**Theorem 2.14.** 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 $k = 1, \ldots, l$. Then the homogeneous multiple harmonic sum

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

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

**Proof.** Congruence for $H$ follows from Eq. (17) and Lemma 2.12. Congruence for $S$ then follows from [13].
Recently, Zhou and Cai obtain an improved version of the above result, see [39].

**Theorem 2.15.** Let \( s \) and \( l \) be two positive integers. Let \( p \) be a prime such that \( p \geq ls + 3 \)

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

Proof. Congruence for \( H \) follows from [39]. Congruence for \( S \) then follows from (13) and an induction on \( l \).

### 2.5 Higher divisibility and distribution of irregular pairs

From Thm. 2.15 we immediately have

**Proposition 2.16.** Let \( p \) be an odd prime. Suppose \((p, p - ls - 2)\) is an irregular pair (so both \( l \) and \( s \) must be odd numbers). Then

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

Suppose \((p, p - ls - 1)\) is an irregular pair. Then

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

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 2.17.** For any fixed positive integer \( M \) and integer \( c \) such that \( 0 \leq c < M \) we have

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

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 Prop. 2.16. In Table II 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 at the end of this paper.

### 3 Non-homogeneous sums

Having dealt with homogeneous multiple harmonic sums we would like to do some initial experiments on the non-homogeneous ones.
| $m$ | 1,000 | 2,000 | 3,000 | 4,000 | 5,000 | 6,000 | 7,000 | 8,000 | 9,000 | 10,000 | 11,000 |
|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|--------|
| $N(0, m)$ | 322 | 664 | 996 | 1318 | 1637 | 1978 | 2310 | 2628 | 2968 | 3310 | 3672 |
| $P(0, m)$ | 32.20 | 33.20 | 33.20 | 32.95 | 32.74 | 32.97 | 33.00 | 32.85 | 32.98 | 33.10 | 33.38 |
| $N(1, m)$ | 343 | 666 | 1005 | 1352 | 1676 | 1999 | 2540 | 2683 | 3017 | 3354 | 3673 |
| $P(1, m)$ | 34.30 | 33.30 | 33.50 | 33.80 | 33.52 | 33.32 | 33.43 | 33.54 | 33.52 | 33.54 | 33.39 |
| $N(2, m)$ | 335 | 670 | 999 | 1330 | 1678 | 2023 | 2550 | 2899 | 3105 | 3336 | 3655 |
| $P(2, m)$ | 33.50 | 33.50 | 33.30 | 33.25 | 33.74 | 33.72 | 33.57 | 33.61 | 33.50 | 33.36 | 33.22 |

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

### 3.1 Non-homogeneous sums of length 2

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

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

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 $0 \leq m, n \leq p - 2$. Then

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

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

$$S(s, t; p - 1) \equiv H(s, t; p - 1) \equiv \frac{(-1)^t}{s + t} \begin{pmatrix} s + t \\ s \end{pmatrix} B_{p - s - t} \pmod{p}.$$ 

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

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

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

Define the formal power series in two variables

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

Exchanging summation we get

$$f(x, y) = \sum_{1 \leq k_1 < k_2 \leq p - 1} e^{k_1 x + k_2 y} = \frac{e^{p(x+y)} - e^{x+y}}{(e^{x+y} - 1)(e^x - 1)} - \frac{(e^{2y} - e^y)e^x}{e^y - 1}$$

$$= \sum_{i = -1}^{\infty} \sum_{j = -1}^{\infty} B_{i+1}(p) - B_{j+1}(1) \frac{B_{i+1}(p) - B_{j+1}(1)}{(i+1)!(j+1)!} \left( B_{i+1} x^i (x + y)^j - B_{i+1} x^i y^j \right)$$

where $B_m(1) = B_m$ if $m \neq 1$ and $B_1(1) = -B_1 = \frac{1}{2}$. We only care about the above sum when $1 \leq i, j \leq p - 2$ since $1 \leq M, N \leq p - 2$. So we may as well replace $B_m(1)$ by $B_m$ everywhere in the
Theorem 3.2. Let we formulated Thm. 3.1 only after we had found these intriguing examples.

Let \( p > s \) that \( p, p \) there is only one irregular pair of the form \( (p, p) \).

Therefore \( H \) verified this on Maple for the only two known irregular pairs of the form \( (p, p) \).

Taking \( m, n \leq 2 \) in the theorem we obtain \( H \) is always congruent to 0 mod \( p \). Otherwise, if \( M + N \geq p - 2 \) then all the terms are in \( pZ \) except when \( N + 1 = p - 1 \).

So finally we arrive at

\[
H(m, n; p - 1) = \sum_{1 \leq k_1 < k_2 \leq p - 1} \frac{1}{k_1!k_2!} \equiv \frac{-(p - m - 1)!B_{p-m-n}}{n!(p - m - n)!} \quad (\text{mod } p).
\]

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 \( S(t) = H(s, t) + H(s + t) \) and Wolstenholme’s theorem.

Taking \( m = 1, n = 2 \) in the theorem we obtain \( H(1, 2; p - 1) \equiv B_{p - 3} \) (mod \( p \)) for \( p \geq 3 \). 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 \( m = 2, n = 3 \) we find that \( H(2, 3; p - 1) \equiv B_{p - 5} \) (mod \( p \)) if \( p \geq 5 \).

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 \( H(2, 3; 36) \equiv 0 \) (mod 37). As a matter of fact, we formulated Thm. 3.1 only after we had found these intriguing examples.

We now can provide an analog of Thm. 3.1 in the non-homogeneous case of length 2.

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

\[
H(s, t; p - 1) \equiv \begin{cases} (-1)^s \frac{s + t + 1}{s} - (-1)^s \frac{s + t + 1}{t} - s - t & B_{p-s-t-1}^{2(s + t + 1)} \quad (\text{mod } p^2) \\ (-1)^s t \frac{s + t + 1}{s} - (-1)^s t \frac{s + t + 1}{t} + s + t & B_{p-s-t-1}^{2(s + t + 1)} \quad (\text{mod } p^2). \end{cases}
\]

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

\[
H(s) \cdot H(t) = H(s, t) + H(t, s) + H(s + t).
\]

By the conditions on \( s_1 \) and \( s_2 \) we know from 7

\[
H(s) \cdot H(t) \equiv 0, H(s + t) \equiv \frac{p(s + t)}{s + t + 1} B_{p-s-t-1} \quad (\text{mod } p^2).
\]

Therefore

\[
H(s, t) + H(t, s) \equiv \frac{-p(s + t)}{s + t + 1} B_{p-s-t-1} \quad (\text{mod } p^2).
\]
Moreover, by the old substitution trick $i, j \to p - i, p - j$

$$H(s, t) = \sum_{1 \leq j < i < p} \frac{1}{(p - i)^s(p - j)^t}$$

$$\equiv \sum_{1 \leq j < i < p} \frac{1}{i^s j^t} \left(1 + \frac{p}{i}\right)^s \left(1 + \frac{p}{j}\right)^t \pmod{p^2} \quad (s + t \text{ is even})$$

$$\equiv \sum_{1 \leq j < i < p} \frac{1}{i^s j^t} \left(1 + \frac{ps}{i} + \frac{pt}{j}\right) \pmod{p^2}$$

$$\equiv H(t, s) + psH(t, s + 1) + ptH(t + 1, s) \pmod{p^2}$$

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

Combined with (4), this completes the proof of the congruence for $H$. Then the $S$ part follows from the identity $S(s, t) = H(s, t) + H(s + t)$.

\[\blacksquare\]

### 3.2 The case of palindrome $s$

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

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

$$H(s; p - 1) \equiv (-1)^{|s|} H(\overline{s}; p - 1) \pmod{p},$$

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

**Proof.** Use the old substitution trick $k_i \to p - k_i$ for all $i$ in the definitions (2) and (3).

An immediate consequence of this lemma is

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

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

On the contrary, a lot of examples show that if the weight $|s| \geq 6$ is even and if the length is bigger than 2, then we often have $H(s; p - 1) \not\equiv 0 \pmod{p}$ when $p$ is large (say, $p \geq 2|s|$), even in the case that $s$ is a palindrome. For example, in length 3 if $s \neq (4, 3, 5), (5, 3, 4)$ then this seems to be always the case (see Problem 3.10). A remarkable different pattern occurs for length 3 weight 4 case which we will consider in subsection 3.4. Clarifying this completely might be a crucial step to understand the structure of $H(s; p - 1)$ in general.

### 3.3 Multiple harmonic sums of length 3 with odd weight

One may want to generalize Thm. 3.1 to multiple harmonic sums 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

$$H(0, m, n; p - 1) \equiv H(m - 1, n; p - 1) - H(m, n; p - 1) \pmod{p},$$

$$H(l, 0, n; p - 1) \equiv H(l, n - 1; p - 1) - H(l, n; p - 1) - H(l - 1, n; p - 1) \pmod{p},$$

$$H(l, m, 0; p - 1) \equiv -H(l, m - 1; p - 1) - H(l, m; p - 1) \pmod{p}.$$

Suppose $l, m, n \geq 1$. Suppose further that $w = l + m + n$ is an odd number. Then

$$H(l, m, n; p - 1) \equiv I(l, m, n) - I(n, m, l) \pmod{p}$$

13
where $I$ is defined as follows. Let $w' = w - (p - 1)$ if $p < w < 2p$ and $w' = w$ otherwise. Then

\[
I(l, m, n) = \begin{cases} 
0 & \text{if } w \geq 2p, \text{ or if } l + m < p \text{ and } p < w < 2p - 1, \\
1/2n & \text{if } w = p, 2p - 1, \\
(-1)^n + 1 \binom{w'}{n} \frac{B_{w-w'}}{2w'} & \text{otherwise.}
\end{cases}
\]

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

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

**Remark 3.6.** In [26] Thm. 6.2] Hoffman gives a easier proof than ours.

**Proof.** The last congruence follows easily from relations (11) and (13) so we only consider the first part. Throughout the proof all congruences are modulo $p$. We leave the trivial cases to the interested readers and assume in the rest of the proof that $l, m, n \geq 1$ and $w = l + m + n$ is odd. Similar to the proof of Thm. 3.1 we put $L = p - l - 1$, $M = p - 1 - m$, and $N = p - 1 - n$. Then $1 \leq L, M, N \leq p - 2$. By Fermat’s Little Theorem

\[
H(s_1, s_2, s_3; p - 1) \equiv H(l, m, n; p - 1) \equiv \sum_{1 \leq k_1 < k_2 < k_3 \leq p - 1} k_1^L k_2^M k_3^N.
\]

Define the formal power series in three variables

\[
f(x, y, z) = \sum_{r,s,t=0}^{\infty} \left( \sum_{1 \leq k_1 < k_2 < k_3 \leq p-1} k_1^r k_2^s k_3^t \right) \frac{x^r y^s z^t}{r!s!t!} = \sum_{1 \leq k_1 < k_2 < k_3 \leq p-1} e^{k_1 x + k_2 y + k_3 z} e^{p(x+y+z) - e^{x+y+z}} - e^{x+y} (e^{pz} - e^z)\]

\[
= \frac{(e^{x+y})(e^{x+y+z} - 1)}{(e^{x+y}-1)(e^{x+y+z} - 1)} - \frac{(e^{y+z})(e^{x+y+z} - 1)}{(e^{x+y}-1)(e^{y+z} - 1)} + \frac{(e^{x+z})(e^{x+y+z} - 1)}{(e^{x+y}-1)(e^{x+z} - 1)}
\]

\[
= \sum_{i,j=-1}^{\infty} \sum_{k=0}^{\infty} B_{i+1} B_{j+1} B_{k+1} (p - B_{k+1}) \frac{x^i y^j z^k}{(i+1)! (j+1)! (k+1)!}.
\]

We are interested in the $x^L y^M z^N$-term of the above sums where $L, M, N \geq 1$. With this in mind we can safely replace all the $B_{m}(1)$ by plain $B_{m}$. It follows that $H(l, m, n; p - 1) \pmod{p}$ is the coefficient of $x^L y^M z^N$-term of the function $L! M! N! g(x, y, z)$ where

\[
g(x, y, z) = \sum_{i,j=-1}^{\infty} \sum_{k=0}^{\infty} p B_{i+1} B_{j+1} B_{k+1} \frac{x^i y^j z^k}{(i+1)! (j+1)! (k+1)!} \left[ (x+y+z)^{k+1} - (y+z)^{k+1} - (x+y)^{k+1} \right].
\]

As $L + M + N = 3(p - 1) - w$ is odd, we know that for a term in (25) to provide a nontrivial contribution to $x^L y^M z^N$ it is necessary that either $i = 0$, or $j = 0$, or $k = 1$ because the only nonzero Bernoulli number with odd index is $B_1 = -1/2$. But $k = 1$ is not an option because all terms corresponding to $x^L y^m z$ cancel out. So we’re left with only two cases (I) $i = 0$ and (J) $j = 0$. We now handle them separately.
(I) When \( i = 0 \) only the following terms really matter:

\[
\sum_{k \geq 2} \frac{pB_1 B_k (x + y + z)^k - z^k}{k!} + \sum_{j \geq 1, k \geq 2} \frac{pB_1 B_{j+1} B_k}{(j+1)!k!} (x + y)^j [(x + y + z)^k - z^k]
\]

\[
= \sum_{1 \leq a < r \leq k} \frac{pB_1 B_k \cdot x^a y^{r-1-a} z^{k-r}}{r! \cdot a! (r-1-a)! (k-r)!} + \sum_{j \geq 1, k \geq 2} \sum_{c=0}^{j} \sum_{a+b=c} \sum_{1 \leq a < r \leq k} \frac{pB_1 B_{j+1} B_k \cdot x^a y^b z^c}{(j+1)!c!(j-c)!a!b!(k-a-b)!}
\]

(26)

where the first sum of \( \mathbb{Z}_p \) comes from setting \( j = -1 \).

\( \text{(II)} \) In the first sum of (26) putting \( L = a, M = r - 1 - a, \) and \( N = k - r \). Then we obtain the unique term (after multiplying \( L!M!/N! \))

\[
\frac{pB_1 B_{L+M+N+1}}{L + M + 1} = \frac{pB_1 B_{3(p-1)-w+1}}{2p - 1 - w + n}.
\]

It is an easy matter to see that the denominator is a \( p \)-unit unless \( l + m = p - 1 \) and the numerator is in \( p\mathbb{Z}_p \) except when \( w = 2p - 1 \) or \( w = p \). So we find the contribution to the coefficient of \( x^L y^M z^N \)-term in \( L!M!/N!g(x,y,z) \) from this case:

\[
I_0 := \frac{pB_1 B_{3(p-1)-w+1}}{2p - 1 - w + n} = \begin{cases} 
0 & \text{if } w \neq p, 2p - 1, \\
-B_1 & \text{if } w = 2p - 1, \\
\frac{n-B_1}{p-1+n} & \text{if } w = p, \\
\frac{B_1 B_{2p-1-n}}{B_{3(p-1)-w+1}} & \text{if } l + m = p - 1.
\end{cases}
\]

Now let’s turn to the second sum in (26). Setting \( L = a + c, M = j + b - c, \) and \( N = k - a - b \) we see that the contribution to the coefficient of \( x^L y^M z^N \)-term is

\[
I' := \sum_{r=1}^{L+M+1} \sum_{a+b=r} \frac{pB_1 B_{L+M+1-r} B_{N+r} L! M!}{(L + M + 1 - r) \cdot (L-a)! (M-b)! r!}
\]

Simple combinatorial argument shows that

\[
\sum_{a+b=r} \frac{L! M!}{(L-a)! (M-b)! r!} = \sum_{a+b=r} \binom{L}{a} \binom{M}{b} = \binom{L+M}{r}.
\]

So we get

\[
I' = \sum_{r=1}^{L+M+1} \frac{pB_1 B_{L+M+1-r} B_{N+r} L!}{L + M + 1 - r} \binom{L+M}{r}.
\]

If \( N + L + M + 1 \leq p - 2 \), i.e., \( w \geq 2p \), then all terms in \( I' \) are in \( p\mathbb{Z}_p \) and we have \( I' \equiv 0 \) \((\text{mod } p)\). Suppose \( w < 2p \). It’s obvious that \( N + r \leq L + M + N + 1 < 3(p-1) \) and \( L + M + 1 - r < 2p - 1 - m - n < 2p - 2 \). Consequently all terms in \( I' \) are in \( p\mathbb{Z}_p \) except when \( (I_1) L + M + 1 - r = p - 1 \), or \( (I_2) N + r = p - 1 \), or \( (I_3) N + r = 2(p-1) \). Note that \( I_1 \) and \( I_2 \) can occur at the same time if and only if \( w = p \).

\( \text{(I}_1) \) Suppose \( w < 2p \) and \( L + M + 1 - r = p - 1 \), i.e., \( r = p - l - m \geq 1 \). This occurs if and only if the followings are satisfied: \( l + m \leq p - 1 \) and \( N + r = 2p - 2 - w \geq 1 \) (so automatically \( w < 2p \)). Then the corresponding term in \( I \) is

\[
I_1 = B_1 B_{L+M+N+2-p} \binom{L+M}{p-2} = B_1 B_{2p-1-w} \binom{2p-2-l-m}{p-2}.
\]

However, \( I_1 \equiv 0 \) unless \( l + m = p - 1 \) or \( w = p \). Hence

\[
I_1 \equiv \begin{cases} 
-B_1 B_{p-n} & \text{if } l + m = p - 1 \text{ and } n \geq 2, \\
-B_1 B_{p-1 - B_1} & \text{if } l + m = p - 1 \text{ and } n = 1, \\
\frac{B_1}{n(n-1)} & \text{if } w = p \text{ and } n \geq 2.
\end{cases}
\]

15
(I2) Suppose \( w < 2p \) and \( N + r = p - 1 \). Because \( L + M \geq r \) we see that \( w \leq 2p - 2 \). Then the contribution is

\[
I_2 \equiv -B_1 B_{L + M + N + 2 - p} \left( \frac{L + M}{L + M + N + 2 - p} (p - 1 - N) \right) \equiv -B_1 B_{2p - 1 - w} \left( \frac{2p - 2 - l - m}{n} \right),
\]

\[
\begin{cases}
0 & \text{if } w = p, \\

\frac{B_1 B_{p-n}}{p - n} & \text{if } l + m < p - 1, \text{ or if } p < w < 2p, \\

\left( -1 \right)^{n+1} \frac{B_1 B_{2p - 1 - w}}{2p - 1 - w} \left( \frac{w + 1}{n} \right) & \text{if } l + m = p - 1 \text{ and } n \geq 2,
\end{cases}
\]

\( \text{by Kummer congruence.} \)

Putting \( I_0, I_1, I_2 \) and \( I_3 \) together we get

\[
I \equiv \begin{cases}
0 & \text{if } w \geq 2p, \\
0 & \text{if } p < w < 2p - 1 \text{ and } l + m < p, \\
\left( -1 \right)^{n+1} \frac{B_1 B_{p-w}}{p-w} \left( \frac{w}{n-1} \right) & \text{if } l + m \geq p \text{ and } w < 2p - 1, \\
\frac{1}{2n} & \text{if } w = p \text{ or } w = 2p - 1, \\
\left( -1 \right)^{n+1} \frac{w}{2w} B_{p-w} & \text{if } w < p.
\end{cases}
\]

(27)

We notice the miracle that when \( l + m = p - 1 \) and \( n \geq 2 \), all the contributions from \( I_0, I_1 \) and \( I_2 \) cancel out because of Kummer congruences!

(J) When \( j = 0 \) in \( 28 \), only the following terms really matter:

\[
\sum_{k \geq 2} \frac{p B_1 B_k (x + y + z)^k - (y + z)^k}{k!} \frac{x^i}{x} \sum_{i \geq 1, k \geq 2} \frac{p B_1 B_{i+1} B_k}{(i + 1)! k!} x^i ((x + y + z)^k - (y + z)^k)
\]

\[
= \sum_{1 \leq b \leq a \leq k} p B_1 B_k x^{a-1} y^b z k-a-b \frac{a! b! (k-a-b)!}{a+b-1, a \geq 1} \sum_{i \geq 1, k \geq 2} \frac{p B_1 B_{i+1} B_k}{(i + 1)! a! b! (k-a-b)!} x^{i+a} y^b z^{k-a-b} \tag{28}
\]

\( \text{(J0) In the first sum of } 28 \text{ put } L = a-1, M = b, \text{ and } N = k-a-b. \text{ After multiplying } L! M! N! \text{ we find the coefficient of } x^i y^M z^N \text{ is} \)

\[
J_0 := \frac{p B_1 B_{3(p-1) - w + 1}}{p-l} = \begin{cases}
0 & \text{if } w \neq p, 2p - 1, \\
-1 & \text{if } w = p, 2p - 1.
\end{cases}
\]

Let’s turn to second sum in \( 28 \). Setting \( L = i+a, M = b, \text{ and } N = k-a-b \) we see that the contribution from this sum is

\[
J' := \sum_{a \geq 1} \frac{p B_1 B_{L+1-a} B_{M+N+a} L!}{(L+1-a)! a!}.
\]

If \( L + M + N + 1 \leq p - 2 \), i.e., \( w \geq 2p \), then all terms are in \( p\mathbb{Z}_p \) and therefore \( J' \equiv 0 \pmod{p} \).

Suppose \( w < 2p \). Clearly \( L+1-a \leq p - 2 \) and \( M + N + a \leq M + N + L + 1 < 3(p-1) \). We know that all terms in \( J' \) are in \( p\mathbb{Z}_p \) except when \( (J_1) M + N + a = p - 1, \text{ or } (J_2) M + N + a = 2(p-1) \).
(J1) Suppose \( w < 2p \) and \( M + N + a = p - 1 \). This can occur if and only if \( M + N \leq p - 2 \), i.e., \( m + n \geq p \), and \( L + 1 - a \geq 1 \) which is equivalent to \( w \leq 2p - 2 \). If this is the case, then the contribution is

\[
J_1 = \frac{-B_1 B_{2p-1-w}(p-1-l)!}{(2p-1-w)!(m + n - p + 1)!} \equiv (-1)^l \frac{B_1 B_{2p-1-w}(w + 1)}{2p-1-w} \binom{w}{l}.
\]

(J2) Suppose \( w < 2p \) and \( M + N + a = 2(p-1) \). This occurs if and only if \( L + 1 - a = L + M + N + 3 - 2p = p - w \geq 1 \), i.e., \( w < p \). In this case \( a = m + n \) and the corresponding term in \( B \) is

\[
J_2 = \frac{-B_1 B_{p-w}(p-1-l)!}{(p-w)!(m + n)!} \equiv (-1)^l \frac{B_1 B_{p-w}(w + 1)}{p-w} \binom{w}{l}.
\]

Combining cases \((J_0), (J_1)\) and \((J_2)\) we have

\[
J = \begin{cases} 
0 & \text{if } w \geq 2p, \\
0 & \text{if } p < w < 2p \text{ and } m + n < p, \\
(1-l)! \left( \frac{w+1}{l} \right) B_{2p-1-w} 2(w+1) & \text{if } w < 2p - 1 \text{ and } m + n \geq p, \\
-1 & \text{if } w = p, 2p - 1, \\
\frac{2l}{(1-l)!} \left( \frac{w}{l} \right) B_{p-w} & \text{if } w < p.
\end{cases}
\]

The theorem now follows from an easy simplification process.

In the case when \( w = r + s + t \) is even the expression is much more complicated. For future reference we provide the following computation when the prime \( p > w + 1 \). The method is similar to that used by Hoffman to compute the length 2 case in \([26]\). Recall that by Bernoulli polynomials we have

\[
\sum_{i=1}^{n} i^d = \sum_{a=0}^{d} \binom{d + 1}{a} B_a d^{d+1-a}.
\]

So modulo \( p \) we have by Fermat’s Little Theorem

\[
H(r, s, t; p - 1) \equiv \sum_{i=1}^{p-1} i^{r-1} \sum_{j=1}^{p-1-s} j^{p-r-s} \sum_{k=1}^{j-1} k^{p-1-r}
\equiv \sum_{i=1}^{p-1} i^{r-1} \sum_{j=1}^{p-1-r} \binom{p-r}{a} \frac{B_a}{p-r} j^{\kappa(a) + p-r-s-a}
\equiv \sum_{i=1}^{p-1} i^{r-1} \sum_{a=0}^{p-r} \binom{p-r}{a} \frac{B_a}{p-r} \sum_{j=1}^{i-1} j^{\kappa(a) + p-r-s-a}
\equiv \sum_{a=0}^{p-r} \sum_{i=1}^{p-1} \binom{p-r}{a} \frac{B_a}{p-r} \sum_{j=0}^{\kappa(a) + p+1-r-s-a} \binom{\kappa(a) + p+1-r-s-a}{b} \frac{B_b}{\kappa(a) + p+1-r-s-a},
\]

where \( \kappa(a) = 0 \) if \( a \leq p - r - s \) 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:

$$H(r, s, t; p - 1) \equiv -\sum_{a=0}^{p+1-w} \left(\frac{p-r}{a}\right) B_a \left(\frac{p+1-r-s-a}{t}\right) \frac{B_{p+1-w-a}}{p+1-r-s-a}$$

$$-\sum_{a=\max\{p+1-r-s, p+2-w\}}^{p+1-w} \left(-1\right)^{a+t} \left(\frac{r+a}{a}\right) B_a \left(\frac{w+a-1}{t}\right) \frac{B_{p+1-w-a}}{w+a-1}$$

$$-\sum_{a=\max\{p+1-r-s, p+2-w\}}^{p+1-w} \left(-1\right)^{a+t} \left(\frac{r+a}{a}\right) B_a \left(\frac{w+a}{t}\right) \frac{B_{2p-w-a}}{w+a}. \quad (30)$$

When $w$ is odd we recover Thm. 3.5 when $p > w + 1$ by noticing that there are only two nontrivial terms in (30) corresponding to $a = 1$ and $a = p - w$.

### 3.4 Some remarkable cases of length 3 with even weight

Applying (24) to $(s_1, s_2) = (1, 3)$ together with shuffle product $H(1, 1; p - 1) \cdot H(2; p - 1)$ we get

$$H(2, 1, 1; p - 1) + H(1, 2, 1; p - 1) + H(1, 1, 2; p - 1) \equiv \frac{4p}{5} B_{p-5} \pmod{p^2}. \quad (31)$$

By Lemma 5.3 we can even see that

$$H(2, 1, 1; p - 1) \equiv H(1, 1, 2; p - 1) \pmod{p}. \quad (32)$$

However, is it true that in fact all of these sums are congruent to 0 mod $p$? Now from (30) we can compute easily that modulo $p$

$$H(1, 2, 1; p - 1) \equiv \sum_{a=0}^{p-3} B_a B_{p-3-a}, \quad (33)$$

$$H(1, 1, 2; p - 1) \equiv -\sum_{a=0}^{p-3} \frac{2+a}{2} B_a B_{p-3-a}, \quad (34)$$

$$H(2, 1, 1; p - 1) \equiv \sum_{a=0}^{p-3} \frac{1+a}{2} B_a B_{p-3-a}. \quad (35)$$

Set

$$A := \sum_{a=0}^{p-3} B_a B_{p-3-a}, \quad B := \sum_{a=0}^{p-3} aB_a B_{p-3-a}. \quad (36)$$

Then from (31), (32) to (36)

$$A/2 \equiv 0 \pmod{p}. \quad (37)$$

Moreover, from (32), (33) and (34)

$$-(A + B/2) \equiv A/2 + B/2 \pmod{p}. \quad (38)$$

Consequently we have

**Corollary 3.7.** For every prime $p \geq 7$ we get

$$\sum_{a=0}^{p-3} B_a B_{p-3-a} \equiv \sum_{a=0}^{p-3} aB_a B_{p-3-a} \equiv 0 \pmod{p}. \quad (39)$$

Therefore we have

$$H(1, 2, 1; p - 1) \equiv H(1, 1, 2; p - 1) \equiv H(2, 1, 1; p - 1) \equiv 0 \pmod{p}. \quad (40)$$
Using Maple we further find the following very stimulating example

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

**Proposition 3.8.** For all prime \( p \geq 7 \) we have

\[
\begin{align*}
H(1, 2, 1; p - 1) &\equiv -\frac{9}{10} p B_{p-5} \pmod{p^2}, \quad (37) \\
H(2, 1, 1; p - 1) &\equiv \frac{3}{5} p B_{p-5} \pmod{p^2}, \quad (38) \\
H(1, 1, 2; p - 1) &\equiv \frac{11}{10} p B_{p-5} \pmod{p^2}. \quad (39)
\end{align*}
\]

And

\[
\begin{align*}
S(1, 2, 1; p - 1) &\equiv -\frac{9}{10} p B_{p-5} \pmod{p^2}, \quad (40) \\
S(2, 1, 1; p - 1) &\equiv \frac{11}{5} p B_{p-5} \pmod{p^2}, \quad (41) \\
S(1, 1, 2; p - 1) &\equiv \frac{3}{10} p B_{p-5} \pmod{p^2}. \quad (42)
\end{align*}
\]

**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 \((31)\) says that

\[
A + B + C \equiv \frac{4}{5} p B_{p-5} \pmod{p^2}. \quad (43)
\]

Now by the shuffle relations

\[
H(1) H(2, 1) = A + 2B + H(3, 1) + H(2, 2), \quad (44)
\]

From Thm. \((32)\) we get

\[
A + 2B \equiv \frac{3}{10} p B_{p-5} \pmod{p^2} \quad (45)
\]

Hence it suffice to show \((37)\). From \((12)\) we see that

\[
S(1, 2, 1) = H(1, 2, 1) + H(3, 1) + H(1, 3) + H(4)
= H(1, 2, 1) + H(1) \cdot H(3) \equiv H(1, 2, 1) \pmod{p^2} \quad (46)
\]

\[
S(2, 2) = H(2, 2) + H(4) = -H(2, 2) + H(2)^2 \equiv -H(2, 2) \pmod{p^2}. \quad (47)
\]

Now because \((1, 2, 1)^* = (2, 2)\) by Thm. \((21)\) we have

\[
-S(2, 2) \equiv S(1, 2, 1) + p \left(H(1, 2, 1, 1) + H(3, 1, 1) + H(1, 3, 1) + H(4, 1)\right) \pmod{p^2}. \quad (48)
\]

By Cor. \((32)\) \(H(1, 3, 1) \equiv 0 \pmod{p}\). So using expressions \((46)\) and \((47)\) we can simplify the preceding congruence to

\[
H(2, 2) \equiv H(1, 2, 1) + p \left(H(1, 2, 1, 1) + H(3, 1, 1) + H(4, 1)\right) \pmod{p^2}. \quad (49)
\]

Now that \((1, 2, 1)^* = (2, 3)\) we find from congruence \((10)\) that modulo \( p \)

\[
-S(2, 3) \equiv S(1, 2, 1, 1) \equiv H(1, 2, 1, 1) + H(3, 1, 1) + H(1, 3, 1)
+ H(1, 2, 2) + H(4, 1) + H(3, 2) + H(1, 4) + H(5) \pmod{p}.
\]

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 \(12\) 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

\[
H(1, 2, 1, 1) \equiv -H(2, 3) - H(3, 2) - H(3, 1, 1) - H(1, 2, 2) \pmod{p} \\
\equiv H(5) - H(3, 1, 1) - H(1, 2, 2) \pmod{p} \\
\equiv -H(3, 1, 1) - H(1, 2, 2) \pmod{p}.
\]

Plugging this into \(19\) we see that

\[
H(2, 2) \equiv H(1, 2, 1) + p \left(H(4, 1) - H(1, 2, 2)\right) \pmod{p^2}.
\]

Using Thm. 2.15 and Thm. 3.2 we can now compute easily that

\[
H(2, 2) \equiv -\frac{2}{5} pB_{p-5} \pmod{p^2}, \quad H(4, 1) \equiv -B_{p-5}, \quad H(1, 2, 2) \equiv -\frac{3}{2} B_{p-5} \pmod{p}.
\]

These lead to congruence \(37\). Then congruence \(40\) follows from \(46\).

We now can solve \(38\) and \(39\) to get congruences \(38\) and \(39\). Finally, \(13\) yields

\[
S(2, 1, 1) = H(1, 1, 2) - H(1)H(1, 2) - H(1, 1)H(2) + H(1)^2 H(2) \equiv \frac{11}{10} pB_{p-5} \pmod{p^2},
\]

\[
S(1, 1, 2) = H(2, 1, 1) - H(2)H(1, 1) - H(2, 1)H(1) + H(2)H(1)^2 \equiv \frac{3}{5} pB_{p-5} \pmod{p^2}.
\]

We have completed the proof of the proposition.

By going through the proof of Thm. 3.9 or the proof leading to \(30\) we can obtain the following result. We leave the details of the proof of it to the interested readers.

**Proposition 3.9.** For all prime \(p \geq 17\) we have

\[
H(4, 3, 5; p-1) \equiv H(5, 3, 4; p-1) \equiv 0 \pmod{p}.
\]

In \(38\), by using the shuffle relations and Hoffman’s convolution we will study the mod \(p\) structure of the multiple harmonic sums for lower weights. In particular, we will prove Prop. \(3.9\) and congruences like

\[
S(2, 3, 2; p-1) \equiv S(2, 3, 3, 2; p-1) \equiv 0 \pmod{p}.
\]

**Problem 3.10.** 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 \(p\mid H(r, s, t; p-1)\). Can one generalize the formula in Thm. 3.9 to prove this?

### 3.5 Some congruences modulo prime squares

We know from Thm. 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 \(k \rightarrow p - k\))

\[
H(r, s, r; p-1) \equiv -H(r, s, r; p-1) - p[2rH(r + 1, s, r; p-1) + sH(r, s + 1, r; p-1)].
\]

Hence

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

(50)
Proposition 3.11. For all prime $p > 5$ we have
\[
H(1, 3, 1; p - 1) \equiv S(1, 3, 1; p - 1) \equiv 0 \pmod{p^2}\]
(51)
\[
H(2, 1, 2; p - 1) \equiv S(2, 1, 2; p - 1) \equiv -\frac{1}{3}B_{p-3}^2 \pmod{p^2}.
\]
(52)
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
\[
H(1, 5, 1; p - 1) \equiv S(1, 5, 1; p - 1) \equiv b_8(p)p \pmod{p^2}.
\]
(53)
\[
H(2, 3, 2; p - 1) \equiv S(2, 3, 2; p - 1) \equiv 4b_8(p)p \pmod{p^2},
\]
(54)
\[
H(3, 1, 3; p - 1) \equiv S(3, 1, 3; p - 1) \equiv b_8(p)p \pmod{p^2}.
\]
(55)
Proof. Notice that
\[
S(r, s; r; p - 1) \equiv H(r, s; r; p - 1) + H(r + s)H(r) \equiv H(r, s; r; p - 1) \pmod{p}.
\]
From (51) we have
\[
2H(1, 3, 1; p - 1) \equiv -p[2H(2, 3, 1; p - 1) + 3H(1, 4, 1; p - 1)] \pmod{p^2},
\]
\[
2H(2, 1, 2; p - 1) \equiv -p[4H(3, 1, 2; p - 1) + H(2, 2, 2; p - 1)] \pmod{p^2},
\]
\[
2H(1, 5, 1; p - 1) \equiv -p[2H(2, 5, 1; p - 1) + 5H(1, 6, 1; p - 1)] \pmod{p^2},
\]
\[
2H(2, 3, 2; p - 1) \equiv -p[4H(3, 3, 2; p - 1) + 3H(2, 4, 2; p - 1)] \pmod{p^2},
\]
\[
2H(3, 1, 3; p - 1) \equiv -p[6H(4, 1, 3; p - 1) + H(3, 2, 3; p - 1)] \pmod{p^2}.
\]
By [26] Thm. 7.2 we know that
\[
S(2, 3, 1; p - 1) \equiv 3S(4, 1, 1; p - 1) \pmod{p},
\]
\[
S(1, 4, 1; p - 1) \equiv -2S(4, 1, 1; p - 1) \pmod{p},
\]
\[
S(3, 1, 2; p - 1) \equiv -S(4, 1, 1; p - 1) \equiv \frac{1}{6}B_{p-3}^2 \pmod{p}
\]
which yield (51) and (52). Similarly, (53) follows from [26] Thm. 7.4] because
\[
2S(2, 5, 1; p - 1) \equiv -2S(5, 2, 1; p - 1) - 2S(5, 1, 2; p - 1) \pmod{p},
\]
\[
= 5S(6, 1, 1; p - 1) - B_{p-5}B_{p-3} \pmod{p},
\]
\[
S(1, 6, 1; p - 1) \equiv -2S(6, 1, 1; p - 1) \pmod{p}.
\]
Also from [26] Thm. 7.4]
\[
S(3, 3, 2; p - 1) \equiv 4b_8(p) \pmod{p},
\]
\[
S(2, 4, 2; p - 1) \equiv -2S(4, 2, 2; p - 1) \equiv -2S(3, 3, 2; p - 1) \pmod{p},
\]
\[
S(3, 2, 3; p - 1) \equiv -2S(3, 3, 2; p - 1) \pmod{p},
\]
\[
S(4, 1, 3; p - 1) \equiv b_8(p) \pmod{p}.
\]
These lead to the last two congruence of the proposition immediately.

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

Proposition 3.12. The following two congruences are equivalent:

(i) For all primes $p > 8$
\[
H(1, 3, 1, 3; p - 1) \equiv -\frac{31}{72}pB_{p-9} \pmod{p^2},
\]
(ii) For all primes $p > 8$
\[
S(6, 1, 1, 1; p - 1) \equiv -\frac{1}{54}B_{p-3}^3 - \frac{1889}{648}B_{p-9} \pmod{p}.
\]

We have verified the congruences in the proposition for all primes $p$ such that $10 < p < 2000$. 

21
3.6 Some congruences of Bernoulli numbers

From Cor. 3.7 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 (30) we have for any even number $n$

$$H(1, n, 1; p - 1) \equiv \sum_{a=0}^{p-n-1} (-1)^a B_a B_{p-n-1-a} + \sum_{a=p-n}^{p-2} (-1)^a B_a B_{2p-n-2-a} \tag{56}$$

Taking $n = 4$ and comparing with (26, Thm. 7.2) we get

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

This proves the proposition. \qed

The following result is straightforward.

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

$$H(1, 1, 1, n; p - 1) \equiv -(-1)^n H(n, 1, 1, 1; p - 1) \equiv (-1)^n S(1, 1, 1, n; p - 1) \equiv -S(n, 1, 1, 1; p - 1)$$

$$\equiv \sum_{a=0}^{p-2} \sum_{b=0}^{p-n-1} (-1)^{b+n} \binom{a+b}{b} \binom{a+b+n}{n} B_a B_{b} B_{p-n-1-a-b} \equiv 0 \pmod{p}.$$ 

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 [27, p.248]):

$$B_m(x) = \sum_{k=0}^{m} \binom{m}{k} B_k x^{m-k} \tag{57}$$

$$B_m'(x) = mB_{m-1}(x) \quad \forall m \geq 1. \tag{58}$$

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

$$\sum_{a,b \geq 0, a+b=p-3n-3} \frac{B_b}{p-b} \binom{p-b}{n+1} \frac{B_a}{p-a} \binom{p-a}{n+2} \equiv 0 \pmod{p}, \tag{59}$$

$$\sum_{a,b \geq 0, a+b=p-3n-3} \frac{B_b}{p-b} \binom{p-b}{n+1} \frac{B_a}{p-a} \binom{p-a}{n+1} \equiv 0 \pmod{p}. \tag{60}$$
Proof. Throughout the proof all congruences are modulo $p$. First we set

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

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

We have

$$A \equiv -\sum_{a,b \geq 0, a+b=p-3n-3} \frac{n+1+a}{n+2} \cdot \frac{B_b}{p-b} \left( \frac{p-b}{n+1} \right) \frac{B_a}{p-a} \left( \frac{p-a}{n+1} \right). \quad (61)$$

Now exchange the index $a$ and $b$ in $A$ we get

$$A = \sum_{a,b \geq 0, a+b=p-3n-3} \frac{B_b}{p-b} \left( \frac{p-b}{n+2} \right) \frac{B_a}{p-a} \left( \frac{p-a}{n+1} \right) \equiv \sum_{a,b \geq 0, a+b=p-3n-3} \frac{2n+2+a}{n+2} \cdot \frac{B_b}{p-b} \left( \frac{p-b}{n+1} \right) \frac{B_a}{p-a} \left( \frac{p-a}{n+1} \right). \quad (62)$$

Adding (61) to (62) we find

$$2A \equiv \sum_{a,b \geq 0, a+b=p-3n-3} \frac{n+1}{n+2} \cdot \frac{B_b}{p-b} \left( \frac{p-b}{n+1} \right) \frac{B_a}{p-a} \left( \frac{p-a}{n+1} \right) = \frac{n+1}{n+2}B. \quad (63)$$

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

$$\left( -1 \right)^{m} \left( \frac{p-b}{m+1} \right) = (-1)^{b} \left( \frac{p-m-1}{b} \right). \quad (64)$$

We get

$$B \equiv n^2 \sum_{a,b \geq 0, a+b=p-3n-3} B_b \left( \frac{p-n-1}{b} \right) B_a \left( \frac{p-n-1}{a} \right) \quad (65)$$

because all the terms with odd index $a$ are zero. Let us denote by $\text{Coeff}[i, f(x)]$ the coefficient of $x^i$ in the polynomial $f(x)$. Then (65) means that

$$B \equiv n^2 \text{Coeff}[p+n+1, B_{p-n-1}^2(x)]$$

$$\equiv \frac{n^2}{p+n+1} \text{Coeff}[p+n, \left( B_{p-n-1}^2(x) \right)']$$

$$\equiv \frac{n^2}{n+1} \text{Coeff}[p+n, 2(p-n-1)B_{p-n-1}(x)B_{p-n-2}(x)]$$

by (65). From (67) this yields

$$B \equiv -2n^2 \sum_{a,b \geq 0, a+b=p-3n-3} B_b \left( \frac{p-n-1}{b} \right) B_a \left( \frac{p-n-2}{a} \right)$$

$$\equiv 2n \frac{n+1}{n} \sum_{a,b \geq 0, a+b=p-3n-3} \frac{B_b}{p-b} \left( \frac{p-b}{n+1} \right) \frac{B_a}{p-a} \left( \frac{p-a}{n+2} \right)$$

by (61). Therefore

$$B \equiv \frac{2n}{n+1}A. \quad (66)$$

Now the lemma follows easily by (63) and (66).
Theorem 3.16. Let $p$ be a prime and $s \in \mathbb{N}$. Assume $p > |s| + 2$. Then

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

if $s$ has the following forms:

1. $s = (1^m, 2, 1^n)$ for $m, n \geq 0$ and $m + n$ is even.
2. $s = (1^n, 2, 1^{n-1}, 2, 1^{n+1})$ where $n \geq 2$ is even.
3. $s = (1^{n+1}, 2, 1^{n-1}, 2, 1^n)$ where $n \geq 0$.
4. $s = (1^n, 2, 1^{n-1}, 2, 1^n)$ where $n \geq 2$ is even.

Furthermore, in the first and last cases we also have $S(s; p - 1) \equiv 0 \pmod{p}$.

Proof. We omit $p - 1$ in $S(\cdot; p - 1)$ and $H(\cdot; p - 1)$ and assume all congruences are modulo $p$ throughout this proof.

Let $s = (1^m, 2, 1^n)$. For future reference we first allow $m$ and $n$ to have different parity. Clearly we have $s^* = (m + 1, n + 1)$. So $|s| = |s^*| = m + n + 2$, $l(s) = m + n + 1$, and $l(s^*) = 2$. By Thm. 6.7 we have

$$S(s^*) \equiv -S(s).$$

(67)

Since $|s^*| - l(s^*) = m + n$ we have by (13)

$$(-1)^{m+n}S(s^*) \equiv (-1)^{|s^*| - l(s^*)}S(s^*) \equiv -H(s^*) + H(m + 1) \cdot H(n + 1) \equiv -H(s^*)$$

(68)

by Thm. 1.3. We now apply (13) to $s$ and get

$$-S(s) \equiv \sum_{\bigcup l_j^0 \cdot s_j = s} (-1)^l \prod_{j=1}^l H(s_j).$$

(69)

Now if $l \geq 2$ then one of $s_j = 1^d$ for some positive $d$ so that $H(s_j) \equiv 0$. Thus

$$S(s) \equiv H(s).$$

Combining this with (67) and (68) we get

$$H(s) \equiv (-1)^{m+n}H(s^*).$$

(70)

When $m + n$ is even we get

$$S(s) \equiv H(s) \equiv H(s^*) \equiv 0.$$

(1)

by Thm. 3.2 which proves case (1).

Let $s = (1^n, 2, 1^{n-1}, 2, 1^{n+1})$ where $n \geq 2$ is even. Then $s^* = (n + 1, n + 1, n + 2)$. So $|s| = |s^*| = 3n + 4$, $l(s) = 3n + 2$, and $l(s^*) = 3$. Since $n$ is even we have by applying (13) to $s^*$

$$S(s^*) \equiv H(s^*) - H(2n + 2, n + 2) - H(n + 1, 2n + 3) + H(3n + 4) \equiv H(s^*)$$

(71)

by Thm. 3.2 and Thm. 1.3. Applying (13) to $s$ and using the fact that $H(1^d) \equiv 0$ for any $d$ we have

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

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

(10)

by (9). Hence by (67) and (1)

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

(72)
We know that for all \( j, k < p \) we have

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

It follows that

\[
\sum_{a=0}^{p-2} H(n+1, a+1) \cdot H(n-a, n+2) = \sum_{a=0}^{p-2} \sum_{1 \leq i < j < p} \sum_{1 \leq k < l < p} \frac{1}{i+n+1} \frac{1}{j+n+1} \\
= -\sum_{1 \leq i < j < k < l < p} \frac{1}{i+n+1} \frac{1}{j+n+1} \\
= -H(n+1, n+1, n+2).
\]

Together with (72) we see that

\[
H(s) \equiv -\sum_{a=n}^{p-2} H(n+1, a+1) \cdot H(n-a, n+2) \\
\equiv -\sum_{a=2n+1}^{p-2} \frac{(-1)^a B_{p-n-2-a}}{n+2+a} \left(\frac{n+2+a}{n+1}\right) \frac{B_{a-2n-1}}{p+2n+1-a} \left(\frac{p+2n+1-a}{n+2}\right)
\]

by Thm. 3.1. Under substitution \( a \to 2n+1+a \) we get:

\[
H(s) \equiv \sum_{a=0}^{p+1-w} (-1)^a \left(\frac{w-1+a}{n+1}\right) \frac{B_{p-1-w-a}}{w-1+a} \left(\frac{p-a}{n+2}\right) \frac{B_a}{p-a} \equiv 0 \pmod{p}
\]  

(73)

by (80). This combined with (74) completes the proof of case (2).

It follows from (2) by taking \( s \).

When \( n = 0 \) or \( n \) is odd this follows from Thm. 2.9 and Lemma 3.3 respectively. When \( n \geq 2 \) is even the proof is almost the same as that of case (2) except at the end one need resort to (60). The congruence for \( S \) follows from the fact that \((1^n, 2^n, 1^n)^*= (n+1, n+2, n+1)\) and therefore

\[
S(s)^* \equiv H(s^*) \equiv 0
\]

by Cor. 3.4.

**Remark 3.17.** Note that in cases (2) and (4) we usually have \( S(s) \not\equiv 0 \pmod{p} \). For example, in case (2) we have \( S(s) \equiv -S(s^*) \equiv -H(s^*) \equiv H(n+1, n+1, n+2) \pmod{p} \) by (11). 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 \( s = \{r, s\}^n \) for some \( r, s \geq 1 \) and \( p \geq |s| \) be a prime. Then

\[
H(s; p-1) \equiv S(s; p-1) \equiv 0 \pmod{p}
\]

if either (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 Thm. 3.4. When \( n = 2 \), this has been confirmed by Hoffman (see the remarks after 20 Thm. 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 (12) it is straightforward to verify that

\[
S(\{r, s\})^n = \sum_{t \leq \{r, s\}} H(t) \\
= H(\{r, s\}) + H(r+s) \cdot \sum_{t \leq \{r, s\}^{n-1}} H(t) \\
= H(\{r, s\}) + H(r+s) \cdot S(\{r, s\})^{n-1} \equiv H(\{r, s\}) \pmod{p}
\]

(74)
by induction assumption. On the other hand, from (13) we find that
\[ S(\{r, s\}^n) \equiv \sum_{\cup i=1, s_i=\{r,s\}^n} (-1)^i H(s_1) \cdots H(s_i) \pmod{p}. \]

Now if \( l > 1 \) then \( s_1 = \{r, s\}^d \) for some \( d < n \) in which case \( H(s_1) \equiv 0 \pmod{p} \) by induction assumption, or else, \( s_1 = \{r, s\}^d \sqcup \{r\} \), in which case \( s_1 \) is a palindrome of odd weight and hence \( H(s_1) \equiv 0 \pmod{p} \) by Cor. 3.21. Consequently
\[ S(\{r, s\}^n) \equiv -H(\{r, s\}^n) \pmod{p}. \]

Together with (74) it shows that \( H(\{r, s\}^n) \equiv S(s; p-1) \equiv 0 \pmod{p} \) and the theorem is proved. \( \Box \)

When both \( r \) and \( s \) are even but \( n > 2 \) the theorem does not hold in general. For example,
\[ H(\{2, 4\}^3; 22) \equiv 21 \pmod{23}, \quad H(\{2, 4\}^4; 28) \equiv 20 \pmod{29}. \]

### 3.8 Some conjectures in general cases

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

**Conjecture 3.20.** Let \( s \in \mathbb{N}^l \) and \( p \geq |s| \) be a prime. Then
\[ H(s; p-1) \equiv 0 \pmod{p} \]

if \( s \) has one of the following forms:

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

We conclude our paper by

**Problem 3.21.** Are there any other \( s \) satisfying Wolstenholme’s type theorem besides those we listed in the paper? More generally is it possible to find a formula similar to Thm. 3.5 for arbitrary \( s \)?

### Appendix: Distribution of Irregular Primes

Table 1 in the paper and the following Table 2 give us some evidence to Conjecture 3.17.

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 \( p - t \equiv k \pmod{3} \) in the top \( m \) irregular pairs, \( 0 \leq k \leq 2 \), and by \( P(k, m) \) the percentage of such pairs. 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 Table 3 and Table 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.
| $i_p = 1, m$ | 3,000 | 6,000 | 9,000 | 12,000 | 15,000 | 18,000 | 21,000 | 24,000 | 27,000 | 30,000 |
|----------------|-------|-------|-------|--------|--------|--------|--------|--------|--------|--------|
| $N_1(0, m)$    | 979   | 1968  | 2954  | 4018   | 5001   | 5993   | 6972   | 7973   | 8968   | 9993   |
| $P_1(0, m)$    | 32.63 | 32.80 | 32.82 | 33.48  | 33.34  | 33.29  | 33.20  | 33.22  | 33.22  | 33.3   |
| $N_1(1, m)$    | 1016  | 2026  | 3049  | 4042   | 5039   | 6075   | 7095   | 8118   | 9090   | 10055  |
| $P_1(1, m)$    | 33.87 | 33.77 | 33.88 | 33.68  | 33.59  | 33.75  | 33.79  | 33.82  | 33.67  | 33.52  |
| $N_1(2, m)$    | 1005  | 2006  | 2997  | 3940   | 4960   | 5932   | 6933   | 7909   | 8942   | 9952   |
| $P_1(2, m)$    | 33.50 | 33.43 | 33.30 | 32.83  | 33.07  | 32.96  | 33.01  | 32.95  | 33.12  | 33.17  |

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

| $i_p = 2, m$ | 3,000 | 6,000 | 9,000 | 12,000 | 15,000 | 18,000 | 21,000 | 24,000 | 27,000 | 30,000 |
|----------------|-------|-------|-------|--------|--------|--------|--------|--------|--------|--------|
| $N_2(0, m)$    | 981   | 2029  | 3033  | 4049   | 5013   | 6024   | 7064   | 8062   | 9085   | 10096  |
| $P_2(0, m)$    | 32.70 | 33.82 | 33.70 | 33.74  | 33.42  | 33.47  | 33.64  | 33.59  | 33.65  | 33.65  |
| $N_2(1, m)$    | 993   | 1977  | 3033  | 4005   | 5001   | 6012   | 6981   | 7962   | 8927   | 9910   |
| $P_2(1, m)$    | 33.10 | 32.95 | 33.70 | 33.38  | 33.40  | 33.24  | 33.18  | 33.06  | 33.03  | 33.03  |
| $N_2(2, m)$    | 1026  | 1994  | 2934  | 3946   | 4986   | 5964   | 6955   | 7976   | 8988   | 9994   |
| $P_2(2, m)$    | 34.20 | 33.23 | 32.60 | 32.88  | 33.24  | 33.13  | 33.23  | 33.23  | 33.29  | 33.31  |

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

| $i_p = 4, m$ | 600   | 1,200 | 1,800 | 2,400  | 3,000  | 3,600  | 4,200  | 4,800  | 5,128  |
|----------------|-------|-------|-------|--------|--------|--------|--------|--------|--------|
| $N_4(0, m)$    | 196   | 388   | 569   | 769    | 948    | 1161   | 1341   | 1537   | 1645   |
| $P_4(0, m)$    | 32.67 | 32.33 | 31.61 | 32.04  | 31.60  | 32.25  | 31.93  | 32.02  | 32.05  |
| $N_4(1, m)$    | 1001  | 1994  | 2968  | 3955   | 4944   | 5956   | 6921   | 7943   | 8974   | 9812   |
| $P_4(1, m)$    | 33.67 | 33.23 | 32.97 | 32.96  | 32.96  | 32.95  | 32.95  | 33.23  | 33.29  | 33.29  |
| $N_4(2, m)$    | 1002  | 1979  | 2967  | 3943   | 4932   | 5953   | 6992   | 7990   | 8980   | 9771   |
| $P_4(2, m)$    | 33.40 | 32.98 | 32.96 | 32.86  | 32.88  | 33.07  | 33.29  | 33.29  | 33.29  | 33.29  |
| $i_p = 5, m$ | 100 | 200 | 300 | 400 | 500 | 600 | 635 |
|----------------|-----|-----|-----|-----|-----|-----|-----|
| $N_5(0, m)$    | 31  | 71  | 111 | 145 | 179 | 218 | 230 |
| $P_5(0, m)$    | 31.00 | 35.50 | 37.00 | 36.25 | 35.80 | 36.33 | 35.94 |
| $N_5(1, m)$    | 33  | 58  | 87  | 115 | 154 | 190 | 200 |
| $P_5(1, m)$    | 33.00 | 29.00 | 29.00 | 28.75 | 30.80 | 31.67 | 31.25 |
| $N_5(2, m)$    | 36  | 71  | 102 | 140 | 167 | 192 | 205 |
| $P_5(2, m)$    | 36.00 | 35.50 | 34.00 | 35.00 | 33.40 | 32.00 | 32.03 |

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

References

[1] E. Alkan, Variations on Wolstenholme’s theorem, Amer. Math. Monthly 101(10) (1994), 1001–1004. MR: 95g:11001.

[2] D.F. Bailey, Two $p^3$ variations of Lucas’ theorem, J. Number Theory 35(2) (1990), 208–215. MR: 91f:11008.

[3] F.L. Bauer, For all primes greater than 3, $\left(\frac{2^p-1}{p-1}\right) \equiv 1 \pmod{p^3}$ holds, Math. Intelligencer 10(3) (1988), p. 42. MR: 89g:11005.

[4] M. Bayat, A generalization of Wolstenholme’s Theorem, Amer. Math. Monthly, 104(6) (1997), 557–560.

[5] J. Blümlein, Harmonic sums, Mellin transforms and Integrals, Int. J. Mod. Phys., A14 (1999), 2037-2076.

[6] J. Blümlein, Algebraic relations between harmonic sums and associated quantities, Comput. Phys. Commun., 159 (2004), 19-54.

[7] D.W. Boyd, A $p$-adic study of the partial sums of the harmonic series, Experimental Math., 3(4) (1994), 287–302.

[8] R. Bruck, Wolstenholme’s theorem, Stirling numbers, and binomial coefficients, available at mathlab.usc.edu/~bruck/research/stirling/.

[9] J.P. Buhler, R.E. Crandall, R. Ernvall, and T. Metsänkylä, Irregular primes and cyclotomic invariants to four million, Math. Comp. 61 (1993), 151–153. MR: 93k:11014.

[10] J.P. Buhler, R.E. Crandall, R. Ernvall, and T. Metsänkylä, and M.A. Shokrollahi, Primes and cyclotomic invariants to 12 million, Computational algebra and number theory (Milwaukee, WI, 1996). J. Symbolic Comput. 31 (2001), 89–96. MR: 2001m:11220.

[11] J.P. Butler, R.E. Crandall, R.W. Sompolski, Irregular primes to one million, Math. Comp. 59 (1992), 717–722. MR: 93k:11014.

[12] R.E. Crandall, Fast evaluation of multiple zeta sum, Math. Comp. 67 (1998), 1163–1172. MR: 98j:11066.

[13] R.E. Crandall and J.P. Buhler, On the evaluation of Euler sums, Experiment. Math. 3 (1994), 275–285. MR: 96e:11113.

[14] K. Dilcher, A bibliography of Bernoulli numbers, www.mscs.dal.ca/~dilcher/bernoulli.html.

[15] R. Ernvall and T. Metsänkylä, Cyclotomic invariants for primes between 125000 and 150000, Math. Comp. 56 (1991), 851–858. MR: 91h:11157
[16] R. Ernvall and T. Metsänkylä, Cyclotomic invariants for primes to one million, Math. Comp. 59 (1992), 249–250. MR: 93a:11108

[17] A. Esswarathasan and E. Levine, $p$-Integral harmonic sums, Discrete Math., 91 (1991), 249–257. MR: 93b:11039.

[18] A. Gardiner, Four problems on prime power divisibility, Amer. Math. Monthly 95 (1988), 926–931.

[19] I.M. Gessel, On Miki’s identity for Bernoulli numbers, J. Number Theory, to be published.

[20] J.W.L. Glaisher, On the residues of the sums of the inverse powers of numbers in arithmetical progression, Quarterly J. Math. 32 (1900), 271–288.

[21] R.L. Graham, D.E. Knuth, and O. Patashnik, Concrete mathematics, Addison-Wesley, Reading, MA 1989.

[22] A. Granville, Arithmetic properties of binomial coefficients I: Binomial coefficients modulo prime powers, Canad. Math. Soc. Conference Proceedings, 20 (1997), 253–275.

[23] R.K. Guy, A quarter century of Monthly unsolved problems, 1969-1993, Amer. Math. Monthly 100 (1993), 945–949.

[24] G.H. Hardy and E.M. Wright, An introduction to the theory of numbers, Clarendon press, Oxford, 1980.

[25] M.E. Hoffman, Algebraic aspects of multiple zeta values, arXiv.org/abs/math.QA/0309425

[26] M.E. Hoffman, Quasi-symmetric functions and mod $p$ multiple harmonic sums, arXiv.org/abs/math.NT/0401319

[27] K. Ireland and M. Rosen, A classical introduction to modern number theory, second edition, Spring-Verlag, 1990.

[28] W. Johnson, Irregular primes and cyclotomic invariants, Math. Comp. 29 (1975), 113–120. MR: 51 #12781.

[29] D.H. Lehmer, E. Lehmer, and H.S. Vandiver, An application of high-speed computing to Fermat’s last theorem, Proc. Nat. Acad. Sci. U.S.A. 40 (1954), 25–33. MR: 15,778f.

[30] E. Lehmer, On Congruences Involving Bernoulli Numbers and the Quotients of Fermat and Wilson, Ann. Math., 2nd Ser., 39 (1938), 350–360.

[31] R.J. McIntosh, On the converse of Wolstenholme’s theorem, Acta Arith. 71(4) (1995), 381–389. MR: 96h:11002.

[32] S. Slavutskii, Leudesdorf’s Theorem and Bernoulli numbers, Archivum Mathematicum (Brno), 35 (1999), 299–303.

[33] J.W. Tanner and S.S. Wagstaff, New congruences for the Bernoulli numbers, Math. Comp. 48 (1987), 341–350. MR: 87m:11017

[34] H. S. Vandiver, An Arithmetical Theory of the Bernoulli Numbers, Trans. Amer. Math. Soc., 51 (3)(1942), 502-531.

[35] S.S. Wagstaff, The irregular primes to 125000, Math. Comp. 32 (1978), 583–591. MR: 58 #10711.

[36] J. Zhao, Multiple harmonic sums II: finiteness of $p$-divisible sets, arxiv.org/abs/math.NT/0303043

[37] J. Zhao, Bernoulli numbers, Wolstenholme’s Theorem, and $p^5$ variations of Lucas’ Theorem, arxiv.org/abs/math.NT/0303332
[38] J. Zhao, Mod $p$ structure of the multiple harmonic sums of lower weights, in preparation.

[39] X. Zhou and T. Cai, A generalization of a curious congruence by Zhao, To appear in Proc. of Amer. Math. Soc.