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Supercongruences Involving Multiple Harmonic Sums and Bernoulli Numbers

Kevin Chen and Jianqiang Zhao
Department of Mathematics
The Bishop's School
La Jolla, CA 92037
USA chenk21@mit.edu, zhaoj@ihes.fr

Abstract

In this paper, we study some supercongruences involving multiple harmonic sums by using Bernoulli numbers. Our main theorem generalizes previous results by many different authors and confirms a conjecture by the authors and their collaborators. In the proof, we will need not only the ordinary multiple harmonic sums in which the indices are ordered, but also some variant forms in which the indices can be unordered or partially ordered. It is a crucial fact that the unordered multiple harmonic sums often behave better than the corresponding ordered sums when one considers congruences. We believe these unordered sums will play important roles in other studies in the future.

1 Introduction

The Bernoulli numbers, defined by the generating series

$$\frac{t}{e^t-1}=\sum_{k=0}^{\infty} B_k \frac{t^k}{k!},$$

have a long and intriguing history in the study of number theory, with over 3000 related papers written so far according to the online Bernoulli Number archive maintained by Dilcher and Slavutskii [3]. In modern mathematics, the Bernoulli numbers have appeared in the Euler-Maclaurin summation formula, Herbrand's theorem concerning the class group of cyclotomic number fields, and even the Kervaire-Milnor formula in topology.

Well-documented history indicates that Jakob Bernoulli, after whom the Bernoulli numbers are named, was very proud of his discovery that sums of powers of positive integers can be quickly calculated by using these numbers. This result was independently discovered by Seki around the same time [1] and by Faulhaber in a few instances some time earlier (so it is now generally called Faulhaber's formula). Classically, it is well-known that Bernoulli numbers play a very important role in studying congruences. For example, Sun [11] discovered a number of fascinating results along this direction. As in the previous work [4, 11], by Fermat's little theorem and Kummer's congruences, Faulhaber's formula quickly leads to many congruences and even supercongruences involving multiple harmonic sums, which were first studied independently by the second author [19, 20] and Hoffman [5]. See [22, Ch. 8] for more details.

Let $\mathbb{N}$ and $\mathbb{N}_0$ be the set of positive integers and nonnegative integers, respectively. For any $n, d \in \mathbb{N}$ and $\mathbf{s} = (s_1, \dots, s_d) \in \mathbb{N}^d$, we define the *multiple harmonic sums* (MHSs) and their p-restricted version for primes p by

$$\mathcal{H}_n(\mathbf{s}) := \sum_{0<k_1<\cdot<k_d<n} \frac{1}{k_1^{s_1} \dots k_d^{s_d}}, \quad \mathcal{H}_n^{(p)}(\mathbf{s}) := \sum_{\substack{0<k_1<\cdot<k_d<n \\ p\nmid k_1,\dots,p\nmid k_d}} \frac{1}{k_1^{s_1} \dots k_d^{s_d}}.$$

Here, d is called the *depth*, and $|\mathbf{s}| := s_1 + \cdots + s_d$ the *weight* of the MHS. For example, $\mathcal{H}_{n+1}(1)$ is often called the nth harmonic number. In general, as $n \to \infty$, we see that $\mathcal{H}_n(\mathbf{s}) \to \zeta(\mathbf{s})$ which are the multiple zeta values (MZVs).

More than a decade ago, the second author [18] discovered the curious congruence

$$\sum_{\substack{i+j+k=p \\ i,j,k>0}} \frac{1}{ijk} \equiv -2B_{p-3} \pmod p \tag{1}$$

for all primes $p \geq 3$. Since then, several different types of generalizations have been found. For example, see the references [8, 10, 13, 14, 16, 21, 23]. In this paper, we will concentrate on congruences of the following type of sums. Let $\mathcal{P}_p$ be the set of positive integers not divisible by p. For all positive integers r and m such that $p \nmid m$, define

$$R_n^{(m)}(p^r) := \sum_{\substack{l_1+l_2+\cdots+l_n=mp^r \\ l_1,\dots,l_n\in\mathcal{P}_p}} \frac{1}{l_1 l_2 \dots l_n}, \tag{2}$$

$$S_n^{(m)}(p^r) := \sum_{\substack{l_1+l_2+\cdots+l_n=mp^r \\ p^r>l_1,\dots,l_n\in\mathcal{P}_p}} \frac{1}{l_1 l_2 \dots l_n}. \tag{3}$$

To put these sums into proper framework, we now recall briefly the definition of the finite MZVs. Let $\mathfrak{P}$ be the set of rational primes. To study the congruences of MHSs, Kaneko and Zagier [6] consider the following ring structure (more precisely, the case $\ell = 1$) first used by

Kontsevich [7]

$$\mathcal{A}_\ell := \prod_{p\in\mathfrak{P}}(\mathbb{Z}/p^\ell\mathbb{Z}) \Big/ \bigoplus_{p\in\mathfrak{P}}(\mathbb{Z}/p^\ell\mathbb{Z}).$$

Two elements in $\mathcal{A}_\ell$ are the same if they differ at only finitely many components. For simplicity, we often write p^r for the element $\left(p^r\right)_{p\in\mathfrak{P}} \in \mathcal{A}_\ell$ for all positive integers $r < \ell$. For other properties and facts of $\mathcal{A}_\ell$ we refer the interested reader to [22, Ch. 8].

One now defines the finite MZVs as the following elements in $\mathcal{A}_\ell$:

$$\zeta_{\mathcal{A}_\ell}(\mathbf{s}) := \Big(\mathcal{H}_p(\mathbf{s}) \pmod{p^\ell}\Big)_{p\in\mathfrak{P}}.$$

It turns out that Bernoulli numbers often play important roles in the study of finite MZVs, as witnessed by the following result [23, p. 1332]:

$$\begin{aligned}
\zeta_{\mathcal{A}_3}(1_n) =& (-1)^{n-1}\frac{(n+1)}{2}\beta_{n+2}\cdot p^2 \quad && \text{if } 2\nmid n;\\
\zeta_{\mathcal{A}_2}(1_n) =& (-1)^n\beta_{n+1}\cdot p && \text{if } 2|n,
\end{aligned}$$

where 1_n is the string $(1,\dots,1)$ with 1 repeating n times, and $\beta_k := \big(-B_{p-k}/k \pmod p\big)_{p>k} \in \mathcal{A}_1$ is the so-called $\mathcal{A}$-Bernoulli number, which is the finite analog of $\zeta(k)$. Note that $\beta_k = 0$ for all even positive integers k while it is still a mystery whether $\beta_k \neq 0$ for all odd integers $k > 2$. In this framework, we can collect $R_n^{(m)}(p^r)$ and $S_n^{(m)}(p^r)$ defined in (2) and (3) for various primes and form a pair of elements in $\mathcal{A}_r$ by putting

$$R_n^{(m,r)} = \big(R_n^{(m)}(p^r)\big)_{p>m}, \quad S_n^{(m,r)} = \big(S_n^{(m)}(p^r)\big)_{p>m}.$$

Previously, the second author and his collaborators [8] made the following conjecture.

Conjecture 1. For any $m, n \in \mathbb{N}$, both $R_n^{(m,1)}$ and $S_n^{(m,1)}$ are elements in the sub-algebra of $\mathcal{A}_1$ generated by the $\mathcal{A}$-Bernoulli numbers.

In this paper, we will prove this conjecture. More precisely, we have the following, our main theorem.

Theorem 2. *Let m, r and n be positive integers. Let $\mathbf{k} \vdash n$ denote any tuple of odd positive integers $\mathbf{k} = (k_1,\dots,k_t)$ such that $k_1+\dots+k_t = n$ and $k_j \geq 3$ for all j. Then for every sufficiently large prime p*

$$R_n^{(m)}(p^r) = \sum_{\substack{l_1+l_2+\dots+l_n=mp^r\\ p\nmid l_1l_2\cdots l_n}} \frac{1}{l_1l_2\cdots l_n} \equiv p^{r-1}\sum_{\mathbf{k}\vdash n} C_{m,\mathbf{k}}B_{p-\mathbf{k}} \pmod{p^r}, \tag{4}$$

$$S_n^{(m)}(p^r) = \sum_{\substack{l_1+l_2+\dots+l_n=mp^r\\ p\nmid l_1l_2\cdots l_n}} \frac{1}{l_1l_2\cdots l_n} \equiv p^{r-1}\sum_{\mathbf{k}\vdash n} C'_{m,\mathbf{k}}B_{p-\mathbf{k}} \pmod{p^r}, \tag{5}$$

where $B_{p-\mathbf{k}} = B_{p-k_1}B_{p-k_2}\cdots B_{p-k_t}$ are products of Bernoulli numbers and the coefficients $C_{m,\mathbf{k}}$ and $C'_{m,\mathbf{k}}$ are polynomials of m independent of p and r.

The coefficients $C_{m,\mathbf{k}}$ and $C'_{m,\mathbf{k}}$ are intimately related, see Conjecture 16.

As a side remark, in our numerical computation, it is crucial to use some generating functions of $R_n^{(m,r)}$ and $S_n^{(m,r)}$, which are certain products of a finite variation of the p-restricted classical polylogarithm function. Unfortunately, it seems difficult to use these generating functions to obtain our main result of this paper.

We conclude this introduction by pointing out that the general congruence structure of (2) and (3) hints at a similar picture to that of the MZVs and their finite version if we consider more general sums by allowing the indices in (2) and (3) to have different exponents. A seminal work was done by Yang and Cai in depth two [17]. It would be very interesting to find out if the Bernoulli numbers are indeed insufficient in the general depth cases, as for MZVs and and their finite version.

2 Preliminary lemmas

In this section, we collect some useful results to be applied in the rest of the paper.

Lemma 3. (cf. [8, Lemma 3.4]) *Let p be a prime, $\kappa, s_1, \dots, s_d$ be positive integers, and γ a non-negative integer. We define the* un-ordered sum

$$U^{(p)}_{\gamma;\kappa}(s_1,\dots,s_d) := \sum_{\substack{\gamma p < l_1,\dots,l_d < (\gamma+\kappa)p \\ l_1,\dots,l_d \in \mathcal{P}_p,\ l_i \neq l_j \forall i \neq j}} \frac{1}{l_1^{s_1}\cdots l_d^{s_d}}.$$

If the weight $w = s_1 + \cdots + s_d \le p-3$ then we have

$$U^{(p)}_{\gamma;\kappa}(s_1,\dots,s_d) \equiv (-1)^{d-1}(d-1)!\frac{\kappa w}{w+1}B_{p-w-1}\cdot p \pmod{p^2}.$$

Lemma 4. *Suppose $a, k, m, n, r \in \mathbb{N}$ and p is a prime. Set*

$$\gamma_n^{(m)}(a) := (-1)^{m+a}\binom{n-2}{m-1}\frac{(a-1)!(n-1-a)!}{(n-1)!}.$$

If $k < n < p-1$ then we have

(i) $S_n^{(k)}(p^r) \equiv (-1)^n S_n^{(n-k)}(p^r) \pmod{p^r}$*;*

(ii) $S_n^{(m)}(p^{r+1}) \equiv p\sum_{a=1}^{n-1}\gamma_n^{(m)}(a)S_n^{(a)}(p^r) \pmod{p^{r+1}}$*;*

(iii) $S_n^{(m)}(p^{r+1}) \equiv (-1)^{m-1}\binom{n-2}{m-1}S_n^{(1)}(p^2)p^{r-1} \pmod{p^{r+1}}$*.*

Proof. Parts (i) and (ii) follow from [8, Lemma 2.3], while part (iii) follows from [2, Lemma 2.2]. ∎

Lemma 5. ([2, Proposition 2.3]) *Let $m, n, r \in \mathbb{N}$. For all $r \geq 2$, we have*

$$R_n^{(m,r)} = m \cdot S_n^{(1,2)} p^{r-2} \in \mathcal{A}_r.$$

Lemma 6. *Suppose $m, n, r \in \mathbb{N}$. Then we have*

$$S_n^{(m,r)} = \sum_{k=0}^{m-1} (-1)^k \binom{n}{k} R_n^{(m-k,r)} \in \mathcal{A}_r. \tag{6}$$

Proof. Equation (6) can be proved using the inclusion-exclusion principle similar to the proof of [15, Lemma 1]. Indeed, for all primes p

$$\begin{aligned}
S_n^{(m)}(p^r) &= \sum_{\substack{l_1+\cdots+l_n=mp^r \\ l_1,\cdots,l_n\in\mathcal{P}_p}} \frac{1}{l_1\cdots l_n} + \sum_{k=1}^{m-1}(-1)^k \sum_{\substack{1\le a_1<\cdots<a_k\le n \\ l_1+\cdots+l_n=mp^r \\ l_1,\cdots,l_n\in\mathcal{P}_p \\ l_{a_1}>p^r,\cdots,l_{a_k}>p^r}} \frac{1}{l_1\cdots l_n} \\
&= \sum_{k=0}^{m-1}(-1)^k \binom{n}{k} \sum_{\substack{l_1+\cdots+l_n=(m-k)p^r \\ l_1,\cdots,l_n\in\mathcal{P}_p}} \frac{1}{(l_1+p^r)\cdots(l_k+p^r)l_{k+1}\cdots l_n} \\
&\equiv \sum_{k=0}^{m-1}(-1)^k \binom{n}{k} \sum_{\substack{l_1+\cdots+l_n=(m-k)p^r \\ l_1,\cdots,l_n\in\mathcal{P}_p}} \frac{1}{l_1\cdots l_n} \pmod{p^r} \\
&\equiv \sum_{k=0}^{m-1}(-1)^k \binom{n}{k} R_n^{(m-k)}(p^r) \pmod{p^r},
\end{aligned}$$

as desired. ∎

We see immediately from Lemmas 5 and 6 that the proof of the Theorem 2 is reduced to its special case of $S_n^{(1,2)}$. The idea is to compute $R_n^{(m,1)}$ first, which leads to $S_n^{(m,1)}$ by the Lemma 6. Then $S_n^{(1,2)}$ can be determined using $S_n^{(m,1)}$ by Lemma 4 (ii).

For the convenience of numerical computation, we list some of the relevant known results.

Lemma 7. ([23, Main Theorem]) *Let $n > 1$ be a positive integer. Then we have*

$$S_n^{(1,1)} = R_n^{(1,1)} = \begin{cases} n!\beta_n, & \text{if } 2 \nmid n; \\ 0, & \text{if } 2 \mid n. \end{cases}$$

Lemma 8. *Let $n > 1$ be a positive integer. Then we have*

$$R_n^{(2,1)} = \begin{cases} \dfrac{(n+1)!}{2}\beta_n, & \text{if } 2 \nmid n; \\ \dfrac{n!}{2} \displaystyle\sum_{(a,b)\vdash n} \beta_a\beta_b, & \text{if } 2 \mid n, \end{cases}$$

and

$$S_n^{(2,1)} = \begin{cases} -\dfrac{n-1}{2} n!\beta_n, & \text{if } 2 \nmid n; \\ \dfrac{n!}{2} \displaystyle\sum_{(a,b)\vdash n} \beta_a\beta_b, & \text{if } 2 \mid n. \end{cases}$$

Proof. The odd cases follow from [8, Lemma 3.5 and Corollary 3.6] respectively. The even cases are proved as [15, Theorem 1 and Corollary 1]. □

Lemma 9. *Let $n > 1$ be a positive integer. Then we have*

$$R_n^{(3,1)} = \begin{cases} \dbinom{n+2}{3} \cdot (n-1)!\beta_n + \dfrac{n!}{6} \displaystyle\sum_{(a,b,c)\vdash n} \beta_a\beta_b\beta_c, & \text{if } 2 \nmid n; \\ \dfrac{n!(n+2)}{4} \displaystyle\sum_{(a,b)\vdash n} \beta_a\beta_b, & \text{if } 2 \mid n, \end{cases}$$

and

$$S_n^{(3,1)} = \begin{cases} \dbinom{n}{3} \cdot (n-1)!\beta_n + \dfrac{n!}{6} \displaystyle\sum_{(a,b,c)\vdash n} \beta_a\beta_b\beta_c, & \text{if } 2 \nmid n; \\ -\dfrac{n!(n-2)}{4} \displaystyle\sum_{(a,b)\vdash n} \beta_a\beta_b, & \text{if } 2 \mid n. \end{cases}$$

Proof. The odd cases follow from [8, Lemma 3.7 and Corollary 3.7] respectively. The even cases are essentially proved as [15, Theorem 2 and Corollary 2]. We only need to observe that if n is even then by exchanging the indices a and b in half of the sums, we get

$$\begin{aligned} R_n^{(3)}(p) \equiv & \frac{n!}{6} \sum_{(a,b)\vdash n} (2n-a+3) \frac{B_{p-a}B_{p-b}}{ab} && \pmod p \\ \equiv & \frac{n!}{12} \sum_{(a,b)\vdash n} (4n-a-b+6) \frac{B_{p-a}B_{p-b}}{ab} && \pmod p \\ \equiv & \frac{n!(n+2)}{4} \sum_{(a,b)\vdash n} \frac{B_{p-a}B_{p-b}}{ab} && \pmod p \end{aligned}$$

since $a + b = n$. Similarly,

$$\begin{aligned} S_n^{(3)}(p) \equiv & -\frac{n!}{6} \sum_{(a,b)\vdash n} (n+a-3) \frac{B_{p-a}B_{p-b}}{ab} && \pmod p \\ \equiv & -\frac{n!}{12} \sum_{(a,b)\vdash n} (2n+a+b-6) \frac{B_{p-a}B_{p-b}}{ab} && \pmod p \\ \equiv & -\frac{n!(n-2)}{4} \sum_{(a,b)\vdash n} \frac{B_{p-a}B_{p-b}}{ab} && \pmod p \end{aligned}$$

as desired. □

3 Sums related to multiple harmonic sums

We are now ready to consider the sums $R_n^{(m,r)}$. The key step is to compute $R_n^{(m,1)}$ for $m \le n/2$, which we now transform using MHSs. By the definition, for all primes p, we have

$$\begin{aligned}
R_n^{(m)}(p) =&\frac{1}{mp}\sum_{\substack{l_1+l_2+\cdots+l_n=mp\\ l_1,\dots,l_n\in\mathcal{P}_p}}\frac{l_1+l_2+\cdots+l_n}{l_1l_2\dots l_n}\\
=&\frac{n}{mp}\sum_{\substack{u_{n-1}=l_1+l_2+\cdots+l_{n-1}<mp\\ l_1,\dots,l_{n-1},u_{n-1}\in\mathcal{P}_p}}\frac{1}{l_1l_2\dots l_{n-1}}\quad\text{(by symmetry of } l_1,\dots,l_n)\\
=&\frac{n}{mp}\sum_{\substack{u_{n-1}=l_1+l_2+\cdots+l_{n-1}<mp\\ l_1,\dots,l_{n-1},u_{n-1}\in\mathcal{P}_p}}\frac{l_1+l_2+\cdots+l_{n-1}}{l_1l_2\dots l_{n-1}u_{n-1}}\\
=&\frac{n(n-1)}{mp}\sum_{\substack{u_{n-2}=l_1+l_2+\cdots+l_{n-2}<u_{n-1}<mp\\ l_1,\dots,l_{n-2}\in\mathcal{P}_p\\ u_{n-1}-u_{n-2},u_{n-1}\in\mathcal{P}_p}}\frac{1}{l_1l_2\dots l_{n-2}u_{n-1}}.
\end{aligned}$$

Continuing this process by using the substitution $u_j = l_1 + l_2 + \cdots + l_j$ for each $j = n-3,\dots,2,1$, we arrive at

$$R_n^{(m)}(p) = \frac{n!}{mp}\sum_{\substack{0<u_1<\cdots<u_{n-1}<mp\\ u_1,u_2-u_1,\dots,u_{n-1}-u_{n-2},u_{n-1}\in\mathcal{P}_p}}\frac{1}{u_1u_2\dots u_{n-1}}.$$

Observe that the indices u_j ($j = 2,\dots,n-2$) are allowed to be multiples of p. Thus we set

$$T_{n,\ell}^{(m)}(p) := \sum_{\substack{2\le a_1<\cdots<a_{\ell-1}\le n-2\\ 1\le k_1<\cdots<k_{\ell-1}<m}}\ \sum_{\substack{0<u_1<\cdots<u_{n-1}<mp\\ u_{a_1}=k_1p,\dots,u_{a_{\ell-1}}=k_{\ell-1}p,\\ u_j\in\mathcal{P}_p\ \forall j\ne a_1,\dots,a_{\ell-1}\\ u_2-u_1,\dots,u_{n-1}-u_{n-2}\in\mathcal{P}_p}}\frac{1}{u_1\dots u_{n-1}}.$$

In this sum, the indices $u_1,\dots,u_{n-1}$ are divided into ℓ-parts by p-multiples so that the indices inside each part (excluding the boundaries) are all prime to p. Hence we can rewrite

$$R_n^{(m)}(p) = \frac{n!}{mp}\sum_{1\le\ell<n/2}T_{n,\ell}^{(m)}(p). \tag{7}$$

So we are naturally led to the study of the following sums. Let $\gamma\in\mathbb{N}_0$, $\kappa, n\in\mathbb{N}$ and p be a prime. Suppose $n>1$. Define

$$\Xi_{\gamma;\kappa}^{(p)}(n) := \sum_{\substack{\gamma p<u_1<\cdots<u_{n-1}<(\gamma+\kappa)p\\ u_1,u_2,\dots,u_{n-1}\in\mathcal{P}_p\\ u_2-u_1,\dots,u_{n-1}-u_{n-2}\in\mathcal{P}_p}}\frac{1}{u_1\dots u_{n-1}}.$$

For convenience, in the above sum if the difference between two adjacent indices is a multiple of p (which is of course not allowed in the definition of Ξ) we then say there is a p-gap between this pair of indices. Let $\gamma \in \mathbb{N}_0$ and $\kappa \in \mathbb{N}$. For all $1 \le g \le \min\{\kappa-1, n-2\}$, define the sum in which at least g p-gaps appear by

$$P^{g;p}_{\gamma;\kappa}(n) := \sum_{1<b_1<\cdots<b_g<n} \sum_{\substack{\gamma p<u_1<\cdots<u_{n-1}<(\gamma+\kappa)p \\ u_1,u_2,\dots,u_{n-1}\in\mathcal{P}_p \\ p|(u_{b_1}-u_{b_1-1}),\dots,p|(u_{b_g}-u_{b_g-1})}} \frac{1}{u_1\dots u_{n-1}}. \tag{8}$$

The following technical result is crucial in the proof of our main theorem, Theorem 2.

Proposition 10. *Let $\gamma \in \mathbb{N}_0$, $\kappa, n \in \mathbb{N}$. Then, for all $1 \le g \le \min\{\kappa-1, n-2\}$, we have*

$$P^{g;p}_{\gamma;\kappa}(n) \equiv P^{g;p}_{0;\kappa}(n) \equiv -(-1)^g \binom{\kappa}{g+1}\binom{n-1}{g}\frac{B_{p-n}}{n}p \pmod{p^2}. \tag{9}$$

We postpone the proof of this proposition to the next section due to its length. A direct consequence is the following corollary.

Corollary 11. *Let $\gamma, \kappa, n \in \mathbb{N}$. Then for all primes $p > n+1$, we have*

$$\Xi^{(p)}_{\gamma;\kappa}(n) \equiv \left(\binom{\kappa}{n} - \binom{\kappa+n-1}{n}\right)\frac{B_{p-n}}{n}p \pmod{p^2}.$$

Proof. Set $\delta_{n>j} = 1$ if $n > j$ and $\delta_{n>j} = 0$ if $n \le j$. By the inclusion-exclusion principle, it is clear that

$$\begin{aligned}
\Xi^{(p)}_{\gamma;\kappa}(n) =& \frac{U^{(p)}_{\gamma;\kappa}(1_{n-1})}{(n-1)!} + \sum_{g=1}^{\kappa-1}(-1)^g \delta_{n>g+1} P^{g;p}_{\gamma;\kappa}(n) \\
\equiv& -\sum_{h=1}^{\kappa} \delta_{n>h}\binom{\kappa}{h}\binom{n-1}{h-1}\frac{B_{p-n}}{n}p \qquad \pmod{p^2} \\
\equiv& \left(\binom{\kappa}{n} - \sum_{h=1}^{\kappa}\binom{\kappa}{h}\binom{n-1}{h-1}\right)\frac{B_{p-n}}{n}p \pmod{p^2}
\end{aligned}$$

by (9) and the congruence (see Lemma 3)

$$\frac{U^{(p)}_{0;\kappa}(1_{n-1})}{(n-1)!} \equiv (-1)^n \frac{\kappa B_{p-n}}{n}p \equiv -\frac{\kappa B_{p-n}}{n}p \pmod{p^2}.$$

Here we used the fact that $B_k = 0$ if $k > 1$ and k is odd. So the proposition follows immediately from the well-known binomial identity

$$\sum_{h=1}^{\kappa}\binom{\kappa}{h}\binom{n-1}{h-1} = \sum_{h=1}^{\kappa}\binom{\kappa}{h}\binom{n-1}{n-h} = \binom{\kappa+n-1}{n}.$$

$\square$

By Corollary 11, it is easy to see that for any fixed $\ell < n/2$

$$T_{n,\ell}^{(m)}(p) \equiv \sum_{\substack{1\le a_1<\cdots<a_{\ell-1}<n\\ 1\le k_1<\cdots<k_{\ell-1}<m}} \left(\prod_{j=1}^{\ell-1}\frac{1}{k_j p}\right)\left(\prod_{j=1}^{\ell}\Xi^{(p)}_{k_{j-1};k_j-k_{j-1}}(a_j-a_{j-1})\right)$$

$$\equiv p \sum_{\substack{k_1+\cdots+k_\ell=m\\ k_1,\dots,k_\ell\ge 1\\ (a_1,\dots,a_\ell)\vdash n}} \prod_{j=1}^{\ell-1}\frac{1}{k_1+\cdots+k_j}\prod_{j=1}^{\ell}\left(\binom{k_j}{a_j}-\binom{k_j+a_j-1}{a_j}\right)\frac{B_{p-a_j}}{a_j} \tag{10}$$

modulo p^2, where we have set $k_0 = a_0 = 0$ and $k_\ell = m, a_\ell = n$. In the last step above, we have used substitutions $k_j \to k_1 + \cdots + k_j$ and $a_j \to a_1 + \cdots + a_j$ for all $j \le \ell - 1$. In view of (7) and Lemma 6, we easily obtain the following result which confirms Conjecture 1.

Theorem 12. *For all positive integer m and n, we have*

$$R_n^{(m,1)} = \frac{n!}{m} \sum_{\substack{1\le \ell\le \lfloor n/3\rfloor\\ k_1+\cdots+k_\ell=m, k_j\ge 1\forall j\\ (a_1,\dots,a_\ell)\vdash n}} \prod_{j=1}^{\ell-1}\frac{1}{k_1+\cdots+k_j}\prod_{j=1}^{\ell}\left(\binom{k_j+a_j-1}{a_j}-\binom{k_j}{a_j}\right)\beta_{a_j}.$$

We only need to remark that $(a_1, \dots, a_\ell) \vdash n$ implies that $3\ell \le a_1 + \cdots + a_\ell = n$.

4 Some numerical examples

Using the formula of Theorem 12, we obtain the following results which extend those in Lemmas 7, 8 and 9. To guarantee accuracy, we have checked these congruences for $m, n \le 20$ and primes $p < 100$ using Maple.

Corollary 13. *For any $\kappa, m, n \in \mathbb{N}$, we have*

$$R_3^{(m,1)} = 3!m\beta_3,\ R_5^{(m,1)} = \frac{5!}{3!}m(m^2+5)\beta_5,\ R_7^{(m,1)} = \frac{7!}{5!}m(m^4+35m^2+84)\beta_7. \tag{11}$$

If $n \ge 9$ is odd, then

$$R_n^{(4,1)} =(n-1)!\binom{n+3}{4}\beta_n + \frac{n!(n+3)}{2\cdot 3!}\sum_{(a,b,c)\vdash n}\beta_a\beta_b\beta_c,$$

$$R_n^{(5,1)} =(n-1)!\binom{n+4}{5}\beta_n + \frac{n!}{5!}\sum_{(a_1,\dots,a_5)\vdash n}\beta_{a_1}\cdots\beta_{a_5}$$

$$+\frac{n!}{4!}\sum_{(a,b,c)\vdash n}\left(\frac{n^2}{2}+4n+7+\frac{a^2}{2}-4\binom{3}{a}\right)\beta_a\beta_b\beta_c,$$

$$
\begin{aligned}
R_n^{(6,1)} =&(n-1)!\binom{n+5}{6}\beta_n + \frac{n!(n+5)}{2\cdot 5!}\sum_{(a_1,\ldots,a_5)\vdash n}\beta_{a_1}\cdots\beta_{a_5}\\
&+\frac{n!}{4\cdot 4!}\sum_{(a,b,c)\vdash n}\left(\frac{n^3}{3}+a^3+2a^2b+5n^2+5a^2+\frac{68n}{3}+30-8\binom{3}{a}(n+5)\right)\beta_a\beta_b\beta_c.
\end{aligned}
$$

If $n \geq 2$ is even, then

$$
\begin{aligned}
R_n^{(4,1)} =&\frac{n!}{4!}\left(\sum_{(a,b)\vdash n}\left(\frac{3}{2}n^2+9n+11+a^2-8\binom{3}{a}\right)\beta_a\beta_b + \sum_{(a,b,c,d)\vdash n}\beta_a\beta_b\beta_c\beta_d\right),\\
R_n^{(5,1)} =&\frac{n!}{3\cdot 4!}\sum_{(a,b)\vdash n}\left(n^3+9n^2+\frac{63}{2}n+30+a^3+6a^2-12(n+4)\binom{3}{a}\right)\beta_a\beta_b\\
&+\frac{n!(n+4)}{2\cdot 4!}\sum_{(a,b,c,d)\vdash n}\beta_a\beta_b\beta_c\beta_d,\\
R_n^{(6,1)} =&\frac{n!}{6!}\sum_{(a,b,c,d,e,f)\vdash n}\beta_a\beta_b\beta_c\beta_d\beta_e\beta_f\\
&+\frac{n!}{6}\sum_{(a,b)\vdash n}\left(\frac{1}{3}\binom{3}{a}\binom{3}{b}-\frac{6}{5}\binom{5}{a}-\frac{n^2+6n-16}{3}\binom{3}{a}+\frac{1}{5!}\left(\frac{8}{3}a^4+\right.\right.\\
&\left.\left.+25a^3+85a^2+\frac{675n}{2}+274+\frac{5}{6}a^3n+\frac{5}{3}n^4+25n^3+\frac{255}{2}n^2\right)\right)\beta_a\beta_b\\
&+\frac{n!}{144}\sum_{(a,b,c,d)\vdash n}\left(a^2+\frac{3n^2}{4}+\frac{15n}{2}+17-8\binom{3}{a}\right)\beta_a\beta_b\beta_c\beta_d.
\end{aligned}
$$

Example 14. When $8 \leq n \leq 12$, we get, respectively,

$$
\begin{aligned}
R_8^{(4,1)} =&16\cdot 8!\beta_3\beta_5, & R_9^{(4,1)} &= 9!(55\beta_9+\beta_3^3),\\
R_{10}^{(5,1)} =&35\cdot 10!(2\beta_3\beta_7+\beta_5^2), & R_{11}^{(5,1)} &= 11!\left(273\beta_{11}+\frac{29}{2}\beta_3^2\beta_5\right),\\
R_{12}^{(6,1)} =&12!\left(333\beta_3\beta_9+321\beta_5\beta_7+\frac{3}{2}\beta_3^4\right).
\end{aligned}
$$

The first three identities were predicted previously [8, Conjecture 5.1]. The last two were also discovered numerically earlier [21, Conjecture 7.2].

Corollary 15. *Let $n \geq 2$ be a positive integer. If n is odd, then*

$$S_n^{(4,1)} = -(n-1)!\binom{n}{4}\beta_n - \frac{n!(n-3)}{12}\sum_{(a,b,c)\vdash n}\beta_a\beta_b\beta_c,$$

$$S_n^{(5,1)} = (n-1)!\binom{n}{5}\beta_n + \frac{n!}{5!}\sum_{(a_1,\dots,a_5)\vdash n}\beta_{a_1}\cdots\beta_{a_5}$$
$$+\frac{n!}{4!}\sum_{(a,b,c)\vdash n}\left(\frac{n^2}{2} - 4n + 7 + \frac{a^2}{2} - 4\binom{3}{a}\right)\beta_a\beta_b\beta_c,$$

$$S_n^{(6,1)} = -(n-1)!\binom{n}{6}\beta_n - \frac{n-5}{2\cdot 5!}\sum_{(a_1,\dots,a_5)\vdash n}\beta_{a_1}\cdots\beta_{a_5}$$
$$-\frac{1}{96}\sum_{(a,b,c)\vdash n}\left(\frac{n^3}{3} + a^3 - 2a^2b - 5n^2 + 5a^2 + \frac{68n}{3} - 30 - 8\binom{3}{a}(n-5)\right)\beta_a\beta_b\beta_c.$$

If n is even, then

$$S_n^{(4,1)} = \frac{n!}{4!}\sum_{(a,b)\vdash n}\left(\frac{3}{2}n^2 - 9n + 11 + a^2 - 8\binom{3}{a}\right)\beta_a\beta_b + \frac{n!}{4!}\sum_{(a,b,c,d)\vdash n}\beta_a\beta_b\beta_c\beta_d,$$

$$S_n^{(5,1)} = \frac{n!}{144}\sum_{(a,b)\vdash n}\left(-2n^3 + 18n^2 - 63n + 60 - 2a^3 + 12a^2 + 24(n-4)\binom{3}{a}\right)\beta_a\beta_b$$
$$-\frac{n!(n-4)}{48}\sum_{(a,b,c,d)\vdash n}\beta_a\beta_b\beta_c\beta_d,$$

$$S_n^{(6,1)} = \frac{n!}{6!}\sum_{(a,b,c,d,e,f)\vdash n}\beta_a\beta_b\beta_c\beta_d\beta_e\beta_f$$
$$+\frac{n!}{6}\sum_{(a,b)\vdash n}\left(\frac{1}{3}\binom{3}{a}\binom{3}{b} - \frac{6}{5}\binom{5}{a} - \frac{n^2-9n-16}{3}\binom{3}{a} + \frac{1}{5!}\left(\frac{8}{3}a^4\right.\right.$$
$$\left.\left.-25a^3 + 85a^2 - \frac{675n}{2} + 274 + \frac{5}{6}a^3n + \frac{5}{3}n^4 - 25n^3 + \frac{255}{2}n^2\right)\right)\beta_a\beta_b$$
$$+\frac{n!}{144}\sum_{(a,b,c,d)\vdash n}\left(a^2 + \frac{3n^2}{4} - \frac{15n}{2} + 17 - 8\binom{3}{a}\right)\beta_a\beta_b\beta_c\beta_d.$$

Proof. By Lemma 6, we see that

$$S_n^{(4,1)} = R_n^{(4,1)} - nR_n^{(3,1)} + \binom{n}{2}R_n^{(2,1)} - \binom{n}{3}R_n^{(1,1)}.$$

Thus the statements concerning $S_n^{(4,1)}$ follow from Lemma 7, 8, 9 and Corollary 13 immediately. The computation of $S_n^{(5,1)}$ and $S_n^{(6,1)}$ can be done similarly. So we leave them to the interested reader. □

By comparing the above two corollaries, we can formulate the following conjecture.

Conjecture 16. For all $m, n \in \mathbb{N}$, suppose

$$R_n^{(m,1)} = n! \sum_{1 \le l \le n/3, 2|(n-l)} \sum_{(a_1,\ldots,a_l) \vdash n} C(a_1, \ldots, a_l)\beta_{a_1} \ldots \beta_{a_l}.$$

Then

$$S_n^{(m,1)} = n! \sum_{1 \le l \le n/3, 2|(n-l)} \sum_{(a_1,\ldots,a_l) \vdash n} C(-a_1, \ldots, -a_l)\beta_{a_1} \ldots \beta_{a_l}.$$

Corollary 17. *For all $r \ge 2$, we have*

$$\begin{aligned}
S_8^{(m,r)} =&(-1)^m \binom{6}{m-1} 5376\beta_3\beta_5 p^{r-1} && \in \mathcal{A}_r \quad \forall m \le 7,\\
S_9^{(m,r)} =&(-1)^{m-1} \binom{7}{m-1} 36(6088\beta_9 + 61\beta_3^3)p^{r-1} && \in \mathcal{A}_r \quad \forall m \le 8,\\
S_{10}^{(m,r)} =&(-1)^m \binom{8}{m-1} 223200(\beta_5^2 + 2\beta_3\beta_7)p^{r-1} && \in \mathcal{A}_r \quad \forall m \le 9,\\
S_{11}^{(m,r)} =&(-1)^{m-1} \binom{9}{m-1} 174240(122\beta_{11} + 3\beta_3^2\beta_5)p^{r-1} && \in \mathcal{A}_r \quad \forall m \le 10,\\
S_{12}^{(m,r)} =&(-1)^m \binom{10}{m-1} 47520(896\beta_3\beta_9 + 872\beta_5\beta_7 + 3\beta_3^4)p^{r-1} && \in \mathcal{A}_r \quad \forall m \le 11.
\end{aligned}$$

Proof. Let p be a prime such that $p \ge 17$. By Lemma 7, 8, 9, and Corollary 15, we have modulo p

$$\begin{aligned}
&S_8^{(1)}(p) \equiv 0,\ S_8^{(2)}(p) \equiv \frac{8!}{15} B_{p-3}B_{p-5},\ S_8^{(3)}(p) \equiv -3S_8^{(2)}(p),\ S_8^{(4)}(p) \equiv 4S_8^{(2)}(p),\\
&S_9^{(1)}(p) \equiv -8!B_{p-9},\ S_9^{(2)}(p) \equiv 4 \cdot 8!B_{p-9},\\
&S_9^{(3)}(p) \equiv -\frac{8!}{18}B_{p-3}^3 - \frac{28 \cdot 8!}{3}B_{p-9}, S_9^{(4)}(p) \equiv \frac{8!}{6}B_{p-3}^3 + 14 \cdot 8!B_{p-9},\\
&S_{10}^{(1)}(p) \equiv 0,\ S_{10}^{(2)}(p) \equiv \frac{1}{2} \cdot 10! \left(\frac{B_{p-5}^2}{25} + \frac{2B_{p-3}B_{p-7}}{21}\right),\\
&S_{10}^{(3)}(p) \equiv -4S_{10}^{(2)}(p), S_{10}^{(4)}(p) \equiv 8S_{10}^{(2)}(p),\ S_{10}^{(5)}(p) \equiv -10S_{10}^{(2)}(p),
\end{aligned}$$

$$\begin{aligned}
S_{11}^{(1)}(p) \equiv& -10!B_{p-11},\ S_{11}^{(2)}(p) \equiv 5\cdot 10!B_{p-11},\\
S_{11}^{(3)}(p) \equiv& -\frac{11!}{90}B_{p-3}^2B_{p-5} - 15\cdot 10!B_{p-11},\\
S_{11}^{(4)}(p) \equiv& \frac{2\cdot 11!}{45}B_{p-3}^2B_{p-5} + 30\cdot 10!B_{p-11},\\
S_{11}^{(5)}(p) \equiv& -\frac{7\cdot 11!}{90}B_{p-3}^2B_{p-5} - 42\cdot 10!B_{p-11},\\
S_{12}^{(1)}(p) \equiv& 0,\ S_{12}^{(2)}(p) \equiv \frac{12!}{27}B_{p-3}B_{p-9} + \frac{12!}{35}B_{p-5}B_{p-7},\ S_{12}^{(3)}(p) \equiv -5S_{12}^{(2)}(p),\\
S_{12}^{(4)}(p) \equiv& \frac{40\cdot 12!B_{p-3}B_{p-9}}{81} + 13\cdot 12!\frac{B_{p-5}B_{p-7}}{35} + \frac{12!}{24}\frac{B_{p-3}^4}{3^4},\\
S_{12}^{(5)}(p) \equiv& -\frac{70\cdot 12!B_{p-3}B_{p-9}}{81} - 22\cdot 12!\frac{B_{p-5}B_{p-7}}{35} - \frac{12!}{6}\frac{B_{p-3}^4}{3^4},\\
S_{12}^{(6)}(p) \equiv& \frac{28\cdot 12!B_{p-3}B_{p-9}}{27} + 26\cdot 12!\frac{B_{p-5}B_{p-7}}{35} + \frac{12!}{4}\frac{B_{p-3}^4}{3^4}.
\end{aligned}$$

Taking $n = 8$ and $r = 1$ in Lemma 4 (i) and (ii), we get

$$\begin{aligned}
S_8^{(1)}(p^2) \equiv& \frac{2p}{7}S_8^{(1)}(p) - \frac{p}{21}S_8^{(2)}(p) + \frac{2p}{105}S_8^{(3)}(p) - \frac{p}{140}S_8^{(4)}(p)\\
\equiv& -\frac{1792}{5}pB_{p-3}B_{p-5} \pmod{p^2}.
\end{aligned}$$

Similarly, taking $9 \le n \le 12$ and $r = 1$ in Lemma 4 (i) and (ii), we see that

$$\begin{aligned}
S_9^{(1)}(p^2) \equiv& \frac{p}{4}S_9^{(1)}(p) - \frac{p}{28}S_9^{(2)}(p) + \frac{p}{84}S_9^{(3)}(p) - \frac{p}{140}S_9^{(4)}(p)\\
\equiv& -288\left(\frac{761B_{p-9}}{9} + \frac{7B_{p-3}^3}{3^3}\right)p \pmod{p^2},\\
S_{10}^{(1)}(p^2) \equiv& \frac{2p}{9}S_{10}^{(1)}(p) - \frac{p}{36}S_{10}^{(2)}(p) + \frac{p}{126}S_{10}^{(3)}(p) - \frac{p}{252}S_{10}^{(4)}(p) + \frac{p}{630}S_{10}^{(5)}(p)\\
\equiv& -194400\left(\frac{B_{p-5}^2}{25} + \frac{2B_{p-3}B_{p-7}}{21}\right)p \pmod{p^2},\\
S_{11}^{(1)}(p^2) \equiv& \frac{p}{5}S_{11}^{(1)}(p) - \frac{p}{45}S_{11}^{(2)}(p) + \frac{p}{180}S_{11}^{(3)}(p) - \frac{p}{420}S_{11}^{(4)}(p) + \frac{p}{630}S_{11}^{(5)}(p)\\
\equiv& -174240\left(\frac{122B_{p-11}}{11} + \frac{3B_{p-3}^2B_{p-5}}{45}\right)p \pmod{p^2},\\
S_{12}^{(1)}(p^2) \equiv& \frac{2p}{11}S_{12}^{(1)}(p) - \frac{p}{55}S_{12}^{(2)}(p) + \frac{2p}{495}S_{12}^{(3)}(p) - \frac{p}{660}S_{12}^{(4)}(p)\\
&+ \frac{p}{1155}S_{12}^{(5)}(p) - \frac{p}{2772}S_{12}^{(6)}(p)\\
\equiv& -47520\left(\frac{896B_{p-3}B_{p-9}}{27} + \frac{872B_{p-5}B_{p-7}}{35} + \frac{3B_{p-3}^4}{3^4}\right)p \pmod{p^2}.
\end{aligned}$$

Now the corollary follows quickly from Lemma 4 (iii). ☐

Corollary 18. *For all positive integers $m \geq 1$, we have*

$$
\begin{aligned}
R_8^{(m,1)} &= 336m(m^2+16)(m^2-1)\beta_3\beta_5,\\
R_9^{(m,1)} &= 12\cdot 7!\binom{m+2}{5}\beta_3^3 + 72m(m^6+126m^4+1869m^2+3044)\beta_9,\\
R_{10}^{(m,1)} &= 360m(m^2-1)(m^4+71m^2+540)(2\beta_3\beta_7+\beta_5^2),\\
R_{11}^{(m,1)} &= 660\cdot 5!\binom{m+2}{5}(m^2+33)\beta_3^2\beta_5\\
&\quad + 110m(m^8+330m^6+16401m^4+152900m^2+193248)\beta_{11},\\
R_{12}^{(m,1)} &= 55\cdot 9!\binom{m+3}{7}\beta_3^4\\
&\quad + 11\cdot 6!\binom{m+1}{3}(m^6+211m^4+6196m^2+32256)\beta_3\beta_9\\
&\quad + 11\cdot 6!\binom{m+1}{3}(m^6+187m^4+6508m^2+31392)\beta_5\beta_7.
\end{aligned}
$$

Proof. Let p be a prime such that $p \geq 11$. By Lemma 5 and Corollary 17, we have

$$R_8^{(m)}(p) \equiv \sum_{a=1}^{7}\binom{m+7-a}{7}S_8^{(a)}(p) \equiv \frac{112}{5}m(m^2+16)(m^2-1)B_{p-3}B_{p-5} \pmod{p}.$$

Similarly,

$$
\begin{aligned}
R_9^{(m)}(p) &\equiv -\frac{8!}{18}\binom{m+2}{5}B_{p-3}^3 - 8m(m^6+126m^4+1869m^2+3044)B_{p-9} \pmod{p},\\
R_{10}^{(m)}(p) &\equiv \frac{10!}{10080}m(m^2-1)(m^4+71m^2+540)\left(\frac{2B_{p-3}B_{p-7}}{21}+\frac{B_{p-5}^2}{25}\right) \pmod{p},\\
R_{11}^{(m)}(p) &\equiv -88\cdot 5!\binom{m+2}{5}(m^2+33)B_{p-3}^2B_{p-5}\\
&\quad - 10m(m^8+330m^6+16401m^4+152900m^2+193248)B_{p-11} \pmod{p},\\
R_{12}^{(m)}(p) &\equiv \frac{55\cdot 8!}{9}\binom{m+3}{7}B_{p-3}^4\\
&\quad + \frac{22\cdot 5!}{9}\binom{m+1}{3}(m^6+211m^4+6196m^2+32256)B_{p-3}B_{p-9}\\
&\quad + \frac{66\cdot 4!}{7}\binom{m+1}{3}(m^6+187m^4+6508m^2+31392)B_{p-5}B_{p-7} \pmod{p}.
\end{aligned}
$$

The corollary now quickly follows from the definition of β_k. ☐

5 Proof of Proposition 10 and Theorem 2

We first deal with the case $\gamma = 0$ and rewrite it as a difference of two sums each of which can be computed more easily.

Let $n, \kappa, g \in \mathbb{N}$ such that $1 \leq g \leq \min\{\kappa - 1, n - 2\}$. Set $d = n - g - 1$. For any prime p, we define

$$V_\kappa^{g;p}(n) := \sum_{\substack{0<a_1<\cdots<a_g<\kappa \\ 0<b_1\leq\cdots\leq b_g\leq d}} \sum_{\substack{0<u_1<\cdots<u_d<(\kappa-a_g)p \\ u_1,u_2,\dots,u_d\in\mathcal{P}_p}} \frac{1}{u_1\dots u_d u_{b_1}\dots u_{b_g}},$$

and

$$M_\kappa^{g;p}(n) := \sum_{\substack{0<a_1<\cdots<a_g<\kappa \\ 0<b_1\leq\cdots\leq b_g\leq d}} \sum_{\substack{0<u_1<\cdots<u_d<(\kappa-a_g)p \\ u_1,u_2,\dots,u_d\in\mathcal{P}_p}} \frac{1}{u_1\dots u_d u_{b_1}\dots u_{b_g}} \left(\frac{a_1}{u_{b_1}} + \frac{a_1}{u_{b_1+1}} + \right.$$
$$\left. \cdots + \frac{a_1}{u_{b_2}} + \frac{a_2}{u_{b_2}} + \cdots + \frac{a_2}{u_{b_3}} + \frac{a_3}{u_{b_3}} + \cdots + \frac{a_{g-1}}{u_{b_g}} + \frac{a_g}{u_{b_g}} + \cdots + \frac{a_g}{u_d}\right).$$

Lemma 19. *We have*

$$V_\kappa^{g;p}(n) \equiv (-1)^{g+1}\binom{\kappa}{g+1}\binom{n-1}{g}\frac{B_{p-n}}{n}p \pmod{p^2}.$$

Proof. Let $d = n-g-1$ and $m \in \mathbb{N}$. For each $0 < b_1 \leq \cdots \leq b_g \leq d$, we write $\mathbf{b} = (b_1, \dots, b_g)$ and define

$$K_{d;m}^{(p)}(\mathbf{b}) := \sum_{\substack{0<u_1<\cdots<u_d<m \\ u_1,u_2,\dots,u_d\in\mathcal{P}_p}} \frac{1}{u_1\dots u_d u_{b_1}\dots u_{b_g}}.$$

Let $[d]^g$ be the set of g-tuples of integers in $\{1, \dots, d\}$. Let $\mathrm{DW}(d, n-1) \subset \mathbb{N}^d$ be the set of d-tuples $\mathbf{s}$ of positive integers with $|\mathbf{s}| = n - 1$. Since every element of $[d]^g$ can be written in the form of $(1_{s_1-1}, 2_{s_2-1}, \dots, d_{s_d-1})$, we may define a map

$$\begin{aligned} \rho : \qquad [d]^g &\longrightarrow \mathrm{DW}(d,n) \\ (1_{s_1-1}, 2_{s_2-1}, \dots, d_{s_d-1}) &\longmapsto (s_1, \dots, s_d). \end{aligned} \tag{12}$$

It is clear that ρ has an inverse so that it provides a 1-1 correspondence. Moreover,

$$K_{d;m}^{(p)}(\mathbf{b}) = \mathcal{H}_m^{(p)}(\rho(\mathbf{b})).$$

Thus, by the substitution $a_j \to \kappa - a_j$, we have

$$V_\kappa^{g;p}(n) = \sum_{\substack{0<a_g<\cdots<a_1<\kappa \\ \mathbf{b}\in[d]^g}} K_{d;a_g p}^{(p)}(\mathbf{b}) = \sum_{\substack{0<a_g<\cdots<a_1<\kappa \\ \mathbf{s}\in\mathrm{DW}(d,n-1)}} \mathcal{H}_{a_g p}^{(p)}(\mathbf{s}).$$

For each $\mathbf{s} \in \mathrm{DW}(d, n-1)$, let γ_d be its permutation group (a symmetry group of d letters), $\mathrm{Orb}(\mathbf{s})$ its orbit under γ_d, and $\mathrm{Stab}(\mathbf{s})$ its stabilizer, i.e., the subgroup of all of the permutations that fix $\mathbf{s}$. It is well-known from group theory that $|\mathrm{Orb}(\mathbf{s})| \cdot |\mathrm{Stab}(\mathbf{s})| = |\gamma_d| = d!$. Thus we have

$$\begin{aligned}
V_\kappa^{g;p}(n) &= \sum_{\substack{0<a_g<\cdots<a_1<\kappa \\ \mathbf{s}\in\mathrm{DW}(d,n-1)}} \frac{1}{|\mathrm{Orb}(\mathbf{s})|} \sum_{\mathbf{t}\in\mathrm{Orb}(\mathbf{s})} \mathcal{H}_{a_g p}^{(p)}(\mathbf{t}) \\
&= \sum_{\substack{0<a_g<\cdots<a_1<\kappa \\ \mathbf{s}\in\mathrm{DW}(d,n-1)}} \frac{1}{|\mathrm{Orb}(\mathbf{s})|} \cdot \frac{U_{0;a_g}^{(p)}(\mathbf{s})}{|\mathrm{Stab}(\mathbf{s})|} = \sum_{\substack{0<a_g<\cdots<a_1<\kappa \\ \mathbf{s}\in\mathrm{DW}(d,n-1)}} \frac{U_{0;a_g}^{(p)}(\mathbf{s})}{d!}. \qquad (13)
\end{aligned}$$

Since $d = n - g - 1$ and $B_{p-n} = 0$ for even n, by Lemma 3,

$$U_{0;a_g}^{(p)}(\mathbf{s}) \equiv a_g(-1)^{g+1}(d-1)!(n-1)\frac{B_{p-n}}{n}p \pmod{p^2}.$$

Noticing that $|\mathrm{DW}(d, n-1)| = \binom{n-2}{d-1}$, we get

$$\begin{aligned}
V_\kappa^{g;p}(n) &\equiv \sum_{0<a_g<\cdots<a_2<a_1<\kappa} a_g(-1)^{g+1}\binom{n-2}{d-1}\frac{n-1}{d}\frac{B_{p-n}}{n}p \pmod{p^2} \\
&\equiv \sum_{0<a_g<\cdots<a_2<a_1<\kappa} a_g(-1)^{g+1}\binom{n-1}{g}\frac{B_{p-n}}{n}p \pmod{p^2}.
\end{aligned}$$

So the lemma follows from (14) at once. ∎

Lemma 20. *For any positive integers $i \le g < \kappa$, we have*

$$\sum_{0<a_1<\cdots<a_g<\kappa} a_i = i\sum_{a=1}^{\kappa-1}\binom{a}{g}.$$

In particular, if $i = g$, then we have

$$\sum_{0<a_g<\cdots<a_2<a_1<\kappa} a_g = \binom{\kappa}{g+1}. \qquad (14)$$

Proof. Clearly

$$\sum_{0<a_1<\cdots<a_i} 1 = \binom{a_i-1}{i-1} = \frac{i}{a_i}\binom{a_i}{i}$$

is the number of ways to choose $i-1$ distinct positive integers from $1, 2, \ldots, a_i - 1$. The lemma follows easily from an induction on g by using the well-known identity

$$\sum_{0<a_i<a_{i+1}} \binom{a_i}{i} = \binom{a_{i+1}}{i+1}.$$

In particular, if $i = g$, then we may take $a_{i+1} = \kappa$ to prove (14). ∎

Lemma 21. *We have*

$$M_\kappa^{g;p}(n) \equiv 0 \pmod p.$$

Proof. Again we let $d = n - g - 1$. By the definition and Lemma 20,

$$M_\kappa^{g;p}(n) = \sum_{\substack{0<a<\kappa \\ 1\le b_1\le\cdots\le b_g\le d}} \binom{a}{g} \sum_{\substack{0<u_1<\cdots<u_d<(\kappa-a)p \\ u_1,u_2,\dots,u_d\in\mathcal{P}_p}} \frac{1}{u_1\dots u_d u_{b_1}\dots u_{b_g}} \Big(\frac{1}{u_{b_1}} + \frac{1}{u_{b_1+1}} + \\ \cdots + \frac{1}{u_{b_2}} + \frac{2}{u_{b_2}} + \cdots + \frac{2}{u_{b_3}} + \frac{3}{u_{b_3}} + \cdots + \frac{g-1}{u_{b_g}} + \frac{g}{u_{b_g}} + \cdots + \frac{g}{u_d} \Big). \tag{15}$$

Because of the terms in the parenthesis, we see that each $\mathbf{b} \in [d]^g$ may produce more than one p-restricted MHSs of weight n. Hence,

$$M_\kappa^{g;p}(n) = \sum_{0<a<\kappa} \binom{a}{g} \sum_{\mathbf{s}\in \mathrm{DW}(d,n)} m(\mathbf{s}) \mathcal{H}^{(p)}_{(\kappa-a)p}(\mathbf{s}).$$

We now show that the multiplicity $m(\mathbf{s}) = g(g+1)/2$ for all $\mathbf{s}$. For simplicity, we set

$$\mathbf{l} = (l_1,\dots,l_d) = (s_1 - 1,\dots,s_d - 1).$$

The idea is to subtract 1 from a component $s_j \ge 2$ of $\mathbf{s}$ and consider the corresponding $\mathbf{b}(j)$ using the 1-1 correspondence ρ defined by (12). Every such $\mathbf{b}(j)$ produced will lead to a p-restricted MHS $\mathcal{H}^{(p)}_{(\kappa-a)p}(\mathbf{s})$ with some multiplicity due to the possible repetition of $1/u_j$-term in the parenthesis of (15). Suppose $s_j \ge 2$. Then we get the corresponding

$$\mathbf{b}(j) = (b_1,\dots,b_g) = (1_{l_1}, 2_{l_2},\dots,(j-1)_{l_{j-1}}, j_{l_j-1}, (j+1)_{l_{j+1}},\dots,d_{l_d}).$$

Set $t = l_1+\cdots+l_{j-1}$. Then we see that $b_{t+i} = j$ for all $i = 1,\dots,l_j-1$. So the contribution to the multiplicity of $m(\mathbf{s})$, denoted by $m_j(\mathbf{s})$, by this particular $\mathbf{b}(j)$ is given by the coefficient of $1/u_j$ in the above (note that $1/u_j$ repeats l_j times with increasing numerators), namely,

$$m_j(\mathbf{s}) = \mu_j(\mathbf{l}) := t + \sum_{i=1}^{l_j-1}(t+i) = \Big(l_1 + \cdots + l_{j-1} + \frac{l_j - 1}{2}\Big) l_j.$$

Remarkably, this is still true even if $s_j = 1$, i.e., $l_j = 0$, because $\mathbf{b}(j)$ does not exist in this case while $m_j(\mathbf{s}) = 0$ according to the formula.

We now show that $\mu(\mathbf{l})$ only depends on $|\mathbf{l}| = n - d = g + 1$. Indeed, let $\mathbf{l}' = (l_1 - 1,\dots,l_{i-1}, l_i + 1, l_{i+1},\dots,l_d)$ for some $i \ge 2$ and let $r_j = \mu_j(\mathbf{l}) - \mu_j(\mathbf{l}')$. If $j = 1$, we have

$$r_1 = \Big(\frac{l_1-1}{2}\Big) l_1 - \Big(\frac{l_1-2}{2}\Big)(l_1 - 1) = l_1 - 1.$$

For $1 < j < i$,

$$r_j = \Big(l_1 + l_2 + \cdots + l_{j-1} + \frac{l_j - 1}{2}\Big)l_j - \Big(l_1 - 1 + l_2 + \cdots + l_{j-1} + \frac{l_j - 1}{2}\Big)l_j = l_j.$$

For $j = i$,

$$\begin{aligned} r_i = \Big(l_1 + l_2 + \cdots + l_{i-1} + \frac{l_i - 1}{2}\Big)l_i - \Big(l_1 - 1 + l_2 + \cdots + l_{i-1} + \frac{l_i}{2}\Big)(l_i + 1) \\ = 1 - (l_1 + \cdots + l_{i-1}). \end{aligned}$$

For $j > i$,

$$r_j = \Big(l_1 + l_2 + \cdots + l_{j-1} + \frac{l_j - 1}{2}\Big)l_j - \Big(l_1 - 1 + l_2 + \cdots + l_{j-1} + 1 + \frac{l_j - 1}{2}\Big)l_j = 0.$$

Therefore

$$\mu(\mathbf{l}) - \mu(\mathbf{l}') = \sum_{j=1}^{d} \Big(\mu_j(\mathbf{l}) - \mu_j(\mathbf{l}')\Big) = \sum_{j=1}^{d} r_j = 0.$$

This implies that $m(\mathbf{s}) = \sum_{j=1}^{d} m_j(\mathbf{s}) = \sum_{j=1}^{d} \mu_j((g+1, 0, \ldots, 0)) = \mu_1((g+1, 0, \ldots, 0)) = g(g+1)/2$ as desired. Consequently, by the idea used to derive (13), we see that

$$\begin{aligned} M_\kappa^{g;p}(n) =& \frac{g(g+1)}{2} \sum_{0<a<\kappa} \binom{a}{g} \sum_{\mathbf{s} \in \mathrm{DW}(d,n)} \mathcal{H}^{(p)}_{(\kappa-a)p}(\mathbf{s}) \\ =& \frac{g(g+1)}{2} \sum_{0<a<\kappa} \binom{a}{g} \sum_{\mathbf{s} \in \mathrm{DW}(d,n)} \frac{U^{(p)}_{0;\kappa-a}(\mathbf{s})}{d!} \equiv 0 \pmod p \end{aligned}$$

by Lemma 3. □

Recall from (8) that

$$P^{g;p}_{\gamma;\kappa}(n) = \sum_{1<b_1<\cdots<b_g<n} \sum_{\substack{\gamma p < u_1 < \cdots < u_{n-1} < (\gamma+\kappa)p \\ u_1, u_2, \ldots, u_{n-1} \in \mathcal{P}_p \\ p | (u_{b_1} - u_{b_1 - 1}), \ldots, p | (u_{b_g} - u_{b_g - 1})}} \frac{1}{u_1 \ldots u_{n-1}}.$$

Lemma 22. *We have*

$$P^{g;p}_{\gamma;\kappa}(n) \equiv P^{g;p}_{0;\kappa}(n) \pmod{p^2}.$$

Proof. As before, we let $d = n - g - 1$. Define

$$E_\kappa^{g;p}(n) := \sum_{\substack{0<a_1<\cdots<a_g<\kappa \\ 1 \le b_1 \le \cdots \le b_g \le d}} \sum_{\substack{0<u_1<\cdots<u_d<(\kappa-a_g)p \\ u_1, u_2, \ldots, u_d \in \mathcal{P}_p}} \frac{1}{u_1 \ldots u_d u_{b_1} \ldots u_{b_g}} \left(\frac{1}{u_1} + \cdots + \frac{1}{u_d}\right),$$

$$F_\kappa^{g;p}(n) := \sum_{\substack{0<a_1<\cdots<a_g<\kappa \\ 1 \le b_1 \le \cdots \le b_g \le d}} \sum_{\substack{0<u_1<\cdots<u_d<(\kappa-a_g)p \\ u_1, u_2, \ldots, u_d \in \mathcal{P}_p}} \frac{1}{u_1 \ldots u_d u_{b_1} \ldots u_{b_g}} \left(\frac{1}{u_{b_1}} + \cdots + \frac{1}{u_{b_g}}\right).$$

Then it is easy to see that

$$P^{g;p}_{0;\kappa}(n) - P^{\kappa}_{\gamma;g}(n;p) \equiv \gamma p\Big(E^{g;p}_{\kappa}(n) + F^{g;p}_{\kappa}(n)\Big) \pmod{p^2}. \tag{16}$$

Indeed, in the definition (8) we may replace every u_j by $u_j + \gamma p$. Then by the geometric series expansion in the p-adic integer ring $\mathbb{Z}_p$, we see that

$$\frac{1}{u_j+\gamma p} \equiv \frac{1}{u_j}\left(1-\frac{\gamma p}{u_j}\right), \quad \frac{1}{u_j+(\gamma+a_i)p} \equiv \frac{1}{u_j}\left(1-\frac{(\gamma+a_i)p}{u_j}\right) \pmod{p^2}. \tag{17}$$

These congruences quickly lead to (16).

We first prove that

$$E^{g;p}_{\kappa}(n) \equiv 0 \pmod{p}. \tag{18}$$

By the proof of Lemma 19, we see that there is a 1-1 correspondence between $[d]^g$ and $\mathrm{DW}(d,n-1)$, where $[d]^g$ is the set of g-tuples of integers in $\{1,\dots,d\}$ and $\mathrm{DW}(d,n-1) \subset \mathbb{N}^d$ is the set of d-tuples $\mathbf{s}$ with $|\mathbf{s}| = n-1$. Let the height of $\mathbf{s}$, denoted by $\mathrm{ht}(\mathbf{s})$, be the number of components of $\mathbf{s}$ which are greater than 1. Let $\mathrm{DW}(d,n,h)$ be the subset of height h elements of $\mathrm{DW}(d,n)$. Since $n-d = g+1 \geq 1$ the height of every element in $\mathrm{DW}(d,n)$ is at least 1. Define

$$\begin{aligned} \lambda_j : &\mathrm{DW}(d,n-1) \longrightarrow \mathrm{DW}(d,n) \\ &(s_1,\dots,s_d) \longmapsto (s_1,\dots,s_{j-1},s_j+1,s_{j+1},\dots,s_d). \end{aligned}$$

It is obvious that the union of the images of λ_j, as a multi-set, covers every element of $\mathrm{DW}(d,n,h)$ exactly h times. Note further that the set $\mathrm{DW}(d,n,h)$ is invariant under every permutation of the components of its elements. By the same idea used to derive (13), we get

$$\begin{aligned} E^{g;p}_{\kappa}(n) &= \sum_{0<a_1<\dots<a_g<\kappa} \sum_{h=1}^{d} h \sum_{\mathbf{s}\in \mathrm{DW}(d,n,h)} \mathcal{H}^{(p)}_{(\kappa-a_g)p}(\mathbf{s}) \\ &= \sum_{0<a_1<\dots<a_g<\kappa} \sum_{h=1}^{d} h \sum_{\mathbf{s}\in \mathrm{DW}(d,n,h)} \frac{U^{(p)}_{0;\kappa-a}(\mathbf{s})}{d!} \equiv 0 \pmod{p} \end{aligned}$$

by Lemma 3.

We now prove that

$$F^{g;p}_{\kappa}(n) \equiv 0 \pmod{p}. \tag{19}$$

We modify the idea used in the proof of Lemma 21. Recall that for any $\mathbf{s} = (s_1,\dots,s_d) \in \mathrm{DW}(d,n-1)$, we set $\rho^{-1}(\mathbf{s}) = (1_{l_1}, 2_{l_2},\dots,d_{l_d})$ where $l_j = s_j - 1$ for all $j = 1,\dots,d$. So we argue similarly as in the proof of Lemma 21 and see that

$$F^{g;p}_{\kappa}(n) = \sum_{0<a_1<\dots<a_g<\kappa} \sum_{\mathbf{s}\in \mathrm{DW}(d,n)} m(\mathbf{s}) \mathcal{H}^{(p)}_{(\kappa-a_g)p}(\mathbf{s}),$$

where the multiplicity

$$m(\mathbf{s}) = l_1 + l_2 + \cdots + l_d = g$$

which is independent of $\mathbf{s}$. Thus

$$\begin{aligned} F_\kappa^{g;p}(n) &= \sum_{0<a_1<\cdots<a_g<\kappa} g \sum_{\mathbf{s}\in \mathrm{DW}(d,n)} \mathcal{H}^{(p)}_{(\kappa-a_g)p}(\mathbf{s}) \\ &= \sum_{0<a_1<\cdots<a_g<\kappa} g \sum_{\mathbf{s}\in \mathrm{DW}(d,n)} \frac{U^{(p)}_{0;\kappa-a}(\mathbf{s})}{d!} \equiv 0 \pmod p \end{aligned}$$

by Lemma 3.

Finally, the lemma follows from (16), (18) and (19). $\square$

We are now ready to prove Proposition 10. By the definition, we have

$$\begin{aligned} P_{0;\kappa}^{g;p}(n) = & \sum_{\substack{0<a_1<\cdots<a_g<\kappa \\ 0<b_1\leq\cdots\leq b_g<n-g}} \sum_{\substack{0<u_1<\cdots<u_d<(\kappa-a_g)p \\ u_1,u_2,\dots,u_d\in\mathcal{P}_p}} \frac{1}{u_1u_2\dots u_{b_1}(u_{b_1}+a_1p)(u_{b_1+1}+a_1p)} \\ & \cdots \frac{1}{(u_{b_2}+a_1p)(u_{b_2}+a_2p)\dots(u_{b_g}+a_{g-1}p)(u_{b_g}+a_gp)\cdots(u_d+a_gp)} \\ \equiv & V_\kappa^{g;p}(n) - pM_\kappa^{g;p}(n) \pmod{p^2} \end{aligned}$$

by (17). Thus, by Lemma 19 and Lemma 21

$$P_{0;\kappa}^{g;p}(n) \equiv (-1)^{g+1}\binom{\kappa}{g+1}\binom{n-1}{g}\frac{B_{p-n}}{n}p \pmod{p^2}.$$

So Proposition 10 follows from Lemma 22.

We can now turn to the proof of our main theorem, Theorem 2. From Theorem 12 and Lemma 6, we see that for all $m,n\in\mathbb{N}$, both $R_n^{(m,1)}$ and $S_n^{(m,1)}$ lie in the sub-algebra $\mathcal{B}$ of $\mathcal{A}_1$ generated by $\mathcal{A}$-Bernoulli numbers. This implies that $S_n^{(m,2)}$ lies in $p\mathcal{B}\subset\mathcal{A}_2$ by Lemma 4 (ii), which in turn yields (5) and (4) by Lemma 4 (iii) and Lemma 5, respectively. We can now conclude the proof of our Theorem 2 and the paper.

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