Quasi-symmetric functions and mod p multiple harmonic sums

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Abstract

We present a number of results about (finite) multiple harmonic sums modulo a prime, which provide interesting parallels to known results about multiple zeta values (i.e., infinite multiple harmonic series). In particular, we prove a "duality" result for mod p harmonic sums similar to (but distinct from) that for multiple zeta values. We also exploit the Hopf algebra structure of the quasi-symmetric functions to do calculations with multiple harmonic sums mod p, and obtain, for each weight $n \leq 9$, a set of generators for the space of weight-n multiple harmonic sums mod p.

1 Introduction

In recent years there has been considerable interest in the multiple zeta values

$$\zeta(i_1, i_2, \ldots, i_k) = \sum_{n_1 > n_2 > \cdots > n_k \geq 1} \frac{1}{n_1^{i_1} n_2^{i_2} \cdots n_k^{i_k}}, \tag{1}$$

which converge for $i_1 > 1$; see, e.g. [2, 13, 14, 17, 16, 27, 28]. The multiple zeta values are limits of the finite harmonic sums

$$A_{(i_1,i_2,\ldots,i_k)}(n) = \sum_{n \geq n_1 > n_2 > \cdots > n_k \geq 1} \frac{1}{n_1^{i_1} n_2^{i_2} \cdots n_k^{i_k}}, \tag{2}$$

as $n \to \infty$. In fact, these finite sums themselves are of interest in physics [1, 26]. Both types of quantities are indexed by the the exponent string $(i_1, \ldots, i_k)$: we refer to k as the length and $i_1 + \cdots + i_k$ as the weight.

The multiple zeta values (1) form an algebra under multiplication. In fact, there are two distinct multiplications on the set of multiple zeta values, the harmonic (or "stuffle") product and the shuffle product, coming from the representation of multiple zeta values as iterated series and as iterated integrals respectively (see §4 of [17] for a discussion). Only the first of these products applies to the finite sums (2).

In this paper we develop a theory of the mod p values (p a prime), of the finite harmonic sums (2) when $n = p-1$. Our main tools are the structure of the algebra QSym of quasi-symmetric functions (which formalizes the harmonic product) and a mod p duality result (Theorem 4.7 below) which corresponds to the duality theorem for multiple zeta values (see, e.g., Corollary 6.2 of [14]). The divisibility properties of finite harmonic sums are considered in [29], and there is some overlap between that paper and this one. But in this paper we focus only on congruences mod p, while [29] also considers congruences mod higher powers of p. A brief account of the results of §4 of this paper appeared earlier in the last section of [16].

The theory of mod p finite harmonic sums has several interesting differences and similarities to the theory of multiple zeta values. While the values of (1) with length $k = 1$ are the classical zeta values $\zeta(i_1)$, it is well known that the mod p value of

$$A_{(i_1)}(p-1) = \sum_{j=1}^{p-1} \frac{1}{j^{i_1}}$$

is zero when $p > i_1 + 1$. But for $k = 2$ we have the relation

$$A_{(i_1,1)}(p-1) \equiv B_{p-i_1-1} \mod p,$$

with Bernoulli numbers (see Theorem 6.1 below). In the case of multiple zeta values, it appears that that multiple zeta values not expressible in terms of the classical zeta values occur first in weight 8 (e.g., $\zeta(6,2)$); for the finite harmonic sums mod p, the first ones not expressible in terms of Bernoulli numbers appear to occur in weight 7 (see §7 below).

As we have already mentioned, there is a duality result in both theories. If we code the exponent strings $(i_1, i_2, \ldots, i_k)$ occurring in (1) and (2) by the monomial $x^{i_1-1}y \cdots x^{i_k-1}y$ in noncommuting variables x and y, then the duality map for multiple zeta values is the anti-automorphism of $\mathbf{Q}\langle x, y\rangle$ that exchanges x and y, while that for the mod p finite harmonic sums is the automorphism ψ of $\mathbf{Z}\langle x, y\rangle$ with $\psi(x) = x + y$ and $\psi(y) = -y$.

The dimension d_n of the rational vector space of multiple zeta values of weight n was conjectured by Zagier [28] to be the Perrin numbers, i.e. $d_1 = 0$, $d_2 = d_3 = 1$, and $d_n = d_{n-2} + d_{n-3}$. The corresponding numbers for the finite harmonic sums (2) are the minimal numbers c_n of weight-n harmonic sums needed to generate all weight-n harmonic sums mod p for $p > n + 1$. From the calculations of §7 below the first few values of c_n seem to be the following.

n	1	2	3	4	5	6	7	8	9
c_n	0	0	1	0	1	1	2	2	3

We do not have a conjecture about the c_n for general n, but we do conjecture that all multiple harmonic sums $A_I(p-1)$ can be written mod p as sums of products of sums of the form $A_{(h,1,\ldots,1)}(p-1)$ (what we call "height one sums"; see §5 below) with h even.

This paper is organized as follows. In §2 we give an exposition of the algebra QSym of quasi-symmetric functions. In §3 we describe the Hopf algebra structure of QSym, particularly the antipode, and introduce some integral bases of QSym important in the sequel. In §4 we define bases A_I and S_I for the set of finite harmonic sums, and prove some basic results about the mod p case. In §5 we discuss a particular class of multiple harmonic sums, the height one sums. In §6 we obtain some results about $S_I(p-1)$ mod p when I has short length. Finally, in §7 we apply the preceding results to find sets of products of height one sums that generate all multiple harmonic sums mod p through weight 9.

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2 Harmonic Algebra and Quasi-Symmetric Functions

Let $\mathfrak{H}$ be the underlying graded abelian group of the noncommutative polynomial algebra $\mathbf{Z}\langle x,y\rangle$, where x and y both have degree 1. For a word w of $\mathfrak{H}$, we refer to the total degree of w as its weight (denoted $|w|$) and its y-degree as its length (denoted $\ell(w)$). We can define a commutative multiplication $*$ on $\mathfrak{H}$ by requiring that it distribute over the addition and that it satisfy the following axioms:

H1. For any word w, $1*w=w*1=w$;

H2. For any word w and integer $n\ge 1$,

$$x^n*w=w*x^n=wx^n;$$

H3. For any words w_1,w_2 and integers $p,q\ge 0$,

$$x^pyw_1*x^qyw_2=x^py(w_1*x^qyw_2)+x^qy(x^pyw_1*w_2)+x^{p+q+1}y(w_1*w_2).$$

Note that axiom (H3) allows the $*$-product of any pair of words to be computed recursively, since each $*$-product on the right has fewer factors of y than the $*$-product on the left-hand side. Induction on length establishes the following.

Theorem 2.1. *The $*$-product is commutative and associative.*

We refer to $\mathfrak{H}$ together with its commutative multiplication $*$ as the (integral) harmonic algebra $(\mathfrak{H},*)$. Let $\mathfrak{H}^1$ be the additive subgroup $\mathbf{Z}1+\mathfrak{H}y$ of $\mathfrak{H}$; it is evidently a subalgebra of $(\mathfrak{H},*)$. Note that any word $w\in\mathfrak{H}^1$ can be written in terms of the elements $z_i=x^{i-1}y$, and that the length $\ell(w)$ is the number of factors z_i of w when expressed this way. We can rewrite the inductive rule (H3) for the $*$-product as

$$z_p w_1 * z_q w_2 = z_p(w_1 * z_q w_2) + z_q(z_p w_1 * w_2) + z_{p+q}(w_1 * w_2). \tag{3}$$

Now for each positive integer n, define a homomorphism $\phi_n : \mathfrak{H}^1 \to \mathbf{Z}[t_1, \dots, t_n]$ of graded abelian groups (where $|t_i| = 1$ for all i) as follows. Let $\phi_n(1) = 1$ and

$$\phi_n(z_{i_1} z_{i_2} \cdots z_{i_k}) = \sum_{1 \le n_1 < n_2 < \cdots < n_k \le n} t_{n_1}^{i_1} t_{n_2}^{i_2} \cdots t_{n_k}^{i_k}$$

for words of length $k \le n$, and let $\phi(w) = 0$ for words of length greater than n; extend ϕ_n additively to $\mathfrak{H}^1$. Because the rule (3) corresponds to multiplication of series, ϕ_n is an algebra homomorphism of $(\mathfrak{H}^1, *)$ into $\mathbf{Z}[t_1, \dots, t_n]$, and ϕ_n is evidently injective through degree n. For each $m \ge n$, there is a restriction map

$$\rho_{m,n} : \mathbf{Z}[t_1, \dots, t_m] \to \mathbf{Z}[t_1, \dots, t_n]$$

defined by

$$\rho_{m,n}(t_i) = \begin{cases} t_i, & i \le n \\ 0, & i > n. \end{cases}$$

The inverse limit

$$\mathfrak{P} = \operatorname*{proj\,lim}_n \mathbf{Z}[t_1, \dots, t_n]$$

is the subalgebra of $\mathbf{Z}[[t_1, t_2, \dots]]$ consisting of those formal power series of bounded degree. The ϕ_n commute with the restriction maps, so they define a homomorphism $\phi : \mathfrak{H}^1 \to \mathfrak{P}$.

Inside $\mathfrak{P}$ is the algebra of symmetric functions

$$\mathrm{Sym} = \operatorname*{proj\,lim}_n \mathbf{Z}[t_1, \dots, t_n]^{\Sigma_n}$$

and also the algebra QSym of quasi-symmetric functions (first described in [9]). We say a formal series $p \in \mathfrak{P}$ is in QSym if the coefficient of $t_{i_1}^{p_1} \cdots t_{i_k}^{p_k}$ in p is the same as the coefficient of $t_{j_1}^{p_1} \cdots t_{j_k}^{p_k}$ in p whenever $i_1 < i_2 < \cdots < i_k$ and $j_1 < j_2 < \cdots < j_k$. Evidently $\mathrm{Sym} \subset \mathrm{QSym}$. An integral basis for QSym is given by the monomial quasi-symmetric functions

$$M_{(p_1, p_2, \dots, p_k)} = \sum_{i_1 < i_2 < \cdots < i_k} t_{i_1}^{p_1} t_{i_2}^{p_2} \cdots t_{i_k}^{p_k},$$

which are indexed by compositions $(p_1, \dots, p_k)$. Since $\phi(z_{i_1} \cdots z_{i_k}) = M_{(i_1, \dots, i_k)}$, we have the following result.

Theorem 2.2. *ϕ is an isomorphism of $(\mathfrak{H}^1, *)$ onto* QSym.

As is well known, the algebra Sym of symmetric functions is generated by the elementary symmetric functions e_i, as well as by the complete symmetric functions h_i. The power-sum symmetric functions p_i generate $\mathrm{Sym}\otimes\mathbf{Q}$, but only generate a subalgebra of Sym over $\mathbf{Z}$. It is easy to see that $\phi(z_1^i)=e_i$ and $\phi(z_i)=p_i$.

A monomial quasi-symmetric function M_I is in Sym exactly when all parts of I are the same. Given $I=(i_1,\dots,i_k)$, the symmetric group Σ_k on k letters acts on I by $\sigma\cdot I=(i_{\sigma(1)},\dots,i_{\sigma(k)})$, and the symmetrization

$$\sum_{\sigma\in\Sigma_k} M_{\sigma\cdot I} \tag{4}$$

of M_I is evidently in Sym. Hence the element (4) can be written as a sum of rational multiples of the power-sums $p_i=M_{(i)}$. But in fact (4) is a sum of products of the $M_{(i)}$ with integral coefficients that can be given explicitly as follows.

Theorem 2.3. *Let $I=(i_1,i_2,\dots,i_k)$ be a composition. Then*

$$\sum_{\sigma\in\Sigma_k} M_{\sigma\cdot I}=\sum_{\text{partitions } \mathcal{B}=\{B_1,\dots,B_l\} \text{ of } \{1,\dots,k\}} (-1)^{k-l}c(\mathcal{B})M_{(b_1)}M_{(b_2)}\cdots M_{(b_l)},$$

where $c(\mathcal{B})=(\operatorname{card}B_1-1)!\cdots(\operatorname{card}B_l-1)!$ and $b_s=\sum_{j\in B_s} i_j$.

Proof. While the argument used to prove Theorem 2.2 of [13] can be adapted to prove this result, we shall use the Möbius inversion formula as follows. The set Π_k of partitions of the set $\{1,\dots,k\}$, with the partial order given by refinement, is a finite semimodular lattice. We also have, for any $\mathcal{C}=\{C_1,\dots,C_p\}\in\Pi_k$,

$$M_{(c_1)}M_{(c_2)}\cdots M_{(c_p)}=\sum_{\mathcal{B}=\{B_1,\dots,B_l\}\preceq\mathcal{C}}\ \sum_{\sigma\in\Sigma_l} M_{\sigma\cdot(b_1,\dots,b_l)},$$

where $b_s=\sum_{j\in B_s} i_j$ and $c_s=\sum_{j\in C_s} i_j$. Then the Möbius inversion formula gives

$$\sum_{\sigma\in\Sigma_p} M_{\sigma\cdot(c_1,\dots,c_p)}=\sum_{\mathcal{B}=\{B_1,\dots,B_l\}\preceq\mathcal{C}} \mu(\mathcal{B},\mathcal{C})M_{(b_1)}\cdots M_{(b_l)}. \tag{5}$$

The conclusion follows by taking $\mathcal{C}=\{\{1\},\{2\},\dots,\{k\}\}$ in equation (5) and noting that in this case $\mu(\mathcal{B},\mathcal{C})=(-1)^{k-l}c(\mathcal{B})$ (see [24], Example 3.10.4). □

The rational algebra of quasi-symmetric functions $\mathrm{QSym}\otimes\mathbf{Q}$ was shown to be a polynomial algebra by Malvenuto and Reutenauer [22]. To describe the generators, we put an order on the words of $\mathfrak{H}$ by setting $x<y$ and extending it lexicographically. A word is called Lyndon if it is smaller than any of its proper right factors, i.e. for w Lyndon we have $w<v$ whenever $w=uv$ for $u,v\neq 1$. Let $\mathcal{L}$ be the set of Lyndon words in $\mathfrak{H}^1$. Then the following result was proved in [22].

Theorem 2.4. $\mathrm{QSym}\otimes\mathbf{Q}$ *is a polynomial algebra on the generators $\phi(w)$, where $w\in\mathcal{L}$.*

The integral structure is more subtle. The result is again that the algebra is polynomial, but one has to use a different set of generators. Let $\mathcal{L}^{mod}$ be the set of modified Lyndon words in $\mathfrak{H}^1$, i.e., whenever $w=z_{i_1}^{p_1}\cdots z_{i_k}^{p_k}\in\mathcal{L}$ has a common factor d dividing all the exponents p_i, replace it with v^d, where $v=z_{i_1}^{p_1/d}\cdots z_{i_k}^{p_k/d}$. The following result was first stated by Ditters, though the first correct proof seems to be due to Hazewinkel [12].

Theorem 2.5. QSym *is a polynomial algebra on the generators $\phi(w)$, where $w\in\mathcal{L}^{mod}$.*

3 Quasi-Symmetric Functions as a Hopf Algebra

For definitions and basic results on Hopf algebras we refer the reader to [23], [25], and [20]. The algebra $(\mathfrak{H}^1, *) \cong \mathrm{QSym}$ has a Hopf algebra structure with coproduct Δ defined by

$$\Delta(z_{i_1} z_{i_2} \cdots z_{i_n}) = \sum_{j=0}^{n} z_{i_1} \cdots z_{i_j} \otimes z_{i_{j+1}} \cdots z_{i_n}, \tag{6}$$

and counit ϵ with $\epsilon(u) = 0$ for all elements u of positive degree. This extends the well-known Hopf algebra structure on the algebra Sym (as described in [7]), in which the elementary symmetric functions e_i ($\leftrightarrow y^i$) and complete symmetric functions h_i are divided powers, while the power sums p_i ($\leftrightarrow z_i$) are primitive. The Hopf algebra $(\mathfrak{H}^1, *, \Delta)$ is commutative but not cocommutative. Its (graded) dual is the Hopf algebra of noncommutative symmetric functions as defined in [8].

Now QSym has various integral bases besides the M_I, also indexed by compositions. For compositions I, J, we say I refines J (denoted $I \succ J$) if J can be obtained from I by combining some of its parts. Then the fundamental quasi-symmetric functions are given by

$$F_I = \sum_{J \succeq I} M_J, \tag{7}$$

and the essential quasi-symmetric functions are given by

$$E_I = \sum_{J \preceq I} M_J. \tag{8}$$

It will be useful to have some additional notations for compositions. We adapt the notation used the previous section for words, so for $I = (i_1, \dots, i_k)$ the weight of I is $|I| = i_1 + \cdots + i_k$, and $k = \ell(I)$ is the length of I. For $I = (i_1, \dots, i_k)$, the reversed composition $(i_k, \dots, i_1)$ will be denoted $\bar{I}$: of course reversal preserves weight, length and refinement (i.e., $I \succeq J$ implies $\bar{I} \succeq \bar{J}$). We write $I \sqcup J$ for the juxtaposition of I and J, so $\overline{I \sqcup J} = \bar{J} \sqcup \bar{I}$.

Compositions of weight n are in 1-to-1 correspondence with subsets of $\{1, 2, \dots, n-1\}$ via partial sums

$$(i_1, i_2, \dots, i_k) \to \{i_1, i_1 + i_2, \dots, i_1 + \cdots + i_{k-1}\}, \tag{9}$$

and this correspondence is an isomorphism of posets, i.e., $I \preceq J$ if and only if the subset corresponding to I contains that corresponding to J. Complementation in the power set thus gives rise to an involution $I \to I^*$; e.g., $(1,1,2)^* = (3,1)$. Evidently $|I^*| = |I|$ and $\ell(I) + \ell(I^*) = |I| + 1$. Also, $I \preceq J$ if and only if $I^* \succeq J^*$. The complementation operation commutes with reversal, so the notation $\bar{I}^*$ is unambiguous.

Because of the correspondence (9) between the poset of compositions of n and the poset of subsets of $\{1, 2, \dots, n-1\}$, it follows that the Möbius function for compositions of n is given by

$$\mu(I, J) = (-1)^{\ell(I) - \ell(J)}.$$

Thus, e.g., the Möbius inversion formula applied to equation (8) is

$$M_I = \sum_{J \preceq I} (-1)^{\ell(I)-\ell(J)} E_J. \tag{10}$$

Since QSym is a commutative Hopf algebra, its antipode S is an automorphism of QSym and $S^2 = \mathrm{id}$. Now S can be given by the following explicit formulas: for proof see [5] or [15].

Theorem 3.1. *The antipode S of* QSym *is given by*

1. $S(M_I) = \sum_{I_1 \sqcup I_2 \sqcup \cdots \sqcup I_l = I} (-1)^l M_{I_1} M_{I_2} \cdots M_{I_l}$;
2. $S(M_I) = (-1)^{\ell(I)} E_{\bar{I}}$.

Part (2) of this result implies a number of facts about the E_I. First, the E_I have almost the same multiplication rules as the M_I: if T is the automorphism of QSym sending M_I to $M_{\bar{I}}$, then ST takes any identity among the M_I to an identity among the E_I that differs only in signs. For example, since

$$M_{(2)} M_{(3)} = M_{(2,3)} + M_{(3,2)} + M_{(5)}$$

we have

$$E_{(2)} E_{(3)} = E_{(2,3)} + E_{(3,2)} - E_{(5)}.$$

Second, the coproduct formula (6), which in terms of the M_I says

$$\Delta(M_I) = \sum_{J \sqcup K = I} M_J \otimes M_K,$$

can also be written

$$\Delta(E_I) = \sum_{J \sqcup K = I} E_J \otimes E_K,$$

because of the standard Hopf algebra relation $\Delta S = (S \otimes S)\Delta^{op}$. Finally, if we apply S to both sides of Theorem 2.3 we obtain, for any composition $I = (i_1, \dots, i_k)$,

$$\sum_{\sigma \in \Sigma_k} E_{\sigma \cdot I} = \sum_{\text{partitions } \mathcal{B} = \{B_1, \dots, B_l\} \text{ of } \{1, \dots, k\}} c(\mathcal{B}) M_{(b_1)} M_{(b_2)} \cdots M_{(b_l)}, \tag{11}$$

where as above $c(\mathcal{B}) = (\operatorname{card} B_1 - 1)! \cdots (\operatorname{card} B_l - 1)!$ and $b_s = \sum_{j \in B_s} i_j$.

Now define an automorphism ψ of $\mathbf{Z}\langle x, y \rangle$ by

$$\psi(x) = x + y, \quad \psi(y) = -y. \tag{12}$$

Evidently $\psi^2 = \mathrm{id}$, and $\psi(\mathfrak{H}^1) = \mathfrak{H}^1$. Thus ψ defines an additive involution of $\mathfrak{H}^1 \cong$ QSym (which is *not*, however, a homomorphism for the $*$-product). We can describe the action of ψ on the integral bases for QSym as follows.

Theorem 3.2. *For any composition I,*

1. $\psi(M_I) = (-1)^{\ell(I)} F_I$;
2. $\psi(E_I) = -E_{I^*}$.

Proof. Suppose $w = w(I)$ is the word in x and y corresponding to a composition I. Then evidently substituting y in place of any particular factor x in w corresponds to splitting a part of I. With this observation, part (1) is clear (there is also one factor of -1 for each occurrence of y in w).

Now we prove part (2). We have

$$\psi(E_I) = \sum_{J \preceq I} \psi(M_J) = \sum_{J \preceq I} (-1)^{\ell(J)} F_J$$

from part (1). From Example 1 of [15], $S(F_I) = (-1)^{|I|} F_{\bar{I}^*}$, where S is the antipode of QSym. Thus

$$\begin{aligned} S\psi(E_I) = \sum_{J \preceq I} (1)^{\ell(J)+|J|} F_{\bar{J}^*} &= -\sum_{J \preceq I} (-1)^{\ell(J^*)} F_{\bar{J}^*} \\ &= -\sum_{\bar{J}^* \succeq \bar{I}^*} (-1)^{\ell(\bar{J}^*)} F_{\bar{J}^*} = -\sum_{K \succeq \bar{I}^*} (-1)^{\ell(K)} F_K. \end{aligned}$$

Now by Möbius inversion of equation (7)

$$M_I = \sum_{I \preceq J} (-1)^{\ell(I)-\ell(J)} F_J,$$

and so

$$S\psi(E_I) = -(-1)^{\ell(\bar{I}^*)} M_{\bar{I}^*}$$

Apply S be both sides to get

$$\psi(E_I) = -(-1)^{\ell(I^*)}(-1)^{\ell(\bar{I}^*)} E_{I^*} = -E_{I^*}.$$

□

4 Finite Multiple Sums and Mod p Results

In this section we consider the finite sums

$$A_{(i_1,\ldots,i_k)}(n) = \sum_{n \geq n_1 > n_2 > \cdots > n_k \geq 1} \frac{1}{n_1^{i_1} \cdots n_k^{i_k}}$$

and

$$S_{(i_1,\ldots,i_k)}(n) = \sum_{n \geq n_1 \geq n_2 \geq \cdots \geq n_k \geq 1} \frac{1}{n_1^{i_1} \cdots n_k^{i_k}},$$

where the notation is patterned after that of [13]; the multiple zeta values are given by

$$\zeta(i_1,\ldots,i_k) = \lim_{n\to\infty} A_{(i_1,\ldots,i_k)}(n),$$

when the limit exists (i.e., when $i_1 > 1$).

Let $\rho_n = eT\phi_n$, where ϕ_n is the map defined in §2, T is the automorphism of QSym sending M_I to $M_{\bar{I}}$, and e is the function that sends t_i to $\frac{1}{i}$. Then $\rho_n : (\mathfrak{H}^1, *) \to \mathbf{R}$ is a homomorphism sending $z_{i_1} z_{i_2} \cdots z_{i_k}$ in $\mathfrak{H}^1$ to $A_{(i_1,\ldots,i_k)}(n)$. We can combine the homomorphisms ρ_n into a homomorphism ρ that sends $w \in \mathfrak{H}^1$ to the real-valued sequence $n \to \rho_n(w)$. We shall write A_I for the real-valued sequence $n \to A_I(n)$ (and similarly for S_I), so $\rho\phi^{-1}$ sends M_I to A_I and E_I to S_I. For example, we can apply $\rho\phi^{-1}$ to equation (10) above to get

$$A_I = \sum_{J \preceq I} (-1)^{\ell(I)-\ell(J)} S_J \tag{13}$$

Applying the homomorphism $\rho_n\phi^{-1}$ to Theorem 2.3 and equation (11), we get formulas for symmetric sums of $A_I(n)$ and $S_I(n)$ in terms of length one sums $S_{(m)}(n)$ (cf. Theorems 2.1 and 2.2 of [13]).

Theorem 4.1. *For any composition $I = (i_1, \cdots, i_k)$,*

$$\sum_{\sigma\in\Sigma_k} S_{\sigma\cdot I}(n) = \sum_{\textit{partitions } \mathcal{B} = \{B_1,\ldots,B_l\} \textit{ of } \{1,\ldots,k\}} c(\mathcal{B}) S_{(b_1)}(n) \cdots S_{(b_l)}(n)$$

$$\sum_{\sigma\in\Sigma_k} A_{\sigma\cdot I}(n) = \sum_{\textit{partitions } \mathcal{B} = \{B_1,\ldots,B_l\} \textit{ of } \{1,\ldots,k\}} (-1)^{k-l} c(\mathcal{B}) S_{(b_1)}(n) \cdots S_{(b_l)}(n),$$

where $c(\mathcal{B}) = (\operatorname{card} B_1 - 1)! \cdots (\operatorname{card} B_l)!$ and $b_s = \sum_{j\in B_s} i_j$.

Remark. If $I = (s, s, \ldots, s)$, the second formula above gives a more explicit version of Lemma 2.11 of [29].

We consider two operators on the space $\mathbf{R}^{\mathbf{N}}$ of real-valued sequences. First, there is the partial-sum operator Σ, given by

$$\Sigma a(n) = \sum_{i=0}^{n} a(i)$$

for $a \in \mathbf{R}^{\mathbf{N}}$. Second, there is the operator ∇ given by

$$\nabla a(n) = \sum_{i=0}^{n} \binom{n}{i} (-1)^i a(i).$$

It is easy to show that Σ and ∇ generate a dihedral group within the automorphisms of $\mathbf{R}^{\mathbf{N}}$, i.e., $\nabla^2 = \mathrm{id}$ and $\Sigma\nabla = \nabla\Sigma^{-1}$. It follows that $(\Sigma\nabla)^2 = \mathrm{id}$. We have the following result on multiple sums.

Theorem 4.2. *For any composition I, $\Sigma\nabla S_I = -S_{I^*}$.*

Proof. We proceed by induction on $|I|$. The weight one case is $\Sigma\nabla S_{(1)} = \nabla\Sigma^{-1}S_{(1)} = -S_{(1)}$, i.e.,

$$\sum_{k=1}^{n} \frac{(-1)^k}{k}\binom{n}{k} = -\sum_{k=1}^{n}\frac{1}{k},$$

a classical (but often rediscovered) formula which actually goes back to Euler [6]. For $I = (i_1, i_2, \dots, i_k)$, it is straightforward to show that $\nabla S_I(n) = \frac{1}{n}f(n)$, where $f \in \mathbf{R}^{\mathbf{N}}$ is given by

$$f(n) = \begin{cases} S_{(i_2,\dots,i_k)}(n), & \text{if } i_1 = 1; \\ \Sigma^{-1}S_{(i_1-1,i_2,\dots,i_k)}(n), & \text{otherwise.} \end{cases}$$

Now suppose the theorem has been proved for all I of weight less than n, and let $I = (i_1, \dots, i_k)$ have weight n. There are two cases: $i_1 = 1$, and $i_1 > 1$. In the first case, let $(i_2, \dots, i_k)^* = J = (j_1, \dots, j_r)$. By the assertion of the preceding paragraph and the induction hypothesis,

$$\Sigma\nabla S_I(n) = \Sigma(\frac{1}{n}\nabla S_{J^*}(n)) = \Sigma(\frac{1}{n}\Sigma^{-1}S_J(n)) = -S_{(j_1+1,j_2,\dots,j_r)}(n).$$

But evidently $I^* = (j_1+1, j_2, \dots, j_r)$, so the theorem holds in this case.

If $i_1 > 1$, we instead write $(i_1 - 1, i_2, \dots, i_k)^* = J = (j_1, \dots, j_r)$. Then

$$\Sigma\nabla S_I(n) = \Sigma(\frac{1}{n}\nabla\Sigma^{-1}S_{J^*}(n)) = \Sigma(\frac{1}{n}\Sigma\nabla S_{J^*}(n)) = -\Sigma(\frac{1}{n}S_J(n)) = -S_{(1,j_1,\dots,j_r)}(n).$$

But in this case $I^* = (1, j_1, \dots, j_r)$, so the theorem holds in this case as well. □

The proof of the preceding result is essentially a formalization of the procedure in App. B of [26]. Recalling the automorphism ψ of $\mathfrak{H}^1$ defined by equation (12), we note that Theorem 4.2, together with part (2) of Theorem 3.2, says that the diagram

$$\begin{array}{ccc} \mathrm{QSym} & \xrightarrow{\psi} & \mathrm{QSym} \\ \rho\downarrow & & \rho\downarrow \\ \mathbf{R}^{\mathbf{N}} & \xrightarrow{\Sigma\nabla} & \mathbf{R}^{\mathbf{N}} \end{array} \tag{14}$$

commutes.

We now turn to mod p results about $S_I(p-1)$ and $A_I(p-1)$, where p is a prime. Since the sums $A_I(p-1)$ and $S_I(p-1)$ contain no factors of p in the denominators, they can be regarded as elements of the field $\mathbf{Z}/p\mathbf{Z}$. The following result about length one harmonic sums is well known (cf. [11], pp. 86-88).

Theorem 4.3. $S_{(k)}(p-1) \equiv 0 \mod p$ *for all prime $p > k+1$.*

Proof. Since the group of units in $\mathbf{Z}/p\mathbf{Z}$ has order $p-1$, we have

$$x^{p-1}-1=(x-1)(x-2)\cdots(x-p+1)$$

in $\mathbf{Z}/p\mathbf{Z}$. Thus, in the expansion

$$x(x-1)\cdots(x-p+1)=\sum_{i=1}^{p}(-1)^{p-i}e_{p-i}(1,2,\dots,p-1)x^i,$$

where e_i is the ith elementary symmetric function, we must have $e_{p-i}(1,\dots,p-1)\equiv 0$ mod p except for $e_0(1,\dots,p-1)\equiv 1$ and $e_{p-1}(1,\dots,p-1)\equiv -1$ mod p. Thus, the Newton formulas

$$\sum_{i=1}^{r}(-1)^{i-1}p_i(1,\dots,p-1)e_{r-i}(1,\dots,p-1)=re_r(1,\dots,p-1),$$

where p_i is the ith power-sum symmetric function, reduce mod p to

$$p_r(1,\dots,p-1)\equiv -re_r(1,\dots,p-1)\equiv 0 \mod p$$

when $p>r+1$. But

$$p_r(1,\dots,p-1)\equiv S_{(r)}(p-1) \mod p$$

since inversion permutes the units of $\mathbf{Z}/p\mathbf{Z}$, so the result follows. □

Combining the preceding result with Theorem 4.1 gives the following.

Theorem 4.4. *For any composition $I=(i_1,\dots,i_k)$ and prime $p>|I|+1$,*

$$\sum_{\sigma\in\Sigma_k}A_{\sigma\cdot I}(p-1)\equiv\sum_{\sigma\in\Sigma_k}S_{\sigma\cdot I}(p-1)\equiv 0 \mod p.$$

In particular it follows that, for $I=(r,r,\dots,r)$ (k repetitions), we have

$$A_I(p-1)\equiv S_I(p-1)\equiv 0 \mod p \tag{15}$$

for prime $p>rk+1$ (cf. Theorem 2.13 of [29]). There is the following result relating sums associated to I and $\bar{I}$ (cf. Lemma 3.2 of [29]).

Theorem 4.5. *For any composition I, $A_I(p-1)\equiv(-1)^{|I|}A_{\bar{I}}(p-1) \mod p$, and similarly $S_I(p-1)\equiv(-1)^{|I|}S_{\bar{I}}(p-1) \mod p$.*

Proof. Let $I=(i_1,\dots,i_k)$. Working mod p, we have

$$\begin{aligned}A_I(p-1)&\equiv\sum_{p>a_1>\cdots>a_k>0}\frac{1}{a_1^{i_1}\cdots a_k^{i_k}}\equiv\sum_{p>a_1>\cdots>a_k>0}\frac{(-1)^{i_1+\cdots+i_k}}{(p-a_1^{i_1})\cdots(p-a_k^{i_k})}\\&\equiv\sum_{0<b_1<\cdots<b_k<p}\frac{(-1)^{i_1+\cdots+i_k}}{b_1^{i_1}\cdots b_k^{i_k}}=(-1)^{|I|}A_{\bar{I}}(p-1),\end{aligned}$$

and similarly for S_I. □

An immediate consequence is that $S_I(p-1) \equiv A_I(p-1) \equiv 0 \mod p$ if $I = \bar{I}$ and $|I|$ is odd. Another consequence is that $S_{(i,j)}(p-1) \equiv A_{(i,j)}(p-1) \equiv 0 \mod p$ when $p > i+j+1$ and $i+j$ is even. This is because

$$S_{(i,j)}(p-1) + S_{(j,i)}(p-1) \equiv 0 \mod p$$

for $p > i+j+1$ by Theorem 4.1, while $S_{(i,j)}(p-1) \equiv S_{(j,i)}(p-1) \mod p$ when $i+j$ is even by Theorem 4.5.

We have the following result relating S_I and S_{I^*}.

Theorem 4.6. $S_I(p-1) \equiv -S_{I^*}(p-1) \mod p$ *for all primes* p.

Proof. Let f be a sequence. From the definition of ∇

$$\Sigma\nabla f(n) = \sum_{i=0}^{n} \binom{n+1}{i+1}(-1)^i f(i),$$

so taking $n = p-1$ gives

$$\Sigma\nabla f(p-1) \equiv (-1)^{p-1} f(p-1) \equiv f(p-1) \mod p.$$

Now take $f = S_I$ and apply Theorem 4.2. $\square$

Define, for each prime p, a map $\chi_p : \mathfrak{H}^1 \to \mathbf{Z}/p\mathbf{Z}$ by $\chi_p(w) = \rho_{p-1}(w)$. Then we can use the commutative diagram (14) to restate Theorem 4.6 in the following "algebraic" form, which corresponds to the duality theorem for multiple zeta values as formulated in Corollary 6.2 of [14].

Theorem 4.7. *As elements of* $\mathbf{Z}/p\mathbf{Z}$*,* $\chi_p(w) = \chi_p(\psi(w))$ *for words* w *of* $\mathfrak{H}^1$.

For example, since $\psi(x^2y^3) = -x^2y^3 - xy^4 - yxy^3 - y^5$, we have

$$A_{(3,1,1)}(p-1) \equiv -A_{(3,1,1)}(p-1) - A_{(2,1,1,1)}(p-1) - A_{(1,2,1,1)}(p-1) - A_{(1,1,1,1,1)}(p-1) \mod p.$$

(In fact, for $p > 6$ it follows from Theorem 7.1 below that both sides are congruent mod p to $\frac{1}{2}B_{p-5}$, where B_i is the ith Bernoulli number.)

5 Harmonic Sums of Height One

Following the terminology of [16], we say a word of $\mathfrak{H}^1$ of the form $x^{h-1}y^k$ has height one. We shall call the corresponding multiple harmonic sums $A_{(h,1,\dots,1)}(n)$ sums of height one. Harmonic sums of this form have a number of special properties, which we discuss in this section.

In this section only we use superscripts for repetition in compositions, so $(n, 1^k)$ means the composition of weight $n+k$ with k repetitions of 1. For compositions of this form, we have the following result relating the two kinds of harmonic sums mod p.

Theorem 5.1. *For any prime $p > k$,*

$$S_{(h,1^{k-1})}(p-1) \equiv (-1)^h A_{(h,1^{k-1})}(p-1) \mod p.$$

Proof. Equate parts (1) and (2) of Theorem 3.1 and apply the homomorphism ρ_{p-1} to get

$$(-1)^{\ell(I)} S_{\bar{I}}(p-1) = \sum_{I_1 \sqcup \cdots \sqcup I_l = I} (-1)^l A_{I_1}(p-1) \cdots A_{I_l}(p-1) \tag{16}$$

for any p. Now set $I = (1^{k-1}, h)$ in equation (16) and reduce both sides mod p. The hypothesis insures that all terms on the right-hand side are zero mod p except the one with $l = 1$, and so we have

$$(-1)^{k-1} S_{(h,1^{k-1})}(p-1) \equiv A_{(1^{k-1},h)}(p-1) \mod p,$$

and the conclusion follows by Theorem 4.5. □

Combining the preceding result with the duality theorem gives the following congruence. It can be compared with Theorem 4.4 of [13], which asserts that $\zeta(h+1, 1^{k-1}) = \zeta(k+1, 1^{h-1})$ for positive integers h and k.

Theorem 5.2. *If p is a prime with $p > \max\{k, h\}$, then*

$$A_{(h,1^{k-1})}(p-1) \equiv A_{(k,1^{h-1})}(p-1) \mod p.$$

Proof. First note that $(h, 1^{k-1})^* = (1^{h-1}, k)$. So, combining Theorems 4.6 and 4.5,

$$S_{(h,1^{k-1})}(p-1) \equiv -S_{(1^{h-1},k)}(p-1) \equiv (-1)^{h+k} S_{(k,1^{h-1})}(p-1) \mod p. \tag{17}$$

Now by the preceding result

$$\begin{aligned} S_{(h,1^{k-1})}(p-1) &\equiv (-1)^h A_{(h,1^{k-1})}(p-1) \mod p, \\ S_{(k,1^{h-1})}(p-1) &\equiv (-1)^k A_{(k,1^{h-1})}(p-1) \mod p, \end{aligned}$$

so the conclusion follows from congruence (17). □

The height one harmonic sums can be written in terms of Stirling numbers. The (unsigned) Stirling numbers of the first kind (Stirling cycle numbers) are given by

$$\begin{bmatrix} n \\ k \end{bmatrix} = \text{number of permutations of } \{1, 2, \ldots, n\} \text{ with } k \text{ disjoint cycles},$$

and the Stirling number of the second kind (Stirling subset numbers) are given by

$$\begin{Bmatrix} n \\ k \end{Bmatrix} = \text{number of partitions of } \{1, 2, \ldots, n\} \text{ with } k \text{ blocks}.$$

For basic properties of Stirling numbers see, e.g., [10]. Note that

$$\begin{bmatrix} n+1 \\ k+1 \end{bmatrix} = e_{n-k}(1,2,\dots,n),$$

since each side is the coefficient of x^k in the expansion of $x(x+1)\cdots(x+n)$. Hence

$$\begin{bmatrix} n+1 \\ k+1 \end{bmatrix} = n! \sum_{n \ge j_1 > \cdots > j_{n-k} \ge 1} \frac{j_1 \cdots j_{n-k}}{n!} = n! \sum_{n \ge i_1 > \cdots > i_k \ge 1} \frac{1}{i_1 \cdots i_k} = n! A_{(1^k)}(n). \tag{18}$$

An immediate consequence is the following result, which expresses height one sums in terms of Stirling numbers of the first kind.

Theorem 5.3. *For positive integers h, k, and n,*

$$A_{(h,1^{k-1})}(n) = \sum_{j=k}^{n} \frac{\begin{bmatrix} j \\ k \end{bmatrix}}{j^{h-1} j!}.$$

Proof. We have

$$A_{(h,1^{k-1})}(n) = \sum_{n \ge i_1 > \cdots > i_k \ge 1} \frac{1}{i_1^h i_2 \cdots i_k} = \sum_{j=k}^{n} \frac{1}{j^h} A_{(1^{k-1})}(j-1) = \sum_{j=k}^{n} \frac{\begin{bmatrix} j \\ k \end{bmatrix}}{j^h (j-1)!}$$

(where we used equation (18) in the last step), from which the conclusion follows. □

In doing computations, the following mod p result is often useful.

Theorem 5.4. *For prime p and positive integers $h, k < p$,*

$$A_{(h,1^{k-1})}(p-1) \equiv \sum_{j=1}^{p-k} (-1)^j (-j)^{p-h} (j-1)! \begin{Bmatrix} p-k \\ j \end{Bmatrix} \mod p.$$

Proof. We start by setting $n = p-1$ and reversing the order of summation in the preceding result:

$$A_{(h,1^{k-1})}(p-1) = \sum_{j=1}^{p-k} \frac{\begin{bmatrix} p-j \\ k \end{bmatrix}}{(p-j)^{h-1}(p-j)!}.$$

By Fermat's theorem, $(p-j)^{1-h} \equiv (p-j)^{p-h} \equiv (-j)^{p-j} \mod p$. Also, since

$$(-1)^{j-1} \equiv \binom{p-1}{j-1} \equiv \frac{(p-1)!}{(j-1)!(p-j)!} \mod p,$$

it follows that

$$\frac{1}{(p-j)!} \equiv (-1)^j (j-1)! \mod p$$

since $(p-1)! \equiv -1 \bmod p$ by Wilson's theorem. Hence

$$A_{(h,1^{k-1})}(p-1) \equiv \sum_{j=1}^{p-k} (-1)^j (j-1)!(-j)^{p-h} \begin{bmatrix} p-j \\ k \end{bmatrix} \mod p. \tag{19}$$

The conclusion then follows from congruence (19) and a mod p relation between the two kinds of Stirling numbers:

$$\begin{bmatrix} n \\ k \end{bmatrix} \equiv \begin{Bmatrix} p-k \\ p-n \end{Bmatrix} \mod p$$

for prime p and $1 \le k \le n \le p-1$, which follows by induction on n using the recurrence relations for the two kinds of Stirling numbers. □

6 Results for Short Lengths

In this section we prove some results about the sums $S_I(p-1)$ for $\ell(I) \le 5$, which will be useful for the calculations of the next section. (Similar results hold for the $A_I(p-1)$, but the $S_I(p-1)$ are more convenient in view of Theorem 4.6.) Henceforth we will assume that all congruences are mod p. The following result expresses $S_I(p-1)$ in terms of a Bernoulli number when $\ell(I) = 2$ (cf. [29], Theorem 3.1).

Theorem 6.1. *For i, j positive and prime $p > i + j + 1$,*

$$S_{(i,j)}(p-1) \equiv \frac{(-1)^i}{i+j} \binom{i+j}{i} B_{p-i-j}.$$

Proof. We use the standard identity expressing sums of powers in terms of Bernoulli numbers (see, e.g., [19]):

$$\sum_{a=1}^{n-1} a^r = \frac{1}{r+1} \sum_{k=0}^{r} \binom{r+1}{k} B_k n^{r+1-k}. \tag{20}$$

Using Fermat's theorem and equation (20), we have

$$\begin{aligned} S_{(i,j)}(p-1) &\equiv A_{(i,j)}(p-1) = \sum_{a=1}^{p-1} \frac{1}{a^i} \sum_{b=1}^{a-1} \frac{1}{b^j} \equiv \sum_{a=1}^{p-1} \frac{1}{a^i} \sum_{b=1}^{a-1} b^{p-1-j} \\ &= \sum_{a=1}^{p-1} \frac{1}{a^j} \frac{1}{p-j} \sum_{k=0}^{p-1-j} \binom{p-j}{k} B_k a^{p-j-k} = \frac{1}{p-j} \sum_{k=0}^{p-1-j} \binom{p-j}{k} B_k \sum_{a=1}^{p-1} a^{p-i-j-k}. \end{aligned}$$

Now $\sum_{a=1}^{p-1} a^{p-i-j-k} \equiv 0$ unless $k = p-i-j$. So the sum reduces to

$$S_{(i,j)}(p-1) \equiv \frac{1}{p-j} \binom{p-j}{p-i-j} B_{p-i-j}(p-1) \equiv \frac{1}{j} \binom{p-j}{i} B_{p-i-j},$$

from which the conclusion follows. □

Since odd Bernoulli numbers are zero, this result implies our earlier observation that $S_{(i,j)}(p-1) \equiv 0$ when $i+j$ is even. Note also that it implies $S_{(i,1)}(p-1) \equiv B_{p-1-i}$ for i even, so we can restate it as

$$S_{(i,j)}(p-1) \equiv \frac{(-1)^i}{i+j}\binom{i+j}{i} S_{(i+j-1,1)}(p-1), \tag{21}$$

i.e., all double sums of odd weight n can be written in terms of $S_{(n-1,1)}(p-1)$. In fact, if the weight is odd we can write all triple sums in terms of the same quantity (cf. [29], Theorem 3.5).

Theorem 6.2. *If $n = i+j+k$ is odd and $p > n+1$, then*

$$S_{(i,j,k)}(p-1) \equiv \frac{1}{2n}\left[(-1)^i\binom{n}{i} + (-1)^{i+j}\binom{n}{i+j}\right] S_{(n-1,1)}(p-1).$$

Proof. From Theorem 3.1 it follows that

$$A_I(m) = \sum_{I_1 \sqcup I_2 \sqcup \cdots \sqcup I_l = I} (-1)^{\ell(I)-l} S_{\bar{I}_1}(m) S_{\bar{I}_2}(m) \cdots S_{\bar{I}_l}(m) \tag{22}$$

for any composition I and positive integer m. In particular, for $\ell(I) = 3$ we have

$$A_{(i,j,k)}(m) = S_{(i)}(m)S_{(j)}(m)S_{(k)}(m) - S_{(j,i)}(m)S_{(k)}(m) - S_{(i)}(m)S_{(k,j)}(m) + S_{(k,j,i)}(m).$$

But also, from equation (13),

$$A_{(i,j,k)}(m) = S_{(i,j,k)}(m) - S_{(i+j,k)}(m) - S_{(i,j+k)}(m) + S_{(i+j+k)}(m).$$

In the case $m = p-1$, this gives the congruence

$$S_{(k,j,i)}(p-1) \equiv S_{(i,j,k)}(p-1) - S_{(i+j,k)}(p-1) - S_{(i,j+k)}(p-1),$$

using Theorem 4.3, and if in addition $i+j+k$ is odd, we have

$$2S_{(i,j,k)}(p-1) \equiv S_{(i+j,k)}(p-1) + S_{(i,j+k)}(p-1)$$

from Theorem 4.5. Now use congruence (21). $\square$

For a composition $I = (i_1, i_2, \ldots, i_k)$ of odd weight and length $k > 1$ it is convenient to define

$$C(I) = \sum_{j=1}^{k-1} (-1)^{i_1+\cdots+i_j} \binom{|I|}{i_1+\cdots+i_j}, \tag{23}$$

so Theorem 6.2 says that

$$S_I(p-1) \equiv \frac{1}{2n} C(I) S_{(n-1,1)}(p-1)$$

when $n = |I|$ is odd and $\ell(I) = 3$. It is easy to show that the function $C(I)$ mirrors the properties of $S_I(p-1)$ with regard to reversal and duality, i.e., $C(\bar{I}) = -C(I)$ and $C(I^*) = -C(I)$.

In the even-weight case, we can express all length-4 sums in terms of triple sums and products of lower-weight sums as follows.

Theorem 6.3. *If $n = i + j + k + l$ is even and $p > n + 1$, then*

$$2S_{(i,j,k,l)}(p-1) \equiv S_{(i+j,k,l)}(p-1) + S_{(i,j+k,l)}(p-1) + S_{(i,j,k+l)}(p-1) + S_{(i,j)}(p-1)S_{(k,l)}(p-1).$$

Proof. From equation (22) with $\ell(I) = 4$,

$$\begin{aligned} A_{(i,j,k,l)}(m) = &-S_{(l,k,j,i)}(m) + S_{(i)}(m)S_{(l,j,k)}(m) + S_{(j,i)}(m)S_{(l,k)}(m) + S_{(k,j,i)}(m)S_{(k)}(m) \\ &- S_{(i)}(m)S_{(j)}(m)S_{(l,k)}(m) - S_{(i)}(m)S_{(k,j)}(m)S_{(l)}(m) - S_{(j,i)}(m)S_{(k)}(m)S_{(l)}(m) \\ &+ S_{(i)}(m)S_{(j)}(m)S_{(k)}(m)S_{(l)}(m). \end{aligned}$$

Set $m = p - 1$ and reduce mod p to get

$$A_{(i,j,k,l)}(p-1) \equiv -S_{(l,k,j,i)}(p-1) + S_{(j,i)}(p-1)S_{(l,k)}(p-1).$$

But equation (13) gives, after reduction mod p,

$$A_{(i,j,k,l)}(p-1) \equiv S_{(i,j,k,l)}(p-1) - S_{(i+j,k,l)}(p-1) - S_{(i,j+k,l)}(p-1) - S_{(i,j,k+l)}(p-1),$$

and the conclusion follows by the use of Theorem 4.5. □

If we specialize the preceding result to the case $k = i, l = j$, we have

$$2S_{(i,j,i,j)}(p-1) \equiv S_{(i+j,i,j)}(p-1) + S_{(i,i+j,j)}(p-1) + S_{(i,j,i+j)}(p-1) + S_{(i,j)}(p-1)^2.$$

But the sum of the first three terms on the right-hand side is zero mod p by Theorem 4.4, so we have

$$2S_{(i,j,i,j)}(p-1) \equiv S_{(i,j)}(p-1)^2. \tag{24}$$

We note that we also have $A_{(i,j,i,j)}(p-1) \equiv S_{(i,j,i,j)}(p-1)$, which follows from equation (13), Theorem 4.4, and the comments following Theorem 4.5. If i and j have the same parity, then $i + j$ is even and the right-hand side of (24) is zero mod p by Theorem 4.5, so in this case

$$S_{(i,j,i,j)}(p-1) \equiv A_{(i,j,i,j)}(p-1) \equiv 0.$$

This proves the case $n = 2$ of the first part of Conjecture 3.9 of [29].

It is evident that the ideas of the two preceding results can be used to write $S_I(p-1)$, where $|I|$ and $\ell(I)$ are of the same parity, in terms of sums of shorter lengths, together with products of sums of lower weight. We state one more result of this type, since we need it for our computations in weight 9; we omit the proof, which is straightforward.

Theorem 6.4. *If $I = (i, j, k, l, m)$ is a composition of odd weight n and $p > n + 1$, then*

$$\begin{aligned} 2S_I(p-1) \equiv &\, S_{(i+j,k,l,m)}(p-1) + S_{(i,j+k,l,m)}(p-1) + S_{(i,j,k+l,m)}(p-1) + S_{(i,j,k,l+m)}(p-1) \\ &- \frac{1}{2n}C(I)S_{(n-1,1)}(p-1) + S_{(i,j)}(p-1)S_{(k,l,m)}(p-1) + S_{(i,j,k)}(p-1)S_{(l,m)}(p-1), \end{aligned}$$

where $C(I)$ is given by equation (23).

7 Calculations in Low Weights

In this section, we find, for $n \leq 9$, sets of quantities that generate all multiple harmonic sums $S_I(p-1)$ of weight n mod p when $p > n+1$. In fact, all our generators will be sums of the form $S_{(2h,1,\dots,1)}(p-1)$ ($\equiv A_{(2h,1,\dots,1)}(p-1)$ by Theorem 5.1), or products of such sums. To make the notation less cumbersome we will use an abbreviated form in referring to specific sums, e.g., we write S_{221} instead of $S_{(2,2,1)}(p-1)$. We will also assume that $p > |I|+1$ in considering any sum $S_I(p-1)$.

The congruence (15) implies $S_I(p-1) \equiv 0$ when I has length 1 or $|I|$, so the only sums $S_I(p-1)$ with $|I| \leq 3$ that are (possibly) nonzero mod p are $S_{21} \equiv B_{p-3}$ and $S_{12} \equiv -B_{p-3}$. Now p divides the numerator of B_{p-3} only for certain irregular primes p, the only examples with $p < 1.2 \times 10^7$ being $p = 16,843$ and $p = 2,124,679$ [18, 4, 3].

For I of weight 4 we have $S_I(p-1) \equiv 0$; this follows from congruence (15) if $\ell(I) = 1$ or 4, by the remarks following Theorem 4.5 if $\ell(I) = 2$, and by duality if $\ell(I) = 3$ (since in that case $\ell(I^*) = 2$).

In weight 5, it suffices by duality to consider $S_I(p-1)$ with $\ell(I) \leq 3$. Theorems 6.1 and 6.2 give the following result, which implies that all weight 5 sums vanish mod p if and only if p divides the numerator of B_{p-5}; the only known p for which this happens is $p = 37$, and this is the only such $p < 1.2 \times 10^7$ [3].

Theorem 7.1. *All $S_I(p-1)$ with $|I| = 5$ are multiples of $S_{41} \equiv B_{p-5}$. In particular, $S_{32} \equiv -2S_{41}$, $S_{311} \equiv -\frac{1}{2}S_{41}$, and $S_{221} \equiv \frac{3}{2}S_{41}$.*

For $|I| = 6$, it follows from the remarks after Theorem 4.5 and duality that $S_I(p-1) \equiv 0$ unless $\ell(I) = 3$ or 4. By duality it suffices to consider length 3. Here we have the following result, which implies that all harmonic sums of weight 6 vanish if and only if p divides B_{p-3}.

Theorem 7.2. *All the $S_I(p-1)$ with $|I| = 6$ are multiples of $S_{411} \equiv -\frac{1}{6}B_{p-3}^2$. In particular, $S_{141} \equiv -2S_{411}$, $S_{312} \equiv -S_{411}$, $S_{321} \equiv -2S_{411}$, and $S_{231} \equiv 3S_{411}$.*

Proof. From Theorem 4.4, the symmetric sum

$$S_{411} + S_{141} + S_{114} \equiv 2S_{411} + S_{141}$$

is congruent to zero, from which the statement about S_{141} follows. For the same reason

$$S_{3111} + S_{1311} + S_{1131} + S_{1113} \equiv 2S_{3111} + 2S_{1311}$$

is congruent to zero; applying duality, we get $S_{411} + S_{312} \equiv 0$. Theorem 4.4 also gives

$$S_{321} + S_{231} \equiv -S_{312} \equiv S_{411} \tag{25}$$

Now multiplying in QSym and reducing mod p, we have

$$\begin{aligned} 0 \equiv& S_1 S_{221} \\ \equiv& S_{1221} + S_{2121} + 2S_{2211} - S_{321} - S_{231} - S_{222} \\ \equiv& S_{2121} + 2S_{2211} - S_{321} - S_{231}. \end{aligned}$$

Apply duality (and Theorem 4.5) to obtain from this

$$3S_{321} + 2S_{231} \equiv 0, \tag{26}$$

and solve congruences (25) and (26) to obtain S_{321} and S_{231} in terms of S_{411}.

Finally, $S_{2121} \equiv \frac{1}{2}S_{21}^2$ by congruence (24), while from duality we have $S_{2121} \equiv -S_{231}$. Since we've already shown $S_{231} \equiv 3S_{411}$, the congruence $S_{21}^2 \equiv -6S_{411}$ follows. □

In weight 7, we need only consider sums of length 4 or less. By Theorems 6.1 and 6.2 we can express all sums of length 2 and 3 in terms of $S_{61} \equiv B_{p-7}$, as follows.

$$S_{52} \equiv -3S_{61} \tag{27}$$
$$S_{43} \equiv 5S_{61} \tag{28}$$
$$S_{511} \equiv -S_{61} \tag{29}$$
$$S_{421} \equiv 3S_{61} \tag{30}$$
$$S_{412} \equiv S_{61} \tag{31}$$
$$S_{241} \equiv 2S_{61} \tag{32}$$
$$S_{331} \equiv -2S_{61} \tag{33}$$
$$S_{322} \equiv -4S_{61} \tag{34}$$

For the length 4 sums we have the following result.

Theorem 7.3. *The length 4 harmonic sums of weight 7 can be written in terms of* $S_{61} \equiv B_{p-7}$ *and* S_{4111}. *In particular* $S_{3121} \equiv S_{2221} \equiv S_{4111}$, *and*

$$\begin{aligned} S_{1411} &\equiv 3S_{61} - 3S_{4111} \\ S_{1321} &\equiv 9S_{61} - 3S_{4111} \\ S_{1312} &\equiv -9S_{61} + 5S_{4111} \\ S_{3211} &\equiv -6S_{61} + S_{4111}. \end{aligned}$$

Proof. Duality gives $S_{1411} \equiv S_{3112}$, $S_{3121} \equiv S_{2311}$, and $S_{2212} \equiv S_{1321}$. Thus, it suffices to consider the seven length-four sums S_{4111}, S_{1411}, S_{3121}, S_{2212}, S_{1312}, S_{2221}, and S_{3211}. We can obtain relations among these sums and S_{61} by multiplying lower-weight sums in QSym, reducing mod p, and then applying congruences (27-34) above to get all terms of length three or less in terms of S_{61}. For example, multiplying S_1 by S_{411} gives

$$3S_{61} \equiv S_{1411} + 3S_{4111}. \tag{35}$$

Similarly, consideration of the products S_2S_{311}, S_2S_{221}, $S_{21}S_{31}$, and $S_{11}S_{32}$ gives respectively

$$-3S_{61} \equiv 2S_{3121} + S_{3211} + S_{1411} \tag{36}$$
$$9S_{61} \equiv 3S_{2221} + S_{2212} \tag{37}$$
$$-3S_{61} \equiv -S_{1312} + 3S_{3121} + 2S_{3211} \tag{38}$$
$$-3S_{61} \equiv S_{1411} + S_{2212} + S_{1312} + S_{3211}. \tag{39}$$

Finally, multiplying S_1 by S_{3111} and using duality gives

$$-3S_{61} \equiv S_{4111} + S_{1411} + S_{3211} + S_{3121} \tag{40}$$

The six congruences (35-40) can then be solved for S_{61} and S_{4111} to obtain the conclusion. □

Remark. While it does not appear that S_{4111} is a multiple of S_{61}, we have not been able to prove this. There is no known prime p for which $B_{p-7} \equiv 0$; in particular, $B_{p-7} \not\equiv 0$ for all $p < 1.2 \times 10^7$ [3].

In weight 8, it suffices by duality to consider I with $\ell(I) \leq 4$. By Theorem 6.3, we can write all length 4 sums in terms of triple sums and $S_{41}S_{21}$, and of course all double sums are zero. So it is enough to consider length 3, where we have the following result.

Theorem 7.4. *All length 3, weight 8 sums can be written in terms of S_{611} and $S_{41}S_{21} \equiv B_{p-5}B_{p-3}$. In particular,*

$$S_{521} \equiv S_{611} + S_{41}S_{21} \tag{41}$$
$$S_{512} \equiv \frac{1}{2}(-7S_{611} - S_{41}S_{21}) \tag{42}$$
$$S_{431} \equiv \frac{1}{2}(-25S_{611} - 9S_{41}S_{21}) \tag{43}$$
$$S_{413} \equiv \frac{1}{2}(5S_{611} + S_{41}S_{21}) \tag{44}$$
$$S_{332} \equiv S_{422} \equiv 10S_{611} + 2S_{41}S_{21}. \tag{45}$$

Proof. Consideration of the products $S_1S_{211111} \equiv 0$ and $S_1S_{121111} \equiv 0$, using duality, gives respectively

$$S_{611} + S_{521} + S_{431} + S_{341} + S_{251} + S_{161} \equiv 0, \tag{46}$$
$$S_{521} + S_{512} + S_{422} + S_{332} + S_{242} + S_{152} \equiv 0. \tag{47}$$

Now from symmetry (Theorem 4.4), $S_{161} = -2S_{611}$, $S_{251} \equiv -S_{521} - S_{512}$, and $S_{341} \equiv -S_{431} - S_{413}$. Using these facts, congruences (46-47) reduce to

$$S_{413} \equiv S_{611} - S_{512}, \tag{48}$$
$$S_{332} \equiv S_{422}. \tag{49}$$

Now consider the product $S_1S_{31111} \equiv 0$. Using duality, this gives

$$5S_{611} + S_{512} \equiv S_{4211} + S_{3311} + S_{2311}.$$

Using Theorem 6.3, the right-hand side can be expressed in terms of triple sums and $S_{41}S_{21}$, and then applying the preceding relations we obtain

$$S_{521} \equiv -6S_{611} - 2S_{512}. \tag{50}$$

Applying similar techniques to the product S_2S_{2111} and using congruences (48-50) gives congruences (41), (42), and (44).

Finally, using duality on the product $S_2S_{2112} \equiv 0$ gives

$$0 \equiv 4S_{1421} + 2S_{4112} + 2S_{2312} + S_{1331}.$$

Now rewrite this using Theorem 6.3 and apply the previously established relations to obtain (43); congruence (45) then follows. □

Remark. It cannot be the case that $S_{611} = uS_{41}S_{21}$, where u is a unit of $\mathbf{Z}/p\mathbf{Z}$ for all $p > 9$, since when $p = 37$ we have $S_{611} \equiv 7$ and $S_{41} \equiv 0$.

For sums of weight 9, duality allows us to restrict attention to $S_I(p-1)$ with $\ell(I) \leq 5$. Using Theorem 6.4 (and Theorem 7.2), we can rewrite the length 5 sums in terms of length 4 sums, S_{81}, and the product $S_{411}S_{21}$. So it is enough to consider the sums $S_I(p-1)$ with $\ell(I) = 4$, for which we have the following result.

Theorem 7.5. *All length 4, weight 9 harmonic sums can be written in terms of the three quantities S_{6111}, $S_{81} \equiv B_{p-9}$, and $S_{21}S_{411} \equiv -\frac{1}{6}B_{p-3}^3$. In particular,*

$$S_{1611} \equiv -3S_{6111} + \frac{80}{9}S_{81} \qquad S_{5211} \equiv S_{6111} - \frac{310}{27}S_{81} + \frac{1}{3}S_{21}S_{411}$$
$$S_{5112} \equiv -4S_{6111} + \frac{190}{27}S_{81} - \frac{1}{3}S_{21}S_{411} \qquad S_{5121} \equiv S_{6111} - \frac{70}{27}S_{81} + \frac{1}{3}S_{21}S_{411}$$
$$S_{2511} \equiv 2S_{6111} - \frac{89}{27}S_{81} - \frac{1}{3}S_{21}S_{411} \qquad S_{2151} \equiv -7S_{6111} + \frac{544}{27}S_{81} - \frac{1}{3}S_{21}S_{411}$$
$$S_{1521} \equiv -3S_{6111} + \frac{137}{9}S_{81} - S_{21}S_{411} \qquad S_{4311} \equiv S_{6111} + \frac{13}{3}S_{81}$$
$$S_{4131} \equiv -6S_{6111} + \frac{56}{3}S_{81} - S_{21}S_{411} \qquad S_{4113} \equiv 7S_{6111} - \frac{133}{9}S_{81} + S_{21}S_{411}$$
$$S_{3411} \equiv -2S_{6111} - \frac{20}{9}S_{81} \qquad S_{3141} \equiv 8S_{6111} - \frac{182}{9}S_{81} + S_{21}S_{411}$$
$$S_{1431} \equiv 4S_{6111} - \frac{64}{3}S_{81} + S_{21}S_{411} \qquad S_{4221} \equiv S_{6111} + \frac{82}{27}S_{81} - \frac{1}{3}S_{21}S_{411}$$
$$S_{4212} \equiv -4S_{6111} + \frac{617}{27}S_{81} - \frac{2}{3}S_{21}S_{411} \qquad S_{4122} \equiv 3S_{6111} - \frac{370}{27}S_{81} + \frac{1}{3}S_{21}S_{411}$$
$$S_{2421} \equiv 2S_{6111} - \frac{124}{27}S_{81} + \frac{4}{3}S_{21}S_{411} \qquad S_{2412} \equiv -2S_{6111} + \frac{110}{9}S_{81}$$
$$S_{2241} \equiv \frac{122}{27}S_{81} - \frac{2}{3}S_{21}S_{411} \qquad S_{3321} \equiv -2S_{6111} + \frac{290}{27}S_{81} - \frac{2}{3}S_{21}S_{411}$$
$$S_{3312} \equiv 2S_{6111} - \frac{289}{27}S_{81} + \frac{1}{3}S_{21}S_{411} \qquad S_{3231} \equiv -\frac{292}{27}S_{81} + \frac{4}{3}S_{21}S_{411}$$
$$S_{2331} \equiv \frac{1}{9}S_{81} - S_{21}S_{411} \qquad S_{3213} \equiv 4S_{6111} - \frac{64}{3}S_{81}$$
$$S_{3132} \equiv -\frac{43}{27}S_{81} - \frac{2}{3}S_{21}S_{411} \qquad S_{2322} \equiv -\frac{28}{3}S_{81}$$
$$S_{3222} \equiv -6S_{81}.$$

Proof. There are 56 length-4 sums, but by reversal (Theorem 4.5) we can reduce to 28 of them. Next we go from 28 length-4 sums to 14 length-4 sums, together with S_{81}, by considering various products in QSym. For example, from the products $S_1 S_{422}$, $S_2 S_{421}$, and $S_2 S_{412}$ respectively, we obtain the relations

$$\begin{aligned}
\frac{23}{3} S_{81} &\equiv -S_{2241} + S_{4122} + S_{4212} + S_{4221} \\
\frac{73}{3} S_{81} &\equiv S_{2421} + 2S_{4221} + S_{4212} \\
\frac{23}{3} S_{81} &\equiv S_{2412} + S_{4212} + 2S_{4122}
\end{aligned}$$

which we can use to write S_{2241}, S_{2421}, and S_{2412} in terms of S_{4221}, S_{4212}, S_{4122}, and S_{81}. Similarly, we eliminate S_{1611}, S_{2511}, S_{2151}, S_{1521}, S_{3411}, S_{3141}, S_{1431}, S_{2331}, S_{3213}, S_{3132}, and S_{2322}. Now we consider the eight products $S_1 S_{311111}$, $S_1 S_{221111}$, $S_1 S_{131111}$, $S_1 S_{113111}$, $S_1 S_{212111}$, $S_1 S_{211211}$, $S_1 S_{211121}$, and $S_1 S_{122111}$. Using duality and rewriting in terms of our 14 length-4 sums, we have the relations

$$\begin{aligned}
\frac{28}{3} S_{81} &\equiv 2S_{6111} + S_{5121} + S_{5112} + S_{4131} + S_{4113} \\
\frac{11}{3} S_{81} &\equiv S_{5211} + S_{4221} + S_{4212} - S_{3321} \\
\frac{29}{3} S_{81} &\equiv -S_{5112} - 2S_{4122} + S_{3312} \\
-\frac{61}{3} S_{81} &\equiv -S_{4113} + S_{4122} + 2S_{3312} \\
\frac{4}{3} S_{81} &\equiv S_{4311} - S_{4221} + S_{3321} + S_{3312} \\
11 S_{81} &\equiv -S_{4113} + S_{3141} + S_{4311} + S_{3321} + S_{3231} + S_{4122} + S_{4212} + S_{4221} \\
-13 S_{81} &\equiv S_{5211} + S_{5112} + S_{5121} + S_{4122} - S_{4221} - S_{3231} - S_{3321} - S_{3312} \\
-6 S_{81} &\equiv S_{3222}.
\end{aligned}$$

We can use these congruences to solve for all the length-4 sums in terms of the seven quantities S_{81}, S_{6111}, S_{5211}, S_{5112}, S_{5121}, S_{4311}, and S_{4221}.

From duality, $S_{41211} \equiv S_{33111}$. Expanding out both sides using Theorem 6.4, we obtain the congruence

$$S_{5211} + S_{4311} + S_{4131} + S_{4122} \equiv S_{6111} + S_{3411} + S_{3321} + S_{3312},$$

which (after rewriting in terms of our seven chosen quantities), allows us to solve for S_{4221} in terms of the remaining six quantities. Now apply Theorem 6.4 similarly to the duality relations $S_{41112} \equiv S_{15111}$, $S_{12411} \equiv S_{31122}$, and $S_{21411} \equiv S_{31131}$ to obtain respectively

$$-S_{4311} + 2S_{5121} + S_{5211} - 2S_{61111} + 21 S_{81} \equiv S_{21} S_{411} \tag{51}$$

$$3S_{4311} - S_{5121} + 4S_{5211} - 6S_{61111} + \frac{91}{3} S_{81} \equiv S_{21} S_{411} \tag{52}$$

$$-3S_{4311} + 2S_{5121} + S_{5211} + \frac{89}{3} S_{81} \equiv S_{21} S_{411}. \tag{53}$$

Add 3 times congruence (51) to congruence (52), and compare the resulting expression for $S_{21}S_{411}$ with that obtained by adding congruence (53) to (52); the result is

$$S_{5121} \equiv S_{5211} + \frac{80}{9} S_{81}. \tag{54}$$

Next substitute congruence (54) into the result of subtracting congruence (52) from (51) to get

$$S_{4311} \equiv S_{6111} + \frac{13}{3} S_{81}. \tag{55}$$

Using congruences (54) and (55), any of the congruences (51-53) can be used to write S_{5211} in terms of S_{6111}, S_{81}, and $S_{21}S_{411}$.

Finally, consideration of the product $S_{11}S_{2221}$ gives the relation

$$\begin{aligned} &3S_{3231} + 3S_{3321} + 3S_{4221} + 2S_{3222} + 2S_{2331} + S_{2241} + S_{2421} \\ &\qquad \equiv 3S_{31221} + 3S_{32121} + 2S_{32211} + 2S_{22131} + S_{21231} + S_{23121}, \end{aligned}$$

which can be used to write S_{5112} in terms of S_{6111}, S_{81}, and $S_{21}S_{411}$. $\square$

Remark. The only primes $p < 1.2 \times 10^7$ with $B_{p-9} \equiv 0$ are $p = 67$ and $p = 877$ [3]. Here is a table of the values of our generators at these primes, and at $p = 16,843$, computed using *Mathematica* and Theorem 5.4.

p	67	877	16,843
S_{6111}	7	253	16,690
S_{81}	0	0	14,820
$S_{21}S_{411}$	4	354	0

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