SUPER CONGRUENCES INVOLVING MULTIPLE HARMONIC SUMS

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Abstract. Let \( p \) be a prime and \( \mathcal{P}_p \) the set of positive integers which are prime to \( p \). Recently, Wang and Cai proved that for every positive integer \( r \) and prime \( p \geq 3 \)

\[
\sum_{i,j,k \in \mathcal{P}_p} \frac{1}{ijk} \equiv -2p^{r-1}B_{p-3} \pmod{p^r},
\]

where \( B_{p-3} \) is the \((p-3)\)-rd Bernoulli number. In this paper we prove the following analogous result: Let \( n = 2 \) or \( 4 \). Then for every positive integer \( r \geq n/2 \) and prime \( p > n \)

\[
\sum_{i_1+\cdots+i_n=p, \ i_1,\ldots, i_n \in \mathcal{P}_p} \frac{1}{i_1i_2\cdots i_n} \equiv \begin{cases} -\frac{n!}{n+1}p^rB_{p-n-1} & \text{mod } p^{r+1}. \end{cases}
\]

Moreover, by using integer relation detecting tool PSLQ we can show that if similar congruence holds for \( n = 6 \), say the right hand side of the above has the form \( c_6 p^r B_{p-7} \), \( c_6 \in \mathbb{Q} \), then both the numerator and the denominator of \( c_6 \) must have at least 60 digits.

1. Introduction.

In the study of congruence properties of multiple harmonic sums in \([7, 8]\) the author of the current paper found the following curious congruence for every prime \( p \geq 3 \):

\[
\sum_{i+j+k=p, \ i,j,k \geq 1} \frac{1}{ijk} \equiv -2B_{p-3} \pmod{p}, \tag{1}
\]

where \( B_j \) is the Bernoulli number defined by the generating power series

\[
\frac{x}{e^x-1} = \sum_{j=0}^{\infty} B_j \frac{x^j}{j!}.
\]

A simpler proof of \((1)\) was presented in \([3]\). Since then this congruence has been generalized along several directions. First, Zhou and Cai \([9]\) showed that

\[
\sum_{l_1+l_2+\cdots+l_n=p, \ l_1,\ldots, l_n \geq 1} \frac{1}{l_1l_2\cdots l_n} \equiv \begin{cases} -(n-1)!B_{p-n} & \text{mod } p, \text{ if } n \text{ is odd;} \\
-\frac{n \cdot n!}{2(n+1)}B_{p-n-1}p^2 & \text{mod } p^2, \text{ if } n \text{ is even.} \end{cases} \tag{2}
\]
Later, Xia and Cai [6] generalized (1) to a super congruence (i.e., with higher prime powers as moduli)

\[ \sum_{i+j+k=p \atop i,j,k \geq 1} \frac{1}{ijk} \equiv -12B_{p-3} \frac{p}{p-3} - 3B_{2p-4} \frac{p}{p-4} \pmod{p^2} \]

for every prime \( p \geq 7 \) while Shen and Cai [4] studied the alternating case. Let \( \mathcal{P}_p \) be the set of positive integers which are prime to \( p \). Recently, Wang and Cai [5] proved for every prime \( p \geq 3 \) and positive integer \( r \)

\[ \sum_{i+j+k=p^r \atop i,j,k \in \mathcal{P}_p} \frac{1}{ijk} \equiv -2p^{r-1}B_{p-3} \pmod{p^r}. \]

By numerical experiment we found the following super congruences.

**Theorem 1.1.** Let \( n = 2 \) or \( 4 \). Then for every positive integer \( r \geq n/2 \) and prime \( p > n \) we have

\[ T_n(p, r) := \sum_{i_1, \ldots, i_n = p^r \atop i_1, \ldots, i_n \in \mathcal{P}_p} \frac{1}{i_1i_2 \cdots i_n} \equiv -\frac{n!}{n+1} p^r B_{p-n-1} \pmod{p^{r+1}}, \]

The main idea of the proof of Theorem 1.1 is to relate \( T_n(p, r) \) to the \( p \)-restricted multiple harmonic sums (MHS for short) defined by

\[ \mathcal{H}_n(s_1, \ldots, s_d) := \sum_{0 < k_1, \ldots, k_d < n, k_1, \ldots, k_d \in \mathcal{P}_p} \frac{1}{k_1^{s_1} \cdots k_d^{s_d}}, \quad (3) \]

for all positive integers \( n, s_1, \ldots, s_d \). We call \( d \) the depth and \( s_1 + \cdots + s_d \) the weight. One of the most important properties of the MHS is that they satisfy the so-called stuffle relations. For example, for all \( a, b, c, n \in \mathbb{N} \) we have

\[ \begin{align*}
\mathcal{H}_n(a)\mathcal{H}_n(b) &= \mathcal{H}_n(a, b) + \mathcal{H}_n(b, a) + \mathcal{H}_n(a + b), \\
\mathcal{H}_n(a, b)\mathcal{H}_n(c) &= \mathcal{H}_n(a, b, c) + \mathcal{H}_n(a, c, b) + \mathcal{H}_n(c, a, b) + \mathcal{H}_n(a + c, b) + \mathcal{H}_n(a, b + c). \\
\end{align*} \quad (4) \]

It turns out the case \( n = 2 \) of Theorem 1.1 is almost trivial whereas the case \( n = 4 \) is much more complicated on which we will concentrate in what follows.

2. **First Step: Reduction to Sub-sums.**

We have

\[ T_4(p, r) = \frac{1}{p^r} \sum_{i_1+i_2+i_3+i_4 = p^r \atop i_1, i_2, i_3, i_4 \in \mathcal{P}_p} \frac{i_1 + i_2 + i_3 + i_4}{i_1i_2i_3i_4} = \frac{4}{p^r} \sum_{u_3 = i_1 + i_2 + i_3 < p^r \atop i_1, i_2, i_3, u_3 \in \mathcal{P}_p} \frac{i_1 + i_2 + i_3}{i_1i_2i_3i_4} \frac{1}{u_3} \]

\[ = \frac{12}{p^r} \sum_{u_2 = i_1 + i_2 < u_3 < p^r \atop i_1, i_2, u_3, u_2 \in \mathcal{P}_p} \frac{i_1 + i_2}{i_1i_2i_3i_4} \frac{1}{u_2u_3} = \frac{24}{p^r} \sigma(p^r), \quad (5) \]
For every prime
Lemma 3.1.
formula of sums of powers (see [2, p. 230]) we have
Proof. Throughout this proof, we suppress the subscript
Clearly we have
Then for all 0 \leq a, b, c \leq 3
Define for all positive integers a, b, c and integers 0 \leq i, j \leq 3
and for all positive integers d, s_1, \ldots, s_d
Then by the Inclusion-Exclusion Principle
In the next few sections we shall evaluate the three sub-sums s_I, s_{II} and s_{III} separately modulo \( p^{2r+1} \).

3. Evaluation of First Sub-sum \( s_I \) in (6).

Set
Clearly we have
Lemma 3.1. For every prime \( p \geq 5 \) and positive integer \( r \geq 2 \) we have
Proof. Throughout this proof, we suppress the subscript \( p^r \) to save space. By the well-known formula of sums of powers (see [2] p. 230) we have
Then for all 0 < a, b, c \leq 2 we have
\[
\mathcal{H}(2=0)(1, 1, 1) = \frac{1}{2} \sum_{0 < u_1 < u_2 < u_3 < p^r} \frac{1}{u_1 u_2 u_3} + \frac{1}{(p^r - u_1)(p^r - u_2)(p^r - u_3)} \equiv -\frac{p^{2r}}{2} \left[ \mathcal{H}(2=0)(1, 1, 2) + \mathcal{H}(2=0)(1, 2, 1) + \mathcal{H}(2=0)(2, 1, 1) \right] - \frac{p^{2r}}{2} \left[ \mathcal{H}(2=0)(1, 1, 3) + \mathcal{H}(2=0)(1, 3, 1) + \mathcal{H}(2=0)(3, 1, 1) \right]
\]
\[ + \mathcal{H}^{(2=0)}(1, 2, 2) + \mathcal{H}^{(2=0)}(2, 2, 1) + \mathcal{H}^{(2=0)}(2, 1, 2) \] \pmod{p^{2r+1}}.

Now if \( u_2 \equiv 0 \pmod{p} \) then we write \( u_2 = vp^\beta \) where \( v \in \mathcal{P}_p \). Then

\[
\mathcal{H}^{(2=0)}(a, b, c) = \sum_{\beta=1}^{r-1} \sum_{v \in \mathcal{P}_p} \left( \sum_{0 < u_1 < vp^\beta < r} \frac{1}{u^a_1(vp^\beta)^b u^c_3} \right)
= \sum_{\beta=1}^{r-1} \sum_{v \in \mathcal{P}_p} \frac{1}{vp^\beta} \left( \sum_{0 < u_1 < vp^\beta} \frac{1}{u^a_1} \right) \left( \sum_{vp^\beta < u_3 < r} \frac{1}{u^c_3} \right).
\]

Let \( m = \varphi(p^{2r+1}) \). Then \( m > 4 \) for every prime \( p \geq 5 \). Thus

\[
\sum_{0 < u < vp^\beta, u \in \mathcal{P}_p} \frac{1}{u^a} \equiv \sum_{u=1}^{vp^\beta-1} u^{m-a} \equiv vp^\beta B_{m-a} + p^2f(v) \pmod{p^{r+1+\beta}}
\]

where \( f(x) \in x\mathbb{Z}_p[x] \) is some polynomial with \( p \)-integral coefficients. Further

\[
\sum_{vp^\beta < u < p^r, u \in \mathcal{P}_p} \frac{1}{u^c} \equiv \sum_{u=1}^{p^r-1} u^{m-c} - \sum_{u=1}^{vp^\beta-1} u^{m-c}
\equiv (p^r - vp^\beta)B_{m-c} + p^2g(v) \pmod{p^{r+1+\beta}}
\]

where \( g(x) \in x\mathbb{Z}_p[x] \) is a polynomial with \( p \)-integral coefficients. Now we divide \( (a, b, c) \) into two cases: (i) \( a + b + c = 4 \) and (ii) \( a + b + c = 5 \).

In case (i) we see that \( B_{m-c}B_{m-a} = 0 \) since \( m \) is even and one of \( a \) or \( c \) is 1. Hence

\[
\mathcal{H}(a, b, c) \equiv \sum_{\beta=1}^{r-1} \sum_{v \in \mathcal{P}_p} v^{m-b} \left[ p^{r-(2-b)} B_{m-c} f(v) - vp^{(2-b)} B_{m-c} f(v) \right]
+ vp^{(3-b)} B_{m-a} g(v) + p^{(4-b)} g(v) f(v) \pmod{p^{r+1}}.
\]

Note that \( m \) is even so \( B_{m-c} \neq 0 \) if and only if \( (a, b, c) = (1, 1, 2) \). Similar arguments for the four terms in the above shows that \( \mathcal{H}(a, b, c) \equiv 0 \pmod{p^{r+1}} \) since \( 1 \leq \beta \leq r - 1 \) and for all \( i \geq 1 \)

\[
\sum_{v=1}^{p^{r-\beta}-1} v^i \equiv 0 \pmod{p^{r-\beta}}.
\]

In case (ii) we only need to show \( \mathcal{H}(a, b, c) \equiv 0 \pmod{p} \) which is much easier than the case (i) so we leave it to the interested reader.

This completes the proof of the lemma. \( \square \)

**Lemma 3.2.** For every prime \( p \geq 5 \) and positive integer \( r \geq 2 \) we have

\[
\mathcal{H}_{p^r}^{11}(1, 1, 1) \equiv \mathcal{H}_{p^r}(1, 1, 1) \equiv -\frac{2}{5} B_{p-5} p^{2r} \pmod{p^{2r+1}}. \tag{9}
\]
Hence by (8) we get
\[ m \text{ by the stuffle relations (4). Noticing that} \]
then we have
\[ \text{Now the lemma follows immediately from the following Kummer congruence} \]
and Lemma 3.1.
\[ \Box \]

Proof. Let \( m = \varphi(p^{2r+1}) - 1 \). Then \( m \geq 2r + 1 \) for every prime \( p \geq 5 \). Thus
\[ H_{p^r}(1, 1, 1) = \sum_{0 < u_1 < u_2 < u_3 < p^r} u_1^m u_2^m u_3^m \equiv H_{p^r}(m, m, m) \]
\[ \equiv \frac{1}{6} \left[ H_{p^r}(m)^3 - 3H_{p^r}(2m)H_{p^r}(m) + 2H_{p^r}(3m) \right] \pmod{p^{2r+1}} \]
by the stuffle relations (4). Noticing that \( m \) is odd, by (8) we get
\[ H_{p^r}(m) \equiv 0 \pmod{p^{r+1}} \text{ and } H_{p^r}(2m) \equiv 0 \pmod{p^r}. \]
Hence by (8) we get
\[ H_{p^r}(1, 1, 1) \equiv \frac{1}{3} H_{p^r}(3m) \equiv \frac{m}{2} p^{2r} B_{3m-1} \equiv -\frac{1}{2} p^{2r} B_{3m-1} \pmod{p^{2r+1}}. \]
Now the lemma follows immediately from the following Kummer congruence
\[ \frac{B_{3m-1}}{3m - 1} \equiv \frac{B_{p-5}}{p-5} \pmod{p} \]
(10)
and Lemma 3.1. \( \Box \)

4. Evaluation of the third sub-sums \( s_{III} \) in (6).

In this section we will use stuffle relations to evaluate the sub-sum \( s_{III} \) of (6) modulo \( p^{2r+1} \). Some parts of the following lemma are similar to (or generalizations) of [5, Lemma 3]. For completeness we provide the details of its proof.

Lemma 4.1. Let \( x \) be an integer in such that \( 0 < x < p \). For all positive integers \( r, k, \) and prime \( p \geq 3 \) we set
\[ S_k(x, p^r) = \sum_{0 < i < p^r, i \equiv x \pmod{p}} \frac{1}{ik}. \]
Then we have
\[ (i) \quad S_k(x, p^2) \equiv pS_k(x, p) \pmod{p^3} \text{ and } S_k(x, p^{r+1}) \equiv pS_k(x, p^r) \pmod{p^{r+2}} \text{ for } r \geq 2 \text{ and } k \geq 1. \]
Moreover, for any integer \( \ell \geq 0 \) and \( r \geq 2 \) we have
\[ \sum_{x=1}^{p-1} x^\ell \left( S_k(x, p^{r+1}) - pS_k(x, p^r) \right) \equiv 0 \pmod{p^{r+3}}. \] (11)
\[ (ii) \quad S_k(x, p^r) \equiv 0 \pmod{p^{r-1}} \text{ for } r \geq 2. \]
\[ (iii) \quad \{S_k(x, p^{r+1})\}^d \equiv p^d \{S_k(x, p^r)\}^d \pmod{p^{d+2}} \text{ for } r \geq 2 \text{ and } d \geq 1. \]
\[ (iv) \quad \{S_k(x, p^r)\}^d \equiv p^{d(r-1)k+d} x^{-dk} + \frac{dk}{2} p^{d(r-1)+1} x^{-dk-1} \pmod{p^{d(r-1)+2}} \text{ for all } d \geq 1 \text{ and } r \geq 2. \]
\[ (v) \quad \text{Let } r \geq 2 \text{ and } d, k \in \mathbb{N} \text{ such that } dk < p - 1. \text{ Then we have} \]
\[ \sum_{x=1}^{p-1} \{S_k(x, p^r)\}^d \equiv \frac{dkp^{d(r-1)+1}}{dk+1} B_{p-1-dk} \pmod{p^{d(r-1)+2}}. \]
\[ (vi) \quad S_1(x, p^{r+1})S_2(x, p^{r+1}) \equiv p^2 S_1(x, p^r)S_2(x, p^r) \pmod{p^{2r+2}} \text{ for } r \geq 2. \text{ Moreover, for every integer } r \geq 2 \text{ we have} \]
\[ \sum_{x=1}^{p-1} S_1(x, p^r)S_2(x, p^r) \equiv 0 \pmod{p^{2r+1}}. \] (12)
Proof. (i) By definition, if \( r = 1 \) we have
\[
S_k(x, p^2) - pS_k(x, p) = \sum_{0<j<p} \frac{1}{(x+jp)^k} - p \sum_{0<j<p} \frac{x}{x^k} \equiv - \sum_{0<j<p} \frac{kjp}{x^k} \equiv 0 \pmod{p^2}.
\]
If \( r \geq 2 \) then
\[
S_k(x, p^{r+1}) - pS_k(x, p^r)
= \sum_{0<j<p^r} \frac{1}{(x+jp)^k} - p \sum_{0<j<p^{r-1}} \frac{1}{(x+ap)^k}
= \sum_{b=1}^{p-1} \left( \sum_{0\leq a<p^{r-1}} \frac{1}{(x+(a+p^{r-1}b)p)^k} - \frac{1}{(x+ap)^k} \right)
= -p^r \sum_{b=1}^{p-1} b \sum_{0\leq a<p^{r-1}} \frac{\sum_{l=0}^{k-1} (x+ap)^l(x+(a+p^{r-1}b)p)^{k-1-l}}{(x+(a+p^{r-1}b)p)^k(x+ap)^k}
\equiv -p^r \sum_{b=1}^{p-1} b \sum_{0\leq a<p^{r-1}} k(x+ap)^{k-1} (x+ap)^{2k} \equiv 0 \pmod{p^{r+2}}
\]
since \( p^r \equiv 0 \pmod{p^2} \), \( \sum_{b=1}^{p-1} b \equiv 0 \pmod{p} \) and
\[
\sum_{0\leq a<p^{r-1}} \frac{k(x+ap)^{k-1}}{(x+ap)^{2k}} \equiv \sum_{0\leq a<p^{r-1}} \frac{k}{x^{k+1}} \equiv \frac{kp^{r-1}}{x^{k+1}} \equiv 0 \pmod{p}.
\]
Further, for any integer \( \ell \geq 0 \) and \( r \geq 2 \) we have modulo \( p^{r+3} \)
\[
\sum_{x=1}^{p-1} x\ell (S_k(x, p^{r+1}) - pS_k(x, p^r)) \equiv -p^r \sum_{x=1}^{p-1} \sum_{b=1}^{p-1} b \sum_{0\leq a<p^{r-1}} \frac{kx\ell}{(x+ap)^{k+1}} \equiv 0
\]
since now for \( m = \varphi(p^2) - k - 1 \) we have
\[
\sum_{x=1}^{p-1} \sum_{0\leq a<p^{r-1}} \frac{x\ell}{(x+ap)^{k+1}} \equiv \sum_{x=1}^{p-1} \sum_{0\leq a<p^{r-1}} x\ell(x+ap)^m \pmod{p^2}
\]
and for any integer \( \alpha, \beta \geq 0 \) we have
\[
\sum_{x=1}^{p-1} x^\alpha \equiv \sum_{0\leq a<p^{r-1}} a^\beta \equiv 0 \pmod{p}.
\]
(ii) This follows from (i) by an easy induction on \( r \).
(iii) This follows from (i) and (ii) by the formula
\[
A^d - B^d = (A - B) \sum_{j=0}^{d-1} A^j B^{d-j}.
\]
(iv) If \(r = 2\) then let \(m = \varphi(p^{d+2}) - k\). We get

\[
S_k(x, p^2) = \sum_{j=0}^{p-1} \frac{1}{(x+jp)} \equiv \sum_{j=0}^{p-1} (x+jp)^m \pmod{p^{d+2}}.
\]

Expanding and noticing that \(m \equiv -k \pmod{p}\) we get

\[
S_k(x, p^2) \equiv px^m + \frac{k}{2} p^2 x^{m-1} + p^3 f(x) \pmod{p^{d+2}}
\]

for some polynomial \(f(x) \in x\mathbb{Z}_p[x]\). Moreover, for each \(x\) we can show that

\[
\{S_k(x, p^2)\}^d \equiv p^d x^{dm} + \frac{dk}{2} p^{d+1} x^{dm-1} \pmod{p^{d+2}}.
\]

Now (iv) follows from induction on \(r\) by using (iii).

(v) This follows from (iv) immediately.

(vi) Set \(m = \varphi(p^5) - 2\). By (iv) there are polynomials \(f(x), g(x), h(x) \in x\mathbb{Z}_p[x]\) such that

\[
\sum_{x=1}^{p-1} S_1(x, p^2) S_2(x, p^2) = \sum_{x=1}^{p-1} \left[ px^{m+1} \right] \left[ px^m + p^3 f(x) \right] = \sum_{x=1}^{p-1} \left[ p^2 x^{2m+1} + \frac{3}{2} p^3 x^{2m} + p^4 h(x) \right]
\]

\[
= \frac{2m + 1}{2} p^4 B_{2m} + \frac{3}{2} p^4 B_{2m} \equiv 0 \pmod{p^5}
\]

since \(2m + 1 \equiv -3 \pmod{p}\). This proves (vi) for \(r = 2\).

For the general case, similar to (iii) we have

\[
S_1(x, p^{r+1}) S_2(x, p^{r+1}) - p^2 S_1(x, p^r) S_2(x, p^r)
= S_2(x, p^{r+1})[S_1(x, p^{r+1}) - p S_1(x, p^r)] + p S_1(x, p^r) [S_2(x, p^{r+1}) - p S_2(x, p^r)]
\]

\[
\equiv 0 \pmod{p^{2r+2}}
\]

by (i) and (ii). Moreover, for each \(x\) there exist \(f(x), g(x) \in \mathbb{Z}_p[x]\) such that

\[
S_2(x, p^{r+1}) = p^r f(x), \quad \text{ and } \quad p S_1(x, p^r) = p^r g(x).
\]

Thus from (iii) and by induction on \(r\) we can show that

\[
\sum_{x=1}^{p-1} S_1(x, p^r) S_2(x, p^r) \equiv p^2 \sum_{x=1}^{p-1} S_1(x, p^{r-1}) S_2(x, p^{r-1})
\]

\[
\equiv \cdots \equiv p^{2r-4} \sum_{x=1}^{p-1} S_1(x, p^2) S_2(x, p^2) \equiv 0 \pmod{p^{2r+1}}
\]

because of (ii).

This completes the proof of the lemma. \(\square\)

We can now consider the second sub-sums of (iii) modulo \(p^{2r+1}\)
Lemma 4.2. For every prime \( p \geq 5 \) and positive integer \( r \geq 2 \) we have
\[
\mathcal{H}_{p^r}^{(2)}(1, 2) + \mathcal{H}_{p^r}^{(2)}(2, 1) \equiv \frac{6}{5} B_{p-5} p^{2r} \pmod{p^{2r+1}},
\]
\[
\mathcal{H}_{p^r}(3) \equiv -\frac{6}{5} B_{p-5} p^{2r} \pmod{p^{2r+1}}.
\]

Proof. It is easy to see that
\[
\mathcal{H}_{p^r}^{(2)}(1, 2) + \mathcal{H}_{p^r}^{(2)}(2, 1) + \mathcal{H}_{p^r}(3) \equiv \sum_{x=1}^{p-1} S_1(x, p^r) S_2(x, p^r) \equiv 0 \pmod{p^{2r+1}}
\]
by (12). Setting \( m = \varphi(p^{2r+1}) - 3 \) and noticing \( m \) is odd we get
\[
\mathcal{H}_{p^r}(3) \equiv \sum_{u=1}^{p-1} u^m \equiv \frac{m}{2} p^{2r} B_{m-1} \equiv -\frac{3}{2} p^{2r} B_{m-1} \equiv -\frac{6}{5} p^{2r} B_{p-5} \pmod{p^{2r+1}}
\]
by the Kummer congruence
\[
\frac{B_{m-1}}{m-1} \equiv \frac{B_{p-5}}{p-5} \pmod{p}.
\]
The lemma now follows at once.

Finally we deal with the sub-sum \( s_{III} \) of (3) modulo \( p^{2r+1} \).

Corollary 4.3. For every prime \( p \geq 5 \) and positive integer \( r \geq 2 \) we have
\[
\mathcal{H}_{p^r}^{(3)}(1, 1, 1) \equiv -\frac{2}{5} B_{p-5} p^{2r} \pmod{p^{2r+1}}.
\]

Proof. By stuffle relation (4) we have
\[
6 \mathcal{H}_{p^r}^{(3)}(1, 1, 1) + 3 \left( \mathcal{H}_{p^r}^{(2)}(1, 2) + \mathcal{H}_{p^r}^{(2)}(2, 1) \right) + \mathcal{H}_{p^r}(3)
\]
\[
= \sum_{x=1}^{p-1} \{ S_1(x, p^r) \}^3 \equiv 0 \pmod{p^{2r+1}}
\]
by Lemma 4.1(v). So the corollary follows quickly from Lemma 4.2.

5. Evaluation of the second sub-sums \( s_{II} \) in (6).

It turns out \( s_{II} \) is the most difficult to evaluate modulo \( p^{2r+1} \). We will use repeatedly (and often implicitly) the fact that
\[
\sum_{w=1}^{p^r} w^\ell \equiv \begin{cases} 0 \pmod{p^s}, & \text{if } \ell \text{ is even;} \\ 0 \pmod{p^{s+1}}, & \text{if } \ell \text{ is odd.} \end{cases}
\]

Lemma 5.1. For every positive integer \( r \geq 2 \) and prime \( p \geq 5 \) we have
\[
\mathcal{H}_{p^r}^{1,3}(1, 1, 1) \equiv -\frac{3}{5} p^{2r} B_{p-5} \pmod{p^{2r+1}}.
\]
Proof. Let $m = \varphi(p^{2r+1}) - 1$. Modulo $p^{2r+1}$ we have

$$H_{p^r}^{1,3}(1, 1, 1) \equiv \sum_{v=1}^{p^{r-1}-1} \sum_{0 < u < u_1 < u + vp^r} u^m u_1^m (u + vp)^m$$

$$\equiv \sum_{v=1}^{p^{r-1}-1} \sum_{0 < u < vp^r - vp} \left[ P(m, u + vp) - u^m - P(m, u) \right] (u + vp)^m u^m,$$

$$\equiv \sum_{v=1}^{p^{r-1}-1} \sum_{0 < u < vp} \left[ P(m, u + p^r - vp) - u^m - P(m, u) \right] (u + p^r - vp)^m u^m,$$

by changing the index $v \to p^{r-1} - v$. Observe

$$P(m, u + p^r - vp) = \sum_{k=0}^{m} \frac{(m+1)}{m+1} (u + p^r - vp)^{m+1-k} B_k$$

$$\equiv \sum_{k=0}^{m} \frac{(m+1)}{m+1} [(u - vp)^{m+1-k} + (m + 1 - k)p^r(u - vp)^{m-k}] B_k$$

$$\equiv \sum_{k=0}^{m} \frac{(m+1)}{m+1} (vp - u)^{m+1-k} B_k + (vp - u)^m + p^r F(u - vp) - \frac{m}{2} p^r (u - vp)^{m-1}$$

$$\equiv P(m, vp - u) + (vp - u)^m + p^r F(u - vp) + \frac{1}{2} p^r (u - vp)^{m-1} \pmod{p^{r+1}}$$

since $B_1 = -1/2$ and $B_k = 0$ for all odd $k > 2$. Here $F(x) \in x\mathbb{Z}_p[x]$ is an odd polynomial in $x$ (i.e., only odd powers of $x$ can appear). It is straight-forward to see that

$$\sum_{v=1}^{p^{r-1}-1} \sum_{0 < u < vp} F(u - vp)(u + p^r - vp)^m u^m \equiv 0 \pmod{p^{r+1}}.$$

Hence modulo $p^{2r+1}$ we have

$$H_{p^r}^{1,3}(1, 1, 1) \equiv \sum_{v=1}^{p^{r-1}-1} \sum_{0 < u < vp} \left[ P(m, vp - u) + (vp - u)^m \right.$$

$$\left. + \frac{1}{2} p^r (u - vp)^{m-1} - u^m - P(m, u) \right] (u + p^r - vp)^m u^m,$$

$$\equiv G(p, r) + \sum_{v=1}^{p^{r-1}-1} \sum_{0 < u < vp} \left\{ \frac{1}{2} p^r (u - vp)^{m-1}(u + p^r - vp)^m u^m \right. + mp^r \left[ P(m, vp - u) + (vp - u)^m - u^m - P(m, u) \right] (u - vp)^{m-1} u^m \left\}$$

$$\equiv G(p, r) + p^r \sum_{v=1}^{p^{r-1}-1} \sum_{0 < u < vp} \left\{ \frac{5}{2} u^{3m-1} + \left[ P(m, u) - P(m, vp - u) \right] u^{2m-1} \right\},$$
where
\[ G(p, r) = \sum_{v=1}^{p^r-1-1} \sum_{0 < u < vp} \left[ P(m, vp - u) + (vp - u)^m - u^m - P(m, u) \right] (u - vp)^m u^m. \]

By change of index \( u \to vp - u \) we see clearly that \( G(p, r) \equiv 0 \pmod{p^{2r+1}} \) since \( m \) is odd. Expanding \( P(m, vp - u) \) and \( P(m, u) \) using (8) and (16) we get
\[
H_{p^r}^{1,3}(1, 1, 1) \equiv p^r \sum_{v=1}^{p^r-1-1} \sum_{0 < u < vp} \left\{ \frac{5}{2} u^{3m-1} + [u^m B_1 - (vp - u)^m B_1] u^{2m-1} \right\} \equiv \frac{3}{2} p^r \sum_{v=1}^{p^r-1-1} u^{3m-1} \equiv \frac{3}{2} p^r \sum_{v=1}^{p^r-1-1} v B_{3m-1} \equiv -\frac{3}{4} p^2 B_{3m-1}.
\]

Now the lemma follows readily from by Kummer congruence
\[
\frac{B_{3m-1}}{3m-1} \equiv \frac{B_{p-5}}{p-5} \pmod{p}.
\]

**Lemma 5.2.** For every positive integer \( r \geq 2 \) and prime \( p \geq 5 \) we have
\[
H_{p^r}^{1,2}(1, 1, 1) + H_{p^r}^{2,3}(1, 1, 1) \equiv -\frac{3}{5} p^2 B_{p-5} \pmod{p^{2r+1}}. \tag{18}
\]

**Proof.** By stuffle relations (14) and Lemma 4.1 we have modulo \( p^{2r+1} \) (suppressing the subscript \( p^r \))
\[
0 \equiv \mathcal{H}(1) \sum_{x=1}^{p^r-1} \left( S_1(x, p^r) \right)^2 = \mathcal{H}(1) \left[ \mathcal{H}(2) + 2 \mathcal{H}^{(2)}(1, 1) \right] = \mathcal{H}(1) \mathcal{H}(2)
\]
\[
+ 2 \left[ \mathcal{H}^{1,2}(1, 1, 1) + \mathcal{H}^{2,3}(1, 1, 1) + \mathcal{H}^{1,3}(1, 1, 1) \right] + 2 \left[ \mathcal{H}^{(2)}(1, 2) + \mathcal{H}^{(2)}(2, 1) \right].
\]

Noticing that \( \mathcal{H}(1) \mathcal{H}(2) \equiv 0 \pmod{p^{2r+1}} \) we can derive (18) from (14) and (17) immediately. \( \square \)

**6. Proof of Theorem 1.1**

Let \( m = \varphi(p^{2r+1}) - 1 \). When \( n = 2 \) and \( r \geq 1 \) we have
\[
\sum_{i+j=p^r, i, j \in P_p} \frac{1}{ij} = \frac{1}{p^r} \sum_{i+j=p^r, i, j \in P_p} \frac{i+j}{ij} = \frac{2}{p^r} \sum_{0 < i < p^r} \frac{1}{i}.
\]

Observing that \( m \) is odd we have
\[
\sum_{0 < i < p^r} \frac{1}{i} \equiv \sum_{i=1}^{p^r-1} i^m \equiv \frac{m}{2} p^{2r} B_{m-1} \equiv -\frac{1}{3} p^{2r} B_{p-3} \pmod{p^{2r+1}}
\]

by Kummer congruence
\[
\frac{B_{m-1}}{m-1} \equiv \frac{B_{p-3}}{p-3} \pmod{p}.
\]
This completes the proof of the theorem when \( n = 2 \).

For the case of \( n = 4 \) we can use (9), (15), and (18) evaluate (6) and get
\[
\sigma(p^r) \equiv -\frac{1}{5}p^{2r}B_{p-5} \pmod{p^{2r+1}}.
\]

So the theorem follows immediately from (5).

7. Numerical computation for larger integers \( n \)

It is natural to ask if one can generalize Theorem 1.1 to the case of \( n = 6 \) and other larger even numbers. By using integer relation detecting tool PSLQ (the partial sum of least squares algorithm) developed originally by Ferguson and Bailey [1] we can show that if similar congruence holds for \( n = 6 \), say
\[
\sum_{\substack{i_1+\cdots+i_6=p^2 \\
i_1,\ldots,i_6 \in \mathbb{P}_p}} \frac{1}{i_1i_2i_3i_4i_5i_6} \equiv c_6p^2B_{p-7} \pmod{p^3}
\]
for some \( c_6 \in \mathbb{Q} \) and for all prime \( p \geq 7 \), then both the numerator and the denominator of \( c_6 \) must have at least 60 digits.

At first glance, it may seem impossible to use PSLQ to work with congruences. However, we may use the following idea, say, in case \( n = 6 \). Let \( S \) be the set of the first 1000 primes greater than 6. Let \( P \) be the product of these primes. By the Chinese Remainder Theorem we can find two integers \( A \) and \( B \), between 0 and \( P^3 \) so that
\[
A \equiv \sum_{\substack{i_1+\cdots+i_6=p^2 \\
i_1,\ldots,i_6 \in \mathbb{P}_p}} \frac{1}{i_1i_2i_3i_4i_5i_6} \pmod{p^3}, \quad B \equiv p^2B_{p-7} \pmod{p^3}
\]
for each prime in \( S \). If (19) were true for some \( c_6 = a/b \) in reduced form with \( a \) and \( b \) both of reasonable sizes, then we would have
\[
A - \frac{a}{b}B = mP^3
\]
for some integer \( m \). Thus we can use PSLQ to discover \( a \) and \( b \).

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