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PROOF OF A CONJECTURAL SUPERCONGRUENCE MODULO p^5

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ABSTRACT. In this paper, we prove the supercongruence

$$\sum_{n=0}^{(p-1)/2} \frac{6n+1}{256^n} \binom{2n}{n}^3 \equiv p(-1)^{(p-1)/2} + (-1)^{(p-1)/2} \frac{7}{24} p^4 B_{p-3} \pmod{p^5}$$

for any prime p>3, where B_0,B_1,\ldots are the Bernoulli numbers. This confirms a conjecture posed by Z.-W. Sun in 2019.

1. Introduction

In 1997, L. van Hamme [25] proposed many conjectural p-adic supercongruences motivated by corresponding Ramanujan-type series for $1/\pi$. For example, he conjectured the supercongruence

$$\sum_{n=0}^{(p-1)/2} \frac{6n+1}{256^n} {2n \choose n}^3 \equiv (-1)^{(p-1)/2} p \pmod{p^4}$$
 (1.1)

for any prime p > 3, inspired by the Ramanujan series (cf. [19])

$$\sum_{n=0}^{\infty} \frac{6n+1}{256^n} \binom{2n}{n}^3 = \frac{4}{\pi}.$$

The congruence (1.1) was confirmed by L. Long [12] in 2011.

In 2011, Z.-W. Sun [21] formulated many conjectural supercongruences involving Bernoulli numbers or Euler numbers. Recall that the Bernoulli numbers B_0, B_1, \ldots and the Euler numbers E_0, E_1, \ldots are defined by

$$\frac{x}{e^x - 1} = \sum_{n=0}^{\infty} B_n \frac{x^n}{n!} (|x| < 2\pi) \text{ and } \frac{2}{e^x + e^{-x}} = \sum_{n=0}^{\infty} E_n \frac{x^n}{n!} (|x| < \frac{\pi}{2})$$

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respectively. For example, for any prime p > 3, he conjectured that

$$\sum_{n=0}^{p-1} \frac{6n+1}{256^n} {2n \choose n}^3 \equiv (-1)^{(p-1)/2} p - p^3 E_{p-3} \pmod{p^4}. \tag{1.2}$$

This was later confirmed by G.-S. Mao and C.-W. Wen [15, Th. 1.2]. In 2019, Z.-W. Sun [23, Conj. 22] conjectured that: for any prime p > 3 and positive odd integer m, we have

$$\frac{16^{m-1}}{(pm)^4 \binom{m-1}{\frac{m-1}{2}}}^3 \left(\sum_{n=0}^{(pm-1)/2} \frac{6n+1}{256^n} \binom{2n}{n}^3 - (-1)^{(p-1)/2} p \sum_{r=0}^{(m-1)/2} \frac{6r+1}{256^r} \binom{2r}{r}^3\right)$$

$$\equiv (-1)^{(p-1)/2} \frac{7}{24} B_{p-3} \pmod{p}.$$

In this paper, we confirm this in the case m = 1. Namely, we establish the following result.

Theorem 1.1. Let p > 3 be a prime. Then

$$\sum_{n=0}^{(p-1)/2} \frac{6n+1}{256^n} {2n \choose n}^3 \equiv (-1)^{(p-1)/2} \left(p + \frac{7}{24} p^4 B_{p-3} \right) \pmod{p^5}. \tag{1.3}$$

For any prime p > 3, Z.-W. Sun [21] also conjectured the congruence

$$\sum_{n=0}^{p-1} \frac{3n+1}{16^n} {2n \choose n}^3 \equiv p + \frac{7}{6} p^4 \pmod{p^5},$$

which was confirmed by C. Wang and D.-W. Hu [26] in 2020. For more studies of such congruences, one may consult [8, 10, 11, 18].

In the next section, we provide some known lemmas. We will use the WZ method to prove Theorem 1.1 in Section 3.

2. Some known Lemmas

In 1862, J. Wolstenholme [27] proved the classical congruence

$$\binom{2p-1}{p-1} \equiv 1 \pmod{p^3}$$

for any prime p > 3. This was refined by J.W.L. Glaisher [3] in 1900.

Lemma 2.1 (Glaisher [3]). For any prime p > 3, we have

$$\binom{2p-1}{p-1} \equiv 1 - \frac{2}{3}p^3 B_{p-3} \pmod{p^4}.$$
 (2.1)

Remark 2.2. For modern references about (2.1), the reader may consult [5] and [16].

In 1895, F. Morley [17] got the following fundamental congruence:

$$\binom{p-1}{(p-1)/2} \equiv (-1)^{(p-1)/2} 4^{p-1} \pmod{p^3}$$

for any prime p > 3. This was refined by L. Carlitz [1] in 1953.

Lemma 2.3 (L. Carlitz [1]). For each odd prime p, we have

$$(-1)^{(p-1)/2} {p-1 \choose (p-1)/2} \equiv 4^{p-1} + \frac{p^3}{12} B_{p-3} \pmod{p^4}.$$

We also need the following result of E. Lehmer established in 1938.

Lemma 2.4 (E. Lehmer [9]). For any prime p > 3, we have

$$\sum_{k=1}^{(p-1)/2} \frac{1}{k} \equiv -2 \sum_{k=1}^{(p-1)/2} \frac{1}{2k-1} \equiv -2q_p(2) + p \, q_p(2)^2 \pmod{p^2}, \quad (2.2)$$

where $q_p(2)$ denotes the Fermat quotient $(2^{p-1}-1)/p$.

Let a_1, a_2, \ldots, a_m be integers. For any integer $n \geq m$, we define the alternating multiple harmonic sum

$$H(a_1, a_2, \dots, a_m; n) := \sum_{1 \le k_1 < k_2 < \dots < k_m \le n} \prod_{i=1}^m \frac{\operatorname{sign}(a_i)^{k_i}}{k_i^{|a_i|}},$$

and call m and $\sum_{i=1}^{m} |a_i|$ its depth and weight respectively.

We need the following known results as lemmas.

Lemma 2.5 ([7]). Let $a, r \in \mathbb{Z}^+ = \{1, 2, 3, ...\}$. For any prime p > ar + 2, we have

$$H(\{a\}^r; p-1) \equiv \begin{cases} (-1)^r \frac{a(ar+1)}{2(ar+2)} p^2 B_{p-ar-2} & \pmod{p^3} & \text{if ar is odd,} \\ (-1)^{r-1} \frac{a}{ar+1} p B_{p-ar-1} & \pmod{p^2} & \text{if ar is even.} \end{cases}$$

Lemma 2.6 ([20]). For any $a \in \mathbb{Z}^+$ and prime p > a + 2, we have

$$H\left(a; \frac{p-1}{2}\right)$$

$$\equiv \begin{cases} -2q_p(2) + pq_p(2)^2 - \frac{2}{3}p^2q_p(2)^3 - \frac{7}{12}p^2B_{p-3} \pmod{p^3} & \text{if } a = 1, \\ -\frac{2^a - 2}{a}B_{p-a} \pmod{p} & \text{if } a > 1 \text{ is odd,} \\ \frac{a(2^{a+1} - 1)}{2(a+1)}pB_{p-a-1} \pmod{p^2} & \text{if } a \text{ is even.} \end{cases}$$

Lemma 2.7 ([6]). Let $a, b \in \mathbb{Z}^+$ with a+b odd. For any prime p > a+b, we have

$$H\left(a, b; \frac{p-1}{2}\right) \equiv \frac{B_{p-a-b}}{2(a+b)} \left((-1)^b \binom{a+b}{a} + 2^{a+b} - 2 \right) \pmod{p}.$$

Lemma 2.8 (R. Tauraso and J. Q. Zhao [24]). For any prime p > 3, we have

$$H(1,-1;p-1) \equiv q_p(2)^2 - p q_p(2)^3 - \frac{13}{24} p B_{p-3} \pmod{p^2}.$$
 (2.3)

We also need the following lemma involving the harmonic numbers

$$H_n := H(1; n) = \sum_{0 < k \le n} \frac{1}{k} \quad (n = 0, 1, 2, \ldots)$$

and the second order harmonic numbers

$$H(2;n) = \sum_{0 < k \le n} \frac{1}{k^2} \quad (n = 0, 1, 2, \ldots).$$

Lemma 2.9. Let p > 3 be a prime. Then we have

$$\sum_{k=1}^{(p-1)/2} \frac{H_k}{k^2} \equiv -\frac{B_{p-3}}{2} \pmod{p},\tag{2.4}$$

$$\sum_{k=1}^{(p-1)/2} \frac{H_{2k}}{k^2} \equiv \frac{3}{2} B_{p-3} \pmod{p},\tag{2.5}$$

$$\sum_{k=1}^{(p-1)/2} \frac{H_{2k}^2}{k} \equiv -\frac{2}{3} q_p(2)^3 + \frac{2}{3} B_{p-3} \pmod{p},\tag{2.6}$$

$$\sum_{k=0}^{(p-3)/2} \frac{H_k^2}{2k+1} \equiv \frac{B_{p-3}}{4} + 4q_p(2)^3 \pmod{p},\tag{2.7}$$

$$\sum_{k=0}^{(p-1)/2} \frac{H_k H_{2k}}{k} \equiv \frac{5}{6} B_{p-3} - \frac{4}{3} q_p(2)^3 \pmod{p}. \tag{2.8}$$

Also,

$$\sum_{k=1}^{(p-1)/2} \frac{H(2:k)}{k} \equiv -\frac{3}{2} B_{p-3} \pmod{p}, \tag{2.9}$$

$$\sum_{k=1}^{(p-1)/2} \frac{H(2;2k)}{k} \equiv -\frac{5}{4} B_{p-3} \pmod{p}. \tag{2.10}$$

Remark 2.10. The congruences (2.4) and (2.5) can be found in [13, Lemma 3.2] and [14, Lemma 2.4], respectively. For (2.6)–(2.8), the reader may consult [14, (3.12) and Theorem 1.3]. (2.9) and (2.10) can be found in [14, (2.2)-(2.3)].

3. Proof of Theorem 1.1

To prove Theorem 1.1, we need a WZ pair found by J. Guillera [4, p. 42]. For $n, k \in \mathbb{N} = \{0, 1, 2, \ldots\}$, we define

$$F(n,k) = \frac{(6n-2k+1)}{2^{8n-2k}} \frac{\binom{2n}{n}\binom{2n+2k}{n+k}\binom{2n-2k}{n-k}\binom{n+k}{n}}{\binom{2k}{k}}$$
(3.1)

and

$$G(n,k) = \frac{n^2 \binom{2n}{n} \binom{2n+2k}{n+k} \binom{2n-2k}{n-k} \binom{n+k}{n}}{2^{8n-2k-4} (2n+2k-1) \binom{2k}{k}}.$$
 (3.2)

Clearly F(n, k) = G(n, k) = 0 if n < k. It is easy to check that

$$F(n, k-1) - F(n, k) = G(n+1, k) - G(n, k)$$
(3.3)

for all $n \in \mathbb{N}$ and $k \in \mathbb{Z}^+$. The WZ pair $\langle F, G \rangle$ first appeared in [4, p. 42], and it was also used in [2] and [28, p. 9].

Summing (3.3) over $n \in \{0, ..., (p-1)/2\}$, we get

$$\sum_{n=0}^{(p-1)/2} F(n,k-1) - \sum_{n=0}^{(p-1)/2} F(n,k) = G\left(\frac{p+1}{2},k\right) - G(0,k) = G\left(\frac{p+1}{2},k\right).$$

Furthermore, summing both side of the above identity over $k \in \{1, \dots, (p-1)/2\}$, we obtain

$$\sum_{n=0}^{(p-1)/2} F(n,0) = F\left(\frac{p-1}{2}, \frac{p-1}{2}\right) + \sum_{k=1}^{(p-1)/2} G\left(\frac{p+1}{2}, k\right).$$
 (3.4)

Lemma 3.1. Let p > 3 be a prime. Then

$$F\left(\frac{p-1}{2}, \frac{p-1}{2}\right)$$

$$\equiv (-1)^{\frac{p-1}{2}} p\left(1 - pq_p(2) + p^2 q_p(2)^2 - p^3 q_p(2)^3 - \frac{7}{12} p^3 B_{p-3}\right) \pmod{p^5}.$$

Proof. By the definition of F(n,k), we have

$$F\left(\frac{p-1}{2}, \frac{p-1}{2}\right) = \frac{2p-1}{2^{3p-3}} \binom{2p-2}{p-1} \binom{p-1}{(p-1)/2} = \frac{p\binom{2p-1}{p-1}\binom{p-1}{(p-1)/2}}{2^{3p-3}}.$$

This, together with Lemma 2.1, Lemma 2.3 and the equality $2^{p-1} = 1 + pq_p(2)$, yields that

$$F\left(\frac{p-1}{2}, \frac{p-1}{2}\right) \equiv \frac{p(1-\frac{2}{3}p^3B_{p-3})(-1)^{(p-1)/2}(4^{p-1}+\frac{1}{12}p^3B_{p-3})}{(1+p\,q_p(2))^3}$$

$$\equiv (-1)^{\frac{p-1}{2}}p\left(1-pq_p(2)+p^2q_p(2)^2-p^3q_p(2)^3-\frac{7}{12}p^3B_{p-3}\right) \pmod{p^5}.$$

This concludes the proof.

Lemma 3.2. For any prime p > 3, we have

$$\sum_{k=1}^{(p-1)/2} \frac{p/2 - k}{(p+1-2k)(p+2k)}$$

$$\equiv \frac{1}{2} q_p(2) - \frac{p}{4} q_p(2)^2 - 2pq_p(2) + \frac{1}{6} p^2 q_p(2)^3 + 4p^2 q_p(2) + p^2 q_p(2)^2 + \frac{7}{48} p^2 B_{p-3} \pmod{p^3}$$

Proof. In view of Lemma 2.4,

$$\sum_{k=1}^{(p-1)/2} \frac{1}{k(2k-1)} = 2 \sum_{k=1}^{(p-1)/2} \frac{1}{2k-1} - H_{(p-1)/2}$$

$$\equiv 4q_p(2) - 2pq_p(2)^2 \pmod{p^2}$$
(3.5)

and

$$\sum_{k=1}^{(p-1)/2} \frac{1}{k(2k-1)^2} = H_{(p-1)/2} - 2 \sum_{k=1}^{(p-1)/2} \frac{1}{2k-1} + 2 \sum_{k=1}^{(p-1)/2} \frac{1}{(2k-1)^2}$$

$$\equiv -4q_p(2) - \frac{1}{2}H(2; (p-1)/2) \equiv -4q_p(2) \pmod{p}.$$
(3.6)

It is easy to see that

$$\sum_{k=1}^{(p-1)/2} \frac{(p/2-k)}{(p+1-2k)(p+2k)}$$

$$= \sum_{k=1}^{(p-1)/2} \frac{k-1/2}{(2k)(2p+1-2k)} = -\frac{1}{4} \sum_{k=1}^{(p-1)/2} \frac{1}{k(1-\frac{2p}{2k-1})}$$

$$\equiv -\frac{1}{4} H_{(p-1)/2} - \frac{p}{2} \sum_{k=1}^{(p-1)/2} \frac{1}{k(2k-1)} - p^2 \sum_{k=1}^{(p-1)/2} \frac{1}{k(2k-1)^2} \pmod{p^3}.$$

Then we immediately obtain the desired result by Lemma 2.6, (3.5) and (3.6).

Lemma 3.3. For any prime p > 3, we have

$$\sum_{k=1}^{(p-1)/2} \frac{(p/2-k)H_k}{(p+1-2k)(p+2k)}$$

$$\equiv 2q_p(2) - q_p(2)^2 - 6pq_p(2) + 2pq_p(2)^2 + pq_p(2)^3 + \frac{7}{12}pB_{p-3} \pmod{p^2}.$$

Proof. By Lemmas 2.5 and 2.6, and (2.3), we have

$$\sum_{k=1}^{(p-1)/2} \frac{H_{2k}}{k} = \sum_{k=1}^{p-1} \frac{(1+(-1)^k)H_k}{k}$$

$$= H(1,1;p-1) + H(1,-1;p-1) + \frac{1}{2}H\left(2;\frac{p-1}{2}\right)$$

$$\equiv q_p(2)^2 - pq_p(2)^3 + \frac{7}{24}pB_{p-3} \pmod{p^2}.$$
(3.7)

Noting $2H(1,1;n) = H_n^2 - H(2;n)$, we get

$$\sum_{k=1}^{(p-1)/2} \frac{H_k}{k} = H(1,1;(p-1)/2) + H(2;(p-1)/2)$$

$$= \frac{1}{2} H_{(p-1)/2}^2 + \frac{1}{2} H(2;(p-1)/2)$$

$$\equiv 2q_p(2)^2 - 2pq_p(2)^3 + \frac{7}{6} pB_{p-3} \pmod{p^2}.$$

It is easy to see that

$$H_{(p+1)/2-k} \equiv \frac{2}{p+1-2k} + 2pH(2;2k) - \frac{p}{2}H(2;k) + H_{(p-1)/2} + 2H_{2k} - H_k \pmod{p^2}.$$

This, together with (3.5)-(3.8), (2.9) and (2.10), yields that

$$\sum_{k=1}^{(p-1)/2} \frac{H_{(p+1)/2-k}}{k} \equiv -8q_p(2) + 4q_p(2)^2 + 4pq_p(2)^2 + 8pq_p(2)$$

$$-4pq_p(2)^3 - \frac{7}{3}pB_{p-3} \pmod{p^2}$$
(3.8)

and

$$\sum_{k=1}^{(p-1)/2} \frac{H_{(p+1)/2-k}}{k(2k-1)} \equiv \sum_{k=1}^{(p-1)/2} \frac{H_k}{k(2k-1)} = 2 \sum_{k=1}^{(p-1)/2} \frac{H_k}{2k-1} - \sum_{k=1}^{(p-1)/2} \frac{H_k}{k}$$

$$\equiv -\sum_{k=1}^{(p-1)/2} \frac{H_{(p+1)/2-k}}{k} - \sum_{k=1}^{(p-1)/2} \frac{H_k}{k}$$

$$\equiv 8q_p(2) - 6q_p(2)^2 \pmod{p}.$$
(3.9)

Since

$$\sum_{k=1}^{(p-1)/2} \frac{(p/2-k)H_k}{(p+1-2k)(p+2k)}$$

$$= \sum_{k=1}^{(p-1)/2} \frac{(k-1/2)H_{(p+1)/2-k}}{(2k)(2p+1-2k)} = -\frac{1}{4} \sum_{k=1}^{(p-1)/2} \frac{H_{(p+1)/2-k}}{k(1-\frac{2p}{2k-1})}$$

$$\equiv -\frac{1}{4} \sum_{k=1}^{(p-1)/2} \frac{H_{(p+1)/2-k}}{k} - \frac{p}{2} \sum_{k=1}^{(p-1)/2} \frac{H_{(p+1)/2-k}}{k(2k-1)} \pmod{p^2},$$

we immediately get the desired result by using (3.8) and (3.9).

Lemma 3.4. Let p > 3 be a prime. Then

$$\sum_{k=1}^{(p-1)/2} \frac{(p/2-k)H_{2k}}{(p+1-2k)(p+2k)}$$

$$\equiv q_p(2) - \frac{1}{4}q_p(2)^2 - 3pq_p(2) + \frac{p}{2}q_p(2)^2 + \frac{p}{4}q_p(2)^3 + \frac{13}{32}pB_{p-3} \pmod{p^2}.$$

Proof. It is easy to check that for each $0 \le k \le p-1$, we have

$$H_{p-1-k} \equiv pH(2;k) + H_k \pmod{p^2},$$

hence

$$H_{p+1-2k} \equiv pH(2; 2k-2) + H_{2k-2} \pmod{p^2}$$
 (3.10)

for each $1 \le k \le (p-1)/2$. So

$$\sum_{k=1}^{(p-1)/2} \frac{H_{p+1-2k}}{k}$$

$$\equiv p \sum_{k=1}^{(p-1)/2} \frac{H(2; 2k-2)}{k} + \sum_{k=1}^{(p-1)/2} \frac{H_{2k-2}}{k}$$

$$= p \left(\sum_{k=1}^{(p-1)/2} \frac{H(2; 2k)}{k} - \sum_{k=1}^{(p-1)/2} \frac{1}{k(2k-1)^2} - \frac{1}{4}H\left(3; \frac{p-1}{2}\right) \right)$$

$$+ \sum_{k=1}^{(p-1)/2} \frac{H_{2k}}{k} - \sum_{k=1}^{(p-1)/2} \frac{1}{k(2k-1)} - \frac{1}{2}H\left(2; \frac{p-1}{2}\right) \pmod{p^2}.$$

Combining the result in the last paragraph with Lemma 2.6, (3.7), (3.5), (3.6) and (2.10), we get

$$\sum_{k=1}^{(p-1)/2} \frac{H_{p+1-2k}}{k} \equiv q_p(2)^2 - 4q_p(2) + 4pq_p(2) + 2pq_p(2)^2 - pq_p(2)^3 - \frac{13}{8}pB_{p-3} \pmod{p^2}.$$

Similarly, by using (3.10) and Lemma 2.4, we get

$$\sum_{k=1}^{(p-1)/2} \frac{H_{p+1-2k}}{k(2k-1)} \equiv \sum_{k=1}^{(p-1)/2} \frac{H_{2k-2}}{k(2k-1)}$$

$$= 2 \sum_{k=1}^{(p-1)/2} \frac{H_{2k}}{2k-1} - \sum_{k=1}^{(p-1)/2} \frac{H_{2k}}{k}$$

$$- \sum_{k=1}^{(p-1)/2} \frac{1}{k(2k-1)^2} - \frac{1}{2} \sum_{k=1}^{(p-1)/2} \frac{1}{k^2(2k-1)}$$

$$\equiv - \sum_{k=1}^{(p-1)/2} \frac{H_{p+1-2k}}{k} - \sum_{k=1}^{(p-1)/2} \frac{H_{2k}}{k} - \sum_{k=1}^{(p-1)/2} \frac{1}{k(2k-1)^2}$$

$$- \frac{1}{2} \sum_{k=1}^{(p-1)/2} \left(\frac{4}{2k-1} - \frac{2}{k} - \frac{1}{k^2} \right)$$

$$\equiv 4q_p(2) - 2q_p(2)^2 \pmod{p}. \tag{3.11}$$

Since

$$\sum_{k=1}^{(p-1)/2} \frac{(p/2-k)H_{2k}}{(p+1-2k)(p+2k)}$$

$$\equiv -\frac{1}{4} \sum_{k=1}^{(p-1)/2} \frac{H_{p+1-2k}}{k} - \frac{p}{2} \sum_{k=1}^{(p-1)/2} \frac{H_{p+1-2k}}{k(2k-1)} \pmod{p^2},$$

we obtain the desired result in view of the last paragraph.

Lemma 3.5. For any prime p > 3, we have

$$\sum_{k=1}^{(p-1)/2} \frac{(p/2-k)H_k^2}{(p+1-2k)(p+2k)} \equiv 4q_p(2) - 6q_p(2)^2 + 2q_p(2)^3 + \frac{1}{8}B_{p-3} \pmod{p}.$$

Proof. It is easy to verify that

$$\sum_{k=1}^{(p-1)/2} \frac{(p/2-k)H_k^2}{(p+1-2k)(p+2k)} \equiv \frac{1}{2} \sum_{k=1}^{(p-1)/2} \frac{H_k^2}{2k-1} = \frac{1}{2} \sum_{k=0}^{(p-3)/2} \frac{H_{k+1}^2}{2k+1}$$

$$= \frac{1}{2} \sum_{k=0}^{(p-3)/2} \frac{H_k^2}{2k+1} + \frac{1}{2} \sum_{k=1}^{(p-1)/2} \frac{1}{(2k-1)k^2} + \sum_{k=1}^{(p-1)/2} \frac{H_{k-1}}{k(2k-1)} \pmod{p}.$$

Observe that

$$\frac{1}{2} \sum_{k=1}^{(p-1)/2} \frac{1}{(2k-1)k^2} = 2 \sum_{k=1}^{(p-1)/2} \frac{1}{2k-1} - H_{(p-1)/2} - \frac{1}{2}H\left(2; \frac{p-1}{2}\right)$$

and

$$\sum_{k=1}^{(p-1)/2} \frac{H_{k-1}}{k(2k-1)}$$

$$= 2 \sum_{k=1}^{(p-1)/2} \frac{H_{k-1}}{2k-1} - \sum_{k=1}^{(p-1)/2} \frac{H_{k-1}}{k}$$

$$= 2 \sum_{k=1}^{(p-1)/2} \frac{H_k}{2k-1} - 2 \sum_{k=1}^{(p-1)/2} \frac{1}{k(2k-1)} - \sum_{k=1}^{(p-1)/2} \frac{H_{k-1}}{k}$$

$$\equiv -\sum_{k=1}^{(p-1)/2} \frac{H_{(p+1)/2-k}}{k} - 2 \sum_{k=1}^{(p-1)/2} \frac{1}{k(2k-1)} - \sum_{k=1}^{(p-1)/2} \frac{H_{k-1}}{k} \pmod{p}.$$

This, together with (2.2), Lemma 2.6, (3.5), (3.8) and (2.7), yields the desired result.

Lemma 3.6. Let p > 3 be a prime. Then

$$\sum_{k=1}^{(p-1)/2} \frac{(p/2-k)H_kH_{2k}}{(p+1-2k)(p+2k)} \equiv 2q_p(2) - \frac{5}{2}q_p(2)^2 + \frac{1}{2}q_p(2)^3 + \frac{5}{16}B_{p-3} \pmod{p}.$$

Proof. By (2.5), (2.6), (3.6) and (3.11), we have

$$\sum_{k=1}^{(p-1)/2} \frac{H_{2k}H_{2k-2}}{k} = \sum_{k=1}^{(p-1)/2} \frac{H_{2k}^2}{k} - \sum_{k=1}^{(p-1)/2} \frac{H_{2k}}{k(2k-1)} - \frac{1}{2} \sum_{k=1}^{(p-1)/2} \frac{H_{2k}}{k^2}$$

$$\equiv -4q_p(2) + 2q_p(2)^2 - \frac{2}{3}q_p(2)^3 - \frac{1}{12}B_{p-3} \pmod{p}.$$
(3.12)

In view of (2.4), (2.8) and (3.9), we have

$$\sum_{k=1}^{(p-1)/2} \frac{H_k H_{2k-2}}{k} = \sum_{k=1}^{(p-1)/2} \frac{H_{2k} H_k}{k} - \sum_{k=1}^{(p-1)/2} \frac{H_k}{k(2k-1)} - \frac{1}{2} \sum_{k=1}^{(p-1)/2} \frac{H_k}{k^2}$$

$$\equiv -8q_p(2) + 6q_p(2)^2 - \frac{4}{3}q_p(2)^3 + \frac{13}{12}B_{p-3} \pmod{p}.$$
(3.13)

For each $1 \le k \le (p-1)/2$, we clearly have

$$H_{(p+1)/2-k} \equiv H_{(p-1)/2} + 2H_{2k-2} - H_{k-1} \pmod{p}$$
.

This, together with (3.10), yields that

$$\sum_{k=1}^{(p-1)/2} \frac{(p/2-k)H_k H_{2k}}{(p+1-2k)(p+2k)}$$

$$\equiv \frac{1}{2} \sum_{k=1}^{(p-1)/2} \frac{H_k H_{2k}}{2k-1} \equiv -\frac{1}{4} \sum_{k=1}^{(p-1)/2} \frac{H_{(p+1)/2-k} H_{p+1-2k}}{k}$$

$$\equiv \frac{1}{2} \sum_{k=1}^{(p-1)/2} \frac{H_{2k-2}}{k(2k-1)} - \frac{1}{4} H_{(p-1)/2} \sum_{k=1}^{(p-1)/2} \frac{H_{2k-2}}{k}$$

$$-\frac{1}{2} \sum_{k=1}^{(p-1)/2} \frac{H_{2k} H_{2k-2}}{k} + \frac{1}{4} \sum_{k=1}^{(p-1)/2} \frac{H_k H_{2k-2}}{k}$$

modulo p holds. Combining this with (3.12), (3.13), (3.11), (3.7), (3.5) and Lemma 2.6, we immediately get the desired result.

Lemma 3.7. For any prime p > 3, we have

$$\sum_{k=1}^{(p-1)/2} \frac{(p/2-k)H_{2k}^2}{(p+1-2k)(p+2k)} \equiv q_p(2) - q_p(2)^2 + \frac{1}{6}q_p(2)^3 + \frac{1}{3}B_{p-3} \pmod{p}.$$

Proof. Replacing k in (3.6) by (p+1)/2 - j, we have

$$\sum_{j=1}^{(p-1)/2} \frac{1}{(2j-1)j^2} \equiv 8q_p(2) \pmod{p}.$$

In view of (2.5) and Lemma 2.6, we can deduce that

$$\sum_{k=1}^{(p-1)/2} \frac{H_{2k-2}}{k^2} \equiv -8q_p(2) + \frac{5}{2}B_{p-3} \pmod{p}.$$

This, together with (3.10), (3.11) and (3.12), yields that

$$\sum_{k=1}^{(p-1)/2} \frac{(p/2-k)H_{2k}^2}{(p+1-2k)(p+2k)}$$

$$\equiv \frac{1}{2} \sum_{k=1}^{(p-1)/2} \frac{H_{2k}^2}{2k-1} \equiv -\frac{1}{4} \sum_{k=1}^{(p-1)/2} \frac{H_{p+1-2k}^2}{k} \equiv -\frac{1}{4} \sum_{k=1}^{(p-1)/2} \frac{H_{2k-2}^2}{k}$$

$$\equiv -\frac{1}{4} \left(\sum_{k=1}^{(p-1)/2} \frac{H_{2k}H_{2k-2}}{k} - \sum_{k=1}^{(p-1)/2} \frac{H_{2k-2}}{k(2k-1)} - \frac{1}{2} \sum_{k=1}^{(p-1)/2} \frac{H_{2k-2}}{k^2} \right)$$

$$\equiv q_p(2) - q_p(2)^2 + \frac{1}{6}q_p(2)^3 + \frac{1}{3}B_{p-3} \pmod{p}.$$

This ends the proof.

Lemma 3.8. Let p > 3 be a prime. Then

$$\sum_{k=1}^{(p-1)/2} \frac{(p/2-k)H(2;2k)}{(p+1-2k)(p+2k)} \equiv q_p(2) - \frac{3}{16}B_{p-3} \pmod{p}$$

and

$$\sum_{k=1}^{(p-1)/2} \frac{(p/2-k)H(2;k)}{(p+1-2k)(p+2k)} \equiv 4q_p(2) - \frac{7}{8}B_{p-3} \pmod{p}.$$

Proof. In view of (2.10), (3.6) and Lemma 2.6, we have

$$\sum_{k=1}^{(p-1)/2} \frac{(p/2-k)H(2;2k)}{(p+1-2k)(p+2k)}$$

$$\equiv \frac{1}{2} \sum_{k=1}^{(p-1)/2} \frac{H(2;2k)}{2k-1} \equiv -\frac{1}{4} \sum_{k=1}^{(p-1)/2} \frac{H(2;p+1-2k)}{k} \equiv \frac{1}{4} \sum_{k=1}^{(p-1)/2} \frac{H(2;2k-2)}{k}$$

$$= \frac{1}{4} \left(\sum_{k=1}^{(p-1)/2} \frac{H(2;2k)}{k} - \sum_{k=1}^{(p-1)/2} \frac{1}{k(2k-1)^2} - \frac{1}{4} \sum_{k=1}^{(p-1)/2} \frac{1}{k^3} \right)$$

$$\equiv q_p(2) - \frac{3}{16} B_{p-3} \pmod{p}.$$
(3.14)

By Lemmas 2.5 and 2.6, we have

$$H(2; (p+1)/2 - k) = \sum_{j=1}^{(p+1)/2 - k} \frac{1}{j^2} \equiv 4 \sum_{j=k}^{(p-1)/2} \frac{1}{(2j-1)^2}$$

$$= 4 \left(H(2; p-1) - \frac{1}{4} H\left(2; \frac{p-1}{2}\right) - H(2; 2k-2) + \frac{1}{4} H(2; k-1) \right)$$

$$\equiv H(2; k-1) - 4H(2; 2k-2) \pmod{p}.$$

Hence,

$$\sum_{k=1}^{(p-1)/2} \frac{(p/2-k)H(2;k)}{(p+1-2k)(p+2k)}$$

$$\equiv \frac{1}{2} \sum_{k=1}^{(p-1)/2} \frac{H(2;(p+1)/2-k)}{p-2k}$$

$$\equiv \sum_{k=1}^{(p-1)/2} \frac{H(2;2k-2)}{k} - \frac{1}{4} \sum_{k=1}^{(p-1)/2} \frac{H(2;k-1)}{k} \pmod{p}.$$

In view of (3.14), we have

$$\sum_{k=1}^{(p-1)/2} \frac{H(2; 2k-2)}{k} \equiv 4q_p(2) - \frac{3}{4}B_{p-3} \pmod{p}.$$

With the aid of Lemma 2.7, we get

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

So

$$\sum_{k=1}^{(p-1)/2} \frac{(p/2-k)H(2;k)}{(p+1-2k)(p+2k)} \equiv 4q_p(2) - \frac{7}{8}B_{p-3} \pmod{p}.$$

Therefore the proof of Lemma 3.8 is complete.

Lemma 3.9. For any primes p > 3, we have

$$\sum_{k=1}^{(p-1)/2} G\left(\frac{p+1}{2}, k\right)$$

$$\equiv (-1)^{(p-1)/2} p^2 \left(q_p(2) - pq_p(2)^2 + p^2 q_p(2)^3 + \frac{7}{8} p^2 B_{p-3}\right) \pmod{p^5}.$$

Proof. For any complex number a, let $(a)_0 = 1$ and $(a)_n = a(a+1)\dots(a+n-1)$ for $n \in \mathbb{Z}^+$. By the definition of G(n,k), we have

$$G(n,k) = \frac{n^2 \binom{2n}{n} \binom{2n+2k}{n+k} \binom{2n-2k}{n-k} \binom{n+k}{n}}{2^{8n-4-2k} (2n+2k-1) \binom{2k}{k}} = \frac{n^2 \binom{2n}{n} \left(\frac{1}{2}\right)_{n+k} \left(\frac{1}{2}\right)_{n-k} \binom{n}{k}}{2^{4n-4-2k} n!^2 (2n+2k-1) \binom{2k}{k}}$$

$$= \frac{n^2 \binom{2n}{n} \left(\frac{1}{2}\right)_n \left(\frac{1}{2}\right)_{n-1} \left(\frac{1}{2}+n\right)_k \binom{n}{k}}{2^{4n-4-2k} n!^2 \left(\frac{1}{2}+n-k\right)_{k-1} (2n+2k-1) \binom{2k}{k}}$$

$$= \frac{n \binom{2n}{n}^2 \binom{2n-2}{n-1} \left(\frac{1}{2}+n\right)_k \binom{n}{k}}{2^{8n-6-2k} \left(\frac{1}{2}+n-k\right)_{k-1} (2n+2k-1) \binom{2k}{k}}, \tag{3.15}$$

where we have used the equalities

$$\frac{\left(\frac{1}{2}\right)_{n+k}}{(n+k)!} = \frac{\binom{2n+2k}{n+k}}{4^{n+k}}, \quad \frac{\left(\frac{1}{2}\right)_{n-k}}{(n-k)!} = \frac{\binom{2n-2k}{n-k}}{4^{n-k}},$$

$$\left(\frac{1}{2}\right)_{n+k} = \left(\frac{1}{2}\right)_n \left(\frac{1}{2} + n\right)_k, \quad \frac{\left(\frac{1}{2}\right)_n}{(n)!} = \frac{\binom{2n}{n}}{4^n}$$

and

$$\left(\frac{1}{2}\right)_{n-k} \left(\frac{1}{2} + n - k\right)_{k-1} = \left(\frac{1}{2}\right)_{n-1} \quad (1 \le k \le n).$$

It is easy to check that

$$\frac{\left(\frac{p}{2}+1\right)_k}{\left(\frac{p}{2}-k\right)_k} \equiv \frac{k!\left(1+\frac{p}{2}H_k+\frac{p^2}{4}\sum_{1\leq i< j\leq k}\frac{1}{ij}\right)}{(-1)^k k!\left(\left(1-\frac{p}{2}H_k+\frac{p^2}{4}\sum_{1\leq i< j\leq k}\frac{1}{ij}\right)}$$

$$\equiv (-1)^k \left(1+pH_k+\frac{p^2}{2}H_k^2\right) \pmod{p^3}.$$

In view of [22, (4.4)], $\binom{(p-1)/2}{k}(-4)^k/\binom{2k}{k}$ is congruent to

$$1 - p \sum_{j=1}^{k} \frac{1}{2j-1} + \frac{p^2}{2} \left(\left(\sum_{j=1}^{k} \frac{1}{2j-1} \right)^2 - \sum_{j=1}^{k} \frac{1}{(2j-1)^2} \right)$$

$$= 1 - p \left(H_{2k} - \frac{1}{2} H_k \right) + \frac{p^2}{2} \left(\left(H_{2k} - \frac{1}{2} H_k \right)^2 - H(2; 2k) + \frac{1}{4} H(2; k) \right)$$

modulo p^3 . By (3.15), we have

$$\begin{split} &\sum_{k=1}^{\frac{p-1}{2}} G\left(\frac{p+1}{2},k\right) \\ &= \frac{(p+1)^2 \binom{p+1}{(p+1)/2}^2 \binom{p-1}{(p-1)/2}}{2^{4p-1}} \sum_{k=1}^{\frac{p-1}{2}} \frac{(p/2+1)_k \binom{(p-1)/2}{k} 4^k (p/2-k)}{(p/2-k)_k \binom{2k}{k} (p+1-2k)(p+2k)} \\ &\equiv \frac{(p+1)^2 \binom{p+1}{(p+1)/2}^2 \binom{p-1}{(p-1)/2}}{2^{4p-1}} \sum_{k=1}^{(p-1)/2} \frac{(p/2-k) a_{p,k}}{(p+1-2k)(p+2k)} \pmod{p^5}, \end{split}$$

where $a_{p,k}$ denotes the expression

$$1 + \frac{3p}{2}H_k - pH_{2k} + \frac{9p^2}{8}H_k^2 - \frac{3p^2}{2}H_kH_{2k} + \frac{p^2}{2}H_{2k}^2 - \frac{p^2}{2}\left(H(2;2k) - \frac{H(2;k)}{4}\right).$$

In light of Lemmas 3.2–3.8 and Lemma 2.3, we have

$$\sum_{k=1}^{(p-1)/2} G\left(\frac{p+1}{2}, k\right)$$

$$\equiv \frac{(p+1)^2 \binom{p+1}{\frac{p+1}{2}}^2 \binom{p-1}{\frac{p-1}{2}}}{2^{4p-1}} \left(\frac{1}{2} q_p(2) - \frac{3}{2} p q_p(2)^2 + 3p^2 q_p(2)^3 + \frac{7}{16} p^2 B_{p-3}\right)$$

$$\equiv \frac{2p^2 \binom{p-1}{(p-1)/2}^3}{2^{4p-4}} \left(\frac{1}{2} q_p(2) - \frac{3}{2} p q_p(2)^2 + 3p^2 q_p(2)^3 + \frac{7}{16} p^2 B_{p-3}\right)$$

$$\equiv 2(-1)^{(p-1)/2} p^2 4^{p-1} \left(\frac{1}{2} q_p(2) - \frac{3}{2} p q_p(2)^2 + 3p^2 q_p(2)^3 + \frac{7}{16} p^2 B_{p-3}\right)$$

$$\pmod{p^5}.$$

$$\pmod{p^5}.$$

Then we obtain the desired result by noting that

$$4^{p-1} = (1 + p q_p(2))^2 = 1 + 2p q_p(2) + p^2 q_p(2)^2.$$

This ends the proof.

Proof of Theorem 1.1. Combining Lemmas 3.1 and 3.9 with (3.4), we immediately get

$$\sum_{n=0}^{(p-1)/2} F(n,0) \equiv p(-1)^{(p-1)/2} + (-1)^{(p-1)/2} \frac{7}{24} p^4 B_{p-3} \pmod{p^5},$$

which is equivalent to our desired result.

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