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Research article

A Ramanujan-type supercongruence related to harmonic numbers

Wenbin Zhang[1], **Yong Zhang**[2,*] **and Jiachen Wu**[2]

[1] Department of Applied Mathematics, Guangzhou Huashang College, Guangzhou, 511300, China

[2] School of Mathematics and Physics, Nanjing Institute of Technology, Nanjing, 211167, China

* **Correspondence:** Email: yongzhang1982@163.com.

Abstract: We prove that, for all primes $p > 5$, positive integers r and m with $p \nmid m$ and $p \nmid \binom{2mp^{r-1}}{mp^{r-1}}$, there holds

$$\frac{1}{m^4 p^{4r}\binom{2mp^{r-1}}{mp^{r-1}}^3}\left(\sum_{k=0}^{mp^r-1}(21k+8)\binom{2k}{k}^3 - p\sum_{k=0}^{mp^{r-1}-1}(21k+8)\binom{2k}{k}^3\right)$$
$$\equiv -6\frac{H_{p-1}}{p^2} \pmod{p^2},$$

where $H_n = \sum_{j=1}^n \frac{1}{j}$ $(n = 1, 2, \cdots)$ are the usual harmonic numbers. This partially confirms a conjecture by Z.-W. Sun.

Keywords: supercongruences; central binomial coefficients; harmonic numbers; Ramanujan-type supercongruences
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1. Introduction

For Ramanujan's and Ramanujan-like series, the reader may consult [7–9, 20, 28] for related work. In the spirit of [35], all known Ramanujan-type formulas for $1/\pi$ and $1/\pi^2$ admit similar p-analogues. For example, Zeilberger [32] discovered the following Ramanujan-type formula:

$$\sum_{k=0}^{\infty}\frac{21k-8}{k^3\binom{2k}{k}^3} = \zeta(2) = \frac{\pi^2}{6}.$$

Sun [24] proposed its p-analogue as follows:

$$\sum_{k=0}^{\frac{p-1}{2}} \frac{21k-8}{k^3\binom{2k}{k}^3} \equiv (-1)^{\frac{p+1}{2}} 4E_{p-3} \pmod{p},$$

where $E_0, E_1, E_2, \cdots$ are the Euler numbers. He also found the above congruence has the following equivalent form:

$$\sum_{k=0}^{\frac{p-1}{2}} (21k+8)\binom{2k}{k}^3 \equiv 8p + \left(\frac{-1}{p}\right) 32p^3 E_{p-3} \pmod{p^4},$$

where $(\frac{\cdot}{\cdot})$ denotes the Jacobi symbol.

In 2011, Sun [26] studied the above summation index k from 0 to $p^r - 1$ and showed that for any prime p and $r \in \mathbb{Z}^+$,

$$\sum_{k=0}^{p^r-1} (21k+8)\binom{2k}{k}^3 \equiv 8p^r + 16p^{r+3} B_{p-3} \pmod{p^{r+4}}, \tag{1.1}$$

where $B_0, B_1, B_2, \cdots$ are the Bernoulli numbers and B_{-1} is regarded as zero. Recall that Glaisher [4, 5] proved that, for any prime $p \geq 5$,

$$H_{p-1} \equiv -\frac{1}{3} p^2 B_{p-3} \pmod{p^3}, \tag{1.2}$$

where H_n $(n = 1, 2, \cdots)$ denotes the usual harmonic number $\sum_{j=1}^{n} \frac{1}{j}$. We refer the reader to [31] for applications of harmonic numbers. Recently, Xia [30] confirmed that, for primes $p \geq 7$,

$$\sum_{k=0}^{p-1} (21k+8)\binom{2k}{k}^3 \equiv 8p - 48p^2 H_{p-1} \pmod{p^6}. \tag{1.3}$$

This, together with (1.2), extends (1.1) to the modulus p^6 case for $r = 1$. Based on the above work, Sun [25, Conjecture 21(i)] proposed the following more general conjecture:

Conjecture 1. *Let $p \neq 2, 5$ be a prime, and let $r \in \mathbb{Z}^+$. Let m be a positive integer with $p \nmid m$. Then*

$$\frac{\sum_{k=0}^{mp^r-1} (21k+8)\binom{2k}{k}^3 - p\sum_{k=0}^{mp^{r-1}-1} (21k+8)\binom{2k}{k}^3}{m^4 p^{4r} \binom{2mp^{r-1}}{mp^{r-1}}^3} \equiv -6\frac{H_{p-1}}{p^2} \pmod{p^2}. \tag{1.4}$$

Remark 1. The case $p \mid \binom{2mp^{r-1}}{mp^{r-1}}$ in Conjecture 1 is somewhat difficult to deal with. In this case, we need to find a more appropriate identity to approximate away this factor $\binom{2mp^{r-1}}{mp^{r-1}}^3$ and achieve modulo greater than $4r + 2$. Conjecture 1 is the Atkin and Swinnerton–Dyer type (see [1]) congruence's extension related to harmonic numbers and Bernoulli numbers. We are all interested in this type of congruence and think it meaningful to study such congruence. That is the motivation for our work.

Here we shall establish the following result, thus partially confirming a weaker version of Conjecture 1, which is the case $p \nmid \binom{2mp^{r-1}}{mp^{r-1}}$ of the congruence (1.4).

Theorem 1. *Let $p > 5$ be a prime and r be a positive integer. Let m be a positive integer with $p \nmid m$ and $p \nmid \binom{2mp^{r-1}}{mp^{r-1}}$. Then the congruence* (1.4) is true.

Remark 2. Clearly, taking $r = m = 1$ in (1.4) yields (1.3). The congruence (1.4) is often called a Ramanujan-type supercongruence. In recent years, many authors have studied Ramanujan-type q-supercongruences; the reader may refer to [10–14, 16, 21, 27, 29]. We think Theorem 1 may be useful to those who are interested in Ramanujan's and Ramanujan–like series, and the Atkin and Swinnerton-Dyer type congruences in combinatorics.

The paper is organized as follows: some lemmas are given in section 2. In section 3, we will give the proof of Theorem 1. The last section is the conclusions.

2. Some lemmas

In order to prove Theorem 1, we need the below eight lemmas. The first one is a result of Beukers [2, Lemma 2 (i)].

Lemma 1. *Let n be an integer, and let p be a prime. Let r and k be positive integers. Then*

$$\binom{p^r n-1}{k} \equiv \binom{p^{r-1}n-1}{\lfloor \frac{k}{p} \rfloor}(-1)^{k-\lfloor \frac{k}{p} \rfloor}\left(1-np^r \sum_{j=1,p\nmid j}^{k} \frac{1}{j}\right) \pmod{p^{2r}}. \tag{2.1}$$

Remark 1. The previous version of (2.1) (also see [2, Lemma 2 (i)]) is very important. We list it out as follows.

$$\binom{p^r n-1}{k} = \binom{p^{r-1}n-1}{\lfloor \frac{k}{p} \rfloor} \prod_{j=1,p\nmid j}^{k} \frac{p^r n-j}{j}. \tag{2.2}$$

The second one is Jacobsthal's binomial congruence (see [18, Lemma 2.1 and the proof of Theorem 1.3]).

Lemma 2. *Let p be a prime. Then, for all integers a, b, and positive integers r, s,*

$$\binom{p^r a}{p^s b} \equiv \binom{p^{r-1}a}{p^{s-1}b}(-1)^{p^s b-p^{s-1}b} \pmod{p^{2r+\min\{r,s\}-\delta_{p,3}-2\delta_{p,2}}}. \tag{2.3}$$

where the Kronecker symbol $\delta_{m,n}$ is defined as 1 if $m = n$ and 0 otherwise.

Remark 2. The $p \geq 5$ case of (2.3) was confirmed by Gessel [3] and Granville [6]. Straub [22] proved the extension to negative integers.

The third result we require is due to Osburn, Sahu, and Straub [18, Lemma 2.2].

Lemma 3. *Let $p > 5$ be a prime, and let n be an even positive integer. Then, for all integers $r \geq 1$,*

$$\sum_{k=1,p\nmid k}^{\frac{p^r-1}{2}} \frac{1}{k^n} \equiv 0 \pmod{p^r}. \tag{2.4}$$

From (2.4) it is easy to see that

$$\sum_{k=1,p\nmid k}^{p^r-1}\frac{1}{k^n}=\sum_{k=1,p\nmid k}^{\frac{p^r-1}{2}}\left(\frac{1}{k^n}+\frac{1}{(p^r-k)^n}\right)\equiv 2\sum_{k=1,p\nmid k}^{\frac{p^r-1}{2}}\frac{1}{k^n}\equiv 0 \pmod{p^r}. \tag{2.5}$$

For any positive integer m, let $H_{n,m}=\sum_{j=1}^{n}\frac{1}{j^m}$ $(n=1,2,...)$ denote the generalized harmonic numbers of order m. Clearly, $H_{n,1}=H_n$. For convenience, we adopt the notation $H'_{n,m}$ to stand for the number $\sum_{j=1,p\nmid j}^{n}\frac{1}{j^m}$ and let $H'_n=H'_{n,1}$. For example, we can revise the congruences (2.4) and (2.5) as follows: $H'_{\frac{p^r-1}{2},n}\equiv 0 \pmod{p^r}$ and $H'_{p^r-1,n}\equiv 0 \pmod{p^r}$.

We need to establish another five lemmas.

Lemma 4. *Let $p>5$ be a prime, and let k be a positive integer. Then, for any positive integer s,*

$$H'_{p^sk-1}\equiv -p^{2s}k^2\left(\frac{B_{2p-4}}{2p-4}-2\frac{B_{p-3}}{p-3}\right) \pmod{p^{2s+2}}, \tag{2.6}$$

and

$$H'_{p^sk-1,2}\equiv kH'_{p^s-1,2} \pmod{p^{2s+\delta_{s,1}}}. \tag{2.7}$$

Proof. For any prime $p\geq 7$, Sun [23, Theorem 5.1] proved that

$$H_{p-1,3}\equiv -\frac{6p^2B_{p-5}}{5} \pmod{p^3}. \tag{2.8}$$

It is easily seen that, for any positive integer s,

$$H'_{p^s-1,3}=\sum_{j=1,p\nmid j}^{p^s-1}\frac{1}{j^3}=\sum_{j=1,p\nmid j}^{p^s-1}\frac{1}{(p^s-j)^3}\equiv -\sum_{j=1,p\nmid j}^{p^s-1}\frac{1}{j^3}\equiv 0 \pmod{p^s}. \tag{2.9}$$

Note that Zhang [33] has given the following result:

$$H'_{p^s-1,2}\equiv 2p^s\left(\frac{B_{2p-4}}{2p-4}-2\frac{B_{p-3}}{p-3}\right) \pmod{p^{s+2}}. \tag{2.10}$$

It follows from (2.5), (2.8), and (2.9) that

$$\begin{aligned}
H'_{p^s-1}&=\frac{1}{2}\sum_{j=1,p\nmid j}^{p^s-1}\left(\frac{1}{j}+\frac{1}{p^s-j}\right)=\frac{p^s}{2}\sum_{j=1,p\nmid j}^{p^s-1}\frac{1}{j(p^s-j)}\\
&\equiv -\frac{p^s}{2}\sum_{j=1,p\nmid j}^{p^s-1}\frac{1}{j^2}\left(1+\frac{p^s}{j}+\frac{p^{2s}}{j^2}\right)\\
&=-\frac{p^s}{2}\left(H'_{p^s-1,2}+p^sH'_{p^s-1,3}+p^{2s}H'_{p^s-1,4}\right)\equiv -\frac{p^s}{2}H'_{p^s-1,2} \pmod{p^{2s+2}},
\end{aligned}$$

and

$$H'_{p^sk-1}=\sum_{i=0}^{k-1}\sum_{j=1,p\nmid j}^{p^s-1}\frac{1}{p^si+j}\equiv\sum_{i=0}^{k-1}\sum_{j=1,p\nmid j}^{p^s-1}\frac{1}{j}\left(1-\frac{p^si}{j}+\frac{p^{2s}i^2}{j^2}-\frac{\delta_{s,1}p^{3s}i^3}{j^3}\right)$$

$$
\begin{aligned}
&= kH'_{p^s-1} - \frac{k(k-1)p^sH'_{p^s-1,2}}{2} + p^{2s}H'_{p^s-1,3}\frac{k(k-1)(2k-1)}{6} \\
&\quad - \delta_{s,1}p^{3s}H'_{p^s-1,4}\sum_{i=1}^{k-1} i^3 \\
&\equiv -\frac{p^sk^2}{2}H'_{p^s-1,2} \equiv -p^{2s}k^2\Big(\frac{B_{2p-4}}{2p-4} - 2\frac{B_{p-3}}{p-3}\Big) \pmod{p^{2s+2}}.
\end{aligned}
$$

Similarly to the proof of (2.6), by using (2.5), (2.8), and (2.9), we can get the following supercongruence:

$$
\begin{aligned}
H'_{p^sk-1,2} &= \sum_{i=0}^{k-1}\sum_{j=1,p\nmid j}^{p^s-1}\frac{1}{(p^si+j)^2} \equiv \sum_{i=0}^{k-1}\sum_{j=1,p\nmid j}^{p^s-1}\frac{1}{j^2}\left(1 - \frac{2p^si}{j} + \frac{3p^{2s}i^2\delta_{s,1}}{j^2}\right) \\
&= kH'_{p^s-1,2} - k(k-1)p^sH'_{p^s-1,3} + \frac{k(k-1)(2k-1)p^{2s}H'_{p^s-1,4}\delta_{s,1}}{2} \\
&\equiv kH'_{p^s-1,2} \pmod{p^{2s+\delta_{s,1}}}.
\end{aligned}
$$

This completes the proof. □

We will use Lemma 5 to handle the sums divisible by p of Theorem 1.

Lemma 5. *Let $p \geq 7$ be a prime, and let m be a positive integer with $p \nmid m$. Then, for any positive integer r,*

$$
\begin{aligned}
&\sum_{k=1}^{mp^{r-1}-1}\binom{-mp^{r-1}}{k}^2\left(2H'_{pk-1} - mp^rH'_{pk-1,2}\right) \\
&\equiv 2m^2p^{2r}(1-\delta_{r,1})(1-(p+2mp)\delta_{r,2})\Big(\frac{B_{2p-4}}{2p-4} - 2\frac{B_{p-3}}{p-3}\Big)\sum_{l=0}^{m-1}\binom{-m-1}{l}^2 \\
&\quad - 2p^{2r}\Big(\frac{B_{2p-4}}{2p-4} - 2\frac{B_{p-3}}{p-3}\Big)\sum_{k=1}^{m-1}\binom{-m}{k}^2 k(k+m) \pmod{p^{2r+2}}.
\end{aligned}
\tag{2.11}
$$

Proof. By (2.6), (2.7), and (2.10), the supercongruence (2.11) is true for $r = 1$.

We now assume that $r \geq 2$. In view of [2, Lemma 1], we have

$$
\sum_{\lfloor \frac{k}{p^r} \rfloor = 0, p\nmid k}\frac{1}{k} \equiv 0 \pmod{p^{2r}},
\tag{2.12}
$$

and so

$$
\sum_{k=1}^{p-1}H_{k-1} \equiv \sum_{k=1}^{p-1}\sum_{j=1}^{k}\frac{1}{j} = \sum_{j=1}^{p-1}\frac{1}{j}\sum_{k=j}^{p-1}1 = \sum_{j=1}^{p-1}\frac{p-j}{j} \equiv 1 - p \pmod{p^2}.
\tag{2.13}
$$

Similarly to the proof of (2.13), by (2.6) and (2.10), we can show that

$$
\sum_{k=1}^{p-1}H_{k,2} = \sum_{j=1}^{p-1}\frac{1}{j^2}\sum_{k=j}^{p-1}1 = pH_{p-1,2} - H_{p-1} \equiv 0 \pmod{p^2}.
\tag{2.14}
$$

Note that for any nonnegative integer l and positive integer k, by (2.6), (2.7), and (2.10), we get

$$\sum_{\lfloor\frac{k-1}{p}\rfloor=l,p\nmid k}\frac{2H'_{pk-1}-mp^2H'_{pk-1,2}}{k^2}\equiv\Big(\frac{B_{2p-4}}{2p-4}-2\frac{B_{p-3}}{p-3}\Big)\sum_{\lfloor\frac{k-1}{p}\rfloor=l,p\nmid k}\Big(-2p^2-\frac{2mp^3}{k}\Big)$$
$$\equiv 2p^2(1-p)\Big(\frac{B_{2p-4}}{2p-4}-2\frac{B_{p-3}}{p-3}\Big)\pmod{p^4} \tag{2.15}$$

and

$$\sum_{\lfloor\frac{k-1}{p}\rfloor=l,p\nmid k}\frac{H'_{k-1}H'_{pk-1}}{k^2}\equiv -p^2\Big(\frac{B_{2p-4}}{2p-4}-2\frac{B_{p-3}}{p-3}\Big)\sum_{\lfloor\frac{k-1}{p}\rfloor=l,p\nmid k}H'_{k-1}\pmod{p^4}. \tag{2.16}$$

With the help of (2.10), (2.13), and (2.14), we can deduce that

$$\sum_{\lfloor\frac{k-1}{p}\rfloor=l,p\nmid k}H'_{k-1}=\sum_{k=1}^{p-1}H'_{pl+k-1}\equiv\sum_{k=1}^{p-1}\sum_{j=1}^{k-1}\frac{1}{pl+j}\equiv\sum_{k=1}^{p-1}\sum_{j=1}^{k-1}\Big(\frac{1}{j}-\frac{pl}{j^2}\Big)$$
$$=\sum_{k=1}^{p-1}\Big(H_{k-1}-plH_{k-1,2}\Big)\equiv 1-p\pmod{p^2}. \tag{2.17}$$

For $r=2$, by (2.1), (2.6), (2.7), (2.10), and (2.15)–(2.17), we have

$$\begin{aligned}&\sum_{k=1,p\nmid k}^{mp-1}\binom{-mp}{k}^2\Big(2H'_{pk-1}-mp^2H'_{pk-1,2}\Big)\\
&\equiv m^2p^2\sum_{k=1,p\nmid k}^{mp-1}\frac{1}{k^2}\binom{-m-1}{\lfloor\frac{k-1}{p}\rfloor}^2\Big(1+2mpH'_{k-1}\Big)\Big(2H'_{pk-1}-mp^2H'_{pk-1,2}\Big)\\
&\equiv m^2p^2\sum_{l=0}^{m-1}\binom{-m-1}{l}^2\sum_{\lfloor\frac{k-1}{p}\rfloor=l,p\nmid k}\frac{2H'_{pk-1}+4mpH'_{k-1}H'_{pk-1}-mp^2H'_{pk-1,2}}{k^2}\\
&\equiv 2m^2p^4(1-p-2mp)\Big(\frac{B_{2p-4}}{2p-4}-2\frac{B_{p-3}}{p-3}\Big)\sum_{l=0}^{m-1}\binom{-m-1}{l}^2\pmod{p^6}.\end{aligned}$$

In light of (2.3), (2.6), (2.7), and (2.10), we can show that

$$\begin{aligned}&\sum_{k=1,p\mid k}^{mp-1}\binom{-mp}{k}^2\Big(2H'_{pk-1}-mp^2H'_{pk-1,2}\Big)\\
&=\sum_{k=1}^{m-1}\binom{-mp}{pk}^2\Big(2H'_{p^2k-1}-mp^2H'_{p^2k-1,2}\Big)\\
&\equiv -2p^4\Big(\frac{B_{2p-4}}{2p-4}-2\frac{B_{p-3}}{p-3}\Big)\sum_{k=1}^{m-1}\binom{-m}{k}^2k(k+m)\pmod{p^6}.\end{aligned}$$

Combining the above two congruences, we arrive at (2.11) with $r = 2$.

Next, we will consider the case $r \geq 3$. For any integer $1 \leq s \leq r-2$ and $1 \leq k \leq mp^{r-s}-1$ with $p \nmid k$, by (2.7) and (2.10), we have $p^r\binom{-mp^{r-1}}{p^{s-1}k}^2 H'_{p^sk-1,2} \equiv 0 \pmod{p^{2r+2}}$. It follows that

$$\begin{aligned}
&\sum_{k=1}^{mp^{r-1}-1}\binom{-mp^{r-1}}{k}^2\left(2H'_{pk-1}-mp^rH'_{pk-1,2}\right)\\
&\equiv 2\sum_{s=1}^{r-2}\sum_{k=1,p\nmid k}^{mp^{r-s}-1}\binom{-mp^{r-1}}{p^{s-1}k}^2 H'_{p^sk-1}\\
&\quad+\sum_{k=1}^{mp-1}\binom{-mp^{r-1}}{p^{r-2}k}^2\left(2H'_{p^{r-1}k-1}-mp^rH'_{p^{r-1}k-1,2}\right) \pmod{p^{2r+2}}.
\end{aligned}\tag{2.18}$$

With the help of (2.3) and (2.6), we obtain

$$\begin{aligned}
&2\sum_{s=1}^{r-2}\sum_{k=1,p\nmid k}^{mp^{r-s}-1}\binom{-mp^{r-1}}{p^{s-1}k}^2 H'_{p^sk-1}\\
&\equiv -2m^2p^{2r}\left(\frac{B_{2p-4}}{2p-4}-2\frac{B_{p-3}}{p-3}\right)\sum_{s=1}^{r-2}\sum_{k=1,p\nmid k}^{mp^{r-s}-1}\binom{-mp^{r-s}-1}{k-1}^2 \pmod{p^{2r+2}}.
\end{aligned}\tag{2.19}$$

For any integer $1 \leq s \leq r-2$, by Lemma 1, we can show that

$$\begin{aligned}
&\sum_{k=1,p\nmid k}^{mp^{r-s}-1}\binom{-mp^{r-s}-1}{k-1}^2\\
&\equiv\sum_{k=1,p\nmid k}^{mp^{r-s}-1}\binom{-mp^{r-s-1}-1}{\lfloor\frac{k-1}{p}\rfloor}^2=\sum_{l=0}^{mp^{r-s-1}-1}\binom{-mp^{r-s-1}-1}{l}^2\sum_{\lfloor\frac{k-1}{p}\rfloor=l,p\nmid k}1\\
&=(p-1)\sum_{l=0}^{mp^{r-s-1}-1}\binom{-mp^{r-s-1}-1}{l}^2 \pmod{p^2}.
\end{aligned}\tag{2.20}$$

If $s = r-2$, then using (2.6), (2.13), and Lemma 1, we have

$$\begin{aligned}
(p-1)\sum_{l=0}^{mp-1}\binom{-mp-1}{l}^2 &\equiv (p-1)\sum_{k=0}^{m-1}\binom{-m-1}{k}^2\sum_{\lfloor\frac{l}{p}\rfloor=k}\left(1+2mpH'_l\right)\\
&\equiv -(1+2m)p\sum_{k=0}^{m-1}\binom{-m-1}{k}^2 \pmod{p^2}.
\end{aligned}\tag{2.21}$$

If $1 \leq s \leq r-3$, then similarly to the proof of (2.20), by (2.21) we get

$$(p-1)\sum_{l=0}^{mp^{r-s-1}-1}\binom{-mp^{r-s-1}-1}{l}^2$$

$$\equiv p(p-1)\sum_{l=0}^{mp^{r-s-2}-1}\binom{-mp^{r-s-2}-1}{l}^2$$
$$\equiv p(p-1)\cdot[s=r-3]\cdot\sum_{l=0}^{mp-1}\binom{-mp-1}{l}^2\equiv 0 \pmod{p^2}. \tag{2.22}$$

It is clear that $[m=n]$ coincides with the Kronecker symbol $\delta_{m,n}$. Substituting (2.20)–(2.22) into (2.19) leads to

$$2\sum_{s=1}^{r-2}\sum_{k=1,p\nmid k}^{mp^{r-s}-1}\binom{-mp^{r-1}}{p^{s-1}k}^2 H'_{p^sk-1}$$
$$\equiv 2m^2(1+2m)p^{2r+1}\Big(\frac{B_{2p-4}}{2p-4}-2\frac{B_{p-3}}{p-3}\Big)\sum_{k=0}^{m-1}\binom{-m-1}{k}^2 \pmod{p^{2r+2}}. \tag{2.23}$$

In light of (2.6)–(2.7), (2.10), (2.13), (2.17), and Lemma 2, we have

$$\sum_{k=1,p\nmid k}^{mp-1}\binom{-mp^{r-1}}{p^{r-2}k}^2\Big(2H'_{p^{r-1}k-1}-mp^rH'_{p^{r-1}k-1,2}\Big)$$
$$\equiv 2m^2p^{2r}\Big(-\frac{B_{2p-4}}{2p-4}+2\frac{B_{p-3}}{p-3}\Big)\Big(\sum_{k=1,p\nmid k}^{mp-1}\binom{-mp-1}{k-1}^2+pm\sum_{k=1,p\nmid k}^{mp-1}\frac{1}{k}\binom{-mp-1}{k-1}^2\Big)$$
$$\equiv 2m^2p^{2r}\Big(-\frac{B_{2p-4}}{2p-4}+2\frac{B_{p-3}}{p-3}\Big)\sum_{l=0}^{m-1}\binom{-m-1}{l}^2\sum_{\lfloor\frac{k-1}{p}\rfloor=l,p\nmid k}\Big(1+2mpH'_{k-1}+\frac{pm}{k}\Big)$$
$$\equiv 2m^2p^{2r}(p-1+2mp)\Big(-\frac{B_{2p-4}}{2p-4}+2\frac{B_{p-3}}{p-3}\Big)\sum_{l=0}^{m-1}\binom{-m-1}{l}^2 \pmod{p^{2r+2}}, \tag{2.24}$$

and

$$\sum_{k=1}^{m-1}\binom{-mp^{r-1}}{p^{r-1}k}^2\Big(2H'_{p^rk-1}-mp^rH'_{p^rk-1,2}\Big)$$
$$\equiv -2p^{2r}\Big(\frac{B_{2p-4}}{2p-4}-2\frac{B_{p-3}}{p-3}\Big)\sum_{k=1}^{m-1}\binom{-m}{k}^2(k^2+km) \pmod{p^{2r+2}}. \tag{2.25}$$

Finally, combining (2.18), (2.23), (2.24) and (2.25), we reach (2.11) with $r\geq 3$. This proves Lemma 5. □

The following Lemma 6 plays an important role in proving Lemma 7.

Lemma 6. *Let $p\geq 7$ be a prime. Then, for any positive integer r,*

$$\sum_{k=0}^{mp^r-1}\binom{-mp^r-1}{k}^2\equiv p^r(1+2m)(1-2mp\delta_{r,1})\sum_{l=0}^{m-1}\binom{-m-1}{l}^2 \pmod{p^{r+2}}. \tag{2.26}$$

Proof. By (2.2), we have

$$\begin{aligned}
&\sum_{k=0}^{mp^r-1}\binom{-mp^r-1}{k}^2-1\\
&=\sum_{k=1}^{mp^r-1}\binom{-mp^{r-1}-1}{\lfloor\frac{k}{p}\rfloor}^2\prod_{j=1,p\nmid j}^{k}\left(1+\frac{mp^r}{j}\right)^2\\
&\equiv\sum_{k=1}^{mp^r-1}\binom{-mp^{r-1}-1}{\lfloor\frac{k}{p}\rfloor}^2\prod_{j=1,p\nmid j}^{k}\left(1+\frac{2mp^r}{j}+\frac{m^2p^{2r}\delta_{r,1}}{j^2}\right)\\
&\equiv\sum_{k=1}^{mp^r-1}\binom{-mp^{r-1}-1}{\lfloor\frac{k}{p}\rfloor}^2\left(1+2mp^rH_k^{'}-m^2p^{2r}\delta_{r,1}H_{k,2}^{'}+2m^2p^{2r}\delta_{r,1}{H_k^{'}}^2\right)\pmod{p^{r+2}}.
\end{aligned}\tag{2.27}$$

In view of (2.6) and the Chu–Vandermonde convolution identity, we get

$$\sum_{k=0}^{p-1}\binom{p-1}{k}^2=\binom{2p-2}{p-1}=\frac{p}{2p-1}\prod_{j=1}^{p-1}\left(1+\frac{p}{j}\right)\equiv-2p^2-p\pmod{p^3}.\tag{2.28}$$

On the other hand,

$$\sum_{k=0}^{p-1}\binom{p-1}{k}^2\equiv1+\sum_{k=1}^{p-1}\left(1-2pH_k-p^2H_{k,2}+2p^2H_k^2\right)\pmod{p^3}.\tag{2.29}$$

Combining (2.6), (2.13), (2.14) and (2.28) with (2.29), we obtain

$$\sum_{k=1}^{p-1}H_k^2\equiv-2\pmod{p}.\tag{2.30}$$

For any nonnegative integer l, by (2.6), (2.13), and (2.14), we have

$$\begin{aligned}
\sum_{\lfloor\frac{k}{p}\rfloor=l}H_k^{'}&\equiv\sum_{k=1}^{p-1}H_{pl+k}^{'}\equiv\sum_{k=1}^{p-1}\sum_{j=1}^{k}\frac{1}{pl+j}\equiv\sum_{k=1}^{p-1}\sum_{j=1}^{k}\left(\frac{1}{j}-\frac{pl}{j^2}\right)\\
&=\sum_{k=1}^{p-1}H_k-pl\sum_{k=1}^{p-1}H_{k,2}\equiv1-p\pmod{p^2},
\end{aligned}$$

$$\sum_{\lfloor\frac{k}{p}\rfloor=l}H_{k,2}^{'}\equiv\sum_{k=1}^{p-1}H_{pl+k,2}^{'}\equiv\sum_{k=1}^{p-1}\sum_{j=1}^{k}\frac{1}{(pl+j)^2}\equiv\sum_{k=1}^{p-1}\sum_{j=1}^{k}\frac{1}{j^2}=\sum_{k=1}^{p-1}H_{k,2}\equiv0\pmod{p},$$

and by (2.30),

$$\sum_{\lfloor\frac{k}{p}\rfloor=l}{H_k^{'}}^2\equiv\sum_{k=1}^{p-1}{H_{pl+k}^{'}}^2\equiv\sum_{k=1}^{p-1}\Big(\sum_{j=1}^{k}\frac{1}{pl+j}\Big)^2\equiv\sum_{k=1}^{p-1}{H_k}^2\equiv-2\pmod{p}.$$

Therefore,

$$\sum_{k=0}^{mp-1}\binom{-mp-1}{k}^2 \equiv \sum_{l=0}^{m-1}\binom{-m-1}{l}^2 \sum_{\lfloor \frac{k}{p}\rfloor = l} 1$$
$$+\sum_{l=0}^{m-1}\binom{-m-1}{l}^2 \sum_{\lfloor \frac{k}{p}\rfloor = l, p\nmid k}\left(2mpH_k^{'} - m^2p^2H_{k,2}^{'} + 2m^2p^2{H_k^{'}}^2\right)$$
$$\equiv p(1+2m)(1-2mp)\sum_{l=0}^{m-1}\binom{-m-1}{l}^2 \pmod{p^3}, \tag{2.31}$$

where we shouldn't accept that $p \mid k$ in sums of the second line in (2.31). This completes the proof of (2.26) for $r = 1$.

Now, we consider the case $r \geq 2$. From (2.27), (2.31), and the above congruences, we can deduce by induction that

$$\sum_{k=0}^{mp^r-1}\binom{-mp^r-1}{k}^2 \equiv \sum_{l=0}^{mp^{r-1}-1}\binom{-mp^{r-1}-1}{l}^2 \sum_{\lfloor \frac{k}{p}\rfloor = l}\left(1+2mp^rH_k^{'}\right)$$
$$\equiv \left(p+2mp^r(1-p)\right)\sum_{l=0}^{mp^{r-1}-1}\binom{-mp^{r-1}-1}{l}^2$$
$$\equiv \prod_{j=2}^{r}\left(p+2mp^j(1-p)\right)\sum_{l=0}^{mp-1}\binom{-mp-1}{l}^2$$
$$\equiv p^r\prod_{j=2}^{r}\left(1+2mp^{j-1}(1-p)\right)(1+2m)(1-2mp)\sum_{l=0}^{m-1}\binom{-m-1}{l}^2$$
$$\equiv p^r(1+2m)\sum_{l=0}^{m-1}\binom{-m-1}{l}^2 \pmod{p^{r+2}},$$

which is just the supercongruence (2.26) for $r \geq 2$. □

We will use Lemma 7 to deal with the sums not divisible by p of Theorem 1.

Lemma 7. *Let $p \geq 7$ be a prime. Then, for any positive integer r,*

$$\sum_{k=1,p\nmid k}^{mp^r-1}\frac{1}{k^2}\binom{-mp^r-1}{k-1}^2 \equiv 2(1+2m+m\delta_{r,1})(1+mp\delta_{r,2})p^r\left(\frac{B_{2p-4}}{2p-4} - 2\frac{B_{p-3}}{p-3}\right)$$
$$\times\sum_{l=0}^{m-1}\binom{-m-1}{l}^2 \pmod{p^{r+2}}. \tag{2.32}$$

Proof. By (2.2), modulo p^{r+2},

$$\sum_{k=1,p\nmid k}^{mp^r-1}\frac{1}{k^2}\binom{-mp^r-1}{k-1}^2 \equiv \sum_{l=0}^{mp^{r-1}-1}\binom{-mp^{r-1}-1}{l}^2$$

$$\times \sum_{\lfloor \frac{k-1}{p} \rfloor = l, p\nmid k} \frac{1 + 2mp^r H'_{k-1} + m^2 p^{2r} \delta_{r,1} (2{H'_{k-1}}^2 - H'_{k-1,2})}{k^2}. \tag{2.33}$$

By (2.7) and (2.10), for any positive integer s and nonnegative integer l, we have

$$\sum_{\lfloor \frac{k}{p^s} \rfloor = l, p\nmid k} \frac{1}{k^2} = \sum_{k=1, p\nmid k}^{p^s l + p^s - 1} \frac{1}{k^2} - \sum_{k=1, p\nmid k}^{p^s l - 1} \frac{1}{k^2} \equiv H'_{p^s-1,2} \equiv p^{s-1} H_{p-1,2} \pmod{p^{s+2}}. \tag{2.34}$$

In light of Lemma 1 and (2.34), by induction, for any positive integer $s \le r-1$, we can conclude that

$$\begin{aligned}
&\sum_{l=0}^{mp^{r-1}-1} \binom{-mp^{r-1}-1}{l}^2 \Big(\sum_{\lfloor \frac{k}{p} \rfloor = l, p\nmid k} \frac{1}{k^2} - H_{p-1,2} \Big) \\
&\equiv \sum_{l=0}^{mp^{r-1}-1} \binom{-mp^{r-2}-1}{\lfloor \frac{l}{p} \rfloor}^2 \Big(\sum_{\lfloor \frac{k}{p} \rfloor = l, p\nmid k} \frac{1}{k^2} - H_{p-1,2} \Big) \\
&= \sum_{l=0}^{mp^{r-2}-1} \binom{-mp^{r-2}-1}{l}^2 \Big(\sum_{\lfloor \frac{k}{p^2} \rfloor = l, p\nmid k} \frac{1}{k^2} - pH_{p-1,2} \Big) \\
&\equiv \sum_{l=0}^{mp^{r-s-1}-1} \binom{-mp^{r-s-1}-1}{l}^2 \Big(\sum_{\lfloor \frac{k}{p^{s+1}} \rfloor = l, p\nmid k} \frac{1}{k^2} - p^s H_{p-1,2} \Big) \\
&\equiv \sum_{l=0}^{m-1} \binom{-m-1}{l}^2 \Big(\sum_{\lfloor \frac{k}{p^r} \rfloor = l, p\nmid k} \frac{1}{k^2} - p^{r-1} H_{p-1,2} \Big) \equiv 0 \pmod{p^{r+2}}.
\end{aligned} \tag{2.35}$$

Recall that Zhao [34, Theorems 1.7 with $s_1 = s_2 = m = n = 2$] proved that for any prime $p \ge 5$,

$$\sum_{k=1}^{p-1} \frac{H_{k-1,2}}{k^2} \equiv 0 \pmod{p}. \tag{2.36}$$

In 2013, Meštrović [17, Theorem 1 and Lemma 6] showed that for any prime $p \ge 7$,

$$\sum_{k=1}^{p-1} \frac{H_k}{k^2} \equiv -\frac{3}{p^2} H_{p-1} \equiv \frac{3}{2p} H_{p-1,2} \equiv 3\Big(\frac{B_{2p-4}}{2p-4} - 2\frac{B_{p-3}}{p-3} \Big) \pmod{p^2}, \tag{2.37}$$

$$\sum_{k=1}^{p-1} \frac{H_{k-1}}{k^3} \equiv 0 \pmod{p} \qquad \text{and} \qquad \sum_{k=1}^{p-1} \frac{{H_k}^2}{k^2} \equiv 0 \pmod{p}. \tag{2.38}$$

In light of (2.6), (2.8), (2.36)-(2.38), and Lemma 6, we obtain

$$\sum_{l=0}^{mp^{r-1}-1} \binom{-mp^{r-1}-1}{l}^2 \sum_{\lfloor \frac{k-1}{p} \rfloor = l, p\nmid k} \frac{H'_{k-1}}{k^2}$$

$$
\begin{aligned}
&= \sum_{l=0}^{mp^{r-1}-1} \binom{-mp^{r-1}-1}{l}^2 \sum_{k=1}^{p-1} \frac{H'_{pl+k-1}}{(pl+k)^2} \\
&\equiv \sum_{l=0}^{mp^{r-1}-1} \binom{-mp^{r-1}-1}{l}^2 \sum_{k=1}^{p-1} \left(\frac{1}{k^2} - \frac{2pl}{k^3}\right) \sum_{j=1}^{k-1} \frac{1}{pl+j} \\
&\equiv \sum_{l=0}^{mp^{r-1}-1} \binom{-mp^{r-1}-1}{l}^2 \sum_{k=1}^{p-1} \left(\frac{H_{k-1}}{k^2} - \frac{2plH_{k-1}}{k^3} - \frac{plH_{k-1,2}}{k^2}\right) \\
&\equiv 3(p(1+2m)\delta_{r,2} + \delta_{r,1}) \left(\frac{B_{2p-4}}{2p-4} - 2\frac{B_{p-3}}{p-3}\right) \sum_{l=0}^{m-1} \binom{-m-1}{l}^2 \pmod{p^2}. \qquad (2.39)
\end{aligned}
$$

By (2.5)–(2.6), (2.10), (2.36), and (2.38), we get

$$
\begin{aligned}
&\sum_{l=0}^{m-1} \binom{-m-1}{l}^2 \sum_{\lfloor \frac{k-1}{p} \rfloor = l, p \nmid k} \frac{2{H'_{k-1}}^2 - H'_{k-1,2}}{k^2} \\
&= \sum_{l=0}^{m-1} \binom{-m-1}{l}^2 \sum_{k=1}^{p-1} \frac{2{H'_{pl+k-1}}^2 - H'_{pl+k-1,2}}{(pl+k)^2} \\
&\equiv \sum_{l=0}^{m-1} \binom{-m-1}{l}^2 \sum_{k=1}^{p-1} \frac{2{H_{k-1}}^2 - H_{k-1,2}}{k^2} \equiv 0 \pmod{p}, \qquad (2.40)
\end{aligned}
$$

where the last congruence comes from

$$
\sum_{k=1}^{p-1} \frac{{H_{k-1}}^2}{k^2} = \sum_{k=1}^{p-1} \frac{(H_k - \frac{1}{k})^2}{k^2} = \sum_{k=1}^{p-1} \frac{{H_k}^2}{k^2} - 2\sum_{k=2}^{p-1} \frac{H_{k-1}}{k^3} - H_{p-1,4} \equiv 0 \pmod{p}.
$$

Finally, combining (2.33), (2.35), (2.39)–(2.40), and Lemma 6, we reach (2.32). □

At the end of proving Theorem 1, we need such a curious identity as follows:

Lemma 8. *For any positive integer m, we have*

$$
\begin{aligned}
2m(1+3m) \sum_{k=0}^{m-1} \binom{-m-1}{k}^2 - 2\sum_{k=1}^{m-1} \binom{-m}{k}^2 k(k+m) \\
-2m^2 \sum_{k=0}^{m-1} \binom{-m}{k}^2 = \frac{3m^2}{2} \binom{2m}{m}^2. \qquad (2.41)
\end{aligned}
$$

Proof. Since

$$
\binom{-m}{k} k = -m \binom{-m-1}{k-1} \quad \text{and} \quad \binom{-m}{k}(k+m) = m\binom{-m-1}{k},
$$

we obtain

$$
\sum_{k=1}^{m-1} \binom{-m}{k}^2 k(k+m) = -m^2 \sum_{k=1}^{m-1} \binom{-m-1}{k}\binom{-m-1}{k-1}
$$

$$= -m^2 \sum_{k=0}^{m-2} \binom{-m-1}{k+1} \binom{-m-1}{k}. \tag{2.42}$$

It is clear that

$$\begin{aligned}
&2\sum_{k=0}^{m-1} \binom{-m-1}{k}^2 - \binom{-m-1}{m-1}^2 \\
&= \sum_{k=0}^{m-2} \left(\binom{-m-1}{k}^2 + \binom{-m-1}{k+1}^2 \right) + 1 \\
&= \sum_{k=0}^{m-2} \left(\binom{-m-1}{k} + \binom{-m-1}{k+1} \right)^2 - 2\sum_{k=0}^{m-2} \binom{-m-1}{k}\binom{-m-1}{k+1} + 1 \\
&= \sum_{k=0}^{m-1} \binom{-m}{k}^2 - 2\sum_{k=0}^{m-2} \binom{-m-1}{k}\binom{-m-1}{k+1}.
\end{aligned} \tag{2.43}$$

By Zeilberger's algorithm (see, e.g., [19, pp. 101–119]), Andersen found the following identity:

$$\sum_{k=0}^{n-1} (21k+8)\binom{2k}{k}^3 = 4n\binom{2n}{n} \sum_{k=0}^{n-1} \binom{-n}{k}^2. \tag{2.44}$$

Let $S(n)$ denote $\frac{1}{\binom{2n}{n}} \sum_{k=0}^{n-1} (21k+8)\binom{2k}{k}^3$. Via Zeilberger's algorithm in Mathematica, we have the recurrence relation

$$-(n+1)S(n) + 2(1+2n)S(n+1) = 4(n+1)(21n+8)\binom{2n-1}{n-1}^2.$$

Let $F(n)$ denote $4n\sum_{k=0}^{n-1}\binom{-n}{k}^2$. Applying the Zeilberger algorithm, we get the same recurrence relation. By induction on n, we can get (2.44).

Taking $n = m, m+1$ in (2.44), we get

$$\begin{aligned}
&8(2m+1)\sum_{k=0}^{m-1} \binom{-m-1}{k}^2 - 4m\sum_{k=0}^{m-1}\binom{-m}{k}^2 \\
&= \frac{2(2m+1)}{(m+1)\binom{2(m+1)}{m+1}} \sum_{k=0}^{m} (21k+8)\binom{2k}{k}^3 - 8(2m+1)\binom{-m-1}{m}^2 \\
&\quad - \frac{1}{\binom{2m}{m}} \sum_{k=0}^{m-1} (21k+8)\binom{2k}{k}^3 = 5m\binom{2m}{m}^2.
\end{aligned} \tag{2.45}$$

Substituting (2.42) and (2.43) into the left-hand side of (2.41) gives

$$2m(1+3m)\sum_{k=0}^{m-1}\binom{-m-1}{k}^2 - 2m^2\sum_{k=0}^{m-1}\binom{-m}{k}^2$$

$$+ m^2\Big(\sum_{k=0}^{m-1}\binom{-m}{k}^2 - 2\sum_{k=0}^{m-1}\binom{-m-1}{k}^2 + \binom{-m-1}{m-1}^2\Big)$$
$$= 2m(1+2m)\sum_{k=0}^{m-1}\binom{-m-1}{k}^2 - m^2\sum_{k=0}^{m-1}\binom{-m}{k}^2 + \frac{m^2}{4}\binom{2m}{m}^2. \tag{2.46}$$

The congruence (2.41) then follows from (2.45) and (2.46). □

3. Proof of Theorem 1

Substituting $n = mp^{r-1+j}$ for $j \in \{0, 1\}$ and $r \geq 1$ in (2.44) yields

$$\frac{1}{m^4p^{4r}\binom{2mp^{r-1}}{mp^{r-1}}^3}\Big(\sum_{k=0}^{mp^r-1}(21k+8)\binom{2k}{k}^3 - p\sum_{k=0}^{mp^{r-1}-1}(21k+8)\binom{2k}{k}^3\Big)$$
$$=\frac{1}{m^3p^{3r}\binom{2mp^{r-1}}{mp^{r-1}}^3}\Big(4\binom{2mp^r}{mp^r}\sum_{k=0}^{mp^r-1}\binom{-mp^r}{k}^2 - 4\binom{2mp^{r-1}}{mp^{r-1}}\sum_{k=0}^{mp^{r-1}-1}\binom{-mp^{r-1}}{k}^2\Big). \tag{3.1}$$

For all nonnegative integers s, t with $t \leq s$ and primes $p \geq 5$, Helou and Terjanian [15] established the following supercongruence:

$$\binom{ps}{pt} \equiv \binom{s}{t}\Big(1 - st(s-t)\Big(\frac{p^3}{2}B_{p^3-p^2-2} - \frac{p^5}{6}B_{p-3}$$
$$+ \frac{s^2-st+t^2}{5}p^5B_{p-5}\Big)\Big) \pmod{p^{6+\nu_p(s-t)+\nu_p(\binom{s}{t})}}, \tag{3.2}$$

where $\nu_p(n)$ is the largest integer k such that $p^k \mid n$. Taking $s = 2mp^{r-1}$ and $t = mp^{r-1}$ into (3.2) gives

$$\binom{2mp^r}{mp^r} - \binom{2mp^{r-1}}{mp^{r-1}} \equiv -\binom{2mp^{r-1}}{mp^{r-1}}m^3p^{3r}B_{p^3-p^2-2} \pmod{p^{3r+2}}. \tag{3.3}$$

Here we will explain why a congruence modulo what might be p^{r+5} (that is (3.2)) can imply a congruence modulo p^{3r+2} (that is (3.3)). Note that

$$\binom{2mp^r}{mp^r}$$
$$= 2\prod_{j=1}^{mp^r-1}\frac{2mp^r-j}{j}$$
$$= (-1)^{mp^{r-1}(p-1)}\binom{2mp^{r-1}}{mp^{r-1}}\prod_{j=1,p\nmid j}^{mp^r-1}\Big(1-\frac{2mp^r}{j}\Big)$$
$$\equiv \binom{2mp^{r-1}}{mp^{r-1}}\Big(1 - 2mp^rH'_{mp^r-1} + 2m^2p^{2r}({H'_{mp^r-1}}^2 - H'_{mp^r-1,2})$$

$$- \sum_{1\le i<j<k\le mp^r-1, p\nmid ijk} \frac{8m^3p^{3r}}{ijk} + \sum_{1\le i<j<k<l\le mp^r-1, p\nmid ijkl} \frac{16m^4p^{4r}\delta_{r,1}}{ijkl}\Bigg) \pmod{p^{3r+2}}. \tag{3.4}$$

If two terms $\binom{2mp^{r-1}}{mp^{r-1}} - \binom{2mp^{r-1}}{mp^{r-1}} m^3 p^{3r} B_{p^3-p^2-2}$ exist in the congruence (3.2) modulo a low power p^{r+5}, they will also exist in the congruence (3.4) modulo a high power p^{3r+2}. So we just bring the special values $s = 2mp^{r-1}$ and $t = mp^{r-1}$ into (3.2) and get the congruence (3.3).

The congruence (3.3) can also be understood in another way. If $r = 1$, we can get (3.3) by taking $s = 2m$ and $t = m$ in (3.2) immediately. Now we suppose that $r \ge 2$. Letting $mp^r - a \to i$, $mp^r - b \to j$, and $mp^r - c \to k$ in the following summation, we see that

$$\begin{aligned}\sum_{1\le i<j<k\le mp^r-1, p\nmid ijk} \frac{1}{ijk} &= \sum_{1\le c<b<a\le mp^r-1, p\nmid cba} \frac{1}{(mp^r-a)(mp^r-b)(mp^r-c)}\\ &\equiv - \sum_{1\le c<b<a\le mp^r-1, p\nmid abc} \frac{1}{cba} \equiv 0 \pmod{p^r}.\end{aligned} \tag{3.5}$$

Recall that Sun [23, Remark 5.1] has obtained the supercongruence: for any prime $p \ge 7$,

$$H_{p-1} \equiv -\Big(\frac{B_{2p-4}}{2p-4} - 2\frac{B_{p-3}}{p-3}\Big)p^2 \pmod{p^4}. \tag{3.6}$$

By Kummer's congruence, we obtain

$$B_{\phi(p^5)-2} \equiv B_{\phi(p^4)-2} \equiv B_{\phi(p^3)-2} = B_{p^3-p^2-2} \pmod{p^2}, \tag{3.7}$$

where $\phi(n)$ denotes the Euler's totient function and $\phi(p^r) = p^r - p^{r-1}$ for any positive integer r. Note that

$$H_{p-1} \equiv -\frac{p^2}{2} B_{\phi(p^5)-2} \pmod{p^4}. \tag{3.8}$$

By (3.6) and (3.7)–(3.8) (also see [33, (3.10) and (3.13)]), we have

$$B_{p^3-p^2-2} \equiv 2\Big(\frac{B_{2p-4}}{2p-4} - 2\frac{B_{p-3}}{p-3}\Big) \pmod{p^2}. \tag{3.9}$$

Substituting (2.6)–(2.7), (2.10), and (3.5) into the rightside of (3.4) gives

$$\binom{2mp^r}{mp^r} \equiv \binom{2mp^{r-1}}{mp^{r-1}}\Big(1 - 2m^3p^{3r}\Big(\frac{B_{2p-4}}{2p-4} - 2\frac{B_{p-3}}{p-3}\Big)\Big) \pmod{p^{3r+2}}. \tag{3.10}$$

Combining (3.9) and (3.10), we deduce the congruence (3.3) in the case $r \ge 2$.

With the help of Lemma 2, by induction, we get

$$\sum_{k=0}^{mp^r-1} \binom{-mp^r}{k}^2 \equiv \sum_{k=0}^{mp^{r-1}-1} \binom{-mp^r}{pk}^2 \equiv \sum_{k=0}^{mp^{r-1}-1} \binom{-mp^{r-1}}{k}^2$$

$$\equiv \sum_{k=0}^{mp-1}\binom{-mp}{k}^2 \equiv \sum_{k=0}^{m-1}\binom{-m}{k}^2 \pmod{p^2}. \tag{3.11}$$

In view of (1.4), (2.3), (3.1), and (3.3)–(3.11), to prove the theorem, it suffices to show that

$$\begin{aligned}&\sum_{k=0}^{mp^r-1}\binom{-mp^r}{k}^2 - \sum_{k=0}^{mp^{r-1}-1}\binom{-mp^{r-1}}{k}^2\\ &\equiv m^3p^{3r}\Big(\frac{B_{2p-4}}{2p-4}-2\frac{B_{p-3}}{p-3}\Big)\Big(\frac{3}{2}\binom{2m}{m}^2+2\sum_{k=0}^{m-1}\binom{-m}{k}^2\Big) \pmod{p^{3r+2}}.\end{aligned} \tag{3.12}$$

Note that

$$\sum_{k=0}^{mp^r-1}\binom{-mp^r}{k}^2 = \sum_{k=1,p\nmid k}^{mp^r-1}\binom{-mp^r}{k}^2 + \sum_{k=0}^{mp^{r-1}-1}\binom{-mp^r}{pk}^2.$$

Now we will divide the sum into two parts: the sum divisible by p and not divisible by p. Since $\binom{-x}{k}(-1)^k = \binom{x+k-1}{k}$ for any nonnegative integer k,we have

$$\binom{-mp}{pk}^2 = \binom{p(m+k)-1}{pk}^2 = \binom{p(m+k)}{pm}^2\frac{m^2}{(m+k)^2}.$$

Moreover, taking $s = m + k$ and $t = m$ in (3.2) gives

$$\binom{p(m+k)}{pm} \equiv \binom{m+k}{m}\Big(1-mk(m+k)p^3\Big(\frac{B_{2p-4}}{2p-4}-2\frac{B_{p-3}}{p-3}\Big)\Big) \pmod{p^5},$$

and so

$$\binom{-mp}{pk}^2 = \binom{-m}{k}^2\Big(1-2mk(m+k)p^3\Big(\frac{B_{2p-4}}{2p-4}-2\frac{B_{p-3}}{p-3}\Big)\Big) \pmod{p^5}. \tag{3.13}$$

Thus, in order to prove (3.12) for $r = 1$, it suffices to prove that

$$\begin{aligned}&-2p\Big(\frac{B_{2p-4}}{2p-4}-2\frac{B_{p-3}}{p-3}\Big)\sum_{k=1}^{m-1}\binom{-m}{k}^2k(k+m)+\sum_{k=1,p\nmid k}^{mp-1}\frac{m}{k^2}\binom{-mp-1}{k-1}^2\\ &\equiv m^2p\Big(\frac{B_{2p-4}}{2p-4}-2\frac{B_{p-3}}{p-3}\Big)\Big(\frac{3}{2}\binom{2m}{m}^2+2\sum_{k=0}^{m-1}\binom{-m}{k}^2\Big) \pmod{p^3},\end{aligned} \tag{3.14}$$

which follows from (2.32) and (2.41). This proves the $r = 1$ case of the theorem. For the sake of convenience, we use the notation $H'(r,s,t;n)$ to denote the number $\sum_{1\le i<j<l\le n,p\nmid ijl}\frac{1}{i^rj^sl^t}$. Similarly to the proof of [34, (3.33)]: using substitution of indices $l\to pk-l$ and $\frac{1}{pk-i}\equiv -(\frac{1}{i}+\frac{pk}{i^2}) \pmod{p^2}$, we have

$$H'(1,1,1;pk-1)$$

$$
\begin{aligned}
&= \sum_{l=1,p\nmid l}^{pk-1} \frac{1}{l} \sum_{j=1,p\nmid j}^{l-1} \frac{1}{j} \sum_{i=1,p\nmid i}^{j-1} \frac{1}{i} \\
&= \sum_{l=1,p\nmid l}^{pk-1} \frac{1}{pk-l} \sum_{j=l+1,p\nmid j}^{pk-1} \frac{1}{pk-j} \sum_{i=j+1,p\nmid i}^{pk-1} \frac{1}{pk-i} \\
&\equiv -H'(1,1,1;pk-1) - pk(2H'(2,1,1;pk-1) + H'(1,2,1;pk-1)) \pmod{p^2}.
\end{aligned}
$$

By Lemma 4, we can prove that

$$
\begin{aligned}
H'(2,1,1;pk-1) &= \sum_{l=1,p\nmid l}^{pk-1} \frac{1}{l} \sum_{j=1,p\nmid j}^{l-1} \frac{1}{j} \sum_{i=1,p\nmid i}^{j-1} \frac{1}{i^2} = \sum_{a=0}^{k-1} \sum_{b=1}^{p-1} \frac{1}{pa+b} \sum_{j=1,p\nmid j}^{pa+b-1} \frac{1}{j} \sum_{i=1,p\nmid i}^{j-1} \frac{1}{i^2} \\
&\equiv kH'(2,1,1;p-1) \pmod{p}
\end{aligned}
$$

and

$$
H'(1,2,1;pk-1) \equiv kH'(1,2,1;p-1) \pmod{p}.
$$

Recall that Zhao [34, (3.20)] has proved the following congruences:

$$
H'(1,2,1;p-1) \equiv H'(2,1,1;p-1) \equiv 0 \pmod{p}.
$$

It follows that $H'(1,1,1;pk-1) \equiv 0 \pmod{p^2}$. For $r \geq 2$, noting that

$$
\begin{aligned}
\frac{\binom{-mp^r}{pk}^2}{\binom{-mp^{r-1}}{k}^2} &= \prod_{j=1,p\nmid j}^{pk-1} \frac{(mp^r+j)^2}{j^2} \\
&\equiv \left(1 + mp^r H'_{pk-1} + \frac{m^2p^{2r}({H'_{pk-1}}^2 - H'_{pk-1,2})}{2} + m^3p^{3r}H'(1,1,1;pk-1)\right)^2 \\
&\equiv 1 + 2mp^rH'_{pk-1} + 2m^2p^{2r}{H'_{pk-1}}^2 - m^2p^{2r}H'_{pk-1,2} \pmod{p^{3r+2}},
\end{aligned}
$$

and

$$
p^{2r}\binom{-mp^{r-1}}{k}^2 {H'_{pk-1}}^2 \equiv 0 \pmod{p^{4r+2+2\nu_p(k)}},
$$

since $\binom{-mp^{r-1}}{k}^2 \equiv 0 \pmod{p^{2(r-1-\nu_p(k))}}$ and ${H'_{pk-1}}^2 \equiv 0 \pmod{p^{4(1+\nu_p(k))}}$ by (2.6), we obtain

$$
\binom{-mp^r}{pk}^2 \equiv \binom{-mp^{r-1}}{k}^2 \left(1 + 2mp^rH'_{pk-1} - m^2p^{2r}H'_{pk-1,2}\right) \pmod{p^{3r+2}}. \tag{3.15}
$$

Thus, to prove (3.12), it suffices to prove that

$$
\begin{aligned}
&\sum_{k=1}^{mp^{r-1}-1} \binom{-mp^{r-1}}{k}^2 \left(2H'_{pk-1} - mp^rH'_{pk-1,2}\right) + \sum_{k=1,p\nmid k}^{mp^r-1} \frac{mp^r}{k^2}\binom{-mp^r-1}{k-1}^2 \\
&\equiv m^2p^{2r}\left(\frac{B_{2p-4}}{2p-4} - 2\frac{B_{p-3}}{p-3}\right)\left(\frac{3}{2}\binom{2m}{m}^2 + 2\sum_{k=0}^{m-1}\binom{-m}{k}^2\right) \pmod{p^{2r+2}}.
\end{aligned}
$$

But the above supercongruence follows from Lemmas 5, 7, and 8. This proves the $r \geq 2$ case of the theorem.

4. Conclusions

In this paper, we make use of some unknown congruences involving the generalized harmonic numbers and Bernoulli numbers and an identity involving sums of binomial coefficients' squares by induction and Zeilberger's algorithm, and partially prove a congruence modulo high powers related to $\sum(21k+8)\binom{2k}{k}^3$. Conjecture 1 in the case $p \mid \binom{2mp^{r-1}}{mp^{r-1}}$ may be solved by finding a suitable identity or seeking a q-analogue of the identity via Mathematica or Maple (As shown in Table 1).

Table 1. A summary table lists all congruences used in this paper and their sources.

All congruences are used	Sources
$H_{p-1} \equiv -\frac{1}{3}p^2 B_{p-3} \pmod{p^3}$	J. W. L. Glaisher [4,5]
$\binom{p^r n-1}{k} = \binom{p^{r-1}n-1}{\lfloor \frac{k}{p} \rfloor} \prod_{j=1,p\nmid j}^{k} \frac{p^r n-j}{j}$	F. Beukers [2]
$\binom{p^r a}{p^s b} \equiv \binom{p^{r-1}a}{p^{s-1}b}(-1)^{p^s b-p^{s-1}b}$ $\pmod{p^{2r+\min\{r,s\}-\delta_{p,3}-2\delta_{p,2}}}$	Gessel [3], Granville [6] and Straub [22]
$\sum_{k=1,p\nmid k}^{\frac{p^r-1}{2}} \frac{1}{k^n} \equiv 0 \pmod{p^r}$ (n is even)	Osburn, Sahu, and Straub [18]
$H_{p-1,3} \equiv -\frac{6p^2 B_{p-5}}{5} \pmod{p^3}$	Sun [23]
$H'_{p^s-1,2} \equiv 2p^s\left(\frac{B_{2p-4}}{2p-4} - 2\frac{B_{p-3}}{p-3}\right)$	Zhang [33]
$\sum_{k=1}^{p-1} \frac{H_k}{k^2} \equiv -\frac{3}{p^2}H_{p-1} \equiv \frac{3}{2p}H_{p-1,2}$ $\equiv 3\left(\frac{B_{2p-4}}{2p-4} - 2\frac{B_{p-3}}{p-3}\right) \pmod{p^2}$	Meštrović [17]
$\sum_{k=1}^{p-1} \frac{H_{k-1}}{k^3} \equiv 0 \pmod{p}$	Meštrović [17]
$\sum_{k=1}^{p-1} \frac{H_k{}^2}{k^2} \equiv 0 \pmod{p}$	Meštrović [17]
$\binom{ps}{pt} \equiv \binom{s}{t}\left(1 - st(s-t)\left(\frac{p^3}{2}B_{p^3-p^2-2} - \frac{p^5}{6}B_{p-3}\right.\right.$ $\left.\left.+\frac{s^2-st+t^2}{5}p^5 B_{p-5}\right)\right) \pmod{p^{6+v_p(s-t)+v_p(\binom{s}{t})}}$	Helou and Terjanian [15]
$H_{p-1} \equiv -\left(\frac{B_{2p-4}}{2p-4} - 2\frac{B_{p-3}}{p-3}\right)p^2 \pmod{p^4}$	Sun [23]
$B_{p^3-p^2-2} \equiv 2\left(\frac{B_{2p-4}}{2p-4} - 2\frac{B_{p-3}}{p-3}\right) \pmod{p^2}$	Zhang [33]
$H'(1,2,1;p-1) \equiv H'(2,1,1;p-1) \equiv 0 \pmod{p}$.	Zhao [34]

Author contributions

Wenbin Zhang: Methodology, writing—review and editing; Jiachen Wu: Investigation, writing—original draft; Yong Zhang: Funding acquisition, supervision, writing—review and editing. All authors have read and agreed to the published version of the manuscript.

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

No potential conflict of interest was reported by the authors.

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