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A NEW SERIES FOR π^3 AND RELATED CONGRUENCES

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Abstract. Let $H_n^{(2)}$ denote the second-order harmonic number $\sum_{0<k\leqslant n} 1/k^2$ for $n=0,1,2,\ldots$. In this paper we obtain the following identity:

$$\sum_{k=1}^{\infty}\frac{2^k H_{k-1}^{(2)}}{k\binom{2k}{k}}=\frac{\pi^3}{48}.$$

We explain how we found the series and develop related congruences involving Bernoulli or Euler numbers; for example, it is shown that

$$\sum_{k=1}^{p-1}\frac{\binom{2k}{k}}{2^k}H_k^{(2)}\equiv -E_{p-3} \pmod p$$

for any prime $p>3$, where $E_0,E_1,E_2,\ldots$ are Euler numbers. Motivated by the Amdeberhan-Zeilberger identity $\sum_{k=1}^{\infty}(21k-8)/(k^3\binom{2k}{k}^3)=\pi^2/6$, we also establish the congruence

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

for each prime $p>3$.

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1. Introduction

Series with summations related to π have a long history. Leibniz and Euler got the famous identities

$$\sum_{k=0}^{\infty}\frac{(-1)^k}{2k+1}=\frac{\pi}{4}\quad\text{and}\quad\sum_{k=1}^{\infty}\frac{1}{k^2}=\frac{\pi^2}{6}$$

respectively. Though there exist many series for π and π^2 (see, e.g., [Ma]), there are very few interesting series for π^3. The most well-known series for π^3 is the following one:

$$\sum_{k=0}^{\infty}\frac{(-1)^k}{(2k+1)^3}=\frac{\pi^3}{32}. \tag{1.1}$$

In 1985 Zucker [Z, (2.23)] showed that

$$\sum_{k=0}^{\infty}\frac{\binom{2k}{k}}{(2k+1)^3 16^k}=\frac{7\pi^3}{216}. \tag{1.2}$$

Recall that harmonic numbers are those rational numbers

$$H_n:=\sum_{0<k\leqslant n}\frac{1}{k}\qquad(n=0,1,2,\ldots),$$

and *harmonic numbers of the second order* are defined by

$$H_n^{(2)}:=\sum_{0<k\leqslant n}\frac{1}{k^2}\qquad(n=0,1,2,\ldots).$$

Now we give our first result which appears to be new and curious.

Theorem 1.1. *We have the following identity:*

$$\sum_{k=1}^{\infty}\frac{2^k H_{k-1}^{(2)}}{k\binom{2k}{k}}=\frac{\pi^3}{48}. \tag{1.3}$$

Remark 1.1. The author noted that `Mathematica 7` could not evaluate the series in (1.3).

By Stirling's formula

$$n!\sim\sqrt{2\pi n}\left(\frac{n}{e}\right)^n\quad(n\to+\infty)$$

and thus

$$\binom{2k}{k} \sim \frac{4^k}{\sqrt{k\pi}} \quad (k \to +\infty).$$

Note also that $H_n^{(2)} \to \zeta(2) = \pi^2/6$ as $n \to +\infty$. Therefore

$$\frac{2^k H_{k-1}^{(2)}}{k\binom{2k}{k}} \sim \frac{\zeta(2)\sqrt{\pi}}{2^k\sqrt{k}} \qquad (k \to +\infty).$$

So the series in (1.3) converges much faster than the series in (1.1) (but slower than the series in (1.2)). Using `Mathematica 7` we found that for $n \geqslant 500$ we have

$$\left|\frac{s_n}{\pi^3/48} - 1\right| < \frac{1}{10^{150}}$$

where $s_n := \sum_{k=1}^n 2^k H_{k-1}^{(2)}/(k\binom{2k}{k})$.

The reader may wonder how the author discovered (1.3) which gives a series for π^3 of a new type. Now we present some explanations.

Let p be an odd prime. In [Su3] and [Su4] the author proved the congruences

$$\sum_{k=0}^{p-1} \frac{\binom{2k}{k}}{2^k} \equiv (-1)^{(p-1)/2} - p^2 E_{p-3} \pmod{p^3} \tag{1.4}$$

and

$$\sum_{k=0}^{p-1} \binom{p-1}{k} \frac{\binom{2k}{k}}{(-2)^k} \equiv (-1)^{(p-1)/2} 2^{p-1} \pmod{p^3} \tag{1.5}$$

respectively, where $E_0, E_1, E_2, \ldots$ are Euler numbers given by $E_0 = 1$ and the recursion

$$\sum_{\substack{k=0\\2\mid k}}^{n} \binom{n}{k} E_{n-k} = 0 \qquad (n = 1, 2, 3, \ldots).$$

For $k = 0, \ldots, p-1$, clearly we have

$$\begin{aligned}\binom{p-1}{k}(-1)^k &= \prod_{0<j\leqslant k}\left(1 - \frac{p}{j}\right)\\ &\equiv 1 - pH_k + \frac{p^2}{2}\sum_{0<i<j\leqslant k}\frac{2}{ij} = 1 - pH_k + \frac{p^2}{2}(H_k^2 - H_k^{(2)}) \pmod{p^3}.\end{aligned}$$

So, in view of (1.4) and (1.5), it is natural to investigate

$$\sum_{k=0}^{p-1} \frac{\binom{2k}{k}}{2^k} H_k^{(2)} \bmod p, \quad \sum_{k=0}^{p-1} \frac{\binom{2k}{k}}{2^k} H_k^2 \bmod p, \quad \sum_{k=0}^{p-1} \frac{\binom{2k}{k}}{2^k} H_k \bmod p^2.$$

This led the author to obtain the following result.

Theorem 1.2. *Let $p>3$ be a prime. Then*
$$\sum_{k=0}^{p-1}\frac{\binom{2k}{k}}{2^k}H_k^{(2)}\equiv -E_{p-3}\pmod{p}. \tag{1.6}$$

Remark 1.2. Let p be an odd prime. We are also able to show that
$$\sum_{k=0}^{p-1}\frac{\binom{2k}{k}}{2^k}H_k^2\equiv\left(\frac{-1}{p}\right)\frac{q_p(2)^2}{2}-\frac{E_{p-3}}{2}\pmod{p}, \tag{1.7}$$
$$\sum_{k=0}^{p-1}\frac{\binom{2k}{k}}{2^k}H_k\equiv\left(\frac{-1}{p}\right)\frac{H_{(p-1)/2}}{2}-pE_{p-3}\pmod{p^2}, \tag{1.8}$$
where $(\frac{\cdot}{p})$ denotes the Legendre symbol, and $q_p(2)$ stands for the Fermat quotient $(2^{p-1}-1)/p$. Recall that in 1938 Lehmer [L] proved the congruence
$$H_{(p-1)/2}\equiv -2q_p(2)+p\,q_p(2)^2\pmod{p^2}. \tag{1.9}$$

In view of certain correspondence between series for the zeta function or powers of π and congruences involving Bernoulli or Euler numbers revealed in the authors' papers [Su2] and [Su3], the congruence (1.6) suggests that we should consider the series $\sum_{k=0}^{\infty}\binom{2k}{k}H_k^{(2)}/2^k$. Since this series diverges, we should seek for certain transformation. Let p be an odd prime. By [Su2, Lemma 2.1] and [T],
$$\frac{1}{p}\binom{2(p-k)}{p-k}\equiv-\frac{2}{k\binom{2k}{k}}\pmod{p}\quad\text{for } k=1,\ldots,\frac{p-1}{2}.$$
Thus, if $p>3$ then
$$\begin{aligned}\sum_{k=0}^{p-1}\frac{\binom{2k}{k}}{2^k}H_k^{(2)}&\equiv\sum_{k=1}^{(p-1)/2}\frac{k\binom{2k}{k}}{k2^k}H_k^{(2)}\equiv\sum_{k=1}^{(p-1)/2}\left(\frac{H_k^{(2)}}{k2^k}\cdot\frac{-2p}{\binom{2(p-k)}{p-k}}\right)\\&\equiv\sum_{p/2<k<p}\left(\frac{H_{p-k}^{(2)}}{(p-k)2^{p-k}}\cdot\frac{-2p}{\binom{2k}{k}}\right)\\&\equiv-p\sum_{p/2<k<p}\frac{2^kH_{k-1}^{(2)}}{k\binom{2k}{k}}\equiv-p\sum_{k=1}^{p-1}\frac{2^kH_{k-1}^{(2)}}{k\binom{2k}{k}}\pmod{p}\end{aligned}$$
since $2^p\equiv 2\pmod{p}$ and
$$-H_{p-k}^{(2)}\equiv H_{p-1}^{(2)}-H_{p-k}^{(2)}\equiv H_{k-1}^{(2)}\pmod{p}.$$

Therefore the congruence in (1.6) is equivalent to

$$p\sum_{k=1}^{p-1}\frac{2^kH_{k-1}^{(2)}}{k\binom{2k}{k}}\equiv E_{p-3}\ (\mathrm{mod}\ p). \tag{1.6$'$}$$

Motivated by (1.6′) the author found (1.3).

Now we state our third theorem which is close to Theorem 1.2.

Theorem 1.3. *Let p be an odd prime. If $p>3$, then*

$$\sum_{k=1}^{p-1}\frac{\binom{2k}{k}}{4^k}H_k\equiv 2-2p+4p^2q_p(2)\ (\mathrm{mod}\ p^3). \tag{1.10}$$

We also have

$$\sum_{k=0}^{(p-1)/2}\frac{\binom{2k}{k}}{4^k}H_k^{(2)}\equiv -4q_p(2)\ (\mathrm{mod}\ p) \tag{1.11}$$

and

$$\sum_{k=1}^{(p-1)/2}\frac{\binom{2k}{k}}{k4^k}H_k^{(2)}\equiv \frac{B_{p-3}}{2}\ (\mathrm{mod}\ p), \tag{1.12}$$

where $B_0, B_1, B_2, \ldots$ are Bernoulli numbers.

In 1997 T. Amdeberhan and D. Zeilberger [AZ] obtained that

$$\sum_{k=1}^{\infty}\frac{21k-8}{k^3\binom{2k}{k}^3}=\zeta(2)=\frac{\pi^2}{6}.$$

We are able to establish the following result related to the Amdeberhan-Zeilberger series.

Theorem 1.4. *Let $p>3$ be a prime. Then*

$$\sum_{k=0}^{(p-1)/2}(21k+8)\binom{2k}{k}^3\equiv 8p+(-1)^{(p-1)/2}32p^3E_{p-3}\ (\mathrm{mod}\ p^4) \tag{1.13}$$

and hence

$$\sum_{k=1}^{(p-1)/2}\frac{21k-8}{k^3\binom{2k}{k}^3}\equiv(-1)^{(p+1)/2}4E_{p-3}\quad(\mathrm{mod}\ p). \tag{1.14}$$

Remark 1.3. In [Su3] the author showed that

$$\sum_{k=0}^{p-1}(21k+8)\binom{2k}{k}^3\equiv 8p+16p^4B_{p-3}\ (\mathrm{mod}\ p^5) \tag{1.15}$$

for any odd prime p. However, (1.13) is much more sophisticated than this congruence involving B_{p-3}.

The next section is devoted to the proof of Theorem 1.1. We are going to show Theorems 1.2–1.3 and Theorem 1.4 in Sections 3 and 4 respectively. Section 5 contains some conjectures of the author for further research.

2. Proof of Theorem 1.1

Set

$$S := \sum_{k=1}^{\infty} \frac{2^k H_{k-1}^{(2)}}{k\binom{2k}{k}}.$$

Then

$$S = \sum_{k=0}^{\infty} \frac{2^{k+1} H_k^{(2)}}{(k+1)\binom{2k+2}{k+1}} = \sum_{k=0}^{\infty} \frac{2^k H_k^{(2)}}{(k+1)\binom{2k+1}{k}} = \sum_{k=0}^{\infty} \frac{2^k H_k^{(2)} \Gamma(k+1)^2}{\Gamma(2k+2)}.$$

Recall the well-known fact that

$$B(a,b) := \int_0^1 x^{a-1}(1-x)^{b-1}dx = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)} \quad \text{for any } a,b>0.$$

So we have

$$\begin{aligned} S =& \sum_{k=0}^{\infty} 2^k H_k^{(2)} \int_0^1 x^k(1-x)^k dx = \sum_{k=0}^{\infty} \frac{H_k^{(2)}}{2^k} \int_0^1 (1-(2x-1)^2)^k dx \\ =& \sum_{k=0}^{\infty} \frac{H_k^{(2)}}{2^{k+1}} \int_{-1}^1 (1-t^2)^k dt = \sum_{k=1}^{\infty} \frac{H_k^{(2)}}{2^k} \int_0^1 (1-t^2)^k dt. \end{aligned}$$

Observe that if $0 \leqslant t \leqslant 1$ then

$$\begin{aligned} \sum_{k=1}^{\infty} H_k^{(2)} \left(\frac{1-t^2}{2}\right)^k =& \sum_{k=1}^{\infty}\sum_{j=1}^{k} \frac{1}{j^2} \left(\frac{1-t^2}{2}\right)^k = \sum_{j=1}^{\infty} \frac{1}{j^2} \sum_{k=j}^{\infty} \left(\frac{1-t^2}{2}\right)^k \\ =& \sum_{j=1}^{\infty} \frac{1}{j^2} \left(\frac{1-t^2}{2}\right)^j \frac{1}{1-(1-t^2)/2} \\ =& \frac{2}{1+t^2} \mathrm{Li}_2\left(\frac{1-t^2}{2}\right), \end{aligned}$$

where the dilogarithm $\mathrm{Li}_2(x)$ is given by

$$\mathrm{Li}_2(x) := \sum_{n=1}^{\infty} \frac{x^n}{n^2} \qquad (|x|<1).$$

Therefore

$$\frac{S}{2} = \int_0^1 \frac{1}{1+t^2} \mathrm{Li}_2\left(\frac{1-t^2}{2}\right) dt = \int_0^1 \mathrm{Li}_2\left(\frac{1-t^2}{2}\right) (\arctan t)' dt.$$

Note that

$$\mathrm{Li}_2'(x) = \sum_{n=1}^{\infty} \frac{x^{n-1}}{n} = -\frac{\log(1-x)}{x}$$

and hence

$$\frac{d}{dt}\mathrm{Li}_2\left(\frac{1-t^2}{2}\right) = -\frac{\log(1-(1-t^2)/2)}{(1-t^2)/2} \times (-t) = \frac{2t}{1-t^2}\log\frac{1+t^2}{2}.$$

Thus, using integration by parts we obtain

$$\begin{aligned}\frac{S}{2} =& \mathrm{Li}_2\left(\frac{1-t^2}{2}\right)\arctan t\,\Big|_{t=0}^{1} - \int_0^1 (\arctan t)\frac{2t}{1-t^2}\log\frac{1+t^2}{2}dt\\ =& \int_0^1 (\arctan t)\left(\frac{1}{1+t} - \frac{1}{1-t}\right)\log\frac{1+t^2}{2}dt\\ =& \int_0^1 \frac{\arctan t}{1+t}\log\frac{1+t^2}{2}dt - \int_0^{-1}\frac{\arctan t}{1+t}\log\frac{1+t^2}{2}dt\\ =& \int_{-1}^1 \frac{\arctan t}{1+t}\log\frac{1+t^2}{2}dt.\end{aligned}$$

Finally, inputting the Mathematica command

```
Integrate[ArcTan[t]Log[(1+t^2)/2]/(1+t),{t,-1,1}]
```

we then obtain from `Mathematica 7` that

$$\int_{-1}^1 \frac{\arctan t}{1+t}\log\frac{1+t^2}{2}dt = \frac{\pi^3}{96}.$$

Thus $S = \pi^3/48$ as desired. We are done.

3. Proofs of Theorems 1.2 and 1.3

We first state some basic facts which will be used very often. For any prime $p > 3$ we have

$$\sum_{k=1}^{(p-1)/2} \frac{1}{k^2} \equiv \frac{1}{2}\sum_{k=1}^{p-1}\frac{1}{k^2} \equiv 0 \pmod p$$

since $\sum_{j=1}^{p-1}(2j)^{-2} \equiv \sum_{k=1}^{p-1} k^{-2} \pmod p$. If p is an odd prime, then

$$\binom{(p-1)/2}{k} \equiv \binom{-1/2}{k} = \frac{\binom{2k}{k}}{(-4)^k} \pmod p \quad \text{for all } k = 0, \ldots, p-1. \tag{3.1}$$

For any $n = 0, 1, 2, \ldots$ we have the identity

$$\sum_{k=0}^{n} (-1)^k \binom{x}{k} = (-1)^n \binom{x-1}{n} \tag{3.2}$$

which can be found in [G, (1.5)].

Lemma 3.1. *For any positive integer n, we have the identities*

$$\sum_{k=1}^{n}\binom{n}{k}\frac{(-1)^{k-1}}{k}=H_n \tag{3.3}$$

and

$$\sum_{k=1}^{n}\binom{n}{k}\frac{(-1)^{k-1}}{k}H_k=H_n^{(2)}. \tag{3.4}$$

Proof. (3.3) and (3.4) follow from [G, (1.45)] and an identity of V. Hernández [He] respectively. Below we give a simple proof of (3.4). In view of the binomial inversion formula (cf. (5.48) of [GKP, pp. 192-193]), (3.4) holds for all $n=1,2,3,\ldots$ if and only if for any positive integer n we have

$$\sum_{k=1}^{n}\binom{n}{k}(-1)^k H_k^{(2)}=-\frac{H_n}{n}. \tag{3.4$'$}$$

In fact, in view of (3.2) and (3.3), we get

$$\begin{aligned}\sum_{k=1}^{n}\binom{n}{k}(-1)^k\sum_{j=1}^{k}\frac{1}{j^2}=&\sum_{j=1}^{n}\frac{1}{j^2}\left(\sum_{k=0}^{n}\binom{n}{k}(-1)^k-\sum_{k=0}^{j-1}\binom{n}{k}(-1)^k\right)\\ =&\sum_{j=1}^{n}\frac{(-1)^j}{j^2}\binom{n-1}{j-1}=\frac{1}{n}\sum_{j=1}^{n}\frac{(-1)^j}{j}\binom{n}{j}=-\frac{H_n}{n}\end{aligned}$$

and hence (3.4$'$) holds. □

Lemma 3.2. *Let $p=2n+1$ be an odd prime and let m be an integer with $m\not\equiv 0,4 \pmod p$. Then*

$$\sum_{k=1}^{n}\frac{\binom{2k}{k}}{m^k}H_k^{(2)}\equiv-\left(\frac{m(m-4)}{p}\right)\sum_{k=1}^{n}\frac{\binom{2k}{k}H_k}{k(4-m)^k} \pmod p. \tag{3.5}$$

In particular,

$$\sum_{k=1}^{(p-1)/2}\frac{\binom{2k}{k}}{2^k}H_k^{(2)}\equiv-\left(\frac{-1}{p}\right)\sum_{k=1}^{(p-1)/2}\frac{\binom{2k}{k}H_k}{k2^k} \pmod p. \tag{3.6}$$

Proof. Clearly it suffices to prove (3.5).

In view of (3.4), we have

$$\begin{aligned}\sum_{k=1}^{n}\binom{n}{k}\left(-\frac{4}{m}\right)^{k}H_k^{(2)}=&\sum_{k=1}^{n}\frac{\binom{n}{k}(-4)^k}{m^k}\sum_{j=1}^{k}\binom{k}{j}\frac{(-1)^{j-1}}{j}H_j\\ =&\sum_{j=1}^{n}\frac{(-1)^{j-1}}{j}H_j\sum_{k=j}^{n}\binom{n}{k}\binom{k}{j}\left(-\frac{4}{m}\right)^{k}\\ =&\sum_{j=1}^{n}\frac{(-1)^{j-1}}{j}H_j\binom{n}{j}\sum_{k=j}^{n}\binom{n-j}{k-j}\left(-\frac{4}{m}\right)^{k}\\ =&\sum_{j=1}^{n}\binom{n}{j}\frac{(-1)^{j-1}}{j}H_j\left(-\frac{4}{m}\right)^{j}\left(1-\frac{4}{m}\right)^{n-j}\\ =&-\frac{1}{m^n}\sum_{j=1}^{n}\binom{n}{j}\frac{4^jH_j}{j}(m-4)^{n-j}.\end{aligned}$$

So, with the help of (3.1), we obtain

$$\sum_{k=1}^{n}\frac{\binom{2k}{k}}{m^k}H_k^{(2)}\equiv-\left(\frac{m(m-4)}{p}\right)\sum_{j=1}^{n}\frac{\binom{2j}{j}(-1)^jH_j}{j(m-4)^j}\pmod{p}.$$

This proves (3.5). We are done. $\square$

Lemma 3.3. *Let n be any positive integer. Then*

$$\sum_{k=1}^{n}\binom{n}{k}\frac{(-2)^k}{k}H_k=-2\sum_{\substack{k=1\\ 2\nmid k}}^{n}\frac{H_n-H_{n-k}}{k}. \tag{3.7}$$

Proof. Let S_n denote the left-hand side of (3.7). Observe that

$$\begin{aligned}S_n=&\sum_{k=1}^{n}\binom{n}{k}\frac{(-2)^k}{k}\sum_{j=1}^{k}\int_0^1x^{j-1}dx=\int_0^1\sum_{k=1}^{n}\binom{n}{k}\frac{(-2)^k}{k}\cdot\frac{x^k-1}{x-1}dx\\ =&\int_0^1\int_0^1\sum_{k=0}^{n}\binom{n}{k}\frac{(-2x)^k-(-2)^k}{x-1}y^{k-1}dydx\\ =&\int_0^1\int_0^1\frac{(1-2xy)^n-(1-2y)^n}{(x-1)y}dydx\\ =&-2\int_0^1\int_0^1\sum_{k=1}^{n}(1-2xy)^{k-1}(1-2y)^{n-k}dxdy.\end{aligned}$$

Clearly,

$$\int_0^1 (1-2xy)^{k-1}dx = \frac{(1-2xy)^k}{-2ky}\bigg|_{x=0}^1 = \frac{(1-2y)^k-1}{k(1-2y-1)} = \frac{1}{k}\sum_{j=1}^k (1-2y)^{j-1}.$$

Therefore

$$\begin{aligned} S_n =& -2\int_0^1 \sum_{k=1}^n \frac{1}{k}\sum_{j=1}^k (1-2y)^{n-k+j-1}dy = \sum_{1\leqslant j\leqslant k\leqslant n} \frac{(1-2y)^{n-k+j}}{k(n-k+j)}\bigg|_{y=0}^1 \\ =& \sum_{1\leqslant j\leqslant k\leqslant n} \frac{(-1)^{n-k+j}-1}{k(n-k+j)} = \sum_{i=1}^n \frac{(-1)^i-1}{i}\sum_{j=1}^i \frac{1}{n+j-i} \\ =& -2\sum_{\substack{i=1\\ 2\nmid i}}^n \frac{1}{i}(H_n - H_{n-i}). \end{aligned}$$

This completes the proof of (3.7). $\square$

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

$$\binom{p-1}{(p-1)/2} \equiv (-1)^{(p-1)/2}4^{p-1} \pmod{p^3}. \tag{3.8}$$

Remark 3.1. (3.8) is a famous congruence of Morley [Mo].

Lemma 3.5. *Let $p>3$ be a prime. Then*

$$\sum_{\substack{k=1\\ 2\nmid k}}^{(p-1)/2} \frac{H_k}{k} \equiv \frac{3}{4}q_p(2)^2 - \left(\frac{-1}{p}\right)\frac{E_{p-3}}{2} \pmod{p} \tag{3.9}$$

and

$$\sum_{\substack{k=1\\ 2\mid k}}^{(p-1)/2} \frac{H_k}{k} \equiv \frac{5}{4}q_p(2)^2 + \left(\frac{-1}{p}\right)\frac{E_{p-3}}{2} \pmod{p}. \tag{3.10}$$

Proof. Set $n=(p-1)/2$. Clearly it suffices to show that

$$\sum_{k=1}^n \frac{H_k}{k} \equiv 2q_p(2)^2 \pmod{p} \tag{3.11}$$

and

$$\sum_{k=1}^n \frac{(-1)^k}{k}H_k \equiv \frac{q_p(2)^2}{2} + \left(\frac{-1}{p}\right)E_{p-3} \pmod{p}. \tag{3.12}$$

Let $\delta \in \{0,1\}$. For $r=0,\ldots,p-1$ we obviously have

$$(-1)^r\binom{p-1}{r}=\prod_{0<s\leqslant r}\left(1-\frac{p}{s}\right)\equiv 1-pH_r \pmod{p^2}.$$

Thus

$$\begin{aligned}p\sum_{k=1}^n\frac{(-1)^{\delta k}}{k}H_{k-1}\equiv&\sum_{k=1}^n\frac{(-1)^{\delta k}}{k}\left(1-(-1)^{k-1}\binom{p-1}{k-1}\right)\\=&\sum_{k=1}^n\frac{(-1)^{\delta k}}{k}+\frac{1}{p}\sum_{k=1}^n(-1)^{(\delta+1)k}\binom{p}{k} \pmod{p^2}\end{aligned}$$

and hence

$$p\sum_{k=1}^n\frac{(-1)^{\delta k}}{k}H_k\equiv\sum_{k=1}^n(-1)^{\delta k}\left(\frac{1}{k}+\frac{p}{k^2}\right)+\frac{1}{p}\sum_{k=1}^n(-1)^{(\delta+1)k}\binom{p}{k} \pmod{p^2}. \tag{3.13}$$

Putting $\delta=0$ in (3.13) and recalling (3.2) and the congruence $\sum_{k=1}^n 1/k^2\equiv 0 \pmod{p}$, we get

$$p\sum_{k=1}^n\frac{H_k}{k}\equiv H_n+\frac{(-1)^n\binom{p-1}{n}-1}{p} \pmod{p^2}.$$

With the helps of (1.9) and (3.8), we have

$$p\sum_{k=1}^n\frac{H_k}{k}\equiv -2q_p(2)+pq_p(2)^2+\frac{(1+p\,q_p(2))^2-1}{p}\equiv 2p\,q_p(2)^2 \pmod{p^2}$$

which yields (3.11). Taking $\delta=1$ in (3.13) and using the congruence $\sum_{k=1}^n 1/k^2\equiv 0 \pmod{p}$, we obtain

$$\begin{aligned}p\sum_{k=1}^n\frac{(-1)^k}{k}H_k\equiv&\sum_{k=1}^n\frac{(-1)^k+1}{k}+p\sum_{k=1}^n\frac{(-1)^k+1}{k^2}-H_n+\frac{2^p-2}{2p}\\=&H_{\lfloor p/4\rfloor}+\frac{p}{2}\sum_{j=1}^{\lfloor p/4\rfloor}\frac{1}{j^2}-H_n+q_p(2) \pmod{p^2}.\end{aligned}$$

Let's recall (1.9) and note that

$$\sum_{k=1}^{\lfloor p/4\rfloor}\frac{1}{k^2}\equiv 4\left(\frac{-1}{p}\right)E_{p-3} \pmod{p} \tag{3.14}$$

and

$$H_{\lfloor p/4\rfloor} \equiv -3q_p(2) + \frac{3}{2}p\,q_p(2)^2 - \left(\frac{-1}{p}\right) pE_{p-3} \pmod{p^2}$$

by Lehmer [L, (20)] and [S2, Corollary 3.3] respectively. Therefore,

$$\begin{aligned} p\sum_{k=1}^{n}\frac{(-1)^k}{k}H_k \equiv& -3q_p(2) + \frac{3}{2}p\,q_p(2)^2 - \left(\frac{-1}{p}\right) pE_{p-3} \\ &+ 2p\left(\frac{-1}{p}\right)E_{p-3} + (2q_p(2) - p\,q_p(2)^2) + q_p(2) \\ =&\frac{p}{2}q_p(2)^2 + \left(\frac{-1}{p}\right)pE_{p-3} \pmod{p^2} \end{aligned}$$

and hence (3.12) holds. We are done. □

Lemma 3.6. *Let p be an odd prime. Then*

$$\sum_{\substack{k=1\\4\mid k-2}}^{p-1}\frac{H_k}{k} \equiv \frac{3}{16}q_p(2)^2 \pmod{p}. \tag{3.15}$$

If $p>3$, then we also have

$$\sum_{\substack{k=1\\4\mid k}}^{p-1}\frac{H_k}{k} \equiv \frac{5}{16}q_p(2)^2 \pmod{p}. \tag{3.16}$$

Proof. As $H_{p-k} = H_{p-1} - \sum_{0<j<k}1/(p-j) \equiv H_{k-1} \pmod{p}$ for $k=1,\ldots,p-1$, we have

$$\begin{aligned} p\sum_{\substack{k=1\\4\mid k-2}}^{p-1}\frac{H_k}{k} =&p\sum_{\substack{k=1\\4\mid k-p+2}}^{p-1}\frac{H_{p-k}}{p-k} \\ \equiv& -\sum_{\substack{k=1\\4\mid k+p}}^{p-1}\frac{pH_{k-1}}{k} \equiv \sum_{\substack{k=1\\4\mid k+p}}^{p-1}\frac{(-1)^{k-1}\binom{p-1}{k-1}-1}{k} \\ =&\sum_{\substack{k=1\\4\mid k+p}}^{p-1}\frac{1}{k}\binom{p-1}{k-1} - \sum_{\substack{k=1\\4\mid k+p}}^{p-1}\frac{1}{k} \pmod{p^2}. \end{aligned}$$

Note that

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

by [Su1, Corollary 3.1] and that

$$\sum_{\substack{k=1\\4\mid k+p}}^{p-1}\frac{1}{k}\equiv\frac{q_p(2)}{4}-\frac{p}{8}q_p(2)^2\pmod{p^2}$$

by [S2, Corollary 3.1]. Therefore

$$\begin{aligned}p\sum_{\substack{k=1\\4\mid k-2}}^{p-1}\frac{H_k}{k}\equiv&\frac{2^{p-1}-(\frac{2}{p})2^{(p-1)/2}}{2p}-\frac{2^{p-1}-1}{4p}+\frac{p}{8}q_p(2)^2\\=&p\left(\frac{(\frac{2}{p})2^{(p-1)/2}-1}{2p}\right)^2+\frac{p}{8}q_p(2)^2\\\equiv&p\left(\frac{2^{p-1}-1}{4p}\right)^2+\frac{p}{8}q_p(2)^2=\frac{3}{16}p\,q_p(2)^2\pmod{p^2}\end{aligned}$$

and hence (3.15) follows. When $p>3$ we can prove (3.16) in a similar way. $\square$

Proof of Theorem 1.2. Set $n=(p-1)/2$. In view of (3.1) and (3.6), it suffices to show

$$\sum_{k=1}^{n}\binom{n}{k}\frac{(-2)^k}{k}H_k\equiv\left(\frac{-1}{p}\right)E_{p-3}\pmod{p}.$$

For each $k=1,\ldots,n$, evidently

$$H_n-H_{n-k}=\sum_{j=0}^{k-1}\frac{1}{n-j}\equiv-2\sum_{j=0}^{k-1}\frac{1}{2j+1}=-2\left(H_{2k}-\frac{H_k}{2}\right)\pmod{p}.$$

Thus, in light of (3.7), (3.15) and (3.9), we have

$$\begin{aligned}\sum_{k=1}^{n}\binom{n}{k}\frac{(-2)^k}{k}H_k\equiv&4\sum_{\substack{k=1\\2\nmid k}}^{n}\left(\frac{H_{2k}}{k}-\frac{H_k}{2k}\right)=8\sum_{\substack{j=1\\4\mid j-2}}^{p-1}\frac{H_j}{j}-2\sum_{\substack{k=1\\2\nmid k}}^{n}\frac{H_k}{k}\\\equiv&\frac{3}{2}q_p(2)^2-\frac{3}{2}q_p(2)^2+\left(\frac{-1}{p}\right)E_{p-3}\pmod{p}\end{aligned}$$

as desired. This concludes the proof. $\square$

Lemma 3.7. *Let $p>3$ be a prime. Then*

$$\sum_{k=1}^{p-1}\frac{H_k}{k^2}\equiv B_{p-3}\pmod{p}\tag{3.17}$$

and

$$\sum_{k=1}^{(p-1)/2}\frac{1}{k^3}\equiv -2B_{p-3}\pmod{p}. \tag{3.18}$$

Remark 3.2. (3.17) appeared as [ST, (5.4)], and (3.18) follows from [S1, Corollary 5.2(b)].

Lemma 3.8. *For any positive integer m and nonnegative integer n we have*

$$\sum_{k=0}^{n}\binom{n}{k}\frac{(-1)^k}{k+m}=\frac{1}{m\binom{m+n}{m}}. \tag{3.19}$$

Remark 3.3. (3.19) can be found in [G, (1.43)].

Proof of Theorem 1.3. Observe that

$$\begin{aligned}\sum_{k=1}^{p-1}\frac{\binom{2k}{k}}{4^k}H_k=&\sum_{k=1}^{p-1}\binom{-1/2}{k}(-1)^k\sum_{j=1}^{k}\frac{1}{j}\\ =&\sum_{j=1}^{p-1}\frac{1}{j}\bigg(\sum_{k=0}^{p-1}\binom{-1/2}{k}(-1)^k-\sum_{k=0}^{j-1}\binom{-1/2}{k}(-1)^k\bigg).\end{aligned}$$

Applying (3.2) we get

$$\begin{aligned}\sum_{k=1}^{p-1}\frac{\binom{2k}{k}}{4^k}H_k=&\sum_{j=1}^{p-1}\frac{1}{j}\bigg((-1)^{p-1}\binom{-1/2-1}{p-1}-(-1)^{j-1}\binom{-1/2-1}{j-1}\bigg)\\ =&\binom{-3/2}{p-1}H_{p-1}-2\sum_{j=1}^{p-1}(-1)^j\frac{-1/2}{j}\binom{-3/2}{j-1}\\ =&\binom{-3/2}{p-1}H_{p-1}-2\bigg(\sum_{j=0}^{p-1}(-1)^j\binom{-1/2}{j}-1\bigg)\\ =&\binom{-3/2}{p-1}H_{p-1}-2\binom{-1/2-1}{p-1}+2.\end{aligned}$$

Now assume $p>3$. Note that

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

since $\binom{2p-1}{p-1} \equiv 1 \pmod{p^3}$ by Wolstenholme's theorem (see, e.g., [HT]). In view of Wolstenholme's congruence $H_{p-1} \equiv 0 \pmod{p^2}$, by the above we have

$$\begin{aligned}\sum_{k=1}^{p-1}\frac{\binom{2k}{k}}{4^k}H_k \equiv& 2-2\binom{-3/2}{p-1} \equiv 2-\frac{2p}{(1+p\,q_p(2))^2}\\ \equiv& 2-2p(1-p\,q_p(2))^2 = 2-2p+4p^2q_p(2) \pmod{p^3}.\end{aligned}$$

So (1.10) holds.

Below we write $p=2n+1$. Combining (3.1), (3.4′) and (1.9), we get

$$\sum_{k=0}^{n}\frac{\binom{2k}{k}}{4^k}H_k^{(2)} \equiv -\frac{H_{(p-1)/2}}{(p-1)/2} \equiv 2H_{(p-1)/2} \equiv -4q_p(2) \pmod{p}.$$

This proves (1.11).

In view of (3.4) and (3.19), we have

$$\begin{aligned}\sum_{k=1}^{n}\binom{n}{k}\frac{(-1)^k}{k}H_k^{(2)} =& \sum_{k=1}^{n}\binom{n}{k}\frac{(-1)^k}{k}\sum_{j=1}^{k}\binom{k}{j}(-1)^{j-1}\frac{H_j}{j}\\ =& -\sum_{j=1}^{n}\frac{H_j}{j}\binom{n}{j}\sum_{k=j}^{n}\frac{(-1)^{k-j}}{k}\binom{n-j}{k-j}\\ =& -\sum_{j=1}^{n}\frac{H_j}{j}\binom{n}{j}\frac{1}{j\binom{n}{j}} = -\sum_{j=1}^{n}\frac{H_j}{j^2}.\end{aligned}$$

Observe that

$$\begin{aligned}\sum_{k=1}^{p-1}\frac{H_k}{k^2} =& \sum_{k=1}^{n}\left(\frac{H_k}{k^2}+\frac{H_{p-k}}{(p-k)^2}\right)\\ \equiv& \sum_{k=1}^{n}\left(\frac{H_k}{k^2}+\frac{H_{k-1}}{k^2}\right) = 2\sum_{k=1}^{n}\frac{H_k}{k^2}-\sum_{k=1}^{n}\frac{1}{k^3} \pmod{p}.\end{aligned}$$

Therefore, with the help of (3.1) we have

$$\sum_{k=1}^{n}\frac{\binom{2k}{k}}{4^k}H_k^{(2)} \equiv -\sum_{k=1}^{n}\frac{H_k}{k^2} \equiv -\frac{1}{2}\left(\sum_{k=1}^{p-1}\frac{H_k}{k^2}+\sum_{k=1}^{n}\frac{1}{k^3}\right) \pmod{p}.$$

Now applying Lemma 3.7 we immediately get the desired (1.12).

The proof of Theorem 1.3 is now complete. □

4. Proof of Theorem 1.4

Lemma 4.1. *For any positive integer n, we have the following identities:*

$$\sum_{k=0}^{n}\binom{n}{k}\binom{n+k}{k}(-1)^k H_k = 2(-1)^n H_n, \tag{4.1}$$

$$\sum_{k=0}^{n}\binom{n}{k}\binom{n+k}{k}(-1)^k H_k^{(2)} = 2(-1)^{n-1}\sum_{k=1}^{n}\frac{(-1)^k}{k^2}. \tag{4.2}$$

Remark 4.1. (4.1) and (4.2) can be found in [OS] and [Pr].

Lemma 4.2. *Let $p=2n+1$ be an odd prime, and let $k\in\{0,\ldots,n\}$. Then*

$$\begin{aligned}\frac{\binom{n+k}{k}}{\binom{2k}{k}/4^k} \equiv & 1+p\sum_{j=1}^{k}\frac{1}{2j-1}+\frac{p^2}{2}\bigg(\sum_{j=1}^{k}\frac{1}{2j-1}\bigg)^2\\ &-\frac{p^2}{2}\sum_{j=1}^{k}\frac{1}{(2j-1)^2} \pmod{p^3}\end{aligned} \tag{4.3}$$

and

$$\begin{aligned}\frac{\binom{n}{k}}{\binom{2k}{k}/(-4)^k} \equiv & 1-p\sum_{j=1}^{k}\frac{1}{2j-1}+\frac{p^2}{2}\bigg(\sum_{j=1}^{k}\frac{1}{2j-1}\bigg)^2\\ &-\frac{p^2}{2}\sum_{j=1}^{k}\frac{1}{(2j-1)^2} \pmod{p^3}.\end{aligned} \tag{4.4}$$

Consequently,

$$\binom{n}{k}\binom{n+k}{k}(-1)^k \equiv \frac{\binom{2k}{k}^2}{16^k} \pmod{p^2}. \tag{4.5}$$

Proof. Observe that

$$\begin{aligned}\frac{\binom{n+k}{k}}{\binom{2k}{k}/4^k} =& \prod_{j=1}^{k}\frac{(n+j)/j}{(2j-1)/(2j)} = \prod_{j=1}^{k}\bigg(1+\frac{p}{2j-1}\bigg)\\ \equiv & 1+p\sum_{j=1}^{k}\frac{1}{2j-1}+\frac{p^2}{2}S_k \pmod{p^3},\end{aligned}$$

where

$$S_k := 2\sum_{1\leqslant i<j\leqslant k}\frac{1}{(2i-1)(2j-1)} = \bigg(\sum_{j=1}^{k}\frac{1}{2j-1}\bigg)^2-\sum_{j=1}^{k}\frac{1}{(2j-1)^2}.$$

This proves (4.3). Similarly,

$$\frac{(-1)^k\binom{n}{k}}{\binom{2k}{k}/4^k}=\prod_{j=1}^k\left(1-\frac{p}{2j-1}\right)\equiv 1-p\sum_{j=1}^k\frac{1}{2j-1}+\frac{p^2}{2}S_k \pmod{p^3}$$

and hence (4.4) holds. Clearly (4.5) follows from (4.3) and (4.4). We are done. □

Remark 4.2. The congruence (4.5) was first observed by van Hamme [vH].

Lemma 4.3. *For any nonnegative integer n we have*

$$\sum_{k=0}^n\binom{n}{k}^2=\binom{2n}{n} \tag{4.6}$$

and

$$\sum_{k=0}^n\binom{n}{k}\frac{\binom{2k}{k}}{(-4)^k}=\frac{\binom{2n}{n}}{4^n}. \tag{4.7}$$

Remark 4.3. As $\binom{n}{k}=\binom{n}{n-k}$ and $\binom{2k}{k}/(-4)^k=\binom{-1/2}{k}$ for all $k=0,\ldots,n$, both (4.6) and (4.7) are special cases of the well-known Chu-Vandermonde identity $\sum_{k=0}^n\binom{x}{k}\binom{y}{n-k}=\binom{x+y}{n}$ (cf. [G, (3.1)] or (5.22) of [GKP, p. 169]). □

Lemma 4.5. *Let n be any positive integer. Then*

$$t_n:=\frac{1}{4n\binom{2n}{n}}\sum_{k=0}^{n-1}(21k+8)\binom{2k}{k}^3$$

coincides with

$$t_n':=\sum_{k=0}^{n-1}\binom{n+k-1}{k}^2.$$

Remark 4.4. In Feb. 2010, the author conjectured that t_n is always an integer and later this was confirmed by Kasper Andersen by getting $t_n=t_n'$ via the Zeilberger algorithm (cf. [Su3, Lemma 4.1]).

Now we are ready to prove the following auxiliary result.

Theorem 4.1. *Let $p>3$ be a prime. Then*

$$\sum_{k=0}^{(p-1)/2}\binom{2k}{k}^2\frac{H_k}{16^k}\equiv 2\left(\frac{-1}{p}\right)H_{(p-1)/2}\pmod{p^2},\tag{4.8}$$

$$\sum_{k=1}^{(p-1)/2}\binom{2k}{k}^2\frac{H_k^{(2)}}{16^k}\equiv -4E_{p-3}\pmod{p},\tag{4.9}$$

$$\sum_{k=1}^{(p-1)/2}\binom{2k}{k}^2\frac{H_k}{k16^k}\equiv 4\left(\frac{-1}{p}\right)E_{p-3}\pmod{p},\tag{4.10}$$

$$\sum_{k=0}^{(p-1)/2}\binom{2k}{k}^2\frac{H_{2k}}{16^k}\equiv\left(\frac{-1}{p}\right)\frac{3}{2}H_{(p-1)/2}+pE_{p-3}\pmod{p^2}.\tag{4.11}$$

Proof. Set $n=(p-1)/2$. In view of (4.5), (4.1) implies (4.8), and (4.2) yields that

$$\sum_{k=0}^{n}\binom{2k}{k}^2\frac{H_k^{(2)}}{16^k}\equiv 2(-1)^{n-1}\sum_{k=1}^{n}\frac{(-1)^k}{k^2}\pmod{p^2}.$$

Since $\sum_{k=1}^n 1/k^2\equiv 0\pmod{p}$, we have

$$\sum_{k=1}^{n}\frac{(-1)^k}{k^2}\equiv\sum_{k=1}^{n}\frac{(-1)^k+1}{k^2}=\frac{1}{2}\sum_{j=1}^{\lfloor p/4\rfloor}\frac{1}{j^2}\equiv 2(-1)^nE_{p-3}\pmod{p}$$

by applying (3.14) in the last step. Now it is clear that (4.9) holds.

Next we deduce (4.10). With the helps of (3.4) and the Chu-Vandermonde identity, we get

$$\begin{aligned}&\sum_{k=0}^{n}\binom{n}{k}\binom{n+k}{k}(-1)^kH_k^{(2)}\\
=&\sum_{k=1}^{n}\binom{n}{k}\binom{n+k}{k}(-1)^k\sum_{j=1}^{k}\binom{k}{j}\frac{(-1)^{j-1}}{j}H_j\\
=&\sum_{j=1}^{n}\binom{n}{j}\frac{(-1)^{j-1}}{j}H_j\sum_{k=j}^{n}\binom{n+k}{k}(-1)^k\binom{n-j}{k-j}\\
=&\sum_{j=1}^{n}\binom{n}{j}\frac{(-1)^{j-1}}{j}H_j\sum_{k=0}^{n}\binom{-n-1}{k}\binom{n-j}{n-k}\\
=&\sum_{j=1}^{n}\binom{n}{j}\frac{(-1)^{j-1}}{j}H_j\binom{-j-1}{n}=(-1)^{n-1}\sum_{j=1}^{n}\binom{n}{j}\binom{n+j}{j}\frac{(-1)^j}{j}H_j.\end{aligned}$$

Thus, by applying (4.5) we obtain (4.10) from (4.9).

Since

$$\begin{aligned}\sum_{k=0}^{n}\binom{n}{k}^2 H_{2k}^{(2)} &= \sum_{k=0}^{n}\binom{n}{k}^2 H_{2(n-k)}^{(2)} = \sum_{k=0}^{n}\binom{n}{k}^2 H_{p-1-2k}^{(2)} \\ &\equiv -\sum_{k=0}^{n}\binom{n}{k}^2 H_{2k}^{(2)} \pmod p,\end{aligned}$$

by (3.1) we have

$$\sum_{k=0}^{n}\frac{\binom{2k}{k}^2}{16^k}H_{2k}^{(2)} \equiv \sum_{k=0}^{n}\binom{n}{k}^2 H_{2k}^{(2)} \equiv 0 \pmod p$$

and hence

$$\begin{aligned}\sum_{k=0}^{n}\frac{\binom{2k}{k}^2}{16^k}\sum_{j=1}^{k}\frac{1}{(2j-1)^2} &= \sum_{k=0}^{n}\frac{\binom{2k}{k}^2}{16^k}\left(H_{2k}^{(2)} - \frac{H_k^{(2)}}{4}\right) \\ &\equiv -\frac{1}{4}\sum_{k=0}^{n}\frac{\binom{2k}{k}^2}{16^k}H_k^{(2)} \pmod p.\end{aligned}$$

Thus (4.9) implies that

$$\sum_{k=0}^{n}\frac{\binom{2k}{k}^2}{16^k}\sum_{j=1}^{k}\frac{1}{(2j-1)^2} \equiv E_{p-3} \pmod p. \tag{4.12}$$

By [Su3, (1.7)],

$$\sum_{k=0}^{n}\frac{\binom{2k}{k}^2}{16^k} \equiv (-1)^n + p^2E_{p-3} \pmod{p^3}, \tag{4.13}$$

Combining this with (4.12), we see that

$$\sum_{k=0}^{n}\frac{\binom{2k}{k}^2}{16^k}\left(1 - p^2\sum_{j=1}^{k}\frac{1}{(2j-1)^2}\right) \equiv (-1)^n \pmod{p^3}.$$

By (4.6) and (4.7), we have

$$\begin{aligned}\left(1-\frac{2}{4^n}\right)\binom{2n}{n} &= \sum_{k=0}^{n}\binom{n}{k}\left(\binom{n}{k} - \frac{2\binom{2k}{k}}{(-4)^k}\right) \\ &= \sum_{k=0}^{n}\frac{\binom{2k}{k}^2}{16^k}\cdot\frac{\binom{n}{k}}{\binom{2k}{k}/(-4)^k}\left(\frac{\binom{n}{k}}{\binom{2k}{k}/(-4)^k} - 2\right).\end{aligned}$$

Combining this with (4.4) we get

$$\left(1-\frac{2}{4^n}\right)\binom{2n}{n}\equiv\sum_{k=1}^n\frac{\binom{2k}{k}^2}{16^k}\left(p^2\left(\sum_{j=1}^k\frac{1}{2j-1}\right)^2-1\right)\pmod{p^3}.$$

By Morley's congruence (3.8),

$$\left(1-\frac{2}{4^n}\right)\binom{2n}{n}+(-1)^n\equiv(-1)^n(4^{2n}-2\cdot4^n+1)=(-1)^np^2q_p(2)^2\pmod{p^3}.$$

Thus, in light of (4.13) we obtain

$$\sum_{k=1}^{(p-1)/2}\frac{\binom{2k}{k}^2}{16^k}\left(\sum_{j=1}^k\frac{1}{2j-1}\right)^2\equiv E_{p-3}+\left(\frac{-1}{p}\right)q_p(2)^2\pmod{p}.\qquad(4.14)$$

By (4.7), (4.4), (4.12) and (4.14),

$$\begin{aligned}&\frac{\binom{2n}{n}}{4^n}-\sum_{k=0}^n\frac{\binom{2k}{k}^2}{16^k}\left(1-p\sum_{j=1}^k\frac{1}{2j-1}\right)\\ \equiv&\frac{p^2}{2}\sum_{k=0}^n\frac{\binom{2k}{k}^2}{16^k}\left(\left(\sum_{j=1}^k\frac{1}{2j-1}\right)^2-\sum_{j=1}^k\frac{1}{(2j-1)^2}\right)\\ \equiv&\frac{p^2}{2}(-1)^nq_p(2)^2\pmod{p^3}.\end{aligned}$$

Combining this with (3.8) and (4.13) we obtain

$$\sum_{k=1}^n\frac{\binom{2k}{k}^2}{16^k}\sum_{j=1}^k\frac{1}{2j-1}\equiv(-1)^n\left(-q_p(2)+\frac{p}{2}q_p(2)^2\right)+pE_{p-3}\pmod{p^2}.\quad(4.15)$$

Therefore, in view of (4.8) and (1.9), we have

$$\begin{aligned}\sum_{k=0}^n\frac{\binom{2k}{k}^2}{16^k}H_{2k}=&\sum_{k=1}^n\frac{\binom{2k}{k}^2}{16^k}\left(\sum_{j=1}^k\frac{1}{2j-1}+\frac{H_k}{2}\right)\\ \equiv&(-1)^n\left(-q_p(2)+\frac{p}{2}q_p(2)^2\right)+pE_{p-3}+(-1)^nH_n\\ \equiv&(-1)^n\frac{3}{2}H_n+pE_{p-3}\pmod{p^2}.\end{aligned}$$

This proves (4.11).

So far we have completed the proof of Theorem 4.1. □

Proof of Theorem 1.4. Write $p=2n+1$. Clearly

$$4(n+1)\binom{2(n+1)}{n+1}=8p\binom{2n}{n}\equiv 8p(-1)^n4^{p-1}\pmod{p^4}$$

by Morley's congruence (3.8), and

$$\begin{aligned}4^{1-p}=&\left(\frac{1}{1+p\,q_p(2)}\right)^2\\ \equiv&(1-p\,q_p(2)+p^2q_p(2)^2)^2\equiv 1-2p\,q_p(2)+3p^2q_p(2)^2\pmod{p^3}.\end{aligned}$$

Thus, in view of Lemma 4.5, (1.13) is reduced to

$$\begin{aligned}\sum_{k=0}^n\binom{n+k}{k}^2\equiv&\frac{4p^2E_{p-3}+(-1)^n}{4^{p-1}}\\ \equiv&4p^2E_{p-3}+(-1)^n(1-2p\,q_p(2)+3p^2q_p(2)^2)\pmod{p^3}.\end{aligned}\tag{4.16}$$

For each $k=0,\ldots,n$, by (4.3) we have

$$\begin{aligned}&\binom{n+k}{k}^2\\ \equiv&\frac{\binom{2k}{k}^2}{16^k}\left(1+p\sum_{j=1}^k\frac{1}{2j-1}+\frac{p^2}{2}\left(\left(\sum_{j=1}^k\frac{1}{2j-1}\right)^2-\sum_{j=1}^k\frac{1}{(2j-1)^2}\right)\right)^2\\ \equiv&\frac{\binom{2k}{k}^2}{16^k}\left(1+2p\sum_{j=1}^k\frac{1}{2j-1}+p^2\left(2\left(\sum_{j=1}^k\frac{1}{2j-1}\right)^2-\sum_{j=1}^k\frac{1}{(2j-1)^2}\right)\right)\\ &\pmod{p^3}.\end{aligned}$$

So we can obtain (4.16) by using (4.12)–(4.15).

Now we deduce (1.14). Combining (1.13) and (1.15) we get

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

i.e.,

$$\sum_{k=1}^{(p-1)/2}(21(p-k)+8)\frac{\binom{2(p-k)}{p-k}^3}{p^3}\equiv(-1)^{(p+1)/2}32E_{p-3}\pmod{p}.$$

By [Su3, Lemma 2.1], for each $k=1,\ldots,(p-1)/2$ we have

$$\frac{\binom{2(p-k)}{p-k}}{p}\equiv\frac{-2}{k\binom{2k}{k}}\pmod{p}.$$

Therefore

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

which gives (1.14).

The proof of Theorem 1.4 is now complete. □

5. Some related conjectures

We first pose the following conjecture similar to (1.6).

Conjecture 5.1. *For any prime $p>3$ we have*

$$\sum_{k=1}^{p-1}\frac{\binom{2k}{k}H_k^{(2)}}{k} \equiv \frac{2}{3}\cdot\frac{H_{p-1}}{p^2}+\frac{76}{135}p^2B_{p-5} \pmod{p^3},$$

$$\sum_{k=1}^{p-1}\frac{\binom{2k}{k}H_k^{(2)}}{k2^k} \equiv -\frac{3}{16}\cdot\frac{H_{p-1}}{p^2}+\frac{479}{1280}p^2B_{p-5} \pmod{p^3},$$

$$\sum_{k=1}^{p-1}\frac{\binom{2k}{k}H_k^{(2)}}{k3^k} \equiv -\frac{8}{9}\cdot\frac{H_{p-1}}{p^2}+\frac{268}{1215}p^2B_{p-5} \pmod{p^3}.$$

Remark 5.1. It is known that

$$\frac{H_{p-1}}{p^2} \equiv -\frac{B_{p-3}}{3} \pmod p \quad \text{for any prime } p>3$$

(see, e.g., [S1]).

The following conjecture is close to Theorem 1.3.

Conjecture 5.2. *Let $p>3$ be a prime. Then*

$$\sum_{k=1}^{p-1}\frac{\binom{2k}{k}}{k4^k}H_k \equiv \frac{7}{6}pB_{p-3} \pmod{p^2},$$

$$\sum_{k=1}^{p-1}\frac{\binom{2k}{k}}{k4^k}H_{2k} \equiv \frac{7}{3}pB_{p-3} \pmod{p^2},$$

$$\sum_{k=1}^{p-1}\frac{4^kH_{k-1}}{k^2\binom{2k}{k}} \equiv \frac{2}{3}B_{p-3} \pmod p,$$

$$\sum_{k=1}^{(p-1)/2}\frac{4^kH_{2k-1}}{k^2\binom{2k}{k}} \equiv \frac{7}{2}B_{p-3} \pmod p,$$

$$\sum_{k=1}^{p-1}\frac{\binom{2k}{k}}{k4^k}H_k^{(2)} \equiv -\frac{3}{2}\cdot\frac{H_{p-1}}{p^2}+\frac{7}{80}p^2B_{p-5} \pmod{p^3}.$$

Also,

$$\sum_{k=1}^{p-1}\frac{\binom{2k}{k}}{k^2 4^k}H_k \equiv \frac{3}{2}B_{p-3} \pmod p,$$
$$\sum_{k=1}^{p-1}\frac{\binom{2k}{k}}{k^2 4^k}H_{2k} \equiv \frac{5}{2}B_{p-3} \pmod p,$$

and

$$\sum_{k=1}^{p-1}\frac{\binom{2k}{k}}{k^2 4^k} \equiv -\frac{H_{(p-1)/2}^2}{2} - \frac{7}{4}\cdot\frac{H_{p-1}}{p} \pmod{p^3} \quad \textit{provided } p > 5.$$

Remark 5.2. The author ever conjectured that

$$\sum_{k=1}^{(p-1)/2}\frac{\binom{2k}{k}}{k4^k}H_{2k} \equiv -2\left(\frac{-1}{p}\right)E_{p-3} \pmod p$$

for any prime $p > 3$; this has been confirmed by his former student Hui-Qin Cao. Using `Mathematica 7` the author found that

$$\sum_{k=1}^{\infty}\frac{4^k H_{k-1}}{k^2\binom{2k}{k}} = 7\zeta(3), \quad \sum_{k=1}^{\infty}\frac{4^k H_{2k-1}}{k^2\binom{2k}{k}} = \frac{21}{2}\zeta(3),$$

$$\sum_{k=1}^{\infty}\frac{\binom{2k}{k}}{k4^k}H_k^{(2)} = \frac{3}{2}\zeta(3), \quad \sum_{k=1}^{\infty}\frac{\binom{2k}{k}}{k^2 4^k} = \frac{\pi^2 - 3\log^2 4}{6}.$$

Motivated by Theorem 4.1, we pose the following conjecture.

Conjecture 5.3. *Let $p > 3$ be a prime. Then*

$$\sum_{k=1}^{p-1}\frac{\binom{2k}{k}^2}{k16^k}H_{2k}^{(2)} \equiv B_{p-3} \pmod p,$$
$$\sum_{k=1}^{(p-1)/2}\frac{\binom{2k}{k}^2}{k16^k}H_{2k}^{(2)} \equiv -\frac{5}{2}B_{p-3} \pmod p,$$
$$\sum_{k=1}^{p-1}\frac{\binom{2k}{k}^2}{k16^k}H_k^{(2)} \equiv -12\frac{H_{p-1}}{p^2} + \frac{7}{10}p^2 B_{p-5} \pmod{p^3},$$
$$\sum_{k=(p+1)/2}^{p-1}\frac{\binom{2k}{k}^2}{k16^k}H_k^{(2)} \equiv \frac{31}{2}p^2 B_{p-5} \pmod{p^3}.$$

Also,

$$\sum_{k=0}^{(p-3)/2}\frac{\binom{2k}{k}^2}{(2k+1)16^k}H_k^{(2)}\equiv -7B_{p-3}\pmod p$$

and

$$\sum_{k=(p+1)/2}^{p-1}\frac{\binom{2k}{k}^2}{(2k+1)16^k}H_k^{(2)}\equiv -\frac{31}{2}p^2B_{p-5}\pmod{p^3}.$$

References

[AZ] T. Amdeberhan and D. Zeilberger, *Hypergeometric series acceleration via the WZ method*, Electron. J. Combin. **4** (1997), no. 2, #R3.

[G] H. W. Gould, *Combinatorial Identities*, Morgantown Printing and Binding Co., 1972.

[GKP] R. L. Graham, D. E. Knuth and O. Patashnik, *Concrete Mathematics*, 2nd ed., Addison-Wesley, New York, 1994.

[HT] C. Helou and G. Terjanian, *On Wolstenholme's theorem and its converse*, J. Number Theory **128** (2008), 475–499.

[He] V. Hernández, *Solution IV of problem 10490 (a reciprocal summation identity)*, Amer. Math. Monthly **106** (1999), 589–590.

[L] E. Lehmer, *On congruences involving Bernoulli numbers and the quotients of Fermat and Wilson*, Ann. of Math. **39** (1938), 350–360.

[Ma] R. Matsumoto, *A collection of formulae for π*, on-line version available from the website http://www.pluto.ai.kyutech.ac.jp/plt/matumoto/pi_small.

[Mo] F. Morley, *Note on the congruence $2^{4n}\equiv(-1)^n(2n)!/(n!)^2$, where $2n+1$ is a prime*, Ann. Math. **9** (1895), 168–170.

[OS] R. Osburn and C. Schneider, *Gaussian hypergeometric series and supercongruences*, Math. Comp. **78** (2009), 275–292.

[Pr] H. Prodinger, *Human proofs of identities by Osburn and Schneider*, Integers **8** (2008), #A10, 8pp (electronic).

[S1] Z.-H. Sun, *Congruences concerning Bernoulli numbers and Bernoulli polynomials*, Discrete Appl. Math. **105** (2000), 193–223.

[S2] Z.-H. Sun, *Congruences involving Bernoulli and Euler numbers*, J. Number Theory **128** (2008), 280–312.

[Su1] Z.-W. Sun, *On the sum $\sum_{k\equiv r\pmod m}\binom{n}{k}$ and related congruences*, Israel J. Math. **128** (2002), 135–156.

[Su2] Z.-W. Sun, *On congruences related to central binomial coefficients*, J. Number Theory **131** (2011), 2219–2238.

[Su3] Z.-W. Sun, *Super congruences and Euler numbers*, Sci. China Math. **54** (2011), 2509–2535.

[Su4] Z.-W. Sun, *On sums of binomial coefficients modulo p^2*, Colloq. Math. **127** (2012), 39–54.

[ST] Z.-W. Sun and R. Tauraso, *New congruences for central binomial coefficients*, Adv. in Appl. Math. **45** (2010), 125–148.

[T] R. Tauraso, *More congruences for central binomial coefficients*, J. Number Theory **130** (2010), 2639–2649.

[vH] L. van Hamme, *Some conjectures concerning partial sums of generalized hypergeometric series*, in: p-adic Functional Analysis (Nijmegen, 1996), pp. 223–236, Lecture Notes in Pure and Appl. Math., Vol., 192, Dekker, 1997.

[Z] I. J. Zucker, *On the series $\sum_{k=1}^{\infty}\binom{2k}{k}^{-1}k^{-n}$ and related sums*, J. Number Theory **20** (1985), 92–102.