Proc. Amer. Math. Soc. 140(2012), no. 2, 415–428.

ARITHMETIC THEORY OF HARMONIC NUMBERS

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Abstract. Harmonic numbers $H_k = \sum_{0<j\leqslant k} 1/j$ $(k = 0, 1, 2, \ldots)$ play important roles in mathematics. In this paper we investigate their arithmetic properties and obtain various basic congruences. Let $p > 3$ be a prime. We show that

$$\sum_{k=1}^{p-1} \frac{H_k}{k2^k} \equiv 0 \pmod p, \ \sum_{k=1}^{p-1} H_k^2 \equiv 2p-2 \pmod{p^2}, \ \sum_{k=1}^{p-1} H_k^3 \equiv 6 \pmod p,$$

and

$$\sum_{k=1}^{p-1} \frac{H_k^2}{k^2} \equiv 0 \pmod p \qquad \text{provided } p > 5.$$

(In contrast, it is known that $\sum_{k=1}^{\infty} H_k/(k2^k) = \pi^2/12$ and $\sum_{k=1}^{\infty} H_k^2/k^2 = 17\pi^4/360$.) Our tools include some sophisticated combinatorial identities and properties of Bernoulli numbers.

1. Introduction

The Riemann zeta function is given by

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} \quad \text{for} \ \ \mathrm{Re}(s) > 1.$$

For $n \in \mathbb{N} = \{0, 1, 2, \ldots\}$ we define

$$H_n = \sum_{0<k\leqslant n} \frac{1}{k}.$$

(Note that $H_0 = 0$ by convention.) These numbers are known as harmonic numbers, and they arise naturally from many fields of mathematics. For example, Euler found that

$$\lim_{n\to+\infty} (H_n - \log n) = \gamma = 0.577\ldots \quad \text{and} \quad \sum_{n=1}^{\infty} \frac{H_n}{n^2} = 2\zeta(3);$$

2010 *Mathematics Subject Classification.* Primary 11B75; Secondary 05A19, 11A07, 11B68.

Keywords. Harmonic numbers, congruences, Bernoulli numbers.

Supported by the National Natural Science Foundation (grant 10871087) of China.

also,

$$\sum_{n=1}^{\infty}\frac{H_n}{n2^n}=\frac{\pi^2}{12}\quad \text{(S. W. Coffman [C], 1987)}$$

and

$$\sum_{n=1}^{\infty}\frac{H_n^2}{n^2}=\frac{17}{360}\pi^4\quad \text{(D. Borwein and J. M. Borwein [BB], 1995).}$$

For $m\in\mathbb{Z}^+=\{1,2,3,\dots\}$, harmonic numbers of order m are those rational numbers

$$H_{n,m}=\sum_{0<k\leqslant n}\frac{1}{k^m}\quad (n=0,1,2,\dots).$$

A famous result of Euler (cf. [IR, pp. 231–232]) states that

$$\lim_{n\to+\infty}H_{n,m}=\zeta(m)=(-1)^{m/2-1}2^{m-1}\pi^m\frac{B_m}{m!}\quad \text{for } m=2,4,6,\dots,$$

where $B_0,B_1,B_2,\dots$, are Bernoulli numbers given by

$$B_0=1\ \text{ and }\ \sum_{k=0}^{n}\binom{n+1}{k}B_k=0\ (n=1,2,3,\dots).$$

In this paper we focus on the arithmetic theory of harmonic numbers. In 1862 Wolstenholme [W] proved that if $p>3$ is a prime then

$$H_{p-1}\equiv 0 \pmod{p^2}\ \text{ and }\ H_{p-1,2}\equiv 0 \pmod{p},$$

hence

$$\binom{2p-1}{p-1}=\prod_{k=1}^{p-1}\left(1+\frac{p}{k}\right)\equiv 1+pH_{p-1}+\frac{p^2}{2}(H_{p-1}^2-H_{p-1,2})\equiv 1 \pmod{p^3}.$$

There are various extensions of the Wolstenholme theorem, see, e.g., [A], [ASVZ], [B], [Gr], [HT] and [Z]; in particular, the paper [ASVZ] contains all Wolstenholme-type congruences of the form $\binom{ap+b}{cp+d}\equiv 1 \pmod{p^3}$ with $a,b,c,d\in\mathbb{Z}$. In 1938 E. Lehmer [L] determined $H_{(p-1)/2}$ mod p^2 for any odd prime p. Though there are many identities and combinatorial interpretations involving harmonic numbers (see, e.g., [BPQ]), it seems that there are very few congruences for harmonic numbers.

In this paper we systematically investigate arithmetic properties of harmonic numbers, and present some basic congruences for sums of terms involving harmonic numbers. Our main result is as follows.

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

$$\sum_{k=1}^{p-1}\frac{H_k}{k2^k}\equiv 0 \pmod{p}, \tag{1.1}$$

$$\sum_{k=1}^{p-1}k^2H_k^2\equiv -\frac{4}{9} \pmod{p}, \tag{1.2}$$

$$\sum_{k=1}^{p-1}H_k^3\equiv 6 \pmod{p}, \tag{1.3}$$

$$\sum_{k=1}^{p-1}H_k^2\equiv 2p-2 \pmod{p^2}. \tag{1.4}$$

When $p>5$ we have

$$\sum_{k=1}^{p-1}\frac{H_k^2}{k^2}\equiv 0 \pmod{p}. \tag{1.5}$$

Remark 1.1. Let $p>3$ be a prime. It is easy to determine $\sum_{k=1}^{p-1}k^mH_k$ mod p for all $m\in\mathbb{Z}$. (See [ST, (5.4)] and its proof.) Note also that

$$\begin{aligned}\sum_{k=1}^{p-1}kH_k&=\sum_{k=1}^{p-1}k\sum_{j=1}^{k}\frac{1}{j}=\sum_{j=1}^{p-1}\frac{1}{j}\sum_{k=j}^{p-1}k=\sum_{j=1}^{p-1}\frac{1}{j}\left(\sum_{k=1}^{p-1}k-\sum_{i=0}^{j-1}i\right)\\&=\frac{p(p-1)}{2}H_{p-1}-\sum_{j=1}^{p-1}\frac{j(j-1)/2}{j}\equiv-\frac{(p-1)(p-2)}{4} \pmod{p^3}.\end{aligned}$$

Here are two consequences of Theorem 1.1.

Corollary 1.1. *Let $p>3$ be a prime. Then*

$$\sum_{k=1}^{p-1}kH_k^2\equiv 1 \pmod{p},\ \sum_{k=1}^{p-1}kH_k^3\equiv -3 \pmod{p},\ \sum_{k=1}^{p-1}k^3H_k^2\equiv\frac{1}{6} \pmod{p}.$$

Corollary 1.2. *Let $p>3$ be a prime. Then*

$$\sum_{\substack{0\leqslant r,s,t<p-1\\ r+s+t\in\{p-1,2p-2\}}}B_rB_sB_t\equiv 5 \pmod{p}. \tag{1.6}$$

Remark 1.2. Let $p>3$ be a prime. By taking $n=p-1$ in an identity of Matiyasevich (cf. [PS, (1.3)]) we get $\sum_{k=1}^{p-2}B_kB_{p-1-k}\equiv 1 \pmod{p}$. Via a symmetric identity on Bernoulli polynomials given in [FPZ] (which is an extension of the main result of [SP]), we may deduce that

$$\sum_{\substack{0\leqslant r,s,t<p-1\\ r+s+t=p-1}} B_rB_sB_t \equiv \frac{5}{2} \pmod p.$$

Our computation suggests the following refinement of (1.1) and (1.5).

Conjecture 1.1. *For any prime $p>3$, we have*

$$\sum_{k=1}^{p-1}\frac{H_k}{k2^k} \equiv \frac{7}{24}pB_{p-3} \pmod{p^2} \quad \text{and} \quad \sum_{k=1}^{p-1}\frac{H_k^2}{k^2} \equiv \frac{4}{5}pB_{p-5} \pmod{p^2}.$$

For harmonic numbers of even order, we have the following conjecture based on our computation via `Mathematica`.

Conjecture 1.2. *Let n be any positive integer. If p is a prime with $p-1\nmid 6n$, then*

$$\sum_{k=1}^{p-1}\frac{H_{k,2n}^2}{k^{2n}} \equiv 0 \pmod p. \tag{1.7}$$

Furthermore, for each prime $p>6n+1$ we have

$$\sum_{k=1}^{p-1}\frac{H_{k,2n}^2}{k^{2n}} \equiv \frac{s(n)}{6n+1}pB_{p-1-6n} \pmod{p^2}, \tag{1.8}$$

where

$$s(n) = \frac{n}{2n+1}\binom{6n+1}{2n} + n.$$

We make the following progress on Conjecture 1.2.

Theorem 1.2. *Let $p>3$ be a prime and let $0<m<p-1$ be an even integer. Set $n=p-1-m$. Then*

$$\begin{aligned}-m^2\sum_{k=1}^{p-1}\frac{H_{k,m}^2}{k^m} \equiv & \sum_{\substack{0\leqslant i,j\leqslant n\\ i+j=3n+2-(p-1)}}\binom{n+1}{i}\binom{n+1}{j}B_iB_j\\ &+\sum_{\substack{0\leqslant i,j\leqslant n\\ i+j=3n+2-2(p-1)}}\binom{n+1}{i}\binom{n+1}{j}B_iB_j \pmod p.\end{aligned} \tag{1.9}$$

Hence $\sum_{k=1}^{p-1} H_{k,m}^2/k^m \equiv 0 \pmod p$ if $2p/3<m<p-1$.

In the next section we provide some lemmas. Section 3 is devoted to the proofs of Theorems 1.1-1.2 and Corollaries 1.1-1.2.

2. Some lemmas

Lemma 2.1. *Let p be an odd prime. Then*

$$H_{p-k} \equiv H_{k-1} \pmod{p} \tag{2.1}$$

and

$$(-1)^k\binom{p-1}{k} \equiv 1 - pH_k + \frac{p^2}{2}(H_k^2 - H_{k,2}) \pmod{p^3} \tag{2.2}$$

for every $k = 1, \ldots, p-1$. If $p > 3$ then

$$\sum_{k=1}^{p-1} H_k \equiv 1 - p \pmod{p^3} \quad \text{and} \quad \sum_{k=1}^{p-1}\frac{H_{k-1}}{k} \equiv 0 \pmod{p}. \tag{2.3}$$

Proof. When $k \in \{1, \ldots, p-1\}$, we clearly have

$$H_{p-k} = \sum_{j=1}^{p-k}\frac{1}{j} = H_{p-1} - \sum_{j=1}^{k-1}\frac{1}{p-k+j} \equiv \sum_{j=1}^{k-1}\frac{1}{k-j} = H_{k-1} \pmod{p}$$

and

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

This proves (2.1) and (2.2).

For the first congruence in (2.3) we observe that

$$\begin{aligned}\sum_{k=1}^{p-1} H_k &= \sum_{k=1}^{p-1}\sum_{j=1}^{k}\frac{1}{j} = \sum_{j=1}^{p-1}\frac{1}{j}\sum_{k=j}^{p-1}1\\ &= \sum_{j=1}^{p-1}\frac{p-j}{j} = pH_{p-1} - (p-1) \equiv 1 - p \pmod{p^3}\end{aligned}$$

since $H_{p-1} \equiv 0 \pmod{p^2}$.

Now we prove the second congruence in (2.3). Note that

$$\sum_{k=1}^{p-1}\frac{p}{k}\binom{p-1}{k-1}(-1)^k = \sum_{k=1}^{p-1}\binom{p}{k}(-1)^k + 1 + (-1)^p = (1-1)^p = 0.$$

Thus,

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

and hence the desired congruence follows. We are done. □

For a prime p and an integer $a\not\equiv 0\pmod p$, as usual we call $q_p(a)=(a^{p-1}-1)/p$ a Fermat quotient.

Lemma 2.2 (Lehmer [L]). *Let $p>3$ be a prime. Then*

$$H_{(p-1)/2}\equiv p\,q_p^2(2)-2q_p(2)\pmod{p^2}. \tag{2.4}$$

Lemma 2.3. *Let $p>3$ be a prime. Then*

$$\sum_{\substack{k=1\\ 2\mid k}}^{p-1}\frac{H_k}{k}\equiv\frac{q_p^2(2)}{2}\pmod p\quad\textit{and}\quad\sum_{\substack{k=1\\ 2\nmid k}}^{p-1}\frac{H_k}{k}\equiv-\frac{q_p^2(2)}{2}\pmod p. \tag{2.5}$$

Proof. In view of (2.3),

$$\sum_{k=1}^{p-1}\frac{H_k}{k}=\sum_{k=1}^{p-1}\frac{H_{k-1}}{k}+\sum_{k=1}^{p-1}\frac{1}{k^2}\equiv 0\pmod p.$$

So it suffices to show the first congruence in (2.5).

For any odd $k\in\{1,\ldots,p-1\}$, clearly

$$-\binom{p-1}{k}=\binom{p-1}{k}(-1)^k\equiv 1-pH_k\pmod{p^2}$$

by (2.2). Thus, with the help of (2.4), we have

$$\begin{aligned}p\sum_{\substack{k=1\\ 2\mid k}}^{p-1}\frac{H_{k-1}}{k}\equiv&\sum_{\substack{k=1\\ 2\mid k}}^{p-1}\frac{1+\binom{p-1}{k-1}}{k}=\frac{H_{(p-1)/2}}{2}+\frac{1}{p}\Bigg(\sum_{\substack{k=0\\ 2\mid k}}^{p}\binom{p}{k}-1\Bigg)\\ \equiv&\frac{p}{2}q_p^2(2)-q_p(2)+\frac{2^{p-1}-1}{p}=\frac{p}{2}q_p^2(2)\pmod{p^2}\end{aligned}$$

and hence

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

since $H_{p-1,2}\equiv 0\pmod p$. We are done. □

Lemma 2.4. *Let n be any positive integer. Then*
$$\sum_{k=0}^{n-1}\frac{2^k}{k+1}=\sum_{\substack{k=1\\ 2\nmid k}}^{n}\frac{1}{k}\binom{n}{k}. \tag{2.6}$$

Proof. Observe that
$$\begin{aligned}\sum_{k=0}^{n-1}\frac{2^k}{k+1}&=\sum_{k=0}^{n-1}2^k\int_0^1 x^k dx=\int_0^1\sum_{k=0}^{n-1}(2x)^k dx\\ &=\int_0^1\frac{(2x)^n-1}{2x-1}dx=\int_0^1\sum_{k=1}^{n}\binom{n}{k}(2x-1)^{k-1}dx\\ &=\sum_{k=1}^{n}\binom{n}{k}\frac{(2x-1)^k}{2k}\Big|_0^1=\sum_{k=1}^{n}\binom{n}{k}\frac{1-(-1)^k}{2k}.\end{aligned}$$
So (2.6) follows. □

Lemma 2.5. *Let $n\in\mathbb{N}$. Then we have*
$$\sum_{k=0}^{n}\binom{n}{k}^2=\binom{2n}{n}\quad\text{and}\quad\sum_{k=0}^{2n}(-1)^k\binom{2n}{k}^3=(-1)^n\frac{(3n)!}{(n!)^3}. \tag{2.7}$$

Proof. The first identity is a special case of the Chu-Vandermonde identity (cf. [St, p.12]). The second identity is due to Dixon (cf. [St, p.45]). □

Lemma 2.6. *Let $p>3$ be a prime. Then*
$$\sum_{k=1}^{p-1}H_kH_{k,2}\equiv 0 \pmod p. \tag{2.8}$$

Proof. Observe that
$$\begin{aligned}\sum_{k=1}^{p-1}H_kH_{k,2}&=\sum_{k=1}^{p-1}H_k\sum_{j=1}^{k}\frac{1}{j^2}=\sum_{j=1}^{p-1}\frac{1}{j^2}\sum_{k=j}^{p-1}H_k\\ &=\sum_{j=1}^{p-1}\frac{1}{j^2}\left(\sum_{k=1}^{p-1}H_k-\sum_{0<s<j}H_s\right)\\ &=H_{p-1,2}\sum_{k=1}^{p-1}H_k-\sum_{j=1}^{p-1}\frac{1}{j^2}\sum_{0<s<j}\sum_{t=1}^{s}\frac{1}{t}\\ &\equiv-\sum_{j=1}^{p-1}\frac{1}{j^2}\sum_{0<t<j}\frac{1}{t}\sum_{t\leqslant s<j}1=-\sum_{j=1}^{p-1}\frac{1}{j^2}\sum_{0<t<j}\frac{j-t}{t}\\ &\equiv-\sum_{j=1}^{p-1}\frac{jH_{j-1}-j+1}{j^2}\equiv-\sum_{k=1}^{p-1}\frac{H_{k-1}}{k} \pmod p.\end{aligned}$$

Applying the last congruence in (2.3) we obtain (2.8) from the above. □

Lemma 2.7. *For $n\in\mathbb{Z}^+$ we have the combinatorial identity*

$$\sum_{k=1}^{2n-1}\frac{(-1)^{k-1}}{\binom{2n}{k}}H_k=\frac{n}{2(n+1)^2}+\frac{H_{2n}}{2n+2}. \tag{2.9}$$

Proof. This is a known identity appeared as (2.18) of Gould [G, p.20]. □

Let us recall some well known properties of Bernoulli numbers (cf. [IR, pp. 230–238]). First,

$$\sum_{j=0}^{k-1}j^n=\frac{1}{n+1}\sum_{j=0}^{n}\binom{n+1}{j}B_jk^{n+1-j}\quad\text{for any } k,n\in\mathbb{Z}^+.$$

Secondly, $B_1=-1/2$ and $B_{2n+1}=0$ for $n=1,2,3,\ldots$. Thirdly, if p is an odd prime and n is a positive integer not divisible by $p-1$, then B_n is a p-adic integer (i.e., its denominator is not divisible by p) by the von Staudt–Clausen theorem.

Lemma 2.8 ([Z, (3.19)])**.** *Let $p>5$ be a prime. Then*

$$\sum_{k=0}^{p-3}B_kB_{p-3-k}\equiv 0 \pmod{p}. \tag{2.10}$$

Proof. Though (2.10) is known, here we provide a simple proof. Recall that $B_0,B_1,\ldots B_{p-3}$ are p-adic integers. By an identity of Matiyasevich (cf. [PS, (1.3)] and [SP]),

$$(p-1)\sum_{k=2}^{p-5}B_kB_{p-3-k}-2\sum_{k=2}^{p-5}\binom{p-1}{k}B_kB_{p-3-k}=(p-2)(p-3)B_{p-3}.$$

For $k\in\{2,\ldots,p-3\}$, we clearly have

$$\binom{p-1}{k}B_k\equiv(-1)^kB_k=B_k \pmod{p}.$$

So, the identity yields

$$\sum_{k=2}^{p-5}B_kB_{p-3-k}\equiv -2B_{p-3} \pmod{p},$$

which is equivalent to (2.10) since $B_{p-4}=0$. □

3. Proofs of Theorems 1.1-1.2 and Corollaries 1.1-1.2

Proof of (1.1). Observe that

$$\sum_{k=1}^{p-1}\frac{H_k}{k2^k}=\sum_{k=1}^{p-1}\frac{H_{p-k}}{(p-k)2^{p-k}}\equiv\sum_{k=1}^{p-1}\frac{2^{k-1}H_{k-1}}{-k}=-\sum_{k=0}^{p-2}\frac{2^kH_k}{k+1}\pmod p$$

and hence

$$p\sum_{k=1}^{p-1}\frac{H_k}{k2^k}\equiv\sum_{k=0}^{p-1}\frac{2^k}{k+1}\left(\binom{p-1}{k}(-1)^k-1\right)=\Sigma\pmod{p^2},$$

where

$$\begin{aligned}\Sigma:=&\frac{1}{p}\sum_{k=0}^{p-2}\binom{p}{k+1}(-2)^k-\sum_{k=0}^{p-2}\frac{2^k}{k+1}\\ =&\frac{1}{-2p}\sum_{j=1}^{p-1}\binom{p}{j}(-2)^j-\sum_{\substack{k=1\\ 2\nmid k}}^{p-1}\frac{1}{k}\binom{p-1}{k}\ \text{(by Lemma 2.4)}\\ =&\frac{(1-2)^p-1+2^p}{-2p}+\sum_{\substack{k=1\\ 2\nmid k}}^{p-1}\frac{\binom{p-1}{k}(-1)^k}{k}.\end{aligned}$$

Thus

$$\begin{aligned}\Sigma+q_p(2)\equiv&\sum_{\substack{k=1\\ 2\nmid k}}^{p-1}\frac{1-pH_k}{k}=H_{p-1}-\frac{H_{(p-1)/2}}{2}-p\sum_{\substack{k=1\\ 2\nmid k}}^{p-1}\frac{H_k}{k}\\ \equiv&-\frac{H_{(p-1)/2}}{2}+\frac{p}{2}q_p^2(2)\equiv q_p(2)\pmod{p^2}\end{aligned}$$

in view of (2.4) and (2.5). So we finally get

$$p\sum_{k=1}^{p-1}\frac{H_k}{k2^k}\equiv\Sigma\equiv 0\pmod{p^2}$$

which yields (1.1). □

Proof of (1.2). By Lemma 2.1,

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

Recall that

$$\sum_{k=0}^{p-1} k^2 = \frac{(p-1)p(2p-1)}{6}.$$

Also,

$$\begin{aligned}&\sum_{k=0}^{p-1}(-1)^k k^2\binom{p-1}{k} = \sum_{k=0}^{p-1}(-1)^k(k+k(k-1))\binom{p-1}{k}\\ =&(p-1)\sum_{k=1}^{p-1}\binom{p-2}{k-1}(-1)^k + (p-1)(p-2)\sum_{k=2}^{p-1}\binom{p-3}{k-2}(-1)^{k-2}\\ =&(1-p)(1-1)^{p-2} + (p-1)(p-2)(1-1)^{p-3} = 0.\end{aligned}$$

Thus

$$\begin{aligned}p^2\sum_{k=0}^{p-1}k^2H_k^2 \equiv&\frac{p(p-1)(2p-1)}{6} + \sum_{k=0}^{p-1}k^2\binom{p-1}{k}^2\\ \equiv&\frac{p}{6}(1-3p) + \sum_{k=1}^{p-1}(p-1)^2\binom{p-2}{k-1}^2 \pmod{p^3}.\end{aligned}$$

With helps of the first identity in (2.7) and the Wolstenholme congruence,

$$\begin{aligned}\sum_{k=1}^{p-1}\binom{p-2}{k-1}^2 =&\sum_{j=0}^{p-2}\binom{p-2}{j}^2 = \binom{2p-4}{p-2} = \binom{2p-1}{p-1}\frac{p(p-1)}{2(2p-1)(2p-3)}\\ \equiv&\frac{p}{2}\cdot\frac{p-1}{3-8p} \equiv \frac{p(p-1)}{18}(3+8p) \equiv -\frac{p}{18}(5p+3) \pmod{p^3}.\end{aligned}$$

Therefore

$$p^2\sum_{k=0}^{p-1}k^2H_k^2 \equiv \frac{p}{6}(1-3p) - (p-1)^2\frac{p}{18}(5p+3) \equiv -\frac{4}{9}p^2 \pmod{p^3}$$

and hence (1.2) follows. □

Proof of (1.3). By Lemma 2.1,

$$\sum_{k=0}^{p-1}H_k^3 \equiv \sum_{k=0}^{p-1}\left(\frac{1-(-1)^k\binom{p-1}{k}}{p}\right)^3 = \frac{\Sigma}{p^3} \pmod{p},$$

where

$$\begin{aligned}\Sigma :=&\sum_{k=0}^{p-1}\left(1-3(-1)^k\binom{p-1}{k} + 3\binom{p-1}{k}^2 - (-1)^{3k}\binom{p-1}{k}^3\right)\\ =&p - 3(1-1)^{p-1} + 3\binom{2p-2}{p-1} - (-1)^n\frac{(3n)!}{(n!)^3} \quad \text{(by Lemma 2.5)}\end{aligned}$$

with $n = (p-1)/2$.

Note that

$$\binom{2p-2}{p-1} = \frac{p}{2p-1}\binom{2p-1}{p-1} \equiv \frac{p}{2p-1} \pmod{p^4}$$

by the Wolstenholme congruence. Also,

$$\begin{aligned}(-1)^n\frac{(3n)!}{(n!)^3} =& (-1)^n\frac{p}{p+n}\prod_{k=1}^{n}\frac{k(p-k)(p+k)}{k^3}\\ =& \frac{p}{p+n}\prod_{k=1}^{n}\left(1-\frac{p^2}{k^2}\right) \equiv \frac{p}{p+n} = \frac{2p}{3p-1} \pmod{p^4}\end{aligned}$$

since $2\sum_{k=1}^{n} 1/k^2 = H_{p-1,2} \equiv 0 \pmod{p}$.

Combining the above, we obtain

$$\sum_{k=0}^{p-1} H_k^3 \equiv \frac{\Sigma}{p^3} \equiv \frac{p+3p/(2p-1)-2p/(3p-1)}{p^3} \equiv 6 \pmod{p}.$$

Note that

$$\sum_{k=1}^{p-1} H_k \equiv 1-p \pmod{p^3} \quad\text{and}\quad \sum_{k=1}^{p-1} H_k H_{k,2} \equiv 0 \pmod p$$

by (2.3) and (2.8). Therefore

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

and hence (1.4) follows with the help of (1.3). □

Proof of (1.5). By Fermat's little theorem and the well-known formula for sums of powers,

$$\begin{aligned}\sum_{k=1}^{p-1}\frac{H_{k-1}^2}{k^2} &\equiv \sum_{k=1}^{p-1}\frac{(\sum_{j=0}^{k-1} j^{p-2})^2}{k^2} = \sum_{k=1}^{p-1}\frac{1}{k^2}\left(\frac{1}{p-1}\sum_{j=0}^{p-2}\binom{p-1}{j}B_j k^{p-1-j}\right)^2\\ &\equiv \sum_{k=1}^{p-1}\frac{1}{k^2}\left(\sum_{j=0}^{p-2}(-1)^j B_j k^{p-1-j}\right)\left(\sum_{i=0}^{p-2}(-1)^{p-2-i}B_{p-2-i}k^{i+1}\right)\\ &= -\sum_{k=1}^{p-1}\sum_{i,j=0}^{p-2}(-1)^{i+j}B_j B_{p-2-i}k^{p-2-j+i} \pmod p.\end{aligned}$$

It is well-known that for each $m\in\mathbb{Z}$ we have

$$\sum_{k=1}^{p-1} k^m \equiv \begin{cases} -1 \pmod p & \text{if } p-1\mid m,\\ 0 \pmod p & \text{otherwise.}\end{cases}$$

(See, e.g., [IR, p.235].) Note also that $B_{p-2}=0$. Thus

$$\sum_{k=1}^{p-1}\frac{H_{k-1}^2}{k^2} \equiv \sum_{j=0}^{p-3}(-1)^{(j+1)+j}B_j B_{p-2-(j+1)} = -\sum_{j=0}^{p-3}B_j B_{p-3-j} \equiv 0 \pmod p.$$

with the help of (2.10).

In view of (2.1) and the above,

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

This concludes the proof of (1.5). □

Proof of Corollary 1.1. If $n \in \mathbb{Z}^+$ then

$$\sum_{k=1}^{p-1} kH_k^n = \sum_{k=1}^{p-1}(p-k)H_{p-k}^n \equiv -\sum_{k=1}^{p} kH_{k-1}^n = -\sum_{j=1}^{p-1}(j+1)H_j^n \pmod p$$

and hence

$$\sum_{k=0}^{p-1} kH_k^n \equiv -\frac{1}{2}\sum_{k=1}^{p-1} H_k^n \pmod p.$$

So the first and the second congruences in Corollary 1.1 follow from (1.4) and (1.3) respectively.

In view of (1.2), (1.4) and the first congruence in Corollary 1.1,

$$\begin{aligned}\sum_{k=1}^{p-1} k^3H_k^2 &= \sum_{k=1}^{p-1}(p-k)^3H_{p-k}^2 \\ &\equiv -\sum_{k=1}^{p} k^3H_{k-1}^2 = -\sum_{k=1}^{p-1}(k+1)^3H_k^2 \\ &= -\sum_{k=1}^{p-1} k^3H_k^2 - 3\sum_{k=1}^{p-1} k^2H_k^2 - 3\sum_{k=1}^{p-1} kH_k^2 - \sum_{k=1}^{p-1} H_k^2 \\ &\equiv -\sum_{k=1}^{p-1} k^3H_k^2 - 3\left(-\frac{4}{9}\right) - 3\times 1 - (-2) \pmod p\end{aligned}$$

and hence the third congruence in Corollary 1.1 also holds. □

Proof of Corollary 1.2. Observe that

$$\begin{aligned}\sum_{k=1}^{p-1} H_k^3 &= \sum_{k=1}^{p-1} H_{p-k}^3 \equiv \sum_{k=1}^{p-1} H_{k-1}^3 \equiv \sum_{k=1}^{p-1}\left(\sum_{j=0}^{k-1} j^{p-2}\right)^3 \\ &\equiv \sum_{k=1}^{p-1}\left(\frac{1}{p-1}\sum_{j=0}^{p-2}\binom{p-1}{j}B_jk^{p-1-j}\right)^3 \\ &\equiv -\sum_{k=1}^{p-1}\left(\sum_{j=0}^{p-2}(-1)^jB_jk^{p-1-j}\right)^3 \\ &= -\sum_{r,s,t=0}^{p-2}(-1)^{r+s+t}B_rB_sB_t\sum_{k=1}^{p-1}k^{3(p-1)-r-s-t} \\ &\equiv \sum_{\substack{0\leqslant r,s,t<p-1 \\ r+s+t\in\{0,p-1,2p-2\}}} B_rB_sB_t \pmod p.\end{aligned}$$

So (1.6) follows from (1.3). $\square$

Proof of Theorem 1.2. For any $k \in \{1, \ldots, p-1\}$, obviously

$$H_{p-k,m} \equiv \sum_{j=1}^{p-1} j^{p-1-m} - \sum_{0<j<k} \frac{1}{(p-k+j)^m}$$
$$\equiv - \sum_{0<j<k} \frac{1}{(k-j)^m} = -H_{k-1,m} \pmod p$$

since $p-1 \nmid m$ and $2 \mid m$. Thus

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

As $n = p-1-m$, we have

$$\sum_{k=1}^{p-1} \frac{H_{k-1,m}^2}{k^m} \equiv \sum_{k=1}^{p-1} \frac{(\sum_{j=0}^{k-1} j^n)^2}{k^m} = \sum_{k=1}^{p-1} \frac{1}{k^m} \left(\frac{1}{n+1} \sum_{j=0}^{n} \binom{n+1}{j} B_j k^{n+1-j} \right)^2$$
$$\equiv \frac{1}{m^2} \sum_{k=1}^{p-1} k^n \left(\sum_{i=0}^{n} \binom{n+1}{i} B_i k^{n+1-i} \right) \sum_{j=0}^{n} \binom{n+1}{j} B_j k^{n+1-j}$$
$$\equiv \frac{1}{m^2} \sum_{i,j=0}^{n} \binom{n+1}{i} \binom{n+1}{j} B_i B_j \sum_{k=1}^{p-1} k^{3n+2-(i+j)} \pmod p.$$

Note that $3n+2 < 3(n+1) = 3(p-m) < 3(p-1)$. So (1.9) follows from the above.

If $2p/3 < m < p-1$, then $3n+2 = 3p-1-3m < p-1$, hence the last two sums in (1.9) vanish and consequently $\sum_{k=1}^{p-1} H_{k,m}^2/k^m \equiv 0 \pmod p$.

The proof of Theorem 1.2 is now complete. $\square$

Acknowledgment. The author would like to thank the referee for helpful comments.

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