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SQUARE-FREE HARMONIC NUMBERS: BASIC PROPERTIES

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Abstract. We study a variant of harmonic numbers defined by restricting the summation to square?free indices, denoted by H_n^{sq}. Using the Mobius function to detect square?free integers, we establish a relation between H_n^{sq} and the ordinary harmonic numbers H_n. We derive an asymptotic expansion for H_n^{sq} with an explicit constant involving the Riemann zeta function. Moreover, we obtain the ordinary generating function, a convolution identity, and the arithmetic mean of these numbers.

Keywords. Harmonic numbers, Mobius function, square-free integers, asymptotic expansion, generating function.
2020 Mathematics Subject Classification. Primary 11A25, 11B99; Secondary 11M06, 11N37.

1. Introduction and preliminaries

Harmonic numbers are defined by

$$H_n = \sum_{k=1}^{n} \frac{1}{k}.$$

They have odd numerators and even denominators when expressed in reduced form. Their ordinary generating function is

$$\sum_{n=1}^{\infty} H_n x^n = -\frac{\ln(1-x)}{1-x}, \qquad |x| < 1.$$

They admit the asymptotic expansion

$$H_n = \log n + \gamma + \frac{1}{2n} - \frac{1}{12n^2} + O\left(\frac{1}{n^4}\right),$$

where γ is the Euler-Mascheroni constant.

Classical harmonic numbers appear in many branches of mathematics, and several variants have been studied, including:

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- Skew harmonic numbers:

$$\mathbf{O}_n = \sum_{k=1}^{n} \frac{1}{2k-1}.$$

- Alternating harmonic numbers:

$$\mathbf{H}_n = \sum_{k=1}^{n} \frac{(-1)^{k-1}}{k}.$$

- Alternating skew harmonic numbers:

$$\overline{\mathbf{O}}_n = \sum_{k=1}^{n} \frac{(-1)^{k-1}}{2k-1}.$$

Additional details on harmonic numbers can be found in the following references [2, 5, 7, 12, 13].

An integer $n > 0$ is square-free if it is not divisible by the square of any prime. Equivalently, in its prime factorization $n = \prod_i p_i^{e_i}$, all exponents satisfy $e_i \in \{0, 1\}$. Its characteristic function is $|\mu(n)|$, where μ is the Möbius function. Let

$$Q(x) = \#\{n \leq x : n \text{ is square-free}\}.$$

The asymptotic density of square-free numbers exists and is given by

$$\lim_{x\to\infty} \frac{Q(x)}{x} = \frac{1}{\zeta(2)} = \frac{6}{\pi^2} \approx 0.607927.$$

A classical estimate (see [3]) is

$$Q(x) = \frac{6}{\pi^2}x + O(\sqrt{x}).$$

The Dirichlet generating function for the square-free indicator is

$$\sum_{n=1}^{\infty} \frac{|\mu(n)|}{n^s} = \frac{\zeta(s)}{\zeta(2s)}, \qquad \Re(s) > 1,$$

where $\zeta(s)$ is the Riemann zeta function. For more information on square-free numbers, the reader is referred to the following papers [1, 4, 8, 12, 13].

In this work we consider the square?free harmonic numbers

$$H_n^{\text{sq}} = \sum_{\substack{k \leq n \\ k \text{ square-free}}} \frac{1}{k}.$$

Figure 1 compares H_n and H_n^{sq} for $1 \leq n \leq 10^4$; both sequences grow logarithmically, but H_n is consistently larger because it includes all integers.

We provide several basic properties: an exact relation with ordinary harmonic numbers, an asymptotic expansion with an explicit constant, the ordinary generating function, a convolution identity, and the arithmetic mean.

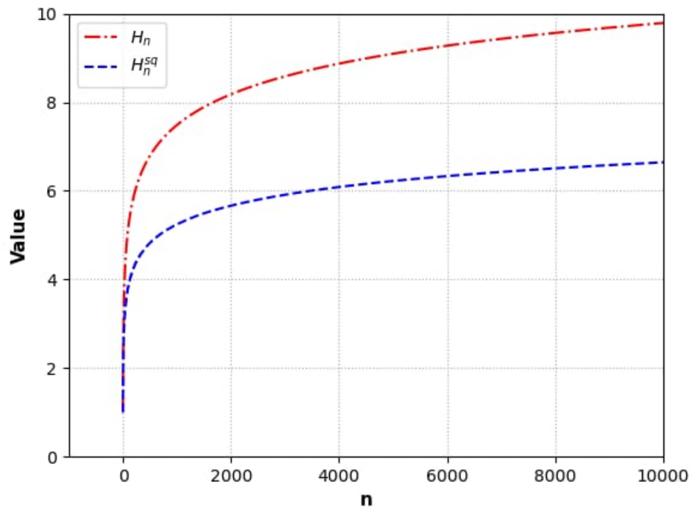

FIGURE 1. Comparison of H_n and H_n^{sq} for $1 \le n \le 10^4$.

2. Relation between H_n^{sq} and H_n

The first result of our work establishes a relation between H_n^{sq} and H_n.

Theorem 2.1. *For any integer $n > 0$,*

$$H_n^{\mathrm{sq}} = \sum_{d=1}^{\lfloor \sqrt{n} \rfloor} \frac{\mu(d)}{d^2} H_{\lfloor n/d^2 \rfloor}. \tag{2.1}$$

Proof. We begin with the well-known Möbius inversion formula for the square-free indicator

$$\mu(k)^2 = \sum_{d^2 | k} \mu(d) = \begin{cases} 1 & \text{if } k \text{ is square?free}, \\ 0 & \text{otherwise}. \end{cases} \tag{2.2}$$

We note that the last sum runs over all positive integers d whose squares divide k. Now, write H_n^{sq} using this indicator:

$$H_n^{\mathrm{sq}} = \sum_{k=1}^{n} \frac{\mu(k)^2}{k} = \sum_{k=1}^{n} \frac{1}{k} \sum_{d^2|k} \mu(d).$$

Interchange the order of summation. The condition $d^2 \mid k$ means $k = d^2 m$ for some integer $m \ge 1$. The inequality $k \le n$ becomes $m \le n/d^2$. Hence

$$H_n^{\mathrm{sq}} = \sum_{d=1}^{\lfloor \sqrt{n} \rfloor} \mu(d) \sum_{m=1}^{\lfloor n/d^2 \rfloor} \frac{1}{d^2 m}.$$

The inner sum simplifies:

$$\sum_{m=1}^{\lfloor n/d^2 \rfloor} \frac{1}{d^2 m} = \frac{1}{d^2} \sum_{m=1}^{\lfloor n/d^2 \rfloor} \frac{1}{m} = \frac{1}{d^2} H_{\lfloor n/d^2 \rfloor}.$$

Therefore

$$H_n^{\mathrm{sq}} = \sum_{d=1}^{\lfloor\sqrt{n}\rfloor} \frac{\mu(d)}{d^2}\, H_{\lfloor n/d^2\rfloor},$$

which completes the proof. □

3. Asymptotic expansion

In our next result, we establish an asymptotic expansion of H_n^{sq}.

Theorem 3.1. *As $n \to \infty$, the square?free harmonic numbers satisfy*

$$H_n^{\mathrm{sq}} = \frac{6}{\pi^2}\log n + C + O\left(\frac{\log n}{\sqrt{n}}\right),$$

where

$$C = \frac{6\gamma}{\pi^2} - \frac{2\zeta'(2)}{\zeta(2)^2}.$$

Proof. We use the classical asymptotic expansion of harmonic numbers (for $m \to \infty$):

$$H_m = \log m + \gamma + \frac{1}{2m} - \frac{1}{12\,m^2} + O\left(\frac{1}{m^4}\right).$$

We apply Theorem 2.1. For fixed d and large n, we set

$$m_d = \lfloor n/d^2\rfloor := \frac{n}{d^2} - \varepsilon_d, \qquad \text{with} \quad 0 \le \varepsilon_d < 1$$

Since $|\log(1-t)| \le 2|t|$ for $|t| < 1$, then

$$\log m_d = \log\left(\frac{n}{d^2}\right) + \log\left(1 - \frac{\varepsilon_d d^2}{n}\right) = \log\frac{n}{d^2} + O\left(\frac{d^2}{n}\right),$$

Moreover,

$$\frac{1}{m_d} = \frac{d^2}{n} + O\left(\frac{d^4}{n^2}\right), \qquad \frac{1}{m_d^2} = O\left(\frac{d^4}{n^2}\right) \qquad \text{and} \qquad \frac{1}{m_d^4} = O\left(\frac{d^8}{n^4}\right).$$

Thus,

$$H_{m_d} = \log\frac{n}{d^2} + \gamma + \frac{d^2}{2n} + O\left(\frac{d^2}{n}\right) + O\left(\frac{d^4}{n^2}\right) + O\left(\frac{d^8}{n^4}\right).$$

The condition $d \le \sqrt{n}$ is equivalent to $d^2 \le n$. So, we get $d^4/n^2 = O\left(\frac{d^2}{n}\right)$ and $d^8/n^4 = O\left(\frac{d^2}{n}\right)$. Hence all errors combine to $O\left(\frac{d^2}{n}\right)$, and we obtain the simpler estimate

$$H_{\lfloor n/d^2\rfloor} = \log\frac{n}{d^2} + \gamma + O\left(\frac{d^2}{n}\right). \tag{3.1}$$

Inserting (3.1) into (2.1), we obtain

$$H_n^{\mathrm{sq}} = \sum_{d\le\sqrt{n}} \frac{\mu(d)}{d^2}\left(\log\frac{n}{d^2} + \gamma\right) + \sum_{d\le\sqrt{n}} \frac{\mu(d)}{d^2}\, O\left(\frac{d^2}{n}\right).$$

On the one hand, the number of square-free integers up to $\sqrt{n}$ is equivalent to $\frac{6}{\pi^2}\sqrt{n} = O(\sqrt{n})$. It becomes that the second sum is bounded by

$$O\left(\frac{1}{n}\sum_{d\le\sqrt{n}}|\mu(d)|\right) = O\left(\frac{1}{n}\cdot\sqrt{n}\right) = O\left(\frac{1}{\sqrt{n}}\right).$$

On the other hand, the first sum splits as

$$\sum_{d\le\sqrt{n}}\frac{\mu(d)}{d^2}\log\frac{n}{d^2} = \log n\sum_{d\le\sqrt{n}}\frac{\mu(d)}{d^2} \;-\; 2\sum_{d\le\sqrt{n}}\frac{\mu(d)\log d}{d^2}.$$

Define the convergent series

$$S_1 = \sum_{d=1}^{\infty}\frac{\mu(d)}{d^2} = \frac{1}{\zeta(2)} = \frac{6}{\pi^2} \qquad \text{and} \qquad S_2 = \sum_{d=1}^{\infty}\frac{\mu(d)\log d}{d^2} = \frac{\zeta'(2)}{\zeta(2)^2}.$$

For any $y > 0$, we have

$$\sum_{d\le y}\frac{\mu(d)}{d^2} = S_1 - \sum_{d>y}\frac{\mu(d)}{d^2}$$

and

$$\left|\sum_{d>y}\frac{\mu(d)}{d^2}\right| \le \sum_{d>y}\frac{1}{d^2} \le \frac{1}{y-1} = O\left(\frac{1}{y}\right).$$

Similarly, using summation by parts, one shows

$$\sum_{d>y}\frac{\mu(d)\log d}{d^2} = O\left(\frac{1}{y}\right),$$

without a logarithmic factor. Indeed, let

$$A(t) = \sum_{d\le t}\frac{\mu(d)}{d^2} = S_1 + O\left(\frac{1}{t}\right).$$

Then,

$$\sum_{d>y}\frac{\mu(d)\log d}{d^2} = \int_y^{\infty}\log t\, dA(t) = -\frac{\log y}{y} + \int_y^{\infty}\frac{A(t)-S_1}{t}\,dt = O\left(\frac{1}{y}\right).$$

Thus,

$$\sum_{d\le\sqrt{n}}\frac{\mu(d)}{d^2} = S_1 + O\left(\frac{1}{\sqrt{n}}\right) \qquad \text{and} \qquad \sum_{d\le\sqrt{n}}\frac{\mu(d)\log d}{d^2} = S_2 + O\left(\frac{1}{\sqrt{n}}\right).$$

Consequently,

$$\begin{aligned} H_n^{\mathrm{sq}} &= (\log n + \gamma)\left(S_1 + O\left(\frac{1}{\sqrt{n}}\right)\right) - 2\left(S_2 + O\left(\frac{1}{\sqrt{n}}\right)\right) + O\left(\frac{1}{\sqrt{n}}\right) \\ &= \frac{6}{\pi^2}\log n + \frac{6\gamma}{\pi^2} - \frac{2\zeta'(2)}{\zeta(2)^2} + (\log n + \gamma)\, O\left(\frac{1}{\sqrt{n}}\right) + O\left(\frac{1}{\sqrt{n}}\right) \\ &= \frac{6}{\pi^2}\log n + \frac{6\gamma}{\pi^2} - \frac{2\zeta'(2)}{\zeta(2)^2} + O\left(\frac{\log n}{\sqrt{n}}\right). \end{aligned}$$

□

Remark 3.2. Figure 2 displays the residual

$$r_n = H_n^{\mathrm{sq}} - \left(\frac{6}{\pi^2}\ln n + C\right)$$

for $n \in [1, 20000]$, together with the envelope $\pm\dfrac{0.9}{\sqrt{n}}$ (dashed red). The residual (solid blue) remains strictly inside the envelope for all $n \geq 1$, exhibits small oscillations for modest n due to the irregular distribution of squarefree integers, and decays visibly toward zero at the rate $\dfrac{1}{\sqrt{n}}$, in full agreement with the error term $O\left(\dfrac{\log n}{\sqrt{n}}\right)$ of Theorem 3.1.

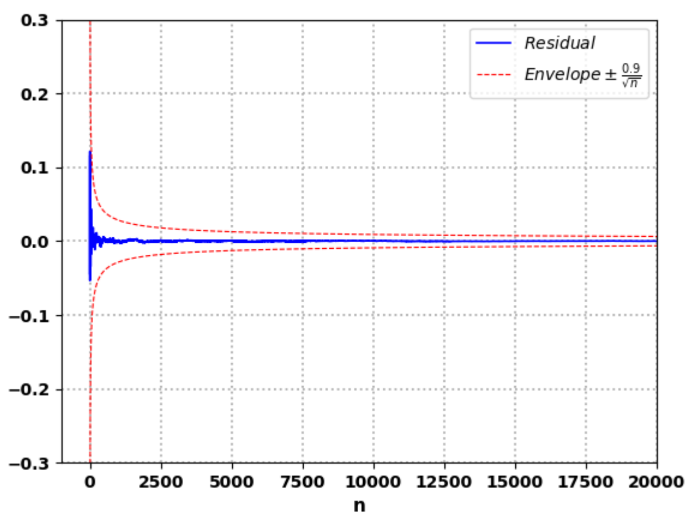

FIGURE 2. Residual r_n and envelope $\pm 0.9/\sqrt{n}$ (dashed red).

4. Generating Function

Now, we turn to the generation function of H_n^{sq}.

Theorem 4.1. *For* $|x| < 1$,

$$\sum_{n=1}^{\infty} H_n^{\mathrm{sq}} x^n = -\frac{1}{1-x}\sum_{d=1}^{\infty}\frac{\mu(d)}{d^2}\ln(1-x^{d^2}). \tag{4.1}$$

Proof. For $|x| < 1$, the ordinary generating function of H_n^{sq} is

$$G(x) = \sum_{n=1}^{\infty} H_n^{\mathrm{sq}} x^n = \sum_{n=1}^{\infty}\left(\sum_{k=1}^{n}\frac{\mu(k)^2}{k}\right)x^n.$$

Since all terms are non-negative when $x \geq 0$ and the series is absolutely convergent for $|x| < 1$, we may interchange the sums:

$$G(x) = \sum_{k=1}^{\infty}\frac{\mu(k)^2}{k}\sum_{n=k}^{\infty}x^n = \frac{1}{1-x}\sum_{k=1}^{\infty}\frac{\mu(k)^2}{k}x^k. \tag{4.1}$$

Substituting (2.2) into (4.1), one gets:

$$\sum_{k=1}^{\infty}\frac{\mu(k)^2}{k}x^k = \sum_{k=1}^{\infty}\frac{x^k}{k}\sum_{d^2|k}\mu(d).$$

Since the double series converges absolutely, we may swap the order:

$$\begin{aligned}
\sum_{k=1}^{\infty}\frac{x^k}{k}\sum_{d^2|k}\mu(d) &= \sum_{d=1}^{\infty}\mu(d)\sum_{\substack{k\geq 1\\ d^2|k}}\frac{x^k}{k} \\
&= \sum_{d=1}^{\infty}\mu(d)\sum_{m=1}^{\infty}\frac{x^{d^2m}}{d^2m} \\
&= \sum_{d=1}^{\infty}\frac{\mu(d)}{d^2}\sum_{m=1}^{\infty}\frac{(x^{d^2})^m}{m} \\
&= -\sum_{d=1}^{\infty}\frac{\mu(d)}{d^2}\ln(1-x^{d^2}).
\end{aligned}$$

Finally,

$$G(x) = -\frac{1}{1-x}\sum_{d=1}^{\infty}\frac{\mu(d)}{d^2}\ln\big(1-x^{d^2}\big).$$

$\square$

5. Convolution identity and arithmetic mean

We begin this section by establishing the convolution identity related to H_n^{sq}.

Theorem 5.1. *For any integer $n \geq 0$,*

$$\sum_{k=0}^{n} H_k^{\mathrm{sq}} H_{n-k}^{\mathrm{sq}} = \sum_{\substack{i,j\geq 1\\ i+j\leq n}} \frac{n+1-i-j}{ij}\,|\mu(i)|^2|\mu(j)|^2.$$

Proof. For $|x|<1$, the ordinary generating function of H_n^{sq} is given by

$$G(x) = \sum_{n=1}^{\infty} H_n^{\mathrm{sq}} x^n = \sum_{n=1}^{\infty} \left(\sum_{\substack{k=1\\ k \text{ square-free}}}^{n} \frac{1}{k} \right) x^n. \tag{5.1}$$

Denoting by

$$S(x) = \sum_{\substack{m\geq 1\\ m \text{ square-free}}} \frac{x^m}{m}$$

and using the square-free indicator (2.2), we can write

$$\begin{aligned} S(x)^2 &= \left(\sum_{\substack{i\geq 1\\ i \text{ square-free}}} \frac{x^i}{i} \right)\left(\sum_{\substack{j\geq 1\\ j \text{ square-free}}} \frac{x^j}{j} \right) \\ &= \sum_{\substack{i,j\geq 1\\ i,j \text{ square-free}}} \frac{x^{i+j}}{ij} \\ &= \sum_{i,j\geq 1} \frac{\mu(i)^2\mu(j)^2}{ij}\, x^{i+j}. \end{aligned}$$

Moreover, interchanging the order of summation in (5.1), gives

$$\begin{aligned} G(x) &= \sum_{\substack{k=1\\ k \text{ square-free}}}^{\infty} \frac{1}{k} \sum_{n=k}^{\infty} x^n \\ &= \frac{1}{1-x} \sum_{\substack{k=1\\ k \text{ square-free}}}^{\infty} \frac{x^k}{k} \\ &= \frac{S(x)}{1-x}. \end{aligned}$$

Now, since $H_0^{\rm sq} = 0$, the convolution sum $\sum_{k=0}^{n} H_k^{\rm sq} H_{n-k}^{\rm sq}$ is exactly the coefficient of x^n in $G(x)^2 = \dfrac{S(x)^2}{(1-x)^2}$. So, expanding

$$\frac{1}{(1-x)^2} = \sum_{t=0}^{\infty} (t+1)x^t$$

it becomes that

$$G(x)^2 = \sum_{i,j\geq 1} \frac{\mu(i)^2\mu(j)^2}{ij} \sum_{t=0}^{\infty} (t+1)x^{t+i+j}.$$

The coefficient of x^n is obtained by setting $t = n-i-j$, which requires $i+j \leq n$. Therefore,

$$\sum_{k=0}^{n} H_k^{\rm sq} H_{n-k}^{\rm sq} = [x^n]F(x)^2 = \sum_{\substack{i,j\geq 1 \\ i+j\leq n}} \frac{n+1-i-j}{ij}\, \mu(i)^2\mu(j)^2.$$

□

The last result of our present work is the arithmetic mean of the $H_k^{\rm sq}$.

Theorem 5.2. *For any integer $n > 0$,*

$$\frac{1}{n}\sum_{k=1}^{n} H_k^{\rm sq} = \Big(1 + \frac{1}{n}\Big) H_n^{\rm sq} - \frac{1}{n}\sum_{i=1}^{n} \frac{1}{i}.$$

Proof. We start with interchanging the order of summation:

$$\begin{aligned}
\textstyle\sum_{k=1}^{n} H_k^{\rm sq} &= \sum_{k=1}^{n} \sum_{\substack{i=1 \\ i \text{ square-free}}}^{k} \frac{1}{i} \\
&= \sum_{\substack{i=1 \\ i \text{ square-free}}}^{n} \frac{1}{i} \sum_{k=i}^{n} 1 \\
&= \sum_{\substack{i=1 \\ i \text{ square-free}}}^{n} \frac{n-i+1}{i} \\
&= (n+1) \sum_{\substack{i=1 \\ i \text{ square-free}}}^{n} \frac{1}{i} - \sum_{\substack{i=1 \\ i \text{ square-free}}}^{n} 1 \\
&= (n+1)H_n^{\rm sq} - Q(n).
\end{aligned}$$

Dividing both sides by n yields the desired formula. □

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