Analogies between identities for Multiple Zeta Values and congruences for Multiple Harmonic Sums

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For $\text{Re}(s) > 1$, the Riemann zeta function is given by

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}.$$ 

Thanks to Euler, we know the formula

$$\zeta(s) = \frac{(2\pi)^s|B_s|}{2 \, s!} \quad \text{for } s = 2, 4, 6, 8, \ldots$$

where Bernoulli numbers $B_s \in \mathbb{Q}$ are defined by generating function

$$\frac{z}{e^z - 1} = \sum_{n=0}^{\infty} \frac{B_n}{n!} z^n \quad \Rightarrow \quad B_n = 1, -\frac{1}{2}, \frac{1}{6}, 0, -\frac{1}{30}, 0, \frac{1}{42}, 0, -\frac{1}{30}, \ldots$$
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- $\zeta(3)$ is irrational [Apery, 1978];
- Infinitely many $\zeta(2n + 1)$ are irrational numbers;
- Conjecture. The numbers $\pi, \zeta(3), \zeta(5), \ldots, \zeta(2n + 1)$ are algebraically independent over $\mathbb{Q}$: for any $n \geq 1$ and for any non-zero polynomial $P \in \mathbb{Z}[x_1, \ldots, x_n],$

$$P(\pi, \zeta(3), \zeta(5), \ldots, \zeta(2n + 1)) \neq 0.$$
Let $d \geq 1$ and let $s = (s_1, \ldots, s_d) \in (\mathbb{N}^*)^d$.

We define the *Multiple Harmonic Sum* (MHS) as

$$H_n(s_1, \ldots, s_d) := \sum_{1 \leq k_1 < k_2 < \ldots < k_d \leq n} \frac{1}{k_1^{s_1} k_2^{s_2} \cdots k_d^{s_d}}.$$
Definitions of MHS and MZV

Let \( d \geq 1 \) and let \( s = (s_1, \ldots, s_d) \in (\mathbb{N}^*)^d \).
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\]

If \( s_d \geq 2 \), the **Multiple Zeta Value** (MZV) is given by

\[
\zeta(s_1, \ldots, s_d) = \lim_{n \to \infty} H_n(s_1, \ldots, s_d).
\]

We call \( d \) and \( w := s_1 + \cdots + s_d \) respectively the **depth** and the **weight** of \( s \).
Representation of MZV as iterated integral

\[ \zeta(s_1, \ldots, s_d) = \int_{0 < t_w < \cdots < t_2 < t_1 < 1} \frac{dt_1 \ dt_2 \cdots \ dt_w}{a_1(t_1)a_2(t_2) \cdots a_w(t_w)} \]

with \( a_i(t) = \begin{cases} 1 - t & \text{for } i \in \{s_d, s_d + s_{d-1}, \ldots, w\}, \\ t & \text{otherwise.} \end{cases} \)

We assign to \( s = (s_1, \ldots, s_d) \) the word

\[ u = x_0^{s_d-1} x_1 x_0^{s_{d-1}-1} x_1 \cdots x_0^{s_1-1} x_1 \]

in non-commuting letters \( x_0, x_1 \), and we write \( \zeta(s) = \zeta(u) \).
For example

\[ \zeta(x_0 x_1 x_1) = \int_0^1 \frac{dt_1}{t_1} \int_0^{t_1} \frac{dt_2}{1 - t_2} \int_0^{t_2} \frac{dt_3}{1 - t_3} \]

\[ = \int_0^1 \frac{dt_1}{t_1} \int_0^{t_1} \frac{dt_2}{1 - t_2} \sum_{j=1}^{\infty} \int_0^{t_2} t_3^{j-1} dt_3 \]

\[ = \int_0^1 \frac{dt_1}{t_1} \int_0^{t_1} \frac{dt_2}{1 - t_2} \sum_{j=1}^{\infty} \frac{t_2^j}{j} \]

\[ = \int_0^1 \frac{dt_1}{t_1} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \int_0^{t_1} \frac{t_2^{j+i-1}}{j} dt_2 \]

\[ = \int_0^1 \frac{dt_1}{t_1} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{t_1^{j+i}}{j(j + i)} \]

\[ = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{1}{j(j + i)^2} = \zeta(1, 2). \]
Duality relation for MZVs

The change of variable

\((t_1, \ldots, t_n) \rightarrow (1 - t_n, \ldots, 1 - t_1)\)

in the iterated integral, yields the *duality relation* for MZVs

\(\zeta(u) = \zeta(u')\),

where \(u'\) is defined by transposing \(x_0\) and \(x_1\) in \(u\),

\[ u = x_0^{s_d-1} x_1 x_0^{s_d-1-1} x_1 \cdots x_0^{s_1-1} x_1 \rightarrow u' = x_0 x_1^{s_1-1} \cdots x_0 x_1^{s_d-1-1} x_0 x_1^{s_d-1}. \]

Notice that \((u')' = u\).
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Notice that \((u')' = u\). For example

\[\zeta(\{1\}^a, 2) = \zeta(x_0 x_1^{a+1}) = \zeta(x_0^{a+1} x_1) = \zeta(a + 2).\]
We define a product \( \shuffle \) between words on alphabet \( \{x_0, x_1\} \) which is distributive over the addition and satisfies the rules

1) \( \forall u, \ 1 \shuffle u = u \shuffle 1 = u \),

2) \( \forall u, v, \ x_i u \shuffle x_j v = x_i (u \shuffle x_j v) + x_j (x_i u \shuffle v) \).

The \( \shuffle \)-product is commutative and associative. Moreover

\[ \zeta(u) \cdot \zeta(v) = \zeta(u \shuffle v). \]
We define a product $\boxdot$ between words on alphabet $\{x_0, x_1\}$ which is distributive over the addition and satisfies the rules

1) $\forall u, 1 \boxdot u = u \boxdot 1 = u$,

2) $\forall u, v, x_i u \boxdot x_j v = x_i (u \boxdot x_j v) + x_j (x_i u \boxdot v)$.

The $\boxdot$-product is commutative and associative. Moreover

$$\zeta(u) \cdot \zeta(v) = \zeta(u \boxdot v).$$

For example

$$x_0 x_1 \boxdot x_0 x_1 = 2x_0 (x_1 \boxdot x_0 x_1) = 2x_0 x_1 (1 \boxdot x_0 x_1) + 2x_0 x_0 (x_1 \boxdot x_1)$$
$$= 2x_0 x_1 x_0 x_1 + 4x_0 x_0 x_1 x_1$$

implies that $\zeta(2)^2 = 2\zeta(2, 2) + 4\zeta(1, 3)$. 
Stuffle product

We define a product $\ast$ between words on alphabet $\{y_i : i \geq 1\}$ which is distributive over the addition and satisfies the rules

1) $\forall u, \ 1 \ast u = u \ast 1 = u$

2) $\forall u, v, \ y_i u \ast y_j v = y_i(u \ast y_j v) + y_j(y_i u \ast v) + y_{i+j}(u \ast v)$.

The $\ast$-product is commutative and associative. Moreover

$H_n(u) \cdot H_n(v) = H_n(u \ast v)$ and $\zeta(u) \cdot \zeta(v) = \zeta(u \ast v)$. 

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The $\ast$-product is commutative and associative. Moreover

\[
H_n(u) \cdot H_n(v) = H_n(u \ast v) \quad \text{and} \quad \zeta(u) \cdot \zeta(v) = \zeta(u \ast v).
\]

For example

\[
y_2 \ast y_2 = 2y_2(1 \ast y_2) + y_4(1 \ast 1) = 2y_2^2 + y_4
\]

implies that

\[
H_n(2)^2 = 2H_n(2, 2) + H_n(4) \quad \text{and} \quad \zeta(2)^2 = 2\zeta(2, 2) + \zeta(4).
\]
Conjectures on MZVs

How many MZVs of weight $w \geq 2$ are there?
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$$\left\{ (s_1, \ldots, s_d) \in (\mathbb{N}^*)^d : d \geq 1, s_d \geq 2, \sum_{i=1}^{d} s_i = w \right\} = 2^{w-2}.$$
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Let $\mathcal{Z}_w$ be the $\mathbb{Q}$-vector space generated by the MZVs of weight $w \geq 2$. What is the dimension of $\mathcal{Z}_w$?
Conjectures on MZVs

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\]

Let \( Z_w \) be the \( \mathbb{Q} \)-vector space generated by the MZVs of weight \( w \geq 2 \). What is the dimension of \( Z_w \)?

**Dimension Conjecture** [Zagier, 1993].

Set \( d_0 = 1, d_1 = 0, d_2 = 1 \) and

\[
d_w = d_{w-2} + d_{w-3} \quad \forall w \geq 3.
\]

Then \( \dim(Z_w) = d_w \) for \( w \geq 2 \).

It is known that \( \dim(Z_w) \leq d_w \), but there is not a single value of \( k \geq 5 \) for which it is known that \( \dim(Z_w) > 1 \).
\[ \zeta_4 = \langle \zeta(4), \zeta(1, 3), \zeta(2, 2), \zeta(1, 1, 2) \rangle. \]

The following relations hold:

\[ \zeta(2)^2 = \left( \frac{\pi^2}{6} \right)^2 = \frac{5}{2} \left( \frac{\pi^4}{90} \right) = \frac{5}{2} \zeta(4), \]

\[ \zeta(1, 1, 2) = \zeta(4), \]

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\]

Therefore \( \mathcal{Z}_4 = \langle \zeta(2, 2) \rangle \) :

\[
\zeta(4) = \zeta(1, 1, 2) = \frac{4}{3} \zeta(2, 2) \quad , \quad \zeta(1, 3) = \frac{1}{3} \zeta(2, 2).
\]
**Basis Conjecture** [Hoffman, 1997].

$\mathcal{Z}_w$ has a basis consisting of

$$\left\{ \zeta(s) : |s| = w, s_i \in \{2, 3\} \text{ for } i \geq 1 \right\}.$$ 

\begin{align*}
d_2 &= 1, \quad \mathcal{Z}_2 = \langle \zeta(2) \rangle, \\
d_3 &= 1, \quad \mathcal{Z}_3 = \langle \zeta(3) \rangle, \\
d_4 &= 1, \quad \mathcal{Z}_4 = \langle \zeta(2, 2) \rangle, \\
d_5 &= 2, \quad \mathcal{Z}_5 = \langle \zeta(2, 3), \zeta(3, 2) \rangle \\
d_6 &= 2, \quad \mathcal{Z}_6 = \langle \zeta(2, 2, 2), \zeta(3, 3) \rangle, \\
d_7 &= 3, \quad \mathcal{Z}_7 = \langle \zeta(2, 2, 3), \zeta(2, 3, 2), \zeta(3, 2, 2) \rangle, \\
d_8 &= 4, \quad \mathcal{Z}_8 = \langle \zeta(2, 2, 2, 2), \zeta(2, 3, 3), \zeta(3, 2, 3), \zeta(3, 3, 2) \rangle, \\
d_9 &= 5, \quad \mathcal{Z}_9 = \langle \zeta(2, 2, 2, 3), \zeta(2, 2, 3, 2), \zeta(2, 3, 2, 2), \\
&\quad \quad \zeta(3, 2, 2, 2), \zeta(3, 3, 3) \rangle.
\end{align*}
Some of the elements of this basis can be expressed in terms of ordinary zeta values:

\[ \zeta(\{2\}^a) = (-1)^a [z^{2a+1}] \left( z \prod_{k=1}^{\infty} \left( 1 - \frac{z^2}{k^2} \right) \right) \]

\[ = (-1)^a [z^{2a+1}] \frac{\sin(\pi z)}{\pi} = \frac{\pi^{2a}}{(2a + 1)!}, \]

\[ \zeta(\{2\}^a, 3, \{2\}^b) = 2 \sum_{r=1}^{a+b+1} c_{r,a,b} \zeta(2r + 1) \zeta(\{2\}^{a+b+1-r}) \]

where \( c_{r,a,b} = (-1)^r \left( \binom{2r}{2a+2} - \left(1 - \frac{1}{4^r}\right) \binom{2r}{2b+1} \right). \]
[Wolstenholme, 1862] For every prime $p \geq 5$ we have

$$H_{p-1}(1) = 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{p-1} \equiv 0 \pmod{p^2}.$$
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$$H_{p-1}(1) = 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{p-1} \equiv 0 \pmod{p^2}.$$ 

[Zhou-Cai, 2007] Let $s, d \geq 1$ and $w = sd$. For every prime $p > w + 2$ we have

$$H_{p-1} \left( \{s\}^d \right) \equiv \begin{cases} (-1)^d \frac{s(w + 1)p^2}{2(w + 2)} B_{p-w-2} \pmod{p^3} & \text{if } 2 \nmid w, \\ (-1)^{d-1} \frac{sp}{w + 1} B_{p-w-1} \pmod{p^2} & \text{if } 2 \mid w. \end{cases}$$

Remark: by Clausen-von Staudt Theorem, the denominator of $B_{2n}$ is the product of primes $p$ such that $p - 1 \mid 2n$. 
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\[
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\]
Relations for MHSs

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\]

Relations for MHSs can be generated by using the stuffle product and the duality relation:

\[
H_{p-1}(s_1, \ldots, s_d) = \sum_{1 \leq k_1 < \ldots < k_d \leq p-1} \frac{1}{k_1^{s_1} \ldots k_d^{s_d}}
\]

\[
= \sum_{1 \leq k_d < \ldots < k_1 \leq p-1} \frac{1}{(p-k_1)^{s_1} \ldots (p-k_d)^{s_d}}
\]

\[
\equiv (-1)^{|s|} H_{p-1}(s_d, \ldots, s_1) \pmod{p}.
\]
Identities involving binomial coefficients

More relations can be obtained by using special binomial identities. For example, let us consider

$$\sum_{k=1}^{n} \frac{1}{k^2} = \sum_{1 \leq i \leq j \leq n} \frac{(-1)^{j-1}}{ij} \binom{n}{j}.$$ 

Since

$$(-1)^{j-1} \binom{p}{j} = (-1)^{j-1} \frac{p \cdot (p-1) \cdots (p-(j-1))}{j \cdot (j-1)!} \equiv \frac{p}{j} \pmod{p^2},$$

by the above identity, it follows that

$$H_{p-1}(2) = p \sum_{1 \leq i \leq j \leq p-1} \frac{1}{ij^2} = pH_{p-1}(1, 2) + pH_{p-1}(3) \pmod{p^2}.$$ 

Hence

$$H_{p-1}(1, 2) \equiv \frac{H_{p-1}(2)}{p} \equiv B_{p-3} \pmod{p}. $$
More binomial identities

[Kh. & T. Hessami Pilehrood and Tauraso, 2012] Let $a, b \geq 0$, $c \geq 2$ and $A_{n,k} = (-1)^{k-1} \binom{n}{k}/\binom{n+k}{k}$. Then

$$H_n^*(\{2\}^a, c, \{2\}^b) = 2 \sum_{k=1}^{n} \frac{A_{n,k}}{k^{2a+2b+c}}$$

$$+ 4 \sum_{\substack{i+j+|s|=c \\ i \geq 1, j \geq 2, |s| \geq 0}} 2^{d(s)} \sum_{k=1}^{n} \frac{A_{n,k} H_{k-1}(2a+i, s)}{k^{2b+j}},$$

where $d(s)$ is the depth of $s$ and

$$H_n^*(s_1, \ldots, s_d) := \sum_{1 \leq k_1 \leq k_2 \leq \ldots \leq k_d \leq n} \frac{1}{k_1^{s_1} k_2^{s_2} \ldots k_d^{s_d}}.$$
Let \( a, b \geq 0 \) and let \( p \) be a prime.
Then the following congruences hold modulo \( p \).
i) For \( p > w = 2a + 2b + 1 \),

\[
H_{p-1}(\{2\}^a, 1, \{2\}^b) \equiv \frac{4(-1)^{a+b}(a - b)(1 - 1/4^{a+b})}{(2a + 1)(2b + 1)} \begin{pmatrix} w - 1 \\ 2a \end{pmatrix} B_{p-w}.
\]

ii) For \( p > w = 2a + 2b + 3 \),

\[
H_{p-1}(\{2\}^a, 3, \{2\}^b) \equiv \frac{(-1)^{a+b}(a - b)}{(a + 1)(b + 1)} \begin{pmatrix} w - 1 \\ 2a + 1 \end{pmatrix} B_{p-w}.
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H_{p-1}(\{2\}^a, 3, \{2\}^b) \equiv \frac{(-1)^{a+b}(a - b)}{(a + 1)(b + 1)} \begin{pmatrix} w - 1 \\ 2a + 1 \end{pmatrix} B_{p-w}.
\]
Moreover, for any prime \( p > 9 \),
\[
H_{p-1}(1, 1, 1, 4) \equiv \frac{27}{16} B_{p-7} \pmod{p},
\]
\[
H_{p-1}(1, 1, 1, 6) \equiv \frac{1889}{648} B_{p-9} + \frac{1}{54} B_{p-3}^3 \pmod{p}.
\]
Conjectures on MHSs

For $n \geq 2$, define the commutative ring

$$\mathbb{Q}(n) := \{ a/b \in \mathbb{Q} : a/b \text{ is reduced and if a prime } p \mid b \text{ then } p \leq n \},$$

and the $\mathbb{Q}(n)$-module $\mathbf{M}(n) := \prod_{p > n} \mathbb{Z}_p$.

Let $H(s) := (H_{p-1}(s) \pmod{p})_{p > n} \in \mathbf{M}(n)$ for some $n \geq |s| + 2$.

Let $\mathcal{H}_w$ be the submodule generated by $H(s)$ of weight $|s| = w$.

What is the rank of $\mathcal{H}_w$?
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Let $H(s) := (H_{p-1}(s) \pmod{p})_{p > n} \in \mathcal{M}(n)$ for some $n \geq |s| + 2$. Let $\mathcal{H}_w$ be the submodule generated by $H(s)$ of weight $|s| = w$. What is the rank of $\mathcal{H}_w$?

**Dimension Conjecture** [Zagier-Zhao, 2013].

Set $r_0 = 1$, $r_1 = 0$, $r_2 = 0$ and

$$r_w = r_{w-2} + r_{w-3} \quad \forall w \geq 3.$$

Then $\text{rank}(\mathcal{H}_w) = r_w$ for $w \geq 1$. 
**Basis Conjecture** [Zhao, 2013].

$\mathcal{H}_w$ has a basis consisting of

$$\left\{ H(s) : |s| = w, s_1 = 1, s_2 = 2, s_i \in \{2, 3\} \text{ for } i \geq 3 \right\}.$$ 

For example,

- $r_1 = 0, \quad \mathcal{H}_1 = \langle 0 \rangle$,
- $r_2 = 0, \quad \mathcal{H}_2 = \langle 0 \rangle$,
- $r_3 = 1, \quad \mathcal{H}_3 = \langle H(1, 2) \rangle$,
- $r_4 = 0, \quad \mathcal{H}_4 = \langle 0 \rangle$,
- $r_5 = 1, \quad \mathcal{H}_5 = \langle H(1, 2, 2) \rangle$,
- $r_6 = 1, \quad \mathcal{H}_6 = \langle H(1, 2, 3) \rangle$,
- $r_7 = 1, \quad \mathcal{H}_7 = \langle H(1, 2, 2, 2) \rangle$,
- $r_8 = 2, \quad \mathcal{H}_8 = \langle H(1, 2, 2, 3), H(1, 2, 3, 2), H(1, 1, 1, 4) \rangle$,
- $r_9 = 2, \quad \mathcal{H}_9 = \langle H(1, 2, 3, 3), H(1, 2, 2, 2, 2), H(1, 1, 1, 6) \rangle$,
- $r_{10} = 3, \quad \mathcal{H}_{10} = \langle H(1, 2, 2, 2, 3), H(1, 2, 2, 3, 2), H(1, 2, 3, 2, 2), H(1, 1, 1, 1, 6), H(2, 2, 1, 4, 1) \rangle$. 
**Basis Conjecture** [Zhao, 2013].

\( \mathcal{H}_w \) has a basis consisting of

\[
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\]

For example,

\[
\begin{align*}
\mathcal{H}_1 &= \langle 0 \rangle, \\
\mathcal{H}_2 &= \langle 0 \rangle, \\
\mathcal{H}_3 &= \langle H(1, 2) \rangle, \\
\mathcal{H}_4 &= \langle 0 \rangle, \\
\mathcal{H}_5 &= \langle H(1, 2, 2) \rangle, \\
\mathcal{H}_6 &= \langle H(1, 2, 3) \rangle, \\
\mathcal{H}_7 &= \langle H(1, 2, 2, 2) \rangle, \\
\mathcal{H}_8 &= \langle H(1, 2, 2, 3), H(1, 2, 3, 2) \rangle, \\
\mathcal{H}_9 &= \langle H(1, 2, 3, 3), H(1, 2, 2, 2, 2) \rangle, \\
\mathcal{H}_{10} &= \langle H(1, 2, 2, 2, 3), H(1, 2, 2, 3, 2), H(1, 2, 3, 2, 2), H(1, 1, 1, 1, 6), H(2, 2, 1, 4, 1) \rangle.
\end{align*}
\]
More examples of series and similar congruences.

The following congruences hold modulo $p^3$, for any prime $p > 5$,

- [Tauraso, 2010]

$$\sum_{k=1}^{\infty} \frac{1}{k^2} \binom{2k}{k}^{-1} = \frac{1}{3} \zeta(2),$$

$$\sum_{k=1}^{\infty} \frac{(-1)^k}{k^3} \binom{2k}{k}^{-1} = -\frac{2}{5} \zeta(3),$$

$$\sum_{k=1}^{p-1} \frac{1}{k^2} \binom{2k}{k}^{-1} \equiv \frac{1}{3} \frac{H_{p-1}(1)}{p},$$

$$\sum_{k=1}^{p-1} \frac{(-1)^k}{k^3} \binom{2k}{k}^{-1} \equiv \frac{2}{5} \frac{H_{p-1}(1)}{p^2}.$$
More examples of series and similar congruences.

The following congruences hold modulo $p^3$, for any prime $p > 5$,

- [Tauraso, 2010]

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

$$\sum_{k=1}^{\infty} \frac{(-1)^k}{k^3} \binom{2k}{k}^{-1} = -\frac{2}{5} \zeta(3), \quad \sum_{k=1}^{p-1} \frac{(-1)^k}{k^3} \binom{2k}{k}^{-1} \equiv \frac{2}{5} \frac{H_{p-1}(1)}{p^2}.$$ 

- [Mattarei-Tauraso, 2012]

$$\sum_{k=1}^{\infty} \frac{(-1)^k}{k} \binom{2k}{k}^{-1} = -\frac{2 \sqrt{5} \ln(\phi)}{5},$$

$$p \sum_{k=1}^{p-1} \frac{(-1)^k}{k} \binom{2k}{k}^{-1} \equiv \frac{1 - L_p F_p}{2} - \frac{2 \sqrt{5} \zeta_2(\phi)}{5} p^2,$$

where $\phi = \frac{1+\sqrt{5}}{2}$ and $\zeta_2(x) = \sum_{k=1}^{p-1} \frac{x^k}{k^2}$. 

Roberto Tauraso

Analogies between MZVs and MHSs
That's all folks!