A note on poly-Bernoulli numbers and multiple zeta values

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Abstract. We review several occurrences of poly-Bernoulli numbers in various contexts, and discuss in particular some aspects of relations of poly-Bernoulli numbers and special values of certain zeta functions, notably multiple zeta values.
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INTRODUCTION

The poly-Bernoulli number $\mathbb{B}_n^{(k)}$ and its modification $C_n^{(k)}$ are defined for any integers $k \in \mathbf{Z}$ and $n \geq 0$ by the generating series

$$\frac{Li_k(1-e^{-x})}{1-e^{-x}} = \sum_{n=0}^{\infty} \mathbb{B}_n^{(k)} \frac{x^n}{n!} \quad \text{and} \quad \frac{Li_k(1-e^{-x})}{e^x-1} = \sum_{n=0}^{\infty} C_n^{(k)} \frac{x^n}{n!}$$

respectively[1]. Here, $Li_k(z)$ denotes the formal power series $\sum_{m=1}^{\infty} z^m/m^k$ (the kth polylogarithm when $k>0$ and the rational function $(z\,d/dz)^{-k}(z/(1-z))$ when $k \leq 0$). When $k=1$, these generating series become

$$\frac{xe^x}{e^x-1} \quad \text{and} \quad \frac{x}{e^x-1}\left(=\frac{xe^x}{e^x-1}-x\right),$$

and hence both $\mathbb{B}_n^{(k)}$ and $C_n^{(k)}$ generalize the classical Bernoulli numbers B_n, via choosing one of the conventions of the sign of $B_1 = \pm 1/2$.

These numbers were introduced in [11] and [4], and studied further in [5], [16], [1]. Most of these investigations are in line with the classical results of Clausen, von Staudt, and Kummer, or pursuits of connections with values of zeta functions. Recently however, the number $\mathbb{B}_n^{(k)}$ with negative k appeared in rather unexpected ways in [8] and [12] as cardinalities of some combinatorial objects.

In the present article, we take up yet other appearances of poly-Bernoulli numbers, namely Hoffman's multiple harmonic sums $\bmod p$ and special values of certain types of

[1] We use the notation $\mathbb{B}_n^{(k)}$ instead of $B_n^{(k)}$, which is often used for Carlitz's Bernoulli number of higher order.

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zeta functions, and discuss some aspects of relations between poly-Bernoulli numbers and multiple zeta values. We also review in the final section the above mentioned combinatorial interpretations of poly-Bernoulli number with negative index.

SPECIAL VALUES OF A CERTAIN ZETA FUNCTION AND MULTIPLE HARMONIC SUMS mod p

In [4], we studied the function $\xi_k(s)$ $(k \geq 1)$ defined by

$$\xi_k(s) := \frac{1}{\Gamma(s)} \int_0^\infty \frac{t^{s-1}}{e^t - 1} Li_k(1 - e^{-t}) dt.$$

The integral converges for $\mathrm{Re}(s) > 0$ and the function $\xi_k(s)$ is meromorphically continued to the whole s-plane. We obtained in [4] the following expression of $\xi_k(s)$ in terms of the (single variable) multiple zeta functions:

$$\begin{aligned}\xi_k(s) &= (-1)^{k-1}[\zeta(s,\underbrace{2,1,\ldots,1}_{k-1}) + \zeta(s,\underbrace{1,2,1,\ldots,1}_{k-1}) + \cdots + \zeta(s,\underbrace{1,\ldots,1,2}_{k-1}) \\ &\quad + s\cdot\zeta(s+1,\underbrace{1,\ldots,1}_{k-1})] + \sum_{j=0}^{k-2}(-1)^j \zeta(k-j)\cdot\zeta(s,\underbrace{1,\ldots,1}_{j}),\end{aligned} \tag{1}$$

where

$$\zeta(s_1,s_2,\ldots,s_n) := \sum_{m_1>m_2>\cdots>m_n>0} \frac{1}{m_1^{s_1} m_2^{s_2} \cdots m_n^{s_n}} \tag{2}$$

is the multiple zeta function (this is meromorphically continued to $\mathbf{C}^n$ ([2]), but we only need the single variable version with all arguments except for the first one fixed). In particular, the values of $\xi_k(s)$ at positive integer arguments (≥ 2) can be written as a linear combination (over $\mathbf{Z}$) of multiple zeta values (= values at positive integers of $\zeta(s_1,s_2,\ldots,s_n)$). As a by-product of his study of so-called Ohno's relation [14], Y. Ohno deduced from the above expression the following simple formula (we shift k by 1 for a reason explained later)

$$\xi_{k-1}(n) = \zeta^\star(k,\underbrace{1,\ldots,1}_{n-1}) \quad (k,n \geq 2), \tag{3}$$

where

$$\zeta^\star(k_1,k_2,\ldots,k_n) := \sum_{m_1\geq m_2\geq\cdots\geq m_n\geq 1} \frac{1}{m_1^{k_1} m_2^{k_2} \cdots m_n^{k_n}}$$

is the "non-strict" multiple zeta value (or multiple zeta-star value).

As for the values at negative integers, we obtained in [4] the formula

$$\xi_{k-1}(-n) = (-1)^n C_n^{(k-1)} \quad (n = 0,1,2,\ldots) \tag{4}$$

in terms of the modified poly-Bernoulli number.

Now, let p be an odd prime number. Following Hoffman [10], we denote by $S_{(k,1^{n-1})}(p-1)$ the finite sum obtained by truncating the series for $\zeta^\star(k,\underbrace{1,\ldots,1}_{n-1})$ right before the prime p enters into denominators:

$$S_{(k,1^{n-1})}(p-1) := \sum_{p-1\geq m_1\geq m_2\geq\cdots\geq m_n\geq 1}\frac{1}{m_1^k m_2\cdots m_n}.$$

If we use a closed formula for the modified poly-Bernoulli number $C_n^{(k)}$,

$$C_n^{(k)} = (-1)^n\sum_{i=0}^{n}(-1)^i\frac{i!\left\{ {n+1 \atop i+1} \right\}}{(i+1)^k}$$

($\left\{ {n+1 \atop i+1} \right\}$ = Stirling number of the second kind = the number of ways to partition a set of $n+1$ elements into $i+1$ nonempty subsets), which can be proved in a similar way as in [11] for the parallel formula for $\mathbb{B}_n^{(k)}$, we easily see that Hoffman's congruence (Theorem 5.4) in [10] is equivalent to the following congruence.

Theorem (Hoffman [10]). For $k,n\geq 1$ and any prime $p>n$, we have

$$S_{(k,1^{n-1})}(p-1) \equiv (-1)^n C_{p-1-n}^{(k-1)} \bmod p. \tag{5}$$

Combining this with the formula (4) for $\xi_{k-1}(-n)$, we obtain

$$S_{(k,1^{n-1})}(p-1) \equiv \xi_{k-1}(-p+1+n) \bmod p. \tag{6}$$

In view of the formula (3), this is quite amusing. That is to say, the value of $\xi_{k-1}(s)$ at positive n is the multiple zeta-star value $\zeta^\star(k,\underbrace{1,\ldots,1}_{n-1})$, and if we truncate this series to get $S_{(k,1^{n-1})}(p-1)$ and reduce it modulo p, then the resulting value is congruent $\bmod\, p$ to the value of $\xi_{k-1}(s)$ at $n-(p-1)$, the shift of n by $p-1$!

Through his study [10] and numerical experiments, Hoffman conjectures the sums $S_{(k,1^{n-1})}(p-1)$ are the "building blocks" of multiple harmonic sums $\bmod\, p$. To be more precise, he considers multiple harmonic sums of general type

$$\sum_{p-1\geq m_1\geq m_2\geq\cdots\geq m_n\geq 1}\frac{1}{m_1^{k_1}m_2^{k_2}\cdots m_n^{k_n}} \quad\text{or}\quad \sum_{p-1\geq m_1>m_2>\cdots>m_n\geq 1}\frac{1}{m_1^{k_1}m_2^{k_2}\cdots m_n^{k_n}} \quad (k_i\geq 1),$$

and he conjectures that all these general sums are congruent $\bmod\, p$ to a polynomial (with rational coefficients, independent of p) of "height 1" sums, i.e., a polynomial of $S_{(k,1^{n-1})}(p-1)$ with various k and n.

Hoffman also proved the duality

$$(-1)^k S_{(k,1^{n-1})}(p-1) \equiv (-1)^n S_{(n,1^{k-1})}(p-1) \bmod p.$$

This can be deduced via (5) from the duality (in $\mathbf{Z}$, not only $\bmod p$)

$$C_{n-1}^{(-k)} = C_{k-1}^{(-n)} \quad (k,n \geq 1)$$

of the modified poly-Bernoulli numbers of negative index (similarly proved as in the case of $\mathbb{B}_n^{(-k)}$, $\mathbb{B}_n^{(-k)} = \mathbb{B}_k^{(-n)}$ $(k,n \geq 0)$, given in [11]).

Recall the (easily proved) congruence of truncated Riemann zeta values

$$1 + \frac{1}{2^n} + \frac{1}{3^n} + \cdots + \frac{1}{(p-1)^n} \equiv 0 \bmod p$$

which is valid for all $p > n$. The above mentioned duality of Hoffman follows from this (as many of the congruences in [10] do) if the difference

$$(-1)^k S_{(k,1^{n-1})}(p-1) - (-1)^n S_{(n,1^{k-1})}(p-1)$$

is expressed as a polynomial in the truncated Riemann zeta values (Hoffman proved the duality in another way and we do not know if this is the case). Inspired by this and suggestive formulas (3), (6), we surmised that the difference of two multiple zeta-star values

$$(-1)^k \zeta^\star(k, \underbrace{1,\ldots,1}_{n-1}) - (-1)^n \zeta^\star(n, \underbrace{1,\ldots,1}_{k-1}) \tag{7}$$

may be written as a polynomial in the Riemann zeta values, and did numerical experiments which were in favor of this. Soon after the author had informed him of this speculation, Yasuo Ohno kindly pointed out that this was indeed the case. In fact, using (3) and (1) together with his main result in [14], we obtain

$$\begin{aligned}
&(-1)^k \zeta^\star(k, \underbrace{1,\ldots,1}_{n-1}) - (-1)^n \zeta^\star(n, \underbrace{1,\ldots,1}_{k-1}) \\
= \ &(n-1)\zeta(n+1, \underbrace{1,\ldots,1}_{k-2}) - (k-1)\zeta(k+1, \underbrace{1,\ldots,1}_{n-2}) \\
- \ &(-1)^k \sum_{j=1}^{k-2} (-1)^j \zeta(k-j) \zeta(n, \underbrace{1,\ldots,1}_{j-1}) + (-1)^n \sum_{j=1}^{n-2} (-1)^j \zeta(n-j) \zeta(k, \underbrace{1,\ldots,1}_{j-1}).
\end{aligned}$$

Since the multiple zeta values of height 1 (= of type $\zeta(m,1,\ldots,1)$) are polynomials in the Riemann zeta values ([3], [9], see also [15]), we conclude that the quantity (7) is a polynomial in the Riemann zeta values.

Note that the duality

$$\zeta(k+1, \underbrace{1,\ldots,1}_{n-1}) = \zeta(n+1, \underbrace{1,\ldots,1}_{k-1})$$

of multiple zeta values of height 1 does not hold for $\zeta^\star$-values as it stands, and no duality-like formula for $\zeta^\star$ is known so far. The assertion

$$(-1)^k \zeta^\star(k, \underbrace{1,\ldots,1}_{n-1}) - (-1)^n \zeta^\star(n, \underbrace{1,\ldots,1}_{k-1}) \in \mathbf{Q}[\zeta(2), \zeta(3), \zeta(5), \ldots]$$

may be regarded as a kind of duality (modulo the ring of Riemann zeta values $\mathbf{Q}[\zeta(2),\zeta(3),\zeta(5),\ldots]$). It may be of interest to note that the correspondence of indices

$$(k,\underbrace{1,\ldots,1}_{n-1}) \longleftrightarrow (n,\underbrace{1,\ldots,1}_{k-1})$$

here is different from the duality of usual multiple zeta values. (For this reason we shifted the index in (3).)

CENTRAL BINOMIAL SERIES

In this section we review another case of appearance of poly-Bernoulli numbers as special values of a certain type of zeta function.

Let $\zeta_{CB}(s)$ be the following Dirichlet series:

$$\zeta_{CB}(s) := \sum_{m=1}^{\infty} \frac{1}{m^s\binom{2m}{m}}.$$

This converges absolutely everywhere. It is shown in [6] that the value $\zeta_{CB}(k)$ for each positive integer $k \geq 2$ is written as a $\mathbf{Q}$-linear combination of multiple zeta values (of height 1) and multiple Clausen and Glaisher values. The latter two are real or imaginary parts (according to the parity of weights) of values at 6th root of unity of the multiple polylogarithm

$$Li_{k_1,\ldots,k_n}(z) := \sum_{m_1>\cdots>m_n>0} \frac{z^{m_1}}{m_1^{k_1}\cdots m_n^{k_n}}.$$

On the other hand, the value $\zeta_{CB}(k)$ for $k \leq 1$ is always a $\mathbf{Q}$-linear combination of 1 and $\pi/\sqrt{3}$. This is a result of D. H. Lehmer [13], who used the formula

$$\frac{2x\arcsin(x)}{\sqrt{1-x^2}} = \sum_{m=1}^{\infty} \frac{(2x)^{2m}}{m\binom{2m}{m}} \quad |x|<1$$

and its successive differentiations to derive it. More precisely, his result is as follows.

Define two sequences of polynomials $\{p_k(t)\}$ and $\{q_k(t)\}$ ($k=-1,0,1,2,\ldots$) by $p_{-1}(t)=0$, $q_{-1}(t)=1$ and the recursion

$$\begin{aligned} p_{k+1}(t) &= 2(kt+1)p_k(t)+2t(1-t)p_k'(t)+q_k(t), \\ q_{k+1}(t) &= (2(k+1)t+1)q_k(t)+2t(1-t)q_k'(t) \quad (k \geq -1). \end{aligned}$$

The first few are $p_0(t)=q_0(t)=1, p_1(t)=3, q_1(t)=2t+1, p_2(t)=8t+7, q_2(t)=4t^2+10t+1,\ldots$. Then we have for $k \geq -1$

$$\sum_{m=1}^{\infty} \frac{(2m)^k(2x)^{2m}}{\binom{2m}{m}} = \frac{x}{(1-x^2)^{k+3/2}}\left(x\sqrt{1-x^2}p_k(x^2)+\arcsin(x)q_k(x^2)\right)$$

and consequently

$$\zeta_{CB}(-k) = \frac{1}{3}\left(\frac{2}{3}\right)^k p_k\left(\frac{1}{4}\right) + \frac{1}{3}\left(\frac{2}{3}\right)^{k+1} q_k\left(\frac{1}{4}\right)\frac{\pi}{\sqrt{3}} \quad (k \geq -1). \tag{8}$$

This means that the values $\zeta_{CB}(-k)$ $(k \geq -1)$ all lie in the two dimensional $\mathbf{Q}$-vector space spanned by 1 and $\pi/\sqrt{3}$. This is reminiscent of the result of Euler for $\zeta(s)$. The values of $\zeta(s)$ at positive integers give variety of (conjecturally) transcendental numbers including powers of π (at even arguments), whereas the values at negative integers all lie in a one dimensional $\mathbf{Q}$-vector space ($\mathbf{Q}$ itself) and are explicitly described by the Bernoulli numbers.

Now, R. Stephan [17] observed that the rational part of this evaluation (8) is nothing but (the third of) the anti-diagonal sum of poly-Bernoulli numbers of negative indices:

$$\left(\frac{2}{3}\right)^k p_k\left(\frac{1}{4}\right) = \sum_{l=0}^{k} \mathbb{B}_{k-l}^{(-l)}.$$

This observation is still conjectural. A possible approach to a proof is to use an explicit formula given in [7].

We do not know whether the coefficient of $\pi/\sqrt{3}$ in (8) has any connection to poly-Bernoulli or allied numbers.

COMBINATORIAL INTERPRETATIONS OF POLY-BERNOULLI NUMBER WITH NEGATIVE INDEX

The numbers $\mathbb{B}_n^{(-k)}$ with $k,n \geq 0$ are positive integers ([11], [5], see also [16]). We end this article with two beautiful combinatorial interpretations of $\mathbb{B}_n^{(-k)}$ due to C. Brewbaker and S. Launois.

A *lonesum matrix* is a matrix with entries 0 and 1 whose row-sums and column-sums determine the matrix uniquely. For instance, the matrix $\begin{pmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 0 \end{pmatrix}$ gives ${}^t(1,2,1)$ and $(3,1)$ as row- and column-sums respectively, and from these two vectors, the original matrix is recovered uniquely. The theorem of Brewbaker states that the number of lonesum matrices of a given size is equal to the poly-Bernoulli number.

Theorem (Brewbaker [8]). *For $k,n \geq 1$, the number of $k \times n$ lonesum matrices is equal to $\mathbb{B}_n^{(-k)}$.*

The second interpretation of $\mathbb{B}_n^{(-k)}$ concerns the number of special type of permutations. Let $\mathfrak{S}_n$ denote the symmetric group of order n, which we identify with the set of all permutations on the set $\{1,2,\ldots,n\}$. S. Launois proved the following.

Theorem (Launois [12]). *Let k and n be positive integers. The cardinality of the set*

$$\{\sigma \in \mathfrak{S}_{k+n} | -k \leq \sigma(i) - i \leq n, 1 \leq \forall i \leq k+n\}$$

is equal to $\mathbb{B}_n^{(-k)}$.

Incidentally, either of these interpretations makes the aforementioned duality formula $\mathbb{B}_n^{(-k)} = \mathbb{B}_k^{(-n)}$ $(k, n \geq 0)$ apparent.

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