Relations for Nielsen polylogarithms (Dedicated to Richard Askey at 80)

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Abstract

Polylogarithms appear in many diverse fields of mathematics. Herein, we investigate relations amongst the restricted class of Nielsen-type (essentially, height one) polylogarithms, both generic and at special arguments including the sixth roots of unity. Numerical computations suggest that the collected relations, partially motivated by a previous study of the authors on log-sine integrals, are complete except in the case when the argument is the fundamental sixth root of unity. For use in other applications, all our results are implemented and accessible for use in symbolic computation or to facilitate numeric computation. In particular, the relations are explicitly exhibited in the case of low weights.

1 Introduction and preliminaries

It is very well-known that the polylogarithmic sums

$$\operatorname{Gl}_{2k}(\tau) := \operatorname{Re} \operatorname{Li}_{2k}(e^{i\tau}) = \sum_{n=1}^{\infty} \frac{\cos(n\tau)}{n^{2k}}$$
(1)

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reduce to polynomials in τ . For instance,

Gl₂(
$$\tau$$
) = $\sum_{n=1}^{\infty} \frac{\cos(n\tau)}{n^2} = \frac{\tau^2}{4} - \frac{\pi\tau}{2} + \frac{\pi^2}{6}$.

These are the simplest instances of (generic) relations among Clausen and Glaisher functions of Nielsen type (these terms will be defined below). In this note, we consider the entirety of these relations. Besides generic relations as above, we will be interested in additional relations at the special arguments $\pi/3$, $\pi/2$ and $2\pi/3$ because of their appearance in applications, see [BS11], both within mathematics (e.g., Apéry-like series for zeta values, multiple Mahler measure [BS13]) and physics (e.g., calculation of higher terms in ε -expansions of Feynman diagrams [DK01, KK10]). We should explicitly mention Broadhurst whose extensive work in [Bro99] on more general polylogarithms in the sixth root of unity, see (29), is indicated in Remark 3.9 and Remark 4.2.

In Sections 2 and 3, we will review the structure of log-sine integrals, and then make the motivating observation that all generic relations amongst Clausen and Glaisher functions of Nielsen type are consequences of previous results on the evaluation of log-sine integrals. The classical evaluation of (1) as a polynomial may then be seen as the special case of the general fact that all Glaisher functions of odd depth (and Nielsen type) may be expressed in terms of Glaisher functions of lower depth.

In [BS11], it was shown that (generalized) log-sine integrals can be expressed in terms of polylogarithms of Nielsen type. Since tools for working with polylogarithmic functions are of practical utility—for instance, in physics—this conversion had been implemented in various computer algebra systems. However, for the (optional) purpose of simplifying results as much as possible, many reductions of multiple polylogarithms were built into our program [BS11]. In particular, a table of reductions at low weight was included. As a consequence of the results herein, we have been able to (almost completely) replace this table by general reductions which also work for higher weight. Numerical computations up to weight 10 suggest that our set of reductions is complete, except in the case of polylogarithms at the (fundamental) sixth root of unity for which, as discussed in Section 4.1, additional relations exist. This suggests that, even for the very restricted class of Nielsen-type polylogarithms, a deeper analysis of the relations at the sixth root of unity remains to be done.

1.1 Preliminaries

In the following, we will denote the *multiple polylogarithm* as studied for instance in [BBK01] and [BBG04, Ch. 3] by

$$\operatorname{Li}_{a_1,\dots,a_k}(z) := \sum_{n_1 > \dots > n_k > 0} \frac{z^{n_1}}{n_1^{a_1} \cdots n_k^{a_k}}.$$
(2)

For our purposes, the a_1, \ldots, a_k will usually be positive integers and $a_1 \geq 2$ so that the sum converges for all $|z| \leq 1$. For example, $\operatorname{Li}_{2,1}(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^2} \sum_{j=1}^{k-1} \frac{1}{j}$. The usual notation will be used for repetitions so that, for instance, $\operatorname{Li}_{2,\{1\}^3}(z) = \operatorname{Li}_{2,1,1,1}(z)$. All such objects are generalizations of Euler's original dilogarithm $\operatorname{Li}_2(z)$ [AAR99, Lew81]. Note that $\operatorname{Li}_1(z) = -\log(1-z)$.

Moreover, *multiple zeta values* [BBG04, Ch. 3] are denoted by

$$\zeta(a_1,\ldots,a_k) := \mathrm{Li}_{a_1,\ldots,a_k}(1)$$

In addition, we consider the multiple Clausen functions (Cl) and multiple Glaisher functions (Gl) of depth k and weight $w = a_1 + \ldots + a_k$ defined as

$$\operatorname{Cl}_{a_1,\dots,a_k}(\tau) := \left\{ \begin{array}{ll} \operatorname{Im} \operatorname{Li}_{a_1,\dots,a_k}(e^{i\tau}) & \text{if } w \text{ even} \\ \operatorname{Re} \operatorname{Li}_{a_1,\dots,a_k}(e^{i\tau}) & \text{if } w \text{ odd} \end{array} \right\},$$
(3)

$$\operatorname{Gl}_{a_1,\dots,a_k}(\tau) := \left\{ \begin{array}{ll} \operatorname{Re}\operatorname{Li}_{a_1,\dots,a_k}(e^{i\tau}) & \text{if } w \text{ even} \\ \operatorname{Im}\operatorname{Li}_{a_1,\dots,a_k}(e^{i\tau}) & \text{if } w \text{ odd} \end{array} \right\}.$$
(4)

This notation goes back to [Lew81] where it is used in the case of depth 1. It will transpire at several occasions that, for the present purposes, a different convention concerning the sign of the Clausen and Glaisher functions, such as in [BBK01], would lead to more appealing formulas. However, we chose to keep the notation used above because of its comparably widespread use in the literature [DK01, CCS09].

Our focus will be on polylogarithms of the form $\operatorname{Li}_{n,\{1\}^k}(z)$ which are said to be of *Nielsen type* (these are polylogarithms of height one; with the height of a polylogarithm indexed by a_1, \ldots, a_k defined as the number of indices $j = 1, \ldots, k$ such that $a_j > 1$). Similar terminology is used for other polylogarithmic quantities such as Clausen and Glaisher functions of Nielsen type: $\operatorname{Cl}_{n,\{1\}^k}(\tau)$ and $\operatorname{Gl}_{n,\{1\}^k}(\tau)$. At some occasions we will use the notation

$$S_{n,p}(z) := \operatorname{Li}_{n+1,\{1\}^{p-1}}(z), \tag{5}$$

as in [KMR70] but shall prefer Li for the most part.

The following notion of reducibility will be used throughout this work: a Clausen value is said to be *(Nielsen) reducible* if it can be written as a linear combination of products of Nielsen-type Clausen values (at the same argument) of either lower weight or values of the same weight and lower depth. (As usual, the empty product is 1.) Here, coefficients are allowed to be polynomials with rational coefficients in π and zeta values $\zeta(k)$. The analogous terminology is used for Glaisher values.

For n = 1, 2, ... and $k \ge 0$, we consider the (generalized) log-sine integrals

$$\operatorname{Ls}_{n}^{(k)}(\sigma) := -\int_{0}^{\sigma} \theta^{k} \log^{n-1-k} \left| 2 \sin \frac{\theta}{2} \right| \,\mathrm{d}\theta.$$
(6)

The modulus is not needed for $0 \le \sigma \le 2\pi$. For k = 0 these are the (basic) log-sine integrals $\operatorname{Ls}_n(\sigma) := \operatorname{Ls}_n^{(0)}(\sigma)$.

Our other notation and usage is largely consistent with that in [Lew81] and that in the newly published DLMF [OLBC10] in which most of the requisite material is described.

2 Evaluations of log-sine integrals

Before recalling some facts about log-sine integrals at general argument, we include an appealing and direct expression for (ordinary) log-sine integrals at argument π . This expression was observed by Richard Crandall in the course of working on [BBC13].¹

Remark 2.1. Crandall observed that, for $n \ge 1$,

$$\frac{(-1)^{n-1}}{n!}\operatorname{Ls}_{n+1}(\pi) = \pi \sum_{k=1}^{n} \frac{1}{k!} \sum_{\substack{m_1+\dots+m_k=n \ m_j>1}} \prod_{j=1}^{k} \frac{\alpha(m_j)}{m_j}$$
(7)

where $\alpha(n) := (1 - 2^{1-n})\zeta(n)$ is the alternating zeta function. The truth of this formula follows from the well-known exponential generating function, [Lew58, Lew81],

$$-\frac{1}{\pi}\sum_{m=0}^{\infty}\operatorname{Ls}_{m+1}(\pi)\frac{\lambda^{m}}{m!} = \frac{\Gamma(1+\lambda)}{\Gamma^{2}\left(1+\frac{\lambda}{2}\right)} = \binom{\lambda}{\lambda/2}$$
(8)

¹Richard Crandall's breadth of insights and skills will be sorely missed by his collaborators and others, see the obituary at http://experimentalmath.info/blog/2012/12/ mathematicianphysicistinventor-richard-crandall-dies-at-64/.

as well as the series

$$f(x) := \log \binom{x}{x/2} = \sum_{n \ge 2} \frac{\alpha(n)}{n} (-x)^n$$

for the logarithm of the central binomial coefficient. Since

$$-\frac{1}{\pi}\operatorname{Ls}_{n+1}(\pi) = \left[D_x^n e^{f(x)}\right]_{x=0},$$

it only remains to apply the general fact that if $g(x) = \sum_{n \ge 1} a(n) x^n$ then

$$e^{g(x)} = \sum_{k=0}^{\infty} \frac{g(x)^k}{k!} = 1 + \sum_{n=1}^{\infty} x^n \sum_{k=1}^n \frac{1}{k!} \sum_{\substack{m_1 + \dots + m_k = n \ m_j \ge 1}} \prod_{j=1}^k a(m_j).$$

We remark that, while Crandall's formula (7) is both beautiful and explicit, for computational purposes one prefers the corresponding recursion due to Lewin.

It would be interesting to determine if formulas similar to (7) can be given for more general log-sine integrals.

We now recollect a method, presented in [BS11] and originating with [Fuc61] and [BBK01], for evaluating the generalized log-sine integrals at arbitrary arguments in terms of Nielsen polylogarithms at related arguments.

Theorem 2.2. For $0 \le \tau \le 2\pi$, and nonnegative integers n, k such that $n - k \ge 2$,

$$\zeta(k+2,\{1\}^{n-k-2}) - \sum_{j=0}^{k} \frac{(-i\tau)^{j}}{j!} \operatorname{Li}_{k-j+2,\{1\}^{n-k-2}}(e^{i\tau})$$
$$= \sum_{r=0}^{n-k-1} \sum_{m=0}^{r} \frac{(-1)^{n-1}i^{k+r+1}2^{-r}(-\pi)^{r-m}}{k!m!(r-m)!(n-1-k-r)!} \operatorname{Ls}_{n-(r-m)}^{(k+m)}(\tau).$$
(9)

Proof. Starting with

$$\operatorname{Li}_{k,\{1\}^n}(\alpha) - \operatorname{Li}_{k,\{1\}^n}(1) = \int_1^\alpha \frac{\operatorname{Li}_{k-1,\{1\}^n}(z)}{z} \, \mathrm{d}z$$

and integrating by parts repeatedly, we obtain

$$\sum_{j=0}^{k-2} \frac{(-1)^j}{j!} \log^j(\alpha) \operatorname{Li}_{k-j,\{1\}^n}(\alpha) - \operatorname{Li}_{k,\{1\}^n}(1)$$
$$= \frac{(-1)^{k-2}}{(k-2)!} \int_1^\alpha \frac{\log^{k-2}(z) \operatorname{Li}_{\{1\}^{n+1}}(z)}{z} \, \mathrm{d}z.$$
(10)

Letting $\alpha = e^{i\tau}$ and changing variables to $z = e^{i\theta}$, as well as using

$$\operatorname{Li}_{\{1\}^n}(z) = \frac{(-\log(1-z))^n}{n!},$$

the right-hand side of (10) can be rewritten as

$$\frac{(-1)^{k-2}}{(k-2)!} \frac{i}{(n+1)!} \int_0^\tau (i\theta)^{k-2} \left(-\log\left(1-e^{i\theta}\right)\right)^{n+1} \,\mathrm{d}\theta.$$
(11)

Since, for $0 \le \theta \le 2\pi$ and the principal branch of the logarithm,

$$\log(1 - e^{i\theta}) = \log\left|2\sin\frac{\theta}{2}\right| + \frac{i}{2}(\theta - \pi),\tag{12}$$

this last integral can now be expanded in terms of generalized log-sine integrals at τ . A change of variables then yields the claim.²

We recall that the real and imaginary parts of the multiple polylogarithms yield Clausen and Glaisher functions as defined in (3) and (4).

Example 2.3 (Ls₄⁽¹⁾(τ)). Using (9) with n = 4, k = 1 and solving for Ls₄⁽¹⁾(τ) yields

$$Ls_{4}^{(1)}(\tau) = 2\zeta(3,1) - 2 \operatorname{Gl}_{3,1}(\tau) - 2\tau \operatorname{Gl}_{2,1}(\tau) + \frac{1}{4} Ls_{4}^{(3)}(\tau) - \frac{1}{2}\pi Ls_{3}^{(2)}(\tau) + \frac{1}{4}\pi^{2} Ls_{2}^{(1)}(\tau) = \frac{1}{180}\pi^{4} - 2 \operatorname{Gl}_{3,1}(\tau) - 2\tau \operatorname{Gl}_{2,1}(\tau) - \frac{1}{16}\tau^{4} + \frac{1}{6}\pi\tau^{3} - \frac{1}{8}\pi^{2}\tau^{2}.$$

For the last equality we used the trivial evaluation $\operatorname{Ls}_{n}^{(n-1)}(\tau) = -\frac{\tau^{n}}{n}$.

 \diamond

In general, we can use (9) recursively to express the log-sine values $Ls_n^{(k)}(\tau)$ in terms of multiple Clausen and Glaisher functions at τ . This approach was used in [BS11] to systematically evaluate log-sine integrals in terms of polylogarithms, and the requisite code is available, see [BS11] and Section 5.

²Here, as elsewhere, the chances of introducing error without using a computer algebra system to verify identity (9) are very high and such errors pervade the literature.

3 Generic relations for Nielsen polylogarithms

3.1 Initial examples and observations

We now reverse the way we apply Theorem 2.2. Instead of using it to evaluate logsine integrals in terms of Nielsen polylogarithms as outlined in Section 2 and studied in [BS11], we start with Nielsen polylogarithms and write them in terms of log-sine integrals. In this way, relations among the Nielsen polylogarithms are deduced. The basic idea is illustrated in the following example.

Example 3.1 (Glaisher evaluation). In each case, one application of Theorem 2.2 and reducing the terms $Ls_n^{(n-1)}(\tau)$ yields

$$Gl_{2,1}(\tau) = -\frac{1}{2} Ls_3(\tau) - \frac{\tau^3}{24} + \frac{\pi\tau^2}{8} - \frac{\pi^2\tau}{8},$$

$$Gl_{3,1}(\tau) = -\frac{1}{2} Ls_4^{(1)}(\tau) + \frac{\tau}{2} Ls_3(\tau) + \frac{\tau^4}{96} - \frac{\pi\tau^3}{24} + \frac{\pi^2\tau^2}{16} + \frac{\pi^4}{360},$$

$$Gl_{2,1,1}(\tau) = -\frac{1}{4} Ls_4^{(1)}(\tau) + \frac{\pi}{4} Ls_3(\tau) - \frac{\tau^4}{192} + \frac{\pi\tau^3}{48} - \frac{\pi^2\tau^2}{32} + \frac{\pi^3\tau}{48} + \frac{\pi^4}{90}.$$

We conclude that

$$Gl_{2,1,1}(\tau) = \frac{1}{2}Gl_{3,1}(\tau) + \frac{\tau - \pi}{2}Gl_{2,1}(\tau) + \frac{\tau^4}{96} - \frac{\pi\tau^3}{24} + \frac{\pi^2\tau^2}{16} - \frac{\pi^3\tau}{24} + \frac{7\pi^4}{720}$$
(13)

 \Diamond

which simplifies upon writing it in terms of $\sigma = \pi - \tau$ as in (19).

In general, there are n-1 Nielsen polylogarithms of weight n, namely the functions $\operatorname{Li}_{m+1,\{1\}^{n-m-1}}(e^{i\tau})$ for $m=1,2,\ldots,n-1$. That makes a total of 2n-2 Clausen and Glaisher functions of weight n and of Nielsen type. On the other hand, there are only n-1 log-sine integrals of weight n, namely $\operatorname{Ls}_{n}^{(k)}(\tau)$ with $k=0,1,\ldots,n-2$. Hence the method illustrated in Example 3.1 should provide n-1 relations among Clausen and Glaisher functions of weight n.

Indeed, we obtain a more precise statement by observing that $\operatorname{Ls}_n^{(k)}(\tau)$ evaluates in terms of Clausen functions if n + k is even and in terms of Glaisher functions otherwise. It follows that at odd weight n = 2m + 1 there are *m* relations among Clausen functions and *m* relations among Glaisher functions. For even weight n = 2m, on the other hand, there are m - 1 relations among Clausen functions and *m* relations.

These observations are a consequence of the following general theorem which uses the notion of reducibility defined in Section 1: Theorem 3.2 (Clausen and Glaisher parity reduction).

- Nielsen-type Clausen functions of even depth are Nielsen reducible.
- Nielsen-type Glaisher functions of odd depth are Nielsen reducible.

The precise reductions implied by Theorem 3.2 will be deduced in the next subsection which also contains the corresponding proofs. We finish this subsection by making these reductions explicit for low weights. Additionally, we include all relations at the arguments $\pi/3$, $\pi/2$ and $2\pi/3$, as will be discussed in Section 4. Throughout, we assume that $0 < \tau < \pi$ and denote $\sigma := \pi - \tau$.

Example 3.3 (Weight 2). We have

$$Gl_2(\tau) = \frac{\sigma^2}{4} - \frac{\pi^2}{12}$$
(14)

 \Diamond

while the Clausen function $Cl_2(\tau)$ appears irreducible.

Example 3.4 (Weight 3). We have the two relations

$$Cl_{2,1}(\tau) = -\frac{1}{2}\sigma Cl_2(\tau) + \frac{1}{2}Cl_3(\tau) + \frac{\zeta(3)}{2},$$
(15)

$$Gl_3(\tau) = \frac{\pi^2 \sigma}{12} - \frac{\sigma^3}{12}.$$
 (16)

There appear to be no further general relations than these expected two. For the special arguments $\tau = \pi/3$, $\tau = \pi/2$ and $\tau = 2\pi/3$ we further find that $\operatorname{Cl}_3(\tau)$ can be expressed as a rational multiple of $\zeta(3)$. Namely, $\operatorname{Cl}_3(\pi/3) = \frac{1}{3}\zeta(3)$, $\operatorname{Cl}_3(\pi/2) = -\frac{3}{32}\zeta(3)$ and $\operatorname{Cl}_3(2\pi/3) = -\frac{4}{9}\zeta(3)$.

Correspondingly, for the Glaisher function: $\operatorname{Gl}_{2,1}\left(\frac{\pi}{3}\right) = \frac{\pi^3}{324}$.

Example 3.5 (Weight 4). We have the three relations

$$Cl_{3,1}(\tau) = \frac{1}{2}\sigma Cl_{3}(\tau) + Cl_{4}(\tau) - \frac{\zeta(3)\sigma}{2},$$
(17)

$$Gl_4(\tau) = -\frac{\sigma^4}{48} + \frac{\pi^2 \sigma^2}{24} - \frac{7\pi^4}{720},$$
(18)

$$Gl_{2,1,1}(\tau) = -\frac{1}{2}\sigma Gl_{2,1}(\tau) + \frac{1}{2}Gl_{3,1}(\tau) + \frac{\sigma^4}{96} - \frac{\pi^4}{1440}.$$
 (19)

For the special argument $\tau = \pi/3$ we find the additional relations

$$\operatorname{Cl}_{2,1,1}\left(\frac{\pi}{3}\right) = \operatorname{Cl}_4\left(\frac{\pi}{3}\right) - \frac{\pi^2}{18}\operatorname{Cl}_2\left(\frac{\pi}{3}\right) - \frac{\pi}{9}\zeta(3) \tag{20}$$

and $\text{Gl}_{3,1}\left(\frac{\pi}{3}\right) = -\frac{23\pi^4}{19440}$. No such relations appear to exist for other special arguments. The reason why additional relations exist at $\pi/3$ is discussed in Section 4.1.

Example 3.6 (Weight 5). We have the four relations

$$Cl_{4,1}(\tau) = -\frac{1}{2}\sigma Cl_4(\tau) + \frac{3}{2}Cl_5(\tau) - \frac{\zeta(3)\sigma^2}{4} + \frac{\zeta(5)}{2} + \frac{\pi^2\zeta(3)}{12},$$
 (21)

$$Cl_{2,1,1,1}(\tau) = -\frac{1}{24}\sigma^{3} Cl_{2}(\tau) + \frac{1}{8}\sigma^{2} Cl_{3}(\tau) - \frac{1}{2}\sigma Cl_{2,1,1}(\tau) + \frac{1}{4}\sigma Cl_{4}(\tau) + \frac{1}{4}\sigma Cl_{4}(\tau) + \frac{1}{4}Cl_{3,1,1}(\tau) - \frac{1}{4}Cl_{5}(\tau) + \frac{\zeta(5)}{2} - \frac{\pi^{2}\zeta(3)}{2},$$
(22)

$$Gl_{5}(\tau) = \frac{\sigma^{5}}{240} - \frac{\pi^{2}\sigma^{3}}{72} + \frac{7\pi^{4}\sigma}{720},$$
(23)

$$Gl_{3,1,1}(\tau) = \frac{1}{2}\sigma Gl_{3,1}(\tau) + Gl_{4,1}(\tau) - \frac{\sigma^5}{480} + \frac{\pi^4\sigma}{1440}.$$
 (24)

At special arguments we have $\operatorname{Cl}_5\left(\frac{\pi}{3}\right) = \frac{25}{54}\zeta(5)$, $\operatorname{Cl}_5\left(\frac{\pi}{2}\right) = -\frac{15}{512}\zeta(5)$, $\operatorname{Cl}_5\left(\frac{2\pi}{3}\right) = -\frac{40}{81}\zeta(5)$ as well as the evaluation of $\operatorname{Cl}_{3,1,1}\left(\frac{\pi}{3}\right)$, given in Example 4.7, and $\operatorname{Gl}_{2,1,1,1}\left(\frac{\pi}{3}\right) = -\frac{\pi^5}{58320}$.

Example 3.7 (Weight 6). There are five generic relations which reduce $Cl_{5,1}(\tau)$, $Cl_{3,1,1,1}(\tau)$, $Gl_6(\tau)$, $Gl_{4,1,1}(\tau)$, $Gl_{2,1,1,1,1}(\tau)$. See Example 5.2 for $Cl_{5,1}(\tau)$. Additionally, for special arguments, we have

$$\operatorname{Cl}_{2,1,1,1,1}\left(\frac{\pi}{3}\right) = \frac{\pi^4 \operatorname{Cl}_2\left(\frac{\pi}{3}\right)}{1944} - \frac{1}{18}\pi^2 \operatorname{Cl}_4\left(\frac{\pi}{3}\right) + \operatorname{Cl}_6\left(\frac{\pi}{3}\right) - \frac{25\pi\zeta(5)}{162} + \frac{\pi^3\zeta(3)}{486}, \quad (25)$$

as well as reductions for $\operatorname{Cl}_{4,1,1}\left(\frac{\pi}{3}\right)$ and $\operatorname{Gl}_{5,1}\left(\frac{\pi}{3}\right)$, given in Example 4.8, and $\operatorname{Gl}_{3,1,1,1}\left(\frac{\pi}{3}\right)$, given in Example 4.7.

3.2 Proof of generic relations

The fact that Nielsen polylogarithms can be expressed in terms of log-sine integrals (and vice versa) was used in the previous section to explain that 'half' of the Clausen and Glaisher functions reduce. The actual reductions follow from solving very simple linear systems of equations as in Example 3.1. Using a general relation amongst Nielsen polylogarithms at arguments x and 1/x due to Nielsen [Nie09] these reductions can be made entirely explicit. Nice references discussing and extending Nielsen's original results are [KMR70] and [Köl86] which also correct many misprints in the literature.

The following is a fully explicit and effective version of Theorem 3.2.

Theorem 3.8 (Effective reduction). Let $n \ge 1$ be an integer and $0 < \tau < \pi$. Let $\varepsilon_m = 1$ if m is even and $\varepsilon_m = 0$ otherwise. For even p,

$$2 \operatorname{Gl}_{n,\{1\}^{p}}(\tau) = -\sum_{s=1}^{p} \sum_{r=0}^{s} \frac{(\tau - \pi)^{r}}{r!} \binom{n + s - r - 2}{s - r} (-1)^{s + nr + \lfloor r/2 \rfloor} \operatorname{Gl}_{n + s - r,\{1\}^{p - s}}(\tau) - \sum_{r=0}^{n-2} \varepsilon_{n+r} (-1)^{p + \lfloor r/2 \rfloor} \frac{(\tau - \pi)^{r}}{r!} C_{n-r-1,p+1} - (-1)^{\lfloor \frac{n+p}{2} \rfloor} \frac{(\tau - \pi)^{n+p}}{(n+p)!}.$$

For odd p,

$$2 \operatorname{Cl}_{n,\{1\}^{p}}(\tau) = -\sum_{s=1}^{p} \sum_{r=0}^{s} \frac{(\tau - \pi)^{r}}{r!} \binom{n + s - r - 2}{s - r} (-1)^{s + nr + \lfloor r/2 \rfloor} \operatorname{Cl}_{n + s - r,\{1\}^{p - s}}(\tau) - \sum_{r=0}^{n-2} \varepsilon_{n+r} (-1)^{p + \lfloor r/2 \rfloor} \frac{(\tau - \pi)^{r}}{r!} C_{n-r-1,p+1}.$$

Here, the numbers $C_{n,p}$, defined below in the proof, can be expressed in terms of (depth-one) zeta values.

Proof. The key ingredient is a relation among Nielsen polylogarithms of argument z and argument 1/z due to Nielsen [Nie09]. In [Köl86, Section 5.2], it is shown that

$$S_{n,p}(z) = (-1)^{n} \sum_{s=0}^{p-1} (-1)^{s} \sum_{r=0}^{s} \frac{\log^{r}(-z)}{r!} {n+s-r-1 \choose s-r} S_{n+s-r,p-s}\left(\frac{1}{z}\right) + (-1)^{p} \left\{ \sum_{r=0}^{n-1} \frac{\log^{r}(-z)}{r!} C_{n-r,p} + \frac{\log^{n+p}(-z)}{(n+p)!} \right\}$$
(26)

where $S_{n,p}$ is as in (5),

$$C_{n,p} := (1 - (-1)^n) \,\sigma_{n,p} - (-1)^n \sum_{s=1}^{p-1} \binom{n+s-1}{s} \sigma_{n+s,p-s}$$

$$\sigma_{n,p} := (-1)^p S_{n,p} (-1).$$

In equation (26), the logarithm is understood to take its principal value and it is assumed that $\text{Im } z \neq 0$ (although the case that z is real is similar and is also discussed in [Köl86]). Therefore, with $z = e^{i\tau}$, $\log(-z) = i(\tau - \pi)$. Moreover,

$$S_{n,p}\left(\frac{1}{z}\right) = \overline{S_{n,p}\left(z\right)}$$

so that taking the real (or imaginary) part of both sides of (26) results in an identity for Clausen or for Glaisher functions. The results are the two asserted identities.

To see that the numbers $C_{n,p}$ can be expressed in terms of zeta values, note the evaluation

$$(-1)^{n}C_{n,p} = (-1)^{\lfloor \frac{n+p}{2} \rfloor} \varepsilon_{n+p} \frac{\pi^{n+p}}{(n+p)(n-1)!p!} - \sum_{k=0}^{p-1} \sum_{j=0}^{\lfloor \frac{n+k-1}{2} \rfloor} (1-(-1)^{n} \delta_{k0}) \binom{n+k-1}{k} \frac{(-1)^{p+k+j} \pi^{2j}}{(2j)!} S_{n+k-2j,p-k}(1),$$

given in [Köl86, Theorem 1], in which δ is denoting the Kronecker symbol and $\varepsilon_m = 1$ if m is even and $\varepsilon_m = 0$ otherwise. It then only remains to recall that Nielsen polylogarithms $S_{n,p}(1)$ evaluate as linear combinations of products of depth-one zeta values and π with rational coefficients, see [Köl82].

Remark 3.9. We note that Theorem 3.8 is an explicit instance of a—largely conjectural—general phenomenon observed, for instance, in [Bro99, Sec. 6.2.4]. Broadhurst considers polylogarithms of the kind (29) with each argument z_j a sixth root of unity. For such a polylogarithm of depth k and weight w, Broadhurst notes that, in each example, a reduction of the real part exists when w - k is odd, and of the imaginary part when w - k is even. In the special case of Euler–Zagier sums, that is when all the z_j are ± 1 , this reduces to the *parity conjecture*, stating that Euler–Zagier sums always reduce when w - k is odd. As reported in [Bro99], massive use of computer algebra has proven this for weights up to 8.

4 Nielsen polylogarithms at special values

Of particular interest are the values of Clausen and Glaisher functions at the special arguments $\pi/3$, $\pi/2$ and $2\pi/3$. Also, in the very interesting cases of arguments 0 or π one is looking at polylogarithms at 1 and -1, respectively.

and

- 1. Nielsen polylogarithms at 1 completely reduce to (depth-one) zeta values. This is made explicit in [Köl82].
- 2. The situation for Nielsen polylogarithms at -1 is as follows. In the depth-one case, one has the classical

$$\operatorname{Li}_{n}(-1) = -(1 - 2^{1-n})\zeta(n)$$

Further, equation (26) also holds for z = -1 and allows us to reduce $S_{n,p}(-1)$ whenever n is odd. Numerical computations up to weight 10 indicate that these are the only relations.

3. For Clausen and Glaisher functions at argument $2\pi/3$, computations up to weight 10 suggest that, apart from the parity reductions of Theorem 3.8, the only source of relations is the identity

$$\operatorname{Cl}_{n}\left(\frac{2\pi p}{q}\right) = \frac{1}{q^{n}} \sum_{k=1}^{q} \zeta\left(n, \frac{k}{q}\right) \left[\frac{1 + (-1)^{n}}{2} \sin\left(\frac{2k\pi p}{q}\right) + \frac{1 - (-1)^{n}}{2} \cos\left(\frac{2k\pi p}{q}\right)\right]$$
(27)

for integers $1 \le p < q$; which is a specialized form [CCS09] of results in [CK95]. Log-sine integrals at $2\pi/3$ are notoriously less tractable than those at $\pi/3$.

4. The same statement applies to Clausen and Glaisher functions at argument $\pi/2$. In this case, (27) implies that, for odd n,

$$\operatorname{Cl}_n\left(\frac{\pi}{2}\right) = \frac{1-2^{n-1}}{2^{2n-1}}\zeta(n).$$

5. The richest setting is that of $\pi/3$ discussed in detail in the next subsection.

4.1 Relations at the sixth root of unity

Throughout, $\omega = e^{i\pi/3}$ will denote the fundamental sixth root of unity. It is the fact that $1 - \omega = \bar{\omega}$ which explains the remarkable wealth of additional relations for polylogarithms at ω .

For instance, the depth-one Clausen functions at $\pi/3$ reduce [Lew81, Section 7.3.3] as

$$\operatorname{Cl}_{2n+1}\left(\frac{\pi}{3}\right) = \frac{1}{2}(1-2^{-2n})(1-3^{-2n})\zeta(2n+1).$$
 (28)

This is another special case of identity (27).

Remark 4.1. We briefly note the values of Nielsen-type polylogarithms at all sixth roots of unity, in light of [BS11], may be expressed in terms of values at ω and ω^2 . \diamond

Remark 4.2. For the importance of polylogarithms at the sixth root unity in the physics of Feynman diagrams we refer to [Bro99] and [KK10]. In [Bro99] much more general polylogarithms involving the sixth root of unity are studied. Indeed, generalizing (2) to

$$\zeta \begin{pmatrix} a_1, \ \dots, \ a_k \\ z_1, \ \dots, \ z_k \end{pmatrix} := \sum_{n_1 > \dots > n_k > 0} \frac{z_1^{n_1} \cdots z_k^{n_k}}{n_1^{a_1} \cdots n_k^{a_k}}, \tag{29}$$

Broadhurst investigates relations among real and imaginary parts of these polylogarithms when each of the z_j are sixth roots of unity. Besides the usual depth-length and weight-length shuffle relations, there are further relations owing to the special properties of the sixth roots of unity, such as the mentioned $1 - \omega = \bar{\omega}$. Thus equipped, Broadhurst deduces all relations among such polylogarithms of weight 3, apart from a single remaining relation which is found by PSLQ but left unproven; similarly, the relations at weight 4 are considered but the study is restricted to depth at most 2, as this is sufficient for the quantum field theoretic considerations of [Bro99].

Relations between multiple polylogarithms at (not necessarily sixth) roots of unity were further studied in [ABS11, Section VI], where these sums arise as the limiting case of (generalized) multiple harmonic sums. Explicit relations are obtained for weights 1 and 2. \diamond

Remark 4.3. The generating function for Nielsen polylogs at the sixth root of unity,

$$\sum_{n,p\geq 1} S_{n,p}(\omega) x^n y^p = 1 - {}_2F_1 \begin{pmatrix} -x, y \\ 1-x \end{vmatrix} \omega \end{pmatrix},$$
(30)

is recorded in [BBK01]. It leads to many curious infinite sums of Nielsen polylogarithms but as the authors of [BBK01] note "is not a very convenient equation for extracting coefficients or proving formulas". Formula (30) may be extended to general argument, see [KMR70]. \diamond

We now turn to a set of reductions at argument ω which may be thought of as corresponding to the famous special case

$$\zeta(2, \{1\}^{n-1}) = \zeta(n+1)$$

of MZV duality [BBBL01].

Theorem 4.4 (Closed forms at $\pi/3$). For any integer $n \ge 1$,

$$\operatorname{Gl}_{2,\{1\}^{n-1}}\left(\frac{\pi}{3}\right) = -(-1)^{n+\lfloor n/2 \rfloor} \frac{(\pi/3)^{n+1}}{2(n+1)!}.$$
(31)

For odd $n \geq 1$,

$$\operatorname{Cl}_{2,\{1\}^{n-1}}\left(\frac{\pi}{3}\right) = -\sum_{m=0}^{n-1} (-1)^{\lfloor \frac{m-1}{2} \rfloor} \frac{(\pi/3)^m}{m!} \operatorname{Cl}_{n-m+1}\left(\frac{\pi}{3}\right).$$
(32)

Note that half of the Clausen functions on the right-hand side of (32) reduce further according to (28). A formula similar to (32) holds for even n. It is omitted here because, by Theorem 3.8, Clausen functions of even depth always reduce.

Proof. Equation (31) is a special case of [BBK01, Theorem 4.5] where two proofs are given. Alternatively, one may combine equation (33) below with the classical

$$\operatorname{Gl}_n(2\pi\tau) = -(-1)^{\lfloor n/2 \rfloor} \frac{2^{n-1}}{n!} B_n(\tau) \pi^n$$

that may be found in [Lew81, Section 7.5.3]. Here, $B_n(\tau)$ denote Bernoulli polynomials. Recall that

$$\operatorname{Li}_{2,\{1\}^{n-1}}(x) = \int_0^x \operatorname{Li}_{\{1\}^n}(t) \frac{\mathrm{d}t}{t}$$

It follows that

$$\operatorname{Li}_{2,\{1\}^{n-1}}(x) = \frac{(-1)^n}{n!} \int_0^x \log(1-t)^n \frac{\mathrm{d}t}{t}$$
$$= \zeta(n+1) - \sum_{m=0}^n \frac{(-1)^{n-m}}{(n-m)!} \log(1-x)^{n-m} \operatorname{Li}_{m+1}(1-x).$$
(33)

To obtain (32) it only remains to set $x = \omega$ and to take imaginary parts.

Example 4.5 (Special cases). In the case n = 3 equation (33) takes the form

$$\operatorname{Li}_{2,1,1}(x) = \frac{\pi^4}{90} - \frac{1}{6}\log(1-x)^3\log x - \frac{1}{2}\log(1-x)^2\operatorname{Li}_2(1-x) + \log(1-x)\operatorname{Li}_3(1-x) - \operatorname{Li}_4(1-x),$$
(34)

as exploited in [BBSW12]. Observe that (34) together with the fact that $1 - \omega = \bar{\omega}$ reveals the additional relation (20) that exists for $\operatorname{Cl}_{2,1,1}\left(\frac{\pi}{3}\right)$.

Finally, we have the following result which yields further reductions at $\pi/3$. In [Köl86, (5.1)] this is given as a functional relation among Nielsen polylogarithms at arguments z and 1 - z.

Theorem 4.6 ([Köl86, (5.1)], [BBK01, Theorem 4.4]). For nonnegative integers a, b, we have

$$\zeta(a+2,\{1\}^b) + \frac{(-1)^a(i\pi/3)^{a+b+2}}{(a+1)!(b+1)!}$$

$$= \sum_{r=0}^a \frac{(-i\pi/3)^r}{r!} \operatorname{Li}_{a+2-r,\{1\}^b}(\omega) + \sum_{r=0}^b \frac{(i\pi/3)^r}{r!} \operatorname{Li}_{b+2-r,\{1\}^a}(\bar{\omega}).$$
(35)

Theorem 4.6 implies "duality relations": a Clausen function $\operatorname{Cl}_{a+2,\{1\}^b}\left(\frac{\pi}{3}\right)$ may be expressed in terms of its dual $\operatorname{Cl}_{b+2,\{1\}^a}\left(\frac{\pi}{3}\right)$ modulo terms of lower weight. The same is true for Glaisher functions. For them, Theorem 4.6 in fact has the added benefit of reducing any self-dual term $\operatorname{Gl}_{a+2,\{1\}^a}\left(\frac{\pi}{3}\right)$. (When a = b, equation (35) is real, so there is no analog for Clausen functions).

Example 4.7 (Consequences of Theorem 4.6). Using Theorem 4.6 we are thus able to deduce a host of reductions, as defined in Section 1, for Clausen and Glaisher functions at $\pi/3$. Specifically, we may reduce $\operatorname{Cl}_{a+2,\{1\}^b}\left(\frac{\pi}{3}\right)$ whenever b > a and $\operatorname{Gl}_{a+2,\{1\}^b}\left(\frac{\pi}{3}\right)$ whenever $b \ge a$. We obtain, for instance,

$$Cl_{3,1,1}\left(\frac{\pi}{3}\right) = -\frac{1}{3}\pi Cl_4\left(\frac{\pi}{3}\right) + \frac{29\zeta(5)}{36} + \frac{\pi^2\zeta(3)}{108},$$
$$Gl_{3,1,1,1}\left(\frac{\pi}{3}\right) = -\frac{1}{3}\pi Gl_{4,1}\left(\frac{\pi}{3}\right) - Gl_{5,1}\left(\frac{\pi}{3}\right) - \frac{\zeta(3)^2}{2} + \frac{5741\pi^6}{7348320},$$

Note that we may also deduce the self-dual $\operatorname{Gl}_{3,1}\left(\frac{\pi}{3}\right) = -\frac{23\pi^4}{19440}$. While the Clausen value $\operatorname{Cl}_{4,1,1}\left(\frac{\pi}{3}\right)$ is self-dual as well, no reduction can be deduced from (35). Still, a reduction is possible in this case as is illustrated in the next example.

Unfortunately, the tools developed so far are not sufficient to deduce all Nielsen reductions symbolically. The next example shows some such Nielsen reductions that were found numerically. Finally, Remark 4.9 gives evidence that these are part of a family of reductions that it is not presented here. Naturally, it would be nice to find the general principle missed here.

Example 4.8 (Extra Clausen and Glaisher reductions). The following are additional relations up to weight 10 for Clausen values; and PSLQ suggests there are no others.

We find one additional Clausen relation at depth three and weight 6, 7, 9, and at depth five and weight 10:

$$Cl_{4,1,1}\left(\frac{\pi}{3}\right) = -\frac{1}{18}\pi^2 Cl_4\left(\frac{\pi}{3}\right) + 3 Cl_6\left(\frac{\pi}{3}\right) - \frac{29\pi\zeta(5)}{108} - \frac{11\pi^3\zeta(3)}{324},$$

$$Cl_{5,1,1}\left(\frac{\pi}{3}\right) = -\frac{2}{3}\pi Cl_6\left(\frac{\pi}{3}\right) + \frac{3229\zeta(7)}{1296} - \frac{25\pi^2\zeta(5)}{972} - \frac{17\pi^4\zeta(3)}{4860},$$

$$Cl_{7,1,1}\left(\frac{\pi}{3}\right) = -\pi Cl_8\left(\frac{\pi}{3}\right) + \text{zeta values},$$

$$Cl_{6,1,1,1,1}\left(\frac{\pi}{3}\right) = 4 Cl_{8,1,1}\left(\frac{\pi}{3}\right) - 21 Cl_{10}\left(\frac{\pi}{3}\right) + \text{lower order terms}.$$

Likewise, we find the additional Glaisher value relation $Gl_{5,1}\left(\frac{\pi}{3}\right) = \frac{209\pi^6}{918540} - \frac{\zeta(3)^2}{6}$ at depth 2 and weight 6, as well as at depth 4 and weights 9 and 10:

$$Gl_{6,1,1,1}\left(\frac{\pi}{3}\right) = -\frac{1}{18}\pi^2 Gl_{6,1}\left(\frac{\pi}{3}\right) + \frac{5}{6}\pi Gl_{7,1}\left(\frac{\pi}{3}\right) + 5 Gl_{8,1}\left(\frac{\pi}{3}\right) + \text{zeta values}$$
$$Gl_{7,1,1,1}\left(\frac{\pi}{3}\right) = -\frac{1}{18}\pi^2 Gl_{7,1}\left(\frac{\pi}{3}\right) - \pi Gl_{8,1}\left(\frac{\pi}{3}\right) + \frac{7}{2} Gl_{9,1}\left(\frac{\pi}{3}\right) + \text{zeta values}.$$

The next remark suggests these relations are part of a set of relations not explained by the identities presented here. But it is possible that for fixed depth this exceptional set is finite with low relative weight as is the case for MZV's [BBG04, Ch. 3]. \diamond

Remark 4.9 (Irreducible Clausen and Glaisher values). The first Glaisher function (of Nielsen type) at $\pi/3$ that appears to be Nielsen irreducible, with reducibility as defined in Section 1, is

$$Gl_{4,1}\left(\frac{\pi}{3}\right) = \sum_{n=1}^{\infty} \frac{\sum_{k=1}^{n-1} \frac{1}{k}}{n^4} \sin\left(\frac{n\pi}{3}\right)$$
(36)

which has weight 5. The only other presumed-irreducible Glaisher values of weight at most 10 are $\operatorname{Gl}_{k,1}\left(\frac{\pi}{3}\right)$ for k = 6, 7, 8, 9. Note that each Nielsen-type polylogarithm is determined by its weight and depth. Figure 1(b) thus gives a graphical representation of Nielsen-type Glaisher values up to weight 16 and their reducibility: the black dot in the upper left represents $\operatorname{Gl}_{4,1}\left(\frac{\pi}{3}\right)$; moving a square to the right increases the weight, while moving a square down increases the depth (while the weight remains constant). The square corresponding to a Glaisher value that is presumed-irreducible is colored black while squares of Nielsen reducible values are gray (light gray if their reduction follows from one of the relations presented here, and dark gray if the reduction does not, as in Example 4.8).

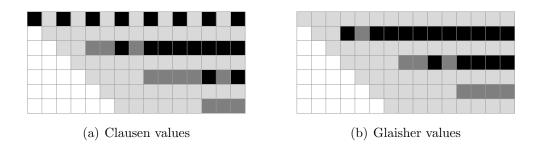


Figure 1: Presumed-irreducible values: weight 2-16 (columns) and depth 1-7 (rows)

Likewise, irreducible Clausen values are represented in Figure 1(a). Here, the upper left black square is $\operatorname{Cl}_2\left(\frac{\pi}{3}\right)$. The depth-one Clausen values $\operatorname{Cl}_{2n}\left(\frac{\pi}{3}\right)$ all appear Nielsen irreducible. Apart from these and up to weight 10, one only finds the two presumed-irreducible Clausen values $\operatorname{Cl}_{6,1,1}\left(\frac{\pi}{3}\right)$ and $\operatorname{Cl}_{8,1,1}\left(\frac{\pi}{3}\right)$ of weight 8 and 10.

Beautiful dimensional formulas for the spaces of irreducible Clausen and Glaisher values (not restricted to Nielsen type) are conjectured in [BBK01, Sec. 5]. \diamond

Remark 4.10. We close with commenting that our restriction to polylogarithms of Nielsen type is a very simplifying one which excludes some complicating phenomena. For instance, we have not observed (at least at weight up to 10) relations such as

$$\operatorname{Gl}_{2,2}\left(\frac{\pi}{3}\right) = \frac{107}{38880}\pi^4 - \operatorname{Cl}_2\left(\frac{\pi}{3}\right)^2$$

where Clausen and Glaisher values are mixed (or occur to higher powers). The above relation can be deduced from [BBK01, Theorem 4.4]. \diamond

5 Implementation

The results presented herein have been added to our $\operatorname{program}^3$ for the evaluation of log-sine integrals as described in [BS11].

Example 5.1. For instance, the evaluation of $\operatorname{Gl}_{3,1}\left(\frac{\pi}{3}\right)$, deduced in Example 4.7, is symbolically computed via

³The packages are freely available for download from http://arminstraub.com/pub/log-sine-integrals

LiReduce[G1[{3,1},Pi/3]]

which results in the output $-\frac{23\pi^4}{19440}$.

Example 5.2. Similarly, the generic reduction, with $\sigma = \pi - \tau$,

$$Cl_{5,1}(\tau) = \frac{1}{2}\sigma Cl_5(\tau) + 2Cl_6(\tau) + \frac{\zeta(3)\sigma^3}{12} - \frac{\zeta(5)\sigma}{2} - \frac{\pi^2\zeta(3)\sigma}{12}$$
(37)

may be symbolically obtained from

LiReduce[Cl[{5,1},tau]]

which yields the right-hand side of (37) with σ replaced by $\pi - \tau$.

Example 5.3. As discussed in Example 4.8 and Remark 4.9, the relations in this paper do not suffice to reduce all Nielsen-type polylogarithms. For the convenience of applications, we have therefore included a table of the additional reductions up to weight 16 which is used by default. To avoid use of this table one may call

```
LiReduce[Cl[{4,1,1},Pi/3], UseReductionTable->False]
```

which results in $\operatorname{Cl}_{4,1,1}\left(\frac{\pi}{3}\right)$ instead of its reduction recorded in Example 4.8.

Finally, we note that our symbolic reduction program also greatly facilitates numerical computation as it reduces the complexity of the objects to be calculated.

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