

COMPUTATION AND STRUCTURE OF CHARACTER POLYLOGARITHMS WITH APPLICATIONS TO CHARACTER MORDELL–TORNHEIM–WITTEN SUMS

D. H. BAILEY AND J. M. BORWEIN

ABSTRACT. This paper extends tools developed to study character polylogarithms. These objects are used to compute Mordell–Tornheim–Witten character sums and to explore their connections with multiple-zeta values (MZVs) and with their character analogues.

1. INTRODUCTION

In [10] we defined an ensemble of extended Mordell–Tornheim–Witten (MTW) zeta function values [7, 12, 18, 24, 25, 32, 34, 36, 38]. There is by now a huge body of literature on these sums; in part because of the many connections with fields such as combinatorics, number theory, and mathematical physics. Unlike previous authors we included *derivatives with respect to the order* of the terms. We investigated interrelations amongst MTW evaluations, and explored some deeper connections with multiple-zeta values (MZVs).

In this article we continue the research in [8, 10] by studying character polylogarithms and applying them to analyze the relations between MTW character sums defined by

$$(1) \quad \mu_{d_1, d_2}(q, r, s) := \sum_{n, m > 0} \frac{\chi_{d_1}(m) \chi_{d_2}(n)}{m^q n^r (m+n)^s},$$

where for $d > 2$, $\chi_{\pm d}(n) := \binom{\pm d}{n}$, and $\chi_{-2}(n) := (-1)^{n-1}$, $\chi_1(n) = 1$. When $d_1 = d_2 = 1$ these devolve to classical Mordell–Tornheim–Witten (MTW) sums, as defined in (2) below for $K = 2$.

1.1. Organization. The organization of this paper is as follows. In Section 2 we record necessary preliminaries regarding (generalized) MTW sums. In Section 3 we examine derivatives of the classical polylogarithm and zeta function. In Section 4 we introduce character polylogarithms (based on classical Dirichlet characters) and in Section 5 we use them to initiate the computational study of character MTW sums. In Section 6 we deduce various reductions, interrelations, and evaluations of our character MTW sums. Finally, in Section 7 we make some concluding remarks.

2. MORDELL–TORNHEIM–WITTEN SUMS

We first recall the definitions of Mordell–Tornheim–Witten (MTW) sums also called Mordell–Tornheim–Witten zeta function values.

Received by the editor February 25, 2014 and, in revised form, June 9, 2014 and June 18, 2014.
2010 *Mathematics Subject Classification*. Primary 11L40, 33F05.

2.1. **Classical MTW sums.** The multidimensional *MTW zeta function*

$$(2) \quad \omega(s_1, \dots, s_{K+1}) := \sum_{m_1, \dots, m_K > 0} \frac{1}{m_1^{s_1} \cdots m_K^{s_K} (m_1 + \cdots + m_K)^{s_{K+1}}}$$

enjoys known relations [29], but remains mysterious with respect to many combinatorial phenomena, especially when we contemplate derivatives with respect to the s_i parameters. We shall refer to $K + 1$ as the *depth* and $\sum_{j=1}^{K+1} s_j$ as the *weight* of ω .

The paper [7] introduced and discussed a novel *generalized MTW zeta function* for positive integers M, N and nonnegative integers s_i, t_j , with constraints $M \geq N \geq 1$, together with a polylogarithm-integral representation:

$$(3) \quad \omega(s_1, \dots, s_M \mid t_1, \dots, t_N) := \sum_{\substack{m_1, \dots, m_M, n_1, \dots, n_N > 0 \\ \sum_{j=1}^M m_j = \sum_{k=1}^N n_k}} \prod_{j=1}^M \frac{1}{m_j^{s_j}} \prod_{k=1}^N \frac{1}{n_k^{t_k}}$$

$$(4) \quad = \frac{1}{2\pi} \int_0^{2\pi} \prod_{j=1}^M \text{Li}_{s_j}(e^{i\theta}) \prod_{k=1}^N \text{Li}_{t_k}(e^{-i\theta}) \, d\theta.$$

Here the *polylogarithm of order s* denotes $\text{Li}_s(z) := \sum_{n \geq 1} z^n/n^s$ and its analytic extensions [28] and the (complex) number s is its *order*.

When some s -parameters are zero, there are convergence issues with this integral representation. One may, however, use principal-value calculus, or alternative representations given in [10] and expanded upon in Section 5.3.

When $N = 1$ the representation (4) devolves to the classic MTW form, in that

$$(5) \quad \omega(s_1, \dots, s_{M+1}) = \omega(s_1, \dots, s_M \mid s_{M+1}).$$

2.2. **Generalized MTW sums.** We also explored a wider *MTW ensemble* involving outer derivatives, introduced in [7], according to

$$(6) \quad \omega \left(\begin{array}{c|c} s_1, \dots, s_M & t_1, \dots, t_N \\ d_1, \dots, d_M & e_1, \dots, e_N \end{array} \right)$$

$$:= \sum_{\substack{m_1, \dots, m_M, n_1, \dots, n_N > 0 \\ \sum_{j=1}^M m_j = \sum_{k=1}^N n_k}} \prod_{j=1}^M \frac{(-\log m_j)^{d_j}}{m_j^{s_j}} \prod_{k=1}^N \frac{(-\log n_k)^{e_k}}{n_k^{t_k}}$$

$$(7) \quad = \frac{1}{2\pi} \int_0^{2\pi} \prod_{j=1}^M \text{Li}_{s_j}^{(d_j)}(e^{i\theta}) \prod_{k=1}^N \text{Li}_{t_k}^{(e_k)}(e^{-i\theta}) \, d\theta,$$

$$(8) \quad = \frac{1}{\pi} \text{Re} \int_0^\pi \prod_{j=1}^M \text{Li}_{s_j}^{(d_j)}(e^{i\theta}) \prod_{k=1}^N \text{Li}_{t_k}^{(e_k)}(e^{-i\theta}) \, d\theta,$$

where the s -th outer derivative of a polylogarithm is denoted $\text{Li}_s^{(d)}(z) := (\frac{\partial}{\partial s})^d \text{Li}_s(z)$. Thus, the effective computation of (7) requires really robust and efficient methods for computing $\text{Li}_s^{(d)}$ as were developed in [8, 10].

3. UNDERLYING SPECIAL FUNCTION TOOLS

We turn to the building blocks of our work:

3.1. Polylogarithms and their derivatives with respect to order. In regard to the needed polylogarithm values, [8] gives formulas such as those below.

Proposition 1. *When $s = n$ is a positive integer,*

$$(9) \quad \text{Li}_n(z) = \sum_{m=0}^{\infty}' \zeta(n - m) \frac{\log^m z}{m!} + \frac{\log^{n-1} z}{(n - 1)!} (H_{n-1} - \log(-\log z)),$$

is valid for $|\log z| < 2\pi$. Here $H_n := 1 + \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{n}$, and the primed sum \sum' means to avoid the singularity at $\zeta(1)$. For any complex order s not a positive integer,

$$(10) \quad \text{Li}_s(z) = \sum_{m \geq 0} \zeta(s - m) \frac{\log^m z}{m!} + \Gamma(1 - s)(-\log z)^{s-1}.$$

(This formula is valid for $s = 0$.)

In formula (9), the condition $|\log z| < 2\pi$ precludes its use when $|z| < e^{-2\pi} \approx 0.0018674$. For such small $|z|$, however, it typically suffices to use the definition

$$(11) \quad \text{Li}_s(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^s}.$$

Note that $\text{Li}_0(z) = z/(1 - z)$ and $\text{Li}_1(z) = -\log(1 - z)$. In fact, we found that formula (11) is generally faster than (9) whenever $|z| < 1/4$, at least for precision levels in the range of 100 to 4000 digits.

3.1.1. Outer derivatives of general polylogarithms. On carefully manipulating (10) for integer $k \geq 0$, we have for $|\log z| < 2\pi$ and $\tau \in [0, 1)$:

$$(12) \quad \text{Li}_{k+1+\tau}(z) = \sum_{0 \leq n \neq k} \zeta(k + 1 + \tau - n) \frac{\log^n z}{n!} + \frac{\log^k z}{k!} \sum_{j=0}^{\infty} c_{k,j}(\mathcal{L}) \tau^j$$

(see [21, §9, eqn. (51)]). Here $\mathcal{L} := \log(-\log z)$ and the c coefficients engage the *Stieltjes constants* γ_n , where $\gamma_0 = \gamma$ [21, §7.1; 26], which occur in the asymptotic expansion

$$\zeta(z) = \frac{1}{z - 1} + \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \gamma_n (z - 1)^n.$$

Precisely,

$$(13) \quad c_{k,j}(\mathcal{L}) = \frac{(-1)^j}{j!} \gamma_j - b_{k,j+1}(\mathcal{L}),$$

where the $b_{k,j}$ terms—corrected from [21, §7.1]—are given by

$$(14) \quad b_{k,j}(\mathcal{L}) := \sum_{\substack{p+t+q=j \\ p,t,q \geq 0}} \frac{\mathcal{L}^p \Gamma^{(t)}(1)}{p! t!} (-1)^t f_{k,q},$$

and $f_{k,q}$ is the coefficient of x^q in $\prod_{m=1}^k \frac{1}{1+x/m}$. This is calculable recursively via $f_{0,0} = 1, f_{0,q} = 0 (q > 0), f_{k,0} = 1 (k > 0)$ and

$$(15) \quad f_{k,q} = \sum_{h=0}^q \frac{(-1)^h}{k^h} f_{k-1,q-h}.$$

Above we used the functional equation for the Gamma function to remove singularities at negative integers. While (12) has little directly to recommend it computationally, it is highly effective in determining derivative values with respect or order, as we shall see in (16). To obtain, for example, the first derivative $\text{Li}_{k+1}^{(1)}(z)$, we differentiate (12) at zero and so require the evaluation $c_{k,1}$.

Theorem 1 (Derivatives for positive order). *Fix $k = 0, 1, 2 \dots$ and $m = 1, 2 \dots$. For $|\log z| < 2\pi$ and $\mathcal{L} = \log(-\log z)$ one has*

$$(16) \quad \text{Li}_{k+1}^{(m)}(z) = \sum_{0 \leq n \neq k} \zeta^{(m)}(k+1-n) \frac{\log^n z}{n!} + m! c_{k,m}(\mathcal{L}) \frac{\log^k z}{k!}.$$

In particular,

$$(17) \quad \text{Li}'_1(z) = \sum_{n=1}^{\infty} \zeta'(1-n) \frac{\log^n z}{n!} - \gamma_1 - \frac{1}{12} \pi^2 - \frac{1}{2} (\gamma + \log(-\log z))^2,$$

which, as before, is valid whenever $|\log z| < 2\pi$.

For $k = -1$, or, in other words, for $\text{Li}_0^{(m)}(z)$, things are simpler, as we may use (10):

Theorem 2 (Derivatives for zero order). *With $\Gamma^{(t)}(1)$ and $\mathcal{L} = \log(-\log z)$ as above for arbitrary z , we have for m any positive integer*

$$(18) \quad \text{Li}_0^{(m)}(z) = \sum_{n \geq 0} \zeta^{(m)}(-n) \frac{\log^n z}{n!} - \sum_{t=0}^m (-1)^t \binom{m}{t} \Gamma^{(t)}(1) \frac{\mathcal{L}^{m-t}}{\log z}.$$

Note that symmetric divided differences allow one to rapidly check (16) or (18) to moderate precision (say 50 digits).

3.2. Values of ζ and its derivatives at positive integer arguments. Effective use of formulas like (9) and (10) typically requires precomputed values of the zeta function and its derivatives at integer arguments (see [5, 19, 26]).

For positive integers, derivatives of the zeta function can be computed via a series-accelerated algorithm for derivatives of the *Dirichlet eta function* (or alternating zeta function), given as

$$(19) \quad \eta(s) := \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n^s} = (1 - 2^{1-s})\zeta(s).$$

For practical computation of eta or its derivatives, any of several alternating series acceleration schemes can be used. The corresponding values of zeta derivatives can then be found by solving (19) for $\zeta(s)$ and then taking formal derivatives, for example,

$$(20) \quad \zeta'(s) = \frac{\eta'(s)}{(1 - 2^{1-s})} - \frac{2^{1-s} \eta(s) \log 2}{(1 - 2^{1-s})^2}.$$

Example 1 (Alternating series acceleration [20, 21]). This is illustrated in the following *Mathematica* code (for argument `ss`, and precision `prec` digits):

```

zetaprime[ss_] :=
Module[{s, n, d, a, b, c}, n = Floor[1.5*prec]; d = (3 + Sqrt[8])^n;
  d = 1/2*(d + 1/d);
  {b, c, s} = {-1, -d, 0};
  Do[c = b - c;
    a = 1/(k + 1)^ss * (-Log[k + 1]);
    s = s + c*a;
    b = (k + n)*(k - n)*b/((k + 1)*(k + 1/2)), {k, 0, n - 1}];
  (s/d - 2^(1 - ss)*Log[2]*Zeta[ss])/(1 - 2^(1 - ss))

```

A similar approach works well for higher derivatives of zeta, although the resulting generalization of (20) becomes progressively more complicated. ◇

3.2.1. *Derivatives of ζ at zero and negative integer arguments.* The functional equation for the zeta function, $\zeta(s) = 2(2\pi)^{s-1} \sin \frac{\pi s}{2} \Gamma(1-s) \zeta(1-s)$, lets one extract $\zeta'(0) = -(\log 2\pi)/2$, and, for even $m = 2, 4, 6, \dots$,

$$(21) \quad \zeta'(-m) := \frac{d}{ds} \zeta(s)|_{s=-m} = \frac{(-1)^{m/2} m!}{2^{m+1} \pi^m} \zeta(m+1)$$

([21, p. 15]), while, for odd $m = 1, 3, 5, \dots$, on the other hand,

$$(22) \quad \zeta'(-m) = \zeta(-m) \left(\gamma + \log 2\pi - H_m - \frac{\zeta'(m+1)}{\zeta(m+1)} \right).$$

In [8, 10] we delineated methods more suited to higher derivatives at negative integers [5] showing for $n = 1, 2, \dots$, with $\kappa := -\log(2\pi) - \frac{1}{2}\pi i$, we have Apostol's finite summation formulas [33, (25.6.13) and (25.6.14)]:

(23a)

$$\begin{aligned}
 & (-1)^k \zeta^{(k)}(1-2n) \\
 &= \frac{2(-1)^n}{(2\pi)^{2n}} \sum_{m=0}^k \sum_{r=0}^m \binom{k}{m} \binom{m}{r} \operatorname{Re}(\kappa^{k-m}) \Gamma^{(r)}(2n) \zeta^{(m-r)}(2n),
 \end{aligned}$$

(23b)

$$\begin{aligned}
 & (-1)^k \zeta^{(k)}(-2n) \\
 &= \frac{2(-1)^n}{(2\pi)^{2n+1}} \sum_{m=0}^k \sum_{r=0}^m \binom{k}{m} \binom{m}{r} \operatorname{Im}(\kappa^{k-m}) \Gamma^{(r)}(2n+1) \zeta^{(m-r)}(2n+1).
 \end{aligned}$$

To compute these values we also need effective algorithms for computation of $\Gamma^{(t)}(n)$ at positive integers, as were given explicitly in [8, 10].

4. CHARACTER POLYLOGARITHMS AND SUMS

We first consider a class of real character L-series (see [15, 17] and [33, §27.8]), which will be denoted as $L_{\pm d}$ for $d \geq 1$. These are based on real multiplicative characters χ modulo d , which we denote $\chi_{\pm d}$ depending as to whether $\chi(d-1) = \pm 1$. Since we only consider real multiplicative characters, $\chi_{\pm d}(k) = \pm 1$ when $(k, d) = 1$ and is zero otherwise. In the following, when we write d without a sign, it denotes $|d|$.

4.1. Character L-series. We shall call upon the series given by the following, for integer $d \geq 3$:

$$(24) \quad L_{\pm d}(s) := \sum_{n>0} \frac{\chi_{\pm d}(n)}{n^s},$$

where $\zeta(s, \nu) := \sum_{n \geq 0} 1/(n + \nu)^s$ is the *Hurwitz zeta function* (see [26] and [9]), so $\zeta(s, 1) = \zeta(s)$. Hence, also for $m = 1, 2, \dots$ and $s \neq 1$ we have

$$(25) \quad L_{\pm d}^{(m)}(s) = \frac{1}{d^s} \sum_{k=1}^{d-1} \chi_{\pm d}(k) \sum_{j=0}^m \binom{m}{j} (-\log d)^j \zeta^{(m-j)}\left(s, \frac{k}{d}\right).$$

This provides access to numerical methods for derivatives of the Hurwitz zeta function for evaluation of quantities like $L_{\pm d}^{(m)}(s)$ with $s > 1$. Various packages such as *Maple* have a good implementation of $\zeta^{(m)}(s, \nu)$ with respect to arbitrary complex s , as we shall see below. For later use we set $\chi_1(n) := 1, \chi_{-2}(n) := (-1)^{n-1}$. Then $L_1 := \zeta$, while $L_{-2} := \eta$, the alternating zeta function.

We say such a character and the corresponding series is *principal* if $\chi(k) = 1$ for all k relatively prime to d . For all other characters $\sum_{k=1}^{d-1} \chi(k) = 0$, and we shall say the character is *balanced*. We say the character and series are *primitive* if it is not induced by a character for a proper divisor of d .

We will be particularly interested in cases when $d = P, 4P$ or $8P$, where P is a *product* of distinct odd primes, since only such d admit primitive characters. It transpires [14, 15, 17] that a unique *primitive* series exists for 1 and each odd prime p , such as $L_{-3}, L_{+5}, L_{-7}, L_{-11}, L_{+13}, \dots$, with the sign determined by the remainder modulo 4, and at 4 and four times primes, while two occur at $8p$, e.g., $L_{\pm 24}$. We then obtain primitive sums for products of distinct odd primes P or $4P$, and again two at $8P$. That is, e.g., $L_{-4}, L_{+12}, L_{-20}, L_{+60}, L_{-84}$. In the primitive cases, $\chi_{\pm d}(n) := \binom{\pm d}{n}$, where $\binom{\pm d}{n}$ is the generalized *Legendre-Jacobi symbol*.

Thence, L_{-2} is an example of an *imprimitive* series, in that it is reducible [33, §27.8] to L_1 via (19). Note the imprimitive series $L_{+6}(s) = \sum_{n>0} (1/(6n + 1)^s + 1/(6n + 5)^s)$ has all positive coefficients, while $L_{-6}(s) = \sum_{n>0} (1/(6n + 1)^s - 1/(6n + 5)^s) = (1 - 1/2^s)L_{-3}(s)$ is imprimitive but balanced, as is $L_{-12}(s) = \sum_{n>0} (1/(12n + 1)^s + 1/(12n + 5)^s - 1/(12n + 7)^s - 1/(12n + 11)^s)$, which, being nonprincipal, has $\sum_{k=1}^{11} \chi_{-12}(k) = 0$.

Recall that the sign determines that $\chi_{\pm d}(d - 1) = \pm 1$. For example, $\chi_{+5}(n) = 1$ for $n = 1, 4$, and $\chi_{+5}(n) = -1$ for $n = 2, 3$.

Remark 1 (An integral representation). A useful integral formula [33, (25.11.27)] is

$$(26) \quad \zeta(s, a) = \frac{a^{1-s}}{s-1} + \frac{1}{2}a^{-s} + \frac{1}{\Gamma(s)} \int_0^\infty \left(\frac{1}{e^x - 1} - \frac{1}{x} + \frac{1}{2} \right) \frac{x^{s-1}}{e^{ax}} dx,$$

valid for $\text{Re } s > -1, s \neq 1, \text{Re } a > 0$; an extension for $\text{Re } s > -(2n + 1), s \neq 1, \text{Re } a > 0$ is given in [33, (25.11.28)]. From (26) we adduce for $d \geq 3$

that

$$(27) \quad L_{\pm d}(s) := \frac{1}{d} \sum_{k=1}^{d-1} \chi_{\pm d}(k) \frac{k^{1-s} - 1}{s - 1} + \frac{1}{2} \sum_{k=1}^{d-1} \frac{\chi_{\pm d}(k)}{k^s} + \int_0^\infty \left(\frac{x^{s-1}}{\Gamma(s)} \right) \left(\frac{1}{e^{dx} - 1} - \frac{1}{dx} + \frac{1}{2} \right) \sum_{k=1}^{d-1} \frac{\chi_{\pm d}(k)}{e^{kx}} dx.$$

For the case L_{-3} we have

$$(28) \quad L_{-3}(s) = \frac{2^{1-s} - 1}{3(1-s)} + \frac{1}{2} \left(1 - \frac{1}{2^s} \right) + \frac{2}{\Gamma(s)} \int_0^\infty x^{s-1} e^{-3x/2} \left(\frac{1}{e^{3x} - 1} - \frac{2}{3x} + \frac{1}{2} \right) \sinh\left(\frac{x}{2}\right) dx.$$

For L_{+5} this simplifies to

$$(29) \quad L_{+5}(s) = \frac{1 - 2^{1-s} - 3^{1-s} + 4^{1-s}}{5(s-1)} + \frac{(1 - 2^{-s} - 3^{-s} + 4^{-s})}{2} + \frac{2}{\Gamma(s)} \int_0^\infty x^{s-1} e^{-5x/2} \left(\frac{1}{e^{5x} - 1} - \frac{1}{5x} + \frac{1}{2} \right) \left(\cosh\left(\frac{3x}{2}\right) - \cosh\left(\frac{x}{2}\right) \right) dx.$$

For all nonprincipal characters, the first-term singularity in (26) at $s = 1$ is removable, leaving an analytic function and so (27) can be used to numerically compute or confirm values of $L_{\pm d}^{(m)}(1)$. Explicitly for $m \geq 1$,

$$(30) \quad L_{\pm d}^{(m)}(1) := \sum_{k=2}^{d-1} \chi_{\pm d}(k) (-\log k)^m \left(\frac{1}{2k} - \frac{\log k}{d(m+1)} \right) + \int_0^\infty \left(\frac{x^{s-1}}{\Gamma(s)} \right)_{s=1}^{(m)} \left(\frac{1}{e^{dx} - 1} - \frac{1}{dx} + \frac{1}{2} \right) \sum_{k=1}^{d-1} \frac{\chi_{\pm d}(k)}{e^{kx}} dx$$

is valid at least for $\text{Re } s > -1$. ◇

Example 2 (Primitive L-series and their derivatives at zero). It helps to know that $\zeta(0, a) = 1/2 - a$, $\zeta'(0, a) = \log \Gamma(a) - \frac{1}{2} \log(2\pi)$ [33]. With $\mu_{\pm d}(1) := \sum_{k=1}^{d-1} \chi_{\pm d}(k)k$, it then follows that $L_{\pm d}(0) = \sum_{k=1}^{d-1} \binom{\pm d}{k} \zeta\left(0, \frac{k}{d}\right) = -\frac{\mu_{\pm d}(1)}{d}$, which is zero for $+d$. Thence,

$$(31) \quad L_{-d}(0) = \sum_{k=1}^{d-1} \binom{-d}{k} \zeta\left(0, \frac{k}{d}\right) = -\frac{\mu_{-d}(1)}{d} \quad \text{and} \quad L_{+d}(0) = 0,$$

since $\sum_{k=1}^{d-1} \chi_{\pm d}(k) = 0$ and $\sum_{k=1}^{d-1} m_{k=1}^{d-1} \chi_{+d}(k)k = 0$ for primitive characters.

Whence, on differentiating the rightmost formula in (24) we have

$$(32) \quad L_{\pm d}^{(1)}(0) = L_{\pm d}(0) \log d + \sum_{k=1}^{d-1} \binom{\pm d}{k} \log \Gamma\left(\frac{k}{d}\right).$$

(See also (34), Remark 3 and the discussion above it.) ◇

Recall also that for $d > 4$, as Dirichlet showed, the class number formula for imaginary quadratic fields is $-\frac{\mu_{-d}(1)}{d} = h(-d)$.

Each such primitive L-series obeys a simple functional equation [4] of the kind seen for ζ in Section 3.2.1:

$$(33) \quad L_{\pm d}(s) = C(s) \begin{Bmatrix} \sin(s\pi/2) \\ \cos(s\pi/2) \end{Bmatrix} L_{\pm d}(1-s), \quad C(s) := 2^s \pi^{s-1} d^{-s+1/2} \Gamma(1-s).$$

Indeed, this is true exactly for primitive series [4]. Moreover, the primitive series can be summed at various integer values:

$$(34) \quad \begin{aligned} L_{\pm d}(1-2m) &= \begin{cases} (-1)^m R(2m-1)!/(2d)^{2m-1}, \\ 0, \end{cases} \\ L_{\pm d}(-2m) &= \begin{cases} 0, \\ (-1)^m R'(2m)!/(2d)^{2m}, \end{cases} \\ L_{+d}(2m) &= Rd^{-1/2}\pi^{2m}, \quad L_{-d}(2m-1) = R'd^{-1/2}\pi^{2m-1}, \end{aligned}$$

where m is a positive integer and R, R' are rational numbers which depend on m, d . For $d = 1$ these engage the Bernoulli numbers, while for $d = -4$ the Euler numbers appear. The precise formulas for R and R' are given in [17, Appendix 1]. Also, notoriously,

$$(35) \quad L_{+p}(1) = 2 \frac{h(p)}{\sqrt{p}} \log \epsilon_0,$$

where $h(p)$ is the class number¹ of the quadratic form with discriminant p and ϵ_0 is the fundamental unit in the real quadratic field $Q(\sqrt{p})$.

4.2. Character polylogarithms. We now introduce our *character polylogarithms*, namely,

$$(36) \quad L_{\pm d}(s; z) := \sum_{n=1}^{\infty} \binom{\pm d}{n} \frac{z^n}{n^s},$$

$$(37) \quad L_{\pm d}^{(m)}(s; z) := \frac{\partial^m}{\partial s^m} L_{\pm d}(s; z).$$

These are well defined for all characters, but of primary interest for primitive ones.

While such objects have been used before, most of the computational tools we provide appear to be new or previously inaccessible. In the sequel, the reader will lose very little if he or she assumes all characters are primitive.

4.3. Character polylogarithms and Lerch's formula. The following parametric version of (10) holds:

$$(38) \quad \sum_{n=0}^{\infty} \frac{z^{(n+\nu)}}{(n+\nu)^s} = \Gamma(1-s)(-\log z)^{s-1} + \sum_{r=0}^{\infty} \zeta(s-r, \nu) \frac{(\log z)^r}{r!}.$$

Here $\zeta(s, \nu)$ is again the *Hurwitz zeta* function, $s \neq 1, 2, 3, \dots, \nu \neq 0, -1, -2, \dots$, and, as before, $|\log z| < 2\pi$ (see [23, Vol 1, p. 29, eqn. (8)]). Then (10) is the case $\nu = 1$. Using (38) it is possible to substantially extend (16).

¹See http://en.wikipedia.org/wiki/List_of_number_fields_with_class_number_one.

We obtain

$$(39) \quad \sum_{n=0}^{\infty} \frac{z^{(dn+k+\varepsilon)}}{(dn+k+\varepsilon)^s} = \frac{1}{d} \Gamma(1-s)(-\log z)^{s-1} + \sum_{r=0}^{\infty} \zeta\left(s-r, \frac{k+\varepsilon}{d}\right) \frac{d^{r-s}(\log z)^r}{r!}.$$

From this we obtain, for $k = 1, 2, \dots, d-1$, $s \neq 1, 2, 3, \dots$, and $0 < \varepsilon < 1$, that provided $\sum_{m=1}^{d-1} \binom{\pm d}{m} = 0$,

$$(40) \quad \sum_{n=1}^{\infty} \binom{\pm d}{n} \frac{z^{(n+\varepsilon)}}{(n+\varepsilon)^s} = \sum_{r=0}^{\infty} \left(\frac{1}{d^{s-r}} \sum_{k=1}^{d-1} \binom{\pm d}{k} \zeta\left(s-r, \frac{k+\varepsilon}{d}\right) \right) \frac{(\log z)^r}{r!}.$$

This holds for all primitive characters and some imprimitive ones such as -12 , and so in these cases any term independent of m vanishes.

We then have a tractable formula for differentiation w.r.t. the order. For $m = 0, 1, 2, \dots$, we can write

$$(41) \quad \begin{aligned} L_{\pm d}^{(m)}(s; z) &:= \sum_{n=1}^{\infty} \binom{\pm d}{n} \frac{(\log n)^m}{n^s} z^n \\ &= \sum_{r=0}^{\infty} \frac{\partial^m}{\partial s^m} \left(\frac{1}{d^{s-r}} \sum_{k=1}^{d-1} \binom{\pm d}{k} \zeta\left(s-r, \frac{k}{d}\right) \right) \frac{(\log z)^r}{r!}. \end{aligned}$$

We can now derive the character counterpart to (16) namely:

Theorem 3 (L-series summations for primitive character polylogarithms). *For primitive $d = -3, -4, 5, \dots$ and all s (since the poles at $s = 1, 2, \dots$ cancel) we have*

$$(42) \quad L_{\pm d}^{(m)}(s; z) = \sum_{r=0}^{\infty} L_{\pm d}^{(m)}(s-r) \frac{(\log z)^r}{r!}$$

when $|\log z| < 2\pi/d$.

Now, however, unlike the case for ζ , this is also applicable at $s = 1, 2, 3, \dots$. By contrast, the integral (7) or (8), is less attractive since it cannot be applied (to the real part) on the full range $[0, \pi]$. It does, however, lead to two attractive Fourier series:

$$(43a) \quad \sum_{n=1}^{\infty} \chi_{\pm d}(n) \frac{\cos n\theta}{n^s} = \sum_{r=0}^{\infty} L_{\pm d}^{(m)}(s-2r) \frac{(-1)^r \theta^{2r}}{(2r)!},$$

$$(43b) \quad \sum_{n=1}^{\infty} \chi_{\pm d}(n) \frac{\sin n\theta}{n^s} = \sum_{r=0}^{\infty} L_{\pm d}^{(m)}(s-2r+1) \frac{(-1)^r \theta^{2r-1}}{(2r-1)!},$$

when $|\theta| < 2\pi/d$.

4.4. L-series derivatives at negative integers. To employ (42) for nonnegative integer order s , we are left with the job of computing $L_{\pm d}^{(m)}(-n)$ at negative integers. This can be achieved from the requisite functional equation in (33) by the methods of [5].

We begin for primitive $d = 1, 2, \dots$, with (33), which we rewrite as:

$$(44) \quad \sqrt{d}L_{\pm d}(1-s) = \Psi_{\pm d}(s)L_{\pm d}(s), \quad \Psi_{\pm d}(s) := \left(\frac{d}{2\pi}\right)^s \left\{ \begin{array}{l} 2 \operatorname{Re} e^{i\pi s/2} \\ 2 \operatorname{Im} e^{i\pi s/2} \end{array} \right\} \Gamma(s).$$

Then for real s and $\kappa_d := -\log \frac{2\pi}{d} + \frac{1}{2}\pi i$,

$$(45a) \quad \sqrt{d}L_{+d}(1-s) = (\operatorname{Re} 2e^{s\kappa_d}) \Gamma(s) L_{+d}(s),$$

$$(45b) \quad \sqrt{d}L_{-d}(1-s) = (\operatorname{Im} 2e^{s\kappa_d}) \Gamma(s) L_{-d}(s).$$

Two applications of Leibnitz' formula for n -fold differentiation with respect to s leads to explicit analogues of (23a) and (23b). We arrive at:

Theorem 4 (L-series derivatives at negative integers). *Let $L_{\pm d}$ be a primitive nonprincipal L-series. For all integers $n \geq 1$,*

$$(46a) \quad L_{+d}^{(m)}(1-2n) = \frac{(-1)^{m+n} d^{2n-1/2}}{2^{2n-1} \pi^{2n}} \times \sum_{k=0}^m \binom{m}{k} \sum_{j=0}^k \binom{k}{j} (\operatorname{Re} \kappa_d^j) \Gamma^{(k-j)}(2n) L_{+d}^{(m-k)}(2n),$$

$$(46b) \quad L_{+d}^{(m)}(2-2n) = \frac{(-1)^{m+n} d^{2n-3/2}}{2^{2n-2} \pi^{2n-1}} \times \sum_{k=0}^m \binom{m}{k} \sum_{j=0}^k \binom{k}{j} (\operatorname{Im} \kappa_d^j) \Gamma^{(k-j)}(2n-1) L_{+d}^{(m-k)}(2n-1),$$

$$(46c) \quad L_{-d}^{(m)}(1-2n) = \frac{(-1)^{m+n} d^{2n-1/2}}{2^{2n-1} \pi^{2n}} \times \sum_{k=0}^m \binom{m}{k} \sum_{j=0}^k \binom{k}{j} (\operatorname{Im} \kappa_d^j) \Gamma^{(k-j)}(2n) L_{-d}^{(m-k)}(2n),$$

$$(46d) \quad L_{-d}^{(m)}(2-2n) = \frac{(-1)^{m+n+1} d^{2n-3/2}}{2^{2n-2} \pi^{2n-1}} \times \sum_{k=0}^m \binom{m}{k} \sum_{j=0}^k \binom{k}{j} (\operatorname{Re} \kappa_d^j) \Gamma^{(k-j)}(2n-1) L_{-d}^{(m-k)}(2n-1),$$

where $\kappa_d = -\log \frac{2\pi}{d} + \frac{1}{2}\pi i$.

Since j is a positive integer, $\operatorname{Re} \kappa_d^j$ and $\operatorname{Im} \kappa_d^j$ can be fully expanded. From the prior result and the known asymptotics, $\Gamma^{(m)}(n) \approx \log^m(n) \Gamma(n)$, one may deduce:

Corollary 1 (L-series derivative asymptotics). *Let $L_{\pm d}$ be a primitive nonprincipal L-series. For all integers $m \geq 0$, as $n \rightarrow +\infty$ we have*

$$(47a) \quad \frac{L_{+d}^{(m)}(1-2n)}{(2n-1)!} \approx 2 \frac{(-1)^{m+n} d^{2n-1/2}}{(2\pi)^{2n}} \operatorname{Re} \left(\frac{\pi i}{2} + \log \left(\frac{(2n)d}{2\pi} \right) \right)^m,$$

$$(47b) \quad \frac{L_{+d}^{(m)}(2-2n)}{(2n-2)!} \approx 2 \frac{(-1)^{m+n} d^{2n-3/2}}{(2\pi)^{2n-1}} \operatorname{Im} \left(\frac{\pi i}{2} + \log \left(\frac{(2n-1)d}{2\pi} \right) \right)^m,$$

$$(47c) \quad \frac{L_{-d}^{(m)}(1-2n)}{(2n-1)!} \approx 2 \frac{(-1)^{m+n} d^{2n-1/2}}{(2\pi)^{2n}} \operatorname{Im} \left(\frac{\pi i}{2} + \log \left(\frac{(2n)d}{2\pi} \right) \right)^m,$$

$$(47d) \quad \frac{L_{-d}^{(m)}(2-2n)}{(2n-2)!} \approx 2 \frac{(-1)^{m+n+1} d^{2n-3/2}}{(2\pi)^{2n-1}} \operatorname{Re} \left(\frac{\pi i}{2} + \log \left(\frac{(2n-1)d}{2\pi} \right) \right)^m.$$

One may use Stirling’s approximation to remove the factorial. For modest n this asymptotic allows an excellent estimate of the size of derivative. For instance,

$$\frac{L_5^{(3)}(-98)}{98!} = -1.157053952 \cdot 10^{-8} \dots$$

while the asymptotic gives $-1.159214401 \cdot 10^{-8} \dots$. Similarly,

$$\frac{L_{-3}^{(5)}(-38)}{38!} = 1.078874094 \cdot 10^{-10} \dots,$$

while the asymptotic gives $-1.092285447 \cdot 10^{-8} \dots$. These are the type of terms we need to compute below.

We note that taking n -th roots on each side of the asymptotics in Corollary 1 shows that the radius of convergence in Theorem 3 is as given. We also observe that $\left(\frac{\pi^2}{4} + \log^2\left(\frac{nd}{\pi}\right)\right)^{m/2}$ provides a useful upper bound for each real and imaginary part in Corollary 1. For example,

$$\sqrt{\left(\frac{L_{-d}^{(m)}(1-2n)}{(2n-1)!}\right)^2 + \left(\frac{L_{+d}^{(m)}(1-2n)}{(2n-1)!}\right)^2} \approx \frac{2}{\sqrt{d}} \left(\frac{\pi^2}{4} + \log^2\left(\frac{nd}{\pi}\right)\right)^{m/2} \left(\frac{d}{2\pi}\right)^{2n}.$$

4.5. Multisectioning character polylogarithms.

Example 3 (Explicit character polylogarithms for small d [17]). With an abuse of notation as above for $d = -2$, for t arbitrary we write

$$(48) \quad \sum_{m=1}^{\infty} \frac{(-1)^{m-1} x^m}{m^t} =: L_{-2}(t; x) := \eta(t; x) = -L_{+1}(t; -x) = -\operatorname{Li}_t(-x),$$

since Theorem 3 holds for any character summing to zero over the period d .

More significantly, for $d = -3$ with $\tau := (-1 + i\sqrt{3})/2$, we have

$$(49) \quad \sum_{m=1}^{\infty} \frac{x^{3m-2}}{(3m-2)^t} - \sum_{m=1}^{\infty} \frac{x^{3m-1}}{(3m-1)^t} = L_{-3}(t; x) = \frac{2}{\sqrt{3}} \operatorname{Im} \operatorname{Li}_t(\tau x),$$

while for $d = -4$,

$$(50) \quad \sum_{m=1}^{\infty} \frac{(-1)^{m-1} x^{2m-1}}{(2m-1)^t} =: \beta(t; x) = L_{-4}(t; x) = \operatorname{Ti}_t(x).$$

It is useful to know [33, (25.11.38)] that for $\operatorname{Re} s > 0$, we have $\beta(s; 1) = \beta(s)$

$$(51) \quad L_{-4}(s) = \beta(s) = \frac{1}{\Gamma(s)} \int_0^{\infty} \frac{x^{s-1}}{2 \cosh(x)} dx,$$

which may be repeatedly differentiated to obtain numerical values of $\beta^{(n)}(s)$ for integers $n \geq 1$.

Herein, $\operatorname{Ti}_t(x)$ is the *inverse tangent integral* of Lewin [27] that he relates to Legendre’s chi-function, confusingly also denoted as $\chi_t(x)$. Note that $\operatorname{Li}_1(x) = -\log(1-x)$, while $\operatorname{Ti}_1(x) = \arctan(x)$.

All character polylogarithms obey the general rule

$$L_{\pm d}(s; x) = \int_0^x \frac{L_{\pm d}(s-1; y)}{y} dy,$$

and, in particular, $Li_n(1) = \zeta(n)$, $Li_n(-1) = -\eta(n)$, and $Ti_n(1) = \beta(n)$. ◇

Indeed, ‘multi-sectioning’ allows us to write all of our character polylogarithms in terms of the classical one. Recall that for integer $d > 0$, given a formal power series $g(z) = \sum_{n \geq 0} a_n z^n$, one may algebraically extract the function $g_{d,q}(z) := \sum_{n \geq 0} a_{nd+q} z^{nd+q}$, for $0 \leq q \leq d-1$ by by the *multi-sectioning* formula

$$g_{d,q}(z) = \frac{1}{d} \sum_{m=0}^{d-1} \omega_d^{-mq} g(\omega_d^m z), \quad \omega_d = e^{2\pi i/d}.$$

Applying this to the polylogarithm of order t , we arrive at:

Theorem 5 (Multi-sectioning for the Hurwitz zeta). *For order t and integers q, d with $0 \leq q \leq d-1$, we have*

$$(52) \quad \sum_{k=1}^{\infty} \frac{x^{dk+q}}{(dk+q)^t} = \frac{1}{d} \sum_{m=0}^{d-1} \omega_d^{-mq} Li_t(\omega_d^m x),$$

and so

$$(53) \quad L_{\pm d}(t; x) = \sum_{m=0}^{d-1} \gamma_{\pm d}(m) Li_t(\omega_d^m x) \quad \text{where} \quad \gamma_{\pm d}(m) := \frac{1}{d} \sum_{q=1}^{d-1} \chi_{\pm d}(q) \omega_d^{-mq}$$

is a Gauss sum (see [3]).

Remark 2 (Examples of multi-sectioning). We directly computed $\gamma_{\pm d}$, defined in (53), for the cases $d = -3, d = +5, d = \pm 8$, and $d = +12$. For $d = -3$, we have $\sqrt{-3}\gamma_3(m) = \chi_{-3}(m)$. For $d = +5$, we have $\sqrt{5}\gamma_5(m) = \chi_{+5}(m)$. For $d = +8$, we have $\sqrt{8}\gamma_8(m) = \chi_{+8}(m)$ and for $d = -8$ we obtain $\sqrt{-8}\gamma_{-8}(m) = \chi_{+8}(m)$. Finally, for $d = +12$ we again have $\sqrt{12}\gamma_{+12}(m) = \chi_{+12}(m)$. From this we have rediscovered the closed form $\gamma_{\pm d}(m) = \frac{\chi_{\pm d}(m)}{\sqrt{\pm d}}$ for primitive characters.

Indeed, in [2, 3]—explicitly for primes and implicitly more generally—we find the proof of the requisite identity. Of course, for any given small $\pm d$ we can verify it directly. The formula fails for imprimitive forms. ◇

Thus we have:

Corollary 2 (Primitive character polylogarithms). *For any primitive character $\chi_{\pm d}$, any nonnegative integer m , and all orders s , we have*

$$(54) \quad L_{\pm d}^{(m)}(s; x) = \frac{\sqrt{\pm d}}{d} \sum_{k=1}^{d-1} \chi_{\pm d}(k) Li_s^{(m)}(\omega_d^k x),$$

valid for $\max_k |\log(x\omega_d^k)| < 2\pi$. In particular, on the unit disk we obtain

$$(55) \quad L_{\pm d}^{(m)}(s; e^{i\theta}) = \frac{\sqrt{\pm d}}{d} \sum_{k=1}^{d-1} \chi_{\pm d}(k) Li_s^{(m)}\left(e^{i(\theta+2k\pi/d)}\right),$$

valid for all θ not equal to $2k\pi/d$ for any $k = 1, \dots, d-1$.

The equation (55) may be used to exploit character generalizations of (6) and (7).

We note that (46b) and (46d) for $n = 1$, express the derivatives at zero in terms of the derivative and values at one. While the quantities are all finite, recall that the Hurwitz form in (24) involves a cancellation of singularities, and so is hard to use directly, while the definition is very slowly convergent at $s = 1$ or near one. We do, however, have recourse to a special case of Corollary 2.

Example 4 (L-series at unity [17]). For any primitive character $\chi_{\pm d}$ and any nonnegative integer m we have

$$(56) \quad L_{\pm d}^{(m)}(s) = \frac{\sqrt{\pm d}}{d} \sum_{k=1}^{d-1} \chi_{\pm d}(k) \operatorname{Li}_s^{(m)}(\omega_d^k).$$

Now we may usefully employ Theorem 1 at roots of unity. Polylogarithms, as well as their order derivatives $\operatorname{Li}_s^{(m)}(\exp(i\theta))$, were studied in some detail in [10], as they resolve Eulerian log Gamma integrals.

We illustrate (56) for $s = 1$ and $m = 1$, or equivalently (55) with $\theta = 0$. Equation (17) summed over the roots becomes

$$(57) \quad \begin{aligned} \frac{d}{\sqrt{\pm d}} L_{\pm d}^{(1)}(1; 1) &= \sum_{n=1}^{\infty} \zeta'(1-n) \sum_{m=1}^{d-1} \chi_{\pm d}(m) \frac{(2\pi mi)^n}{d^n n!} \\ &\quad - \frac{1}{2} \sum_{m=1}^{d-1} \chi_{\pm d}(m) \left(\gamma + \log\left(\frac{2\pi mi}{d}\right) \right)^2, \end{aligned}$$

while the term $\gamma_1 + \frac{1}{12} \pi^2$ having dropped out when summing. With more massaging, on separating real and imaginary terms, we end up with

$$(58a) \quad \sqrt{d} L_{+d}^{(1)}(1) = \sum_{n=1}^{\infty} \zeta'(1-2n) \mu_{+d}(2n) \frac{(-1)^n (2\pi)^{2n}}{d^{2n} (2n)!} - \gamma \left(\lambda_{+d}(1) + \frac{1}{2} \lambda_{+d}(2) \right),$$

$$(58b) \quad \sqrt{d} L_{-d}^{(1)}(1) = \sum_{n=1}^{\infty} \zeta'(-2n) \mu_{-d}(2n-1) \frac{(-1)^n (2\pi)^{2n-1}}{d^{2n-1} (2n-1)!},$$

where $\mu_{\pm d}(n) := \sum_{k=1}^{d-1} \chi_{\pm d}(k) k^n$ is the n -th moment of the character [2] and $\lambda_{\pm d}(n) := \sum_{k=1}^{d-1} \chi_{\pm d}(k) \log^n k$ is the n -th logarithmic moment.

Thus, $\mu_{-3}(n) = 1 - 1/2^n$ and $\mu_{+5}(n) = 1 - 1/2^n - 1/3^n + 1/4^n$, while $\lambda_5(1) := \log 2 - \log 3 + \log 4 = \log(8/3)$ and $\lambda_5(2) := 3 \log^2 2 - \log^2 3$. Also, on appealing to (35) we have evaluated the infinite series in (58a) in closed form. \diamond

Example 5 (Symbolic recovery of values). The L-series derivative with local notation $\lambda(m, \pm d, s) := L_{\pm d}^{(m)}(s)$ in (24) implements very neatly in *Maple*. We use

```

Ls:=(m,d,s)->add(numtheory[jacobi](d,k)*Zeta(m,s,k/abs(d)),
k=1..abs(d)-1)/abs(d)^s:
ie:=exp->identify(evalf[20](exp)):
A:=[lambda(0,-4,3)=ie(Ls(0,-4,3)),lambda(0,-3,5)=ie(Ls(0,-3,5)),
lambda(0,-4,5)=ie(Ls(0,-4,5))]:
B:=convert([lambda(1,5,0)=ie(Ls(1,5,0)),lambda(1,13,0)=ie(Ls(1,13,0)),
lambda(1,17,0)=ie(Ls(1,17,0))],ln);
latex(A);latex(B):
    
```

This accesses the ‘identify’ function and produces—after a little prettification—three evaluations given in (34):

$$\left[\lambda(0, -4, -3) = \frac{1}{32} \pi^3, \lambda(0, -3, 5) = \frac{4\sqrt{3}}{2187} \pi^5, \lambda(0, -4, 5) = \frac{5}{1536} \pi^5 \right]$$

and three first-derivative values at zero, discussed in the next remark:

$$\left[\lambda(1, 5, 0) = \log\left(\frac{1}{2} + \frac{1}{2}\sqrt{5}\right), \lambda(1, 13, 0) = \log\left(\frac{3}{2} + \frac{1}{2}\sqrt{13}\right), \right. \\ \left. \lambda(1, 17, 0) = \log\left(4 + \sqrt{17}\right) \right].$$

The ease of such manipulations highlights the value of modern numeric-symbolic experimentation. One may similarly use (56) when $s = 1$. Interestingly using ‘sum’ rather than ‘add’ led to some problems with large values of $\pm 8P$ such as ± 120 . \diamond

Remark 3 (Derivatives at zero and one revisited). The (derivative) trigonometric series $\sum_{n>0} \frac{\log n}{n} \cos(2\pi n\theta)$ occurs naturally when one desires to compute $L_{\pm d}^{(1)}(1)$, and is studied intensively in [22]. In [22, eqn. (3.4)] a classical relation is recovered for $L_{-d}^{(1)}(1)$ (see (59a) below) and in [22, eqn. (3.6)] a corresponding formula for $L_{+d}^{(1)}(1)$ is presented (engaging a then new auxiliary function). As is observed in [1, Lemma 3.1 and eqn. (4.6)], one obtains $L_{+5}^{(1)}(0) = \log \frac{1+\sqrt{5}}{2}$ as a pretty specialization. We record a version of [1, Lemma 3.1]: for integer $k \geq 1$ one has

$$(59a) \quad \frac{2(-1)^k (2k-3)! d^{2k-5/2}}{(2\pi)^{2k-3}} L_{-d}(2k-2) = L_{-d}^{(1)}(1-2k),$$

$$(59b) \quad \frac{2(-1)^k (2k-2)! d^{2k-3/2}}{(2\pi)^{2k-2}} L_{+d}(2k-1) = L_{+d}^{(1)}(2-2k),$$

and since for positive characters (35) applies; we evaluate $L_{+5}^{(1)}(0), L_{+13}^{(1)}(0), L_{+17}^{(1)}(0)$ and so on (all three having class number one). The asymptotics implicit in (59a) and (59a) are consistent with the domain of convergence given in Theorem 3. \diamond

Example 6 (An order-one generating function). For v, w in the open complex unit disc, [27, A.2.8. (1)] leads to:

$$(60) \quad \sum_{k=2}^{\infty} \left(\frac{v^k}{k} \sum_{j=1}^{k-1} \frac{w^j}{j} \right) = \text{Li}_2\left(\frac{w}{w-1}\right) - \text{Li}_2\left(\frac{w(1-v)}{w-1}\right) + \log(1-v) \log(1-w).$$

This can also be used as a basis for multi-sectioning in one or both variables. \diamond

5. CHARACTER MORDELL–TORNHEIM–WITTEN SUMS

On this foundation, one may then analyse extended *character MTW sums*, in which more general character polylogarithms replace the classical one defined earlier

in (7). That is, we may consider, for real $q, r, s \geq 1$,

$$(61) \quad \mu_{\pm d_1, \pm d_2}(q, r, s) := \sum_{n, m > 0} \frac{\chi_{\pm d_1}(m)}{m^q} \frac{\chi_{\pm d_2}(n)}{n^r} \frac{1}{(m+n)^s}$$

$$(62) \quad = \frac{1}{\Gamma(s)} \int_0^1 L_{\pm d_1}(q; x) L_{\pm d_2}(r; x) (-\log x)^{s-1} \frac{dx}{x},$$

where as before for $d > 2$, $\chi_{\pm d}(n) := \binom{\pm d}{n}$, and $\chi_{-2}(n) := (-1)^{n-1}$, $\chi_{+1}(n) := 1$. We may now also take derivatives in (61) and (62) and indeed so doing is the source of much of our computational interest. Explicitly, we write

$$(63) \quad (\mu_{\pm d_1, \pm d_2})_{a,b,c}(q, r, s) := \sum_{n, m > 0} \frac{(-\log m)^a \chi_{\pm d_1}(m)}{m^q} \frac{(-\log n)^b \chi_{\pm d_2}(n)}{n^r} \frac{(-\log(m+n))^c}{(m+n)^s}$$

$$(64) \quad = \int_0^1 L_{\pm d_1}^{(a)}(q; x) L_{\pm d_2}^{(b)}(r; x) \left(\frac{(-\log x)^{s-1}}{\Gamma(s)} \right)^{(c)} \frac{dx}{x}.$$

5.1. Related work. Such sums do not appear to have been studied in detail, and never with derivatives. The case of $\chi_{-2}(n)$ or $\chi_{-2}(m+n)$ has been studied *ab initio* [35, 37, 39, 40], while [41] provides some q -analogues.

More interesting is a series of papers by Nakamura including [30–32], in which the Lerch transcendent of Section 4.3 is used, so as to study sums of the form

$$(65) \quad \mathcal{N}(\alpha, \beta, \gamma; q, r, s) := \sum_{n, m > 0} \frac{e^{\alpha\pi i m}}{m^q} \frac{e^{\beta\pi i n}}{n^r} \frac{e^{\gamma\pi i(m+n)}}{(m+n)^s}.$$

Note that the γ term can be absorbed in the α, β terms. All of our character sums (61) can be expressed in terms of (65) but the natural arithmetic structure we set up will be lost. We record that (60) evaluates

$$\begin{aligned} \mathcal{N}(\alpha, 0, \gamma; 1, 0, 1) &= \text{Li}_2\left(\frac{e^{i\gamma\pi}}{e^{i\gamma\pi} - 1}\right) - \text{Li}_2\left(\frac{e^{i\gamma\pi}(1 - e^{i\alpha\pi})}{e^{i\gamma\pi} - 1}\right) \\ &\quad + \log(1 - e^{i\alpha\pi}) \log(1 - e^{i\gamma\pi}), \end{aligned}$$

which simplifies nicely when $\gamma = \pm\alpha$.

5.2. First examples. As explained, for Euler sums in [17], there is an impediment to getting a general integral representation if one attempts to add a nontrivial character to the $m+n$ variable other than $(\pm 1)^{n-1}$. In the context of MTWs, this asymmetry is better explained.

Example 7 (Some explicit character polylogarithms and sums of order one [17]). Various cases of (53) give explicit forms.

1. Character polylogarithms of order one. We have

$$(66) \quad L_{+1}(1; x) = -\log(1 - x),$$

$$(67) \quad L_{-3}(1; x) = \frac{2}{\sqrt{3}} \arctan\left(\frac{\sqrt{3}x}{x+2}\right),$$

$$(68) \quad \sqrt{5} L_5(1; x) = \log(x^2 + \omega x + 1) - \log(x^2 - x/\omega + 1), \quad \omega := \frac{\sqrt{5} + 1}{2},$$

$$(69) \quad \sqrt{12} L_{12}(1; x) = \log(x^2 + \sqrt{3}x + 1) - \log(x^2 - \sqrt{3}x + 1),$$

yielding closed forms for order one.

In general, for primitive $\pm d$, Corollary 2 implies that

$$(70) \quad L_{\pm d}(1; x) = -\frac{\sqrt{\pm d}}{d} \log\left(\frac{\prod_j (1 - \omega_d^j x) : \chi_{\pm d}(j) = +1}{\prod_k (1 - \omega_d^k x) : \chi_{\pm d}(k) = -1}\right).$$

It is instructive to verify that

$$(71a) \quad \sqrt{8} L_{+8}(1; x) = -\log\left(\frac{1 - \sqrt{2}x + x^2}{1 + \sqrt{2}x + x^2}\right),$$

$$(71b) \quad \sqrt{8} L_{-8}(1; x) = \arctan\left(\sqrt{8}x(1 - x^2), 1 - 4x^2 + x^4\right).$$

Here $\arctan(y, x) := -i \log\left(\frac{x+iy}{\sqrt{x^2+y^2}}\right)$, so as to assure a value in $(\pi, \pi]$. Correspondingly

$$(72) \quad \sqrt{20} L_{-20}(1; x) = i \log\left(\frac{1 - i\sqrt{5}x - 3x^2 + i\sqrt{5}x^3 + x^4}{1 + i\sqrt{5}x - 3x^2 - i\sqrt{5}x^3 + x^4}\right).$$

2. Some simple character sums. From some of the formulas above, integrals for μ sums follow. Thence,

$$(73) \quad \mu_{-3,1}(1, 1, s) = \frac{2/\sqrt{3}}{\Gamma(s)} \int_0^1 \arctan\left(\frac{\sqrt{3}x}{x+2}\right) (-\log(1-x)) (-\log x)^{s-1} \frac{dx}{x}$$

and

$$(74) \quad \mu_{-3,-3}(1, 1, s) = \frac{4/3}{\Gamma(s)} \int_0^1 \arctan^2\left(\frac{\sqrt{3}x}{x+2}\right) (-\log x)^{s-1} \frac{dx}{x}.$$

For example, $\mu_{-3,-3}(1, 1, 1) \approx 0.259589$ and $\mu_{-3,-3}(1, 1, 3) \approx 0.0936667862$. Similarly,

$$(75) \quad \begin{aligned} \mu_{-12,-12}(1, 1, 3) &= -\frac{1}{72} \int_0^1 \log^2\left(\frac{x^2 + \sqrt{3}x + 1}{x^2 - \sqrt{3}x + 1}\right) \log^3(x) \frac{dx}{x} \\ &= 0.062139235322359770447911814351\dots \end{aligned}$$

and, with $\omega = \frac{\sqrt{5}+1}{2}$ as above, we have

$$(76) \quad \begin{aligned} \mu_{+5,+5}(1, 1, 5) &= \frac{1}{120} \int_0^1 \log^2 \left(\frac{x^2 + \omega x + 1}{x^2 - x/\omega + 1} \right) \log^4(x) \frac{dx}{x} \\ &= 0.026975379493214862581276332615 \dots \end{aligned}$$

We also recall that polylogarithms and Euler sums based primarily on mixes of the characters χ_{-4} and χ_1 are studied at length in [17]. ◇

Example 8 (Some explicit character polylogarithms of order two). As we saw, various cases of (53) give clean explicit forms. For higher order, less can be hoped for explicitly.

That said, [27, A.2.5. (1)] shows that in terms of the *Clausen function*, $\text{Cl}_2(\theta) := \sum_{n>0} \sin(n\theta)/n^2$, we have

$$(77) \quad \text{L}_{-3}(2; x) = \frac{1}{2} \text{Cl}_2(2w) + \frac{1}{2} \text{Cl}_2\left(\frac{4\pi}{3}\right) - \frac{1}{2} \text{Cl}_2\left(2w + \frac{4\pi}{3}\right) + w \log x,$$

where $w := \arctan\left(\frac{\sqrt{3}x}{x+2}\right)$.

We also record a pretty functional equation for $\text{L}_{-4}(2; x) = \text{Im Li}_2(ix)$ given in [27, eqn. (2.3.9)], namely

$$(78) \quad \begin{aligned} \frac{1}{3} \text{Ti}_2(\tan 3\theta) &= \text{Ti}_2(\tan \theta) + \text{Ti}_2(\tan(\pi/6 - \theta)) - \text{Ti}_2(\tan(\pi/6 + \theta)) \\ &+ \frac{\pi}{6} \log \left(\frac{\tan(\pi/6 + \theta)}{\tan(\pi/6 - \theta)} \right). \end{aligned}$$

Since $\text{Ti}_2(\pi/4) = \text{G}$, Catalan’s constant, (78) produces a formula known to Ramanujan:

$$\text{Ti}_2(\pi/12) = \frac{2}{3}\text{G} + \frac{\pi}{12} \log \tan(\pi/12),$$

while $\theta = \pi/24$ yields an interesting linear relation. Also for all real x , $\text{Ti}_2(x) - \text{Ti}_2(1/x) = \text{sign}(x) \log|x|$. Note that $\tan(\pi/8) = \sqrt{2} - 1$, $\tan(5\pi/8) = \sqrt{2} + 1$, $\tan(\pi/12) = 2 - \sqrt{3}$ and $\tan(5\pi/12) = 2 + \sqrt{3}$.

A substantial study of Ti_t , especially Ti_2 , is made in [27]. It is a sign of the greater complexity of nonprincipal primitive character polylogarithms that the cleanest known functional equation for Ti_2 is actually for $\chi_2(x) := i \text{Ti}_2(ix)$, which satisfies

$$(79) \quad \chi_2(x) + \chi_2\left(\frac{1-x}{1+x}\right) = \frac{1}{2} \log\left(\frac{1-x}{1+x}\right) \log x - \frac{\pi^2}{8},$$

for all real x [27, eqn. (1.67)]. Compare [27, eqn. (1.11)], first found by Euler, namely

$$(80) \quad \text{Li}_2(x) + \text{Li}_2(1-x) = \frac{\pi^2}{6} - \frac{1}{2} \log(1-x) \log x,$$

valid at least for $-1 \leq x \leq 1$, which produces the famous result $\text{Li}_2(\frac{1}{2}) = \frac{\pi^2}{12} - \frac{1}{2} \log^2 2$.

More complex functional equations for Li_{-4} lead to relations such as

$$6 \text{Ti}_2(1) - 4 \text{Ti}_2(1/2) - 2 \text{Ti}_2(1/3) - \text{Ti}_2(3/4) = \pi \log 2,$$

see [27, eqn. (2.28)] in which all terms appear to be algebraically independent; recall $\text{Ti}_2(1) = \beta(2) = \text{G}$.

For $d = +5$ we obtain

$$(81) \quad \sqrt{5} L_{+5}(2; x) = \int_0^x \log \left(\frac{1 + r \left(\frac{1+\sqrt{5}}{2} \right) + r^2}{1 + r \left(\frac{1-\sqrt{5}}{2} \right) + r^2} \right) \frac{dr}{r},$$

by integration or by exploiting $\operatorname{Re} \operatorname{Li}_2(re^{i\theta}) = -\frac{1}{2} \int_0^r \log(1 - 2w \cos \theta + w^2) \frac{dw}{w}$; see [27, A.2.5 (1)].

For larger $\pm d$, more cumbersome versions of some of the formulas above can still be given. \diamond

5.3. Values of character sums including order zero. Integral representation (7) is used freely only when $d \leq 2$, and all s_j, t_k numerator (nonlogarithmic) parameters are nonzero; so we must attend to such more general or degenerate cases. In our current three-variable setting, we may freely use formulas such as

$$(82) \quad \omega_{a,b,c}(q, r, s) = \omega \left(\begin{array}{c|c} q, r & s \\ a, b & c \end{array} \right) = \int_0^\infty \left(\frac{x^{s-1}}{\Gamma(s)} \right)^{(c)} \operatorname{Li}_q^{(a)}(e^{-x}) \operatorname{Li}_r^{(b)}(e^{-x}) dx,$$

which is valid when $q \geq 0, r \geq 0, s > 0$, with $q + r + s > 2$, and $a \geq 0, b \geq 0, c \geq 0$. Here the notation $(\cdot)^{(c)}$ denotes the c -th partial derivative of the expression in parentheses with respect to s . This may be seen by expanding the integrand and using $\frac{1}{\Gamma(s)} \int_0^\infty e^{-wx} x^{s-1} dx = \frac{1}{w^s}$, for $s, w > 0$.

It is helpful to split the integral in two, and set $u = e^{-x}$ in the second integral:

$$(83) \quad \begin{aligned} \omega_{a,b,c}(q, r, s) &= \int_0^1 \left(\frac{x^{s-1}}{\Gamma(s)} \right)^{(c)} \operatorname{Li}_q^{(a)}(e^{-x}) \operatorname{Li}_r^{(b)}(e^{-x}) dx \\ &+ \int_0^{1/e} \left(\frac{(-\log u)^{s-1}}{\Gamma(s)} \right)^{(c)} \operatorname{Li}_q^{(a)}(u) \operatorname{Li}_r^{(b)}(u) \frac{du}{u}. \end{aligned}$$

We were able to use formula (83), together with formulas (16) through (18), and related machinery described in [8] to produce high-precision numerical values of all the degenerate omega constants needed in our earlier study.

Alternatively, for ω or μ , one may directly substitute $u = e^{-x}$ in the analogue of formula (82) and obtain the following result, which provides an efficient evaluation method.

For this we require the *incomplete Gamma function*,

$$(84) \quad \Gamma(s, z) := \int_z^\infty t^{s-1} e^{-t} dt,$$

so that $\Gamma(s, 0) = \Gamma(s)$; see [33, Chapter 8] and [9]. Since the size of d determines the domain of validity of (42), we replace e by a general parameter $\sigma > 1$.

Proposition 2 (Depth three character sum computation). *Fix character series $L_1 := L_{\pm d_1}$ and $L_2 := L_{\pm d_2}$. For $q \geq 0, r \geq 0, s > 0$, with $q + r + s > 2$, and*

$a \geq 0, b \geq 0, c \geq 0$. In the notation of (63) we have, for $\sigma > 1$ that

$$\begin{aligned}
 (\mu_{d_1, d_2})_{a, b, c}(q, r, s) &= \int_0^1 \left(\frac{(-\log u)^{s-1}}{\Gamma(s)} \right)^{(c)} L_1^{(a)}(q; u) L_2^{(b)}(r; u) \frac{du}{u} \\
 &= \int_0^{1/\sigma} \left(\frac{(-\log u)^{s-1}}{\Gamma(s)} \right)^{(c)} L_1^{(a)}(q; u) L_2^{(b)}(r; u) \frac{du}{u} \\
 (85) \qquad &+ \int_{1/\sigma}^1 \left(\frac{(-\log u)^{s-1}}{\Gamma(s)} \right)^{(c)} L_1^{(a)}(q; u) L_2^{(b)}(r; u) \frac{du}{u}.
 \end{aligned}$$

Thence,

$$\begin{aligned}
 &(\mu_{d_1, d_2})_{a, b, c}(q, r, s) \\
 &= \sum_{m, n > 0} \left(\frac{\Gamma(s, (m+n) \log \sigma)}{\Gamma(s) (m+n)^s} \right)^{(c)} \frac{\chi_{\pm d_1}(m) (-\log m)^a}{m^q} \frac{\chi_{\pm d_2}(n) (-\log n)^b}{n^r} \\
 (86) \qquad &+ \int_{1/\sigma}^1 \left(\frac{(-\log u)^{s-1}}{\Gamma(s)} \right)^{(c)} L_1^{(a)}(q; u) L_2^{(b)}(r; u) \frac{du}{u},
 \end{aligned}$$

where in (86) we express the result in terms of the incomplete Gamma function of (84).

It is a happy consequence of Theorem 3 that when it applies to both L_1, L_2 we arrive at effective integral free summations.

Theorem 6 (Explicit sum computation). *Suppose L_1 and L_2 satisfy Theorem 3. For $q \geq 0, r \geq 0, s > 0$, with $q + r + s > 2$, and $a \geq 0, b \geq 0, c \geq 0$ we have, for σ chosen so that as necessary $1/\sigma$ does not exceed $\exp(-2\pi/d)$ for either character, that*

$$\begin{aligned}
 &(\mu_{\pm d_1, \pm d_2})_{a, b, c}(q, r, s) \\
 &= \sum_{m, n > 0} \left(\frac{\Gamma(s, (m+n) \log \sigma)}{\Gamma(s) (m+n)^s} \right)^{(c)} \chi_{\pm d_1}(m) \chi_{\pm d_2}(n) \frac{(-\log m)^a}{m^q} \frac{(-\log n)^b}{n^r} \\
 (87) \qquad &+ \sum_{j, k \geq 0} \frac{L_1^{(a)}(q-j)}{j!} \frac{L_2^{(b)}(r-k)}{k!} \int_{1/\sigma}^1 \left(\frac{(-\log u)^{s-1}}{\Gamma(s)} \right)^{(c)} (\log u)^{j+k} \frac{du}{u},
 \end{aligned}$$

where the final integral may now be evaluated symbolically, since $\int_{1/\sigma}^1 \frac{\log^{n-1} u}{u} du = -\frac{(-\log)^n \sigma}{n}$.

Note that $\sigma = e$ may be used when neither of d_1, d_2 exceeds six. In general, to determine the truncation needed in the final term (87), we have proceeded by precomputing the needed L-series and using only those summands which are larger than the desired error. We note that Corollary 1 provides excellent estimates for these L-series terms. For truncation of the first term on the right of (87), the next remark yields an effective *a priori* estimate (when $c = 0$) which decays exponentially in z .

Remark 4 (Error estimates for $\Gamma(s, z)$). For fixed positive integer n and real s , with $u_k = (-1)^k (1 - a)_k = (a - 1)(a - 2) \cdots (a - k)$, we have [33, §8.11] that

$$(88) \quad \Gamma(s, z) = z^{s-1} e^{-z} \left(\sum_{k=0}^{n-1} \frac{u_k}{z^k} + R_n(s, z) \right),$$

where for real z $R_n(s, z) = O(z^{-n})$, is bounded in absolute value by the first neglected term u_n/z^n and has the same sign provided only that $n \geq s - 1$. \diamond

As Crandall [21] observed, for the case of $L_1 = L_2 = L_{-2}$, some seemingly more difficult character sums can now be computed more easily than classical ones, contrary to what one might expect:

Example 9 (Alternating MTWs [21]). For example, $L_{-2}(z, s) = \sum_{m \geq 0} \eta(s - m) \frac{\log^m z}{m!}$ and so we may write

$$(89) \quad (\mu_{-2,-2})_{1,1,0}(q, r, s) = \sum_{n,m>0} \left(\frac{\Gamma(s, n+m)}{\Gamma(s)(n+m)^s} \right) \frac{(-1)^n \log n}{n^q} \frac{(-1)^m \log m}{m^r} + \frac{1}{\Gamma(s)} \sum_{j,k \geq 0} \frac{\eta^{(1)}(q-j)}{j!} \frac{\eta^{(1)}(r-k)}{k!} \frac{(-1)^{j+k}}{j+k+s}.$$

For positive integer s , the incomplete Gamma function value used above is elementary; see [33, Ch. 8] and [9].

Using Theorem 6 with $q = r = s = 1$ and summing say, $m, n, j, k \leq 240$, yields

$$(90) \quad (\mu_{-2,-2})_{0,0,0}(1, 1, 1) := \sum_{m,n \geq 1} \frac{(-1)^{m+n}}{mn(m+n)}$$

$$(91) \quad = 0.3005142257898985713499345403778624976912465730851247 \dots,$$

agreeing with $(\mu_{-2,-2,0})_{0,0,0}(1, 1, 1) = \frac{1}{4}\zeta(3)$, a known evaluation. Likewise, using the first derivative of the η function,

$$(92) \quad (\mu_{-2,-2})_{1,1,0}(1, 1, 1) := \sum_{m,n \geq 1} (-1)^{m+n} \frac{\log m \log n}{m n(m+n)}$$

$$(93) \quad = 0.0084654591832435660002204654836228807098258834876951 \dots$$

Both evaluations are correct to the precision shown. \diamond

For primitive characters with $3 \leq d_1, d_2 \leq 5$, we have

$$(94) \quad \begin{aligned} & (\mu_{\pm d_1, \pm d_2})_{a,b,0}(q, r, s) \\ &= \sum_{m,n \geq 1} \chi_{\pm d_1}(m) \chi_{\pm d_2}(n) \frac{(-\log m)^a (-\log n)^b}{m^r n^q (m+n)^s} \\ &= \sum_{n,m>0} \left(\frac{\Gamma(s, n+m)}{\Gamma(s)(n+m)^s} \right) \frac{\chi_{\pm d_1}(m) (-\log m)^a}{m^q} \frac{\chi_{\pm d_2}(n) (-\log n)^b}{n^r} \\ &+ \frac{1}{\Gamma(s)} \sum_{j,k \geq 0} \frac{L_{\pm d_1}^{(a)}(q-j)}{j!} \frac{L_{\pm d_2}^{(b)}(r-k)}{k!} \frac{(-1)^{j+k}}{j+k+s}, \end{aligned}$$

in analogy with Example 9.

Example 10 (Character MTWs). For $d = -4$ we obtain quite similar evaluations with $\beta := L_{-4}$ replacing $\eta := L_{-2}$. Precisely we get,

$$(95) \quad (\mu_{-4,-4})_{1,1,0}(q, r, s) = \sum_{n,m>0} \left(\frac{\Gamma(s, n+m)}{\Gamma(s)(n+m)^s} \right) \frac{\chi_{-4}(n) \log n}{n^q} \frac{\chi_{-4}(m) \log m}{m^r} + \frac{1}{\Gamma(s)} \sum_{j,k \geq 0} \frac{\beta^{(1)}(q-j)}{j!} \frac{\beta^{(1)}(r-k)}{k!} \frac{(-1)^{j+k}}{j+k+s}.$$

Hence

$$(96) \quad (\mu_{-4,-4})_{1,1,0}(1, 1, 1) := \sum_{m,n \geq 1} \chi_{-4}(n)\chi_{-4}(m) \frac{\log m \log n}{m n(m+n)}$$

$$(97) \quad = 0.00832512075015357521062197448271 \dots$$

To compute the requisite value of $\beta^{(1)}(1) = 0.1929013167969124293 \dots$, we may use (51), and for $\beta^{(1)}(-n)$ with $n \geq 0$, we can use one of many methods including (25). We also computed the same value to the precision shown directly from the sum expressed in terms of Ψ functions.

In like vein, from Theorem 6 or (94), we compute various sums:

$$(98a) \quad (\mu_{-4,-4})_{2,1,0}(1, 1, 5) := - \sum_{m,n \geq 1} \chi_{-4}(m)\chi_{-4}(n) \frac{\log^2 m \log n}{m n(m+n)^5} = -0.00001237144966467 \dots,$$

$$(98b) \quad (\mu_{-4,-4})_{2,1,0}(1, 1, 8) := - \sum_{m,n \geq 1} \chi_{-4}(m)\chi_{-4}(n) \frac{\log^2 m \log n}{m n(m+n)^8} = -7.238940044699712819 \cdot 10^{-8} \dots,$$

$$(98c) \quad (\mu_{-4,-3})_{2,0,0}(1, 1, 7) := \sum_{m,n \geq 1} \chi_{-4}(m)\chi_{-3}(n) \frac{\log^2 m}{m n(m+n)^7} = -0.206867464 \cdot 10^{-8} \dots,$$

$$(98d) \quad (\mu_{-4,-3})_{2,1,0}(1, 1, 7) := - \sum_{m,n \geq 1} \chi_{-4}(m)\chi_{-3}(n) \frac{\log^2 m \log n}{m n(m+n)^7} = -0.150314175 \cdot 10^{-5} \dots,$$

$$(98e) \quad (\mu_{-4,-3})_{2,2,0}(1, 1, 6) := \sum_{m,n \geq 1} \chi_{-4}(m)\chi_{-3}(n) \frac{\log^2 m \log^2 n}{m n(m+n)^6} = 0.45467644545 \cdot 10^{-5} \dots,$$

$$(98f) \quad (\mu_{+5,+5})_{2,2,0}(1, 1, 4) := \sum_{m,n \geq 1} \chi_{+5}(m)\chi_{+5}(n) \frac{\log^2 m \log^2 n}{m n(m+n)^4} = 0.00035650565 \dots,$$

and higher-order variants such as

$$(98g) \quad (\mu_{-4,-4})_{2,2,0}(2, 2, 4) := \sum_{m,n \geq 1} \chi_{+4}(m)\chi_{+4}(n) \frac{\log^2 m \log^2 n}{m^2 n^2 (m+n)^4} \\ = 0.921829712836 \cdot 10^{-5} \dots,$$

$$(98h) \quad (\mu_{-4,-4})_{3,3,0}(3, 3, 3) := \sum_{m,n \geq 1} \chi_{+4}(m)\chi_{+4}(n) \frac{\log^3 m \log^3 n}{m^3 n^3 (m+n)^3} \\ = 0.69071031171 \cdot 10^{-5} \dots,$$

and so on. In each case the precision shown has been confirmed directly from the definitional sum. Note that for the purpose of formula and code validation, it is often useful to use larger values of parameters such as s . \diamond

6. REDUCTIONS AND RELATIONS FOR CHARACTER MTW SUMS

Armed with these computational and analytic tools, we continue our study.

6.1. Reduction of MTW values and derivatives. Again we define the shorthand notation

$$\omega_{a,b,c}(r, s, t) := \omega \left(\begin{array}{cc|c} r & s & t \\ a & b & c \end{array} \right).$$

Partial fraction manipulations allow one to relate partial derivatives of MTWs. Such a relation in the classical three parameter setting, is based on

$$\frac{1}{n^q} \frac{1}{m^r} \frac{1}{(n+m)^s} = \frac{1}{n^{q-1}} \frac{1}{m^r} \frac{1}{(n+m)^{s+1}} + \frac{1}{n^q} \frac{1}{m^{r-1}} \frac{1}{(n+m)^{s+1}}.$$

This yields that for arbitrary a, b, c , the function $\delta = \omega_{a,b,c}$ satisfies

$$(99) \quad \delta(q, r, s) = \delta(q-1, r, s+1) + \delta(q, r-1, s+1),$$

for real positive q, r, s . That in turn, for integers q, r, s , leads to:

Theorem 7 (Reduction of MTW derivatives [7]). *Let nonnegative integers a, b, c and q, r, s , be given. Set $N := q + r + s$. Then for $\delta := \omega_{a,b,c}$ we have*

$$(100) \quad \delta(q, r, s) = \sum_{i=1}^q \binom{q+r-i-1}{r-1} \delta(i, 0, N-i) \\ + \sum_{i=1}^r \binom{q+r-i-1}{q-1} \delta(0, i, N-i).$$

In the case that $\delta = \omega$, this shows that each classical MTW value is a finite positive integer combination of *Euler sums* (character multi-zeta values (MZVs)), as discussed below.

Example 11 (Concrete MTW reductions). It is well known that for $N = r + s + t$ odd, the evaluation is reducible entirely to sums of products of Riemann zeta values [13]. Espinosa and Moll [24, 25] record, with attributions, that

$$(101a) \quad \omega(2n + 1, 2n + 1, 2n + 1) = -4 \sum_{k=0}^n \binom{4n - 2k - 3}{2n} \zeta(2k) \zeta(6n - 2k - 3),$$

$$(101b) \quad \omega(2n, 2n, 2n) = \frac{4}{3} \sum_{k=0}^n \binom{4n - 2k - 1}{2n - 1} \zeta(2k) \zeta(6n - 2k).$$

Then (101b) shows that further cancellation can take place, and seemingly irreducible terms such as $\zeta(10, 2)$ never appear. Another reduction is

$$(102) \quad \omega(n, n, m) = (-1)^n \left(\sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n + m - 2k - 1}{m - 1} + \sum_{k=0}^{\lfloor m/2 \rfloor} \binom{n + m - 2k - 1}{n - 1} \right) \zeta(2k) \zeta(2p + m - 2k).$$

In Tornheim’s [34] original paper one finds

$$(103a) \quad \omega(1, 1, n - 2) = (n - 1) \zeta(n) - \sum_{k=2}^{n-2} \zeta(k) \zeta(n - k),$$

$$(103b) \quad \omega(n - 2, 1, 1) = \frac{1}{2} \omega(1, 1, n - 2) + \zeta(n),$$

and like equations for integral n . See also [8] for a proof that (100) and similar equations hold for all complex values of n . Similar reductions for combinations of ω values, such as $\omega(a, b, s) + (-1)^b \omega(b, s, a) + (-1)^a \omega(s, a, b, s)$ and variants including alternations with L_{-2} , can be found in [30, 31]. \diamond

6.2. Twisted and pure character Euler sums. We now return to the character MTW sums. To do so, we introduce the *twisted and pure character Euler sums*. Here we use notation consistent with [17], namely denote twisted character sums:

$$(104) \quad \langle d_1, d_2 \rangle(a, b) := \sum_{m, n > 0} \frac{\chi_{d_2}(n)}{n^b} \frac{\chi_{d_1}(m)}{(m + n)^a} = \sum_{k=1}^{\infty} \frac{1}{k^a} \sum_{j=1}^{k-1} \frac{\chi_{d_1}(k - j) \chi_{d_2}(j)}{j^b}$$

and pure character sums

$$(105) \quad [d_1, d_2](a, b) := \sum_{m, n > 0} \frac{\chi_{d_2}(n)}{n^b} \frac{\chi_{d_1}(m + n)}{(m + n)^a} = \sum_{k=1}^{\infty} \frac{\chi_{d_1}(k)}{k^a} \sum_{j=1}^{k-1} \frac{\chi_{d_2}(j)}{j^b}.$$

Example 12 (Twisted and pure character Euler sums). For instance, [17, Table 3] provides

$$\langle -2, -2 \rangle(2, 1) = \sum_{m, n > 0} \frac{(-1)^n}{n} \frac{(-1)^m}{(m + n)^2} = [-2, 1](2, 1) = \frac{1}{8} \zeta(3),$$

while

$$[-2, -2](2, 1) = \sum_{m, n > 0} \frac{1}{n} \frac{(-1)^m}{(m + n)^2} = \frac{\pi^2}{4} \log 2 - \frac{13}{8} \zeta(3).$$

Also,

$$\begin{aligned} \langle -4, -4 \rangle(2, 1) &= \sum_{m,n>0} \frac{\chi_{-4}(n)}{n} \frac{\chi_{-4}(m)}{(m+n)^2} = \frac{1}{4} \sum_{m=0}^{\infty} \left(\sum_{n=0}^{\infty} \frac{(-1)^{m+n}}{(m+n+1)^2 (2n+1)} \right) \\ &= -\frac{7}{16} \zeta(3) + \frac{\pi G}{4} \neq [-4, 1](2, 1), \end{aligned}$$

while

$$[-4, -4](2, 1) = \sum_{m,n>0} \frac{\chi_{-4}(n)}{n} \frac{\chi_{-4}(m+n)}{(m+n)^2} = -\frac{7}{16} \zeta(3) + \frac{\pi^2}{16} \log 2,$$

where again these evaluations are in or derivable from [17, Table 3]. Note that integral forms for $[d_1, d_2](s, t)$ for the eight choices $d_1, d_2 = 1, -2, -4$ are given in [17, Table 2]. ◇

6.3. Reduction of character MTW sums to twisted Euler sums. Now (100) holds for any δ satisfying the recursion (99) without being restricted to partial derivatives. In particular, it applies to sums of the form $\sum_{m,n>0} \frac{a_m}{m^a} \frac{b_n}{n^b} \frac{c_{n+m}}{(n+m)^c}$. Thence, Theorem 7 above extends to show that:

Theorem 8 (Reduction of character sums). *For any two characters d_1 and d_2 , each sum $\mu_{d_1, d_2}(q, r, s)$ is a superposition of twisted character Euler sums of the form $\langle d_1, d_2 \rangle(a, b) = \sum_{m,n>0} \frac{\chi_{d_2}(n)}{n^a} \frac{\chi_{d_1}(m)}{(m+n)^b}$, as in (104), with the reduction given by (100).*

Here the χ_{d_2} term is not usually coincident with that seen in [17], which considered instead $[d_1, d_2](a, b)$ as in (105). But note that

$$(106) \quad [1, d_2](a, b) = \langle 1, d_2 \rangle(a, b).$$

The result above has extensions to derivatives $(\mu_{d_1, d_2})_{a,0,c}(q, r, s)$, but we forfend.

Example 13 (Representative character sum reductions). We illustrate with

$$\begin{aligned} \mu_{d_1, d_2}(2, 1, 1) &= \mu_{d_1, d_2}(2, 0, 2) + \mu_{d_1, d_2}(1, 1, 2) \\ &= \mu_{d_1, d_2}(2, 0, 2) + \mu_{d_1, d_2}(1, 0, 3) + \mu_{d_1, d_2}(0, 1, 3). \end{aligned}$$

Thus

$$\mu_{d_1, d_2}(2, 1, 1) = \langle d_1, d_2 \rangle(2, 2) + \langle d_1, d_2 \rangle(3, 1) + \langle d_2, d_1 \rangle(3, 1),$$

and so on. In Example 10 we listed an abbreviated version of

$$(107) \quad (\mu_{-4, -4})_{3,3,0}(3, 3, 3) = 0.690710311713441241214787656159 \cdot 10^{-5},$$

and we similarly compute

$$(108) \quad (\mu_{-4, -4})_{3,3,0}(3, 1, 5) = 0.167646883093693896852765820595 \cdot 10^{-5},$$

while

$$(109) \quad (\mu_{-4, -4})_{3,3,0}(2, 1, 6) = 8.88541363815133618773139117241 \cdot 10^{-7}.$$

The underlying recursion leads to

$$\begin{aligned}
 (110) \quad (\mu_{-4,-4})_{3,3,0}(3, 3, 3) &= 2 (\mu_{-4,-4})_{3,3,0}(3, 2, 4) \\
 &= 2 (\mu_{-4,-4})_{3,3,0}(3, 1, 5) + 2 (\mu_{-4,-4})_{3,3,0}(2, 2, 5) \\
 &= 2 (\mu_{-4,-4})_{3,3,0}(3, 1, 5) + 4 (\mu_{-4,-4})_{3,3,0}(2, 1, 6),
 \end{aligned}$$

and so on. One may check that (107)=2·(108)+4·(109) to the computed 30 places as predicted.

Correspondingly, we also gave

$$(111) \quad (\mu_{+5,+5})_{2,2,0}(1, 1, 4) = 0.000356505653610023,$$

and computed

$$(112) \quad (\mu_{+5,+5})_{2,2,0}(1, 0, 5) = 0.000178252826805198.$$

The underlying recursion leads to

$$(113) \quad (\mu_{+5,+5})_{2,2,0}(1, 1, 4) = 2 (\mu_{+5,+5})_{2,2,0}(1, 0, 5),$$

and one may check that (111)=2·(112) to 16 places. In each case, we used derivatives up to $n = -128$, which for L_{+5} decrease more slowly than for L_{-4} . Increasing the number of derivative terms used to get $n = -256$ leads to $(\mu_{+5,+5})_{2,2,0}(1, 1, 4) = 2 (\mu_{+5,+5})_{2,2,0}(1, 0, 5) = 0.00035650565361002353206435$, which is correct to all places shown.

Finally, we illustrate two much higher precision sums

$$\begin{aligned}
 (114) \quad &(\mu_{-4,-4})_{2,2,0}(1, 1, 4) = \\
 &0.000065079205320893012446595684990042272900528250434096839965346720780 \\
 &85812813651555390159928214387452572766912562913627737004397885757003044 \\
 &5562666574186136298500580253843059981738739583846236751230099872,
 \end{aligned}$$

and

$$\begin{aligned}
 (115) \quad &(\mu_{-4,-4})_{2,2,0}(1, 1, 1) = \\
 &0.00633802199298997495285569331466149967623586882429821383039501211425 \\
 &4520853068931486273015616135520762600461424773493842826729486603855923 \\
 &3192564711049043329230490341942301545096666157132361663200374743,
 \end{aligned}$$

each correct to 200 places by using (95) with all four indices taken to $N = 1024$. \diamond

6.4. Interrelations for character sums. We start by listing information for the MZV cases to which our derivative free character sums reduce. For the principal character we have

$$(116) \quad \omega \left(\begin{array}{c|c} r & s \\ \hline a & b \end{array} \right) = \zeta^{(a+b)}(r + s).$$

Now let $\zeta_{a,b}$ denote the partial derivative of the multi-zeta function

$$\zeta_{a,b}(r, s) := \sum_{k>j>0} \frac{(-\log k)^a}{k^r} \frac{(-\log j)^b}{j^s}.$$

(We shall sometimes use the term MZV for the principal character and Euler sums for the more general case.)

From the definition we derive:

Proposition 3 (Depth three ω reductions). *For $s, t > 0, a, b \geq 0$ we have*

$$(117) \quad \omega \left(\begin{array}{cc|c} 0, & 0 & t \\ 0, & 0 & b \end{array} \right) = \zeta^{(b)}(t) - \zeta^{(b)}(t - 1),$$

$$(118) \quad \omega \left(\begin{array}{cc|c} s, & 0 & t \\ a, & 0 & b \end{array} \right) = \zeta_{b,a}(t, s),$$

$$(119) \quad \omega \left(\begin{array}{cc|c} s, & t & 0 \\ a, & b & 0 \end{array} \right) = \zeta^{(a)}(s) \zeta^{(b)}(t).$$

Moreover, from Euler’s reflection formula, (see [11]),

$$(120) \quad \zeta(s, t) + \zeta(t, s) = \zeta(s)\zeta(t) - \zeta(t + s),$$

we obtain

$$(121) \quad \omega \left(\begin{array}{cc|c} s, & 0 & t \\ a, & 0 & b \end{array} \right) + \omega \left(\begin{array}{cc|c} t, & 0 & s \\ a, & 0 & b \end{array} \right) = \zeta^{(a)}(s) \zeta^{(b)}(t) - \zeta^{(a+b)}(t + s),$$

or, equivalently,

$$(122) \quad \omega \left(\begin{array}{cc|c} s, & t & 0 \\ a, & b & 0 \end{array} \right) - \omega \left(\begin{array}{cc|c} t, & 0 & s \\ a, & 0 & b \end{array} \right) - \omega \left(\begin{array}{cc|c} s, & 0 & t \\ a, & 0 & b \end{array} \right) = \zeta^{(a+b)}(t + s).$$

When $s = 1$, (121) has singularities and must be handled with care. We fully addressed this issue in [8]. We emphasize that when computing quantities such as $\omega_{2,2,0}(1, 1, 2)$, we require the full version of (83).

For twisted character sums we record the special cases corresponding to Proposition 3.

Proposition 4 (Depth three μ reductions). *For $s, t > 0, a, b, c, q, r \geq 0$ we have:*

$$(123) \quad (\mu_{\pm d_1, \pm d_2})_{0,0,c}(0, 0, t) = \sum_{m,n>0} \frac{\chi_{\pm d_1}(n)\chi_{\pm d_2}(m)}{(m+n)^c},$$

$$(124) \quad (\mu_{\pm d_1, \pm d_2})_{a,0,b}(s, 0, t) = \langle d_2, d_1 \rangle_{b,a}(t, s),$$

$$(125) \quad (\mu_{\pm d_1, \pm d_2})_{a,b,0}(q, r, 0) = L_{\pm d_1}^{(a)}(q) L_{\pm d_1}^{(b)}(r).$$

There are many character analogues of Euler’s reflection for (105) given [17]. For instance, using the second sum in (105) we have

$$[d_1, d_2](a, b) + [d_2, d_1](b, a) = L_{d_1}(a) L_{d_2}(b) - L_{\chi_{d_1}\chi_{d_2}}(a + b),$$

so that for $d_1 = d_2$ and $a = b$ we deduce

$$[d, d](a, a) = \frac{1}{2} L_d(a)^2 - \frac{1}{2} L_{\chi_d^2}(2a).$$

For example,

$$[-3, -3](2, 2) = \frac{1}{2} L_{-3}(2)^2 - \frac{15}{32} \zeta(4),$$

$$[-3, -3](3, 3) = \frac{1}{2} L_{-3}(3)^2 - \frac{63}{128} \zeta(6) = -\frac{4}{32805} \pi^6.$$

The case of the twisted sum, when $d_1 \neq 1$, is less clear. By contrast, in Theorem 6 we have provided an effective integral form for general $\langle d_1, d_2 \rangle$ (the case $r = 0$), while none such is known for $[d_1, d_2]$ except when $d_2(n) = (\pm 1)^{n-1}$.

6.5. Character sum ladders. Rather than proceeding as in Theorem 6, we may use instead, for $c \geq 1$,

$$\Gamma(t)\zeta_{0,a}(t, s) = \int_0^1 (-\log x)^{t-1} \frac{\text{Li}_s^{(a)}(x)}{1-x} dx,$$

and as before, employ Leibnitz' formula to obtain

(126)

$$\zeta_{b,a}(t, s) = - \sum_{k=0}^{b-1} \binom{b}{k} \frac{\Gamma^{(b-k)}(b)}{\Gamma(b)} \zeta_{k,a}(t, s) + \int_0^1 \frac{\text{Li}_s^{(a)}(x)}{1-x} \frac{\log^b(-\log x)}{\Gamma(b)} (-\log x)^{t-1} dx,$$

which leads to a nice *ladder* for $\zeta_{k,a}$ values using the algorithms already provided for $\Gamma^{(k)}(b)$.

The same process leads, more generally, for $q + r + s > 2$ and $a, b, q, r \geq 0$, $c \geq 1, s > 0$, for Dirichlet characters d_1 and d_2 , to the ladder

$$\begin{aligned} (\mu_{\pm d_1, \pm d_2})_{a,b,c}(q, r, s) &= - \sum_{k=0}^{c-1} \binom{c}{k} \frac{\Gamma^{(c-k)}(c)}{\Gamma(c)} (\mu_{\pm d_1, \pm d_2})_{a,b,k}(q, r, s) \\ (127) \quad &+ \frac{1}{\Gamma(c)} \int_0^1 \frac{\text{L}_1^{(a)}(q; x) \text{L}_2^{(b)}(r; x)}{x} \log^c(-\log x) (-\log x)^{s-1} dx. \end{aligned}$$

As in (87), this final term may be split at $1/\sigma$.

For simplicity, we give details only for e , which is relevant for $d_1, d_2 = -2, -3, -4, +5$, and is notationally somewhat cleaner. We have

$$\frac{1}{\Gamma(c)} \int_{1/\sigma}^1 \frac{(-\log(-\log x))^c (-\log x)^{n-1}}{x} dx = \frac{c}{n^{c+1}},$$

whence with $\mathcal{I}_{s,c}(k) := \int_0^{1/e} \log^c(-\log x) (-\log x)^{s-1} x^{k-1} dx$ we adduce

$$\begin{aligned} (\mu_{\pm d_1, \pm d_2})_{a,b,c}(q, r, s) &= - \sum_{k=0}^{c-1} \binom{c}{k} \frac{\Gamma^{(c-k)}(c)}{\Gamma(c)} (\mu_{\pm d_1, \pm d_2})_{a,b,k}(q, r, s) \\ &+ c \sum_{j,k>0} \frac{\text{L}_1^{(a)}(q-j)}{j!} \frac{\text{L}_2^{(b)}(r-k)}{k!} \frac{(-1)^{j+k}}{(j+k+s)^{c+1}} \\ (128) \quad &+ \sum_{m,n>0} \chi_{\pm d_1}(m) \chi_{\pm d_2}(n) \frac{(-\log m)^a}{m^q} \frac{(-\log n)^b}{n^r} \mathcal{I}_{s,c}(m+n). \end{aligned}$$

The $c = 0$ case which ignites the ladder is also covered by the simplest case of (87). Also,

$$(129) \quad \mathcal{I}_{s,0}(k) = \frac{1}{k^s} \int_k^\infty z^{s-1} e^{-z} dz = \frac{\Gamma(s, k)}{k^s}$$

and $\mathcal{I}_{s,c}(k) = \mathcal{I}_{s,0}^{(c)}(k)$. By [33, eqn. (8.7.3)] we have

$$(130) \quad \frac{\Gamma(s, z)}{z^s} = \frac{\Gamma(s)}{z^s} - \sum_{j=0}^\infty \frac{(-1)^j z^j}{j!(s+j)},$$

which can easily be symbolically differentiated with respect to s , using methods described in [8] for the derivation of $\Gamma(s)$.

On combining more general forms of (128) and (129) with Theorem 3, we have effective series ladders for $(\mu_{\pm d_1, \pm d_2})_{a,b,c}(q, r, s)$ for characters to which Theorem 3 applies; so certainly not $d_1 = 1$ which needs the intervention of Theorem 1.

In the forthcoming paper [9] we record more information on computation of incomplete Gamma and Hurwitz zeta functions.

7. CONCLUSION

Needless to say, the tools used above are equally applicable for evaluating character MTW sums with $K > 2$, and to some degree for $N > 1$. For instance,

(131)

$$\begin{aligned} \sqrt{8} \sum_{m,n,p>0} \frac{\chi_{+8}(m)\chi_{+8}(n)\chi_{+8}(p)}{mnp(m+n+p)^8} &= \frac{1}{8!} \int_0^1 \log^3 \left(\frac{1 - \sqrt{2}x + x^2}{1 + \sqrt{2}x + x^2} \right) \log^7 x \frac{dx}{x}, \\ &= \underline{0.000423776563719585317405092} \dots \end{aligned}$$

on using (71a) and the four variable analogue of (62). Summing for $n, m, p \leq 200$ gives agreement of the underlined digits with the displayed integral.

Since, as we have in part illustrated, the polylogarithms and their relatives are central to a great deal of mathematics and mathematical physics [6, 16, 28], such efforts to provide robust high precision algorithms are bound to find many applications in the near future. Indeed, providing a suite of such tools is the basis for a 2014 to 2016 Australian Research Council Discovery Project by the current authors in tandem with Richard Brent.

As we proceed with our research we intend, *inter alia*, to:

- Look for effective integral evaluation methods for general $[a, b](s, t)$.
- Search for evaluations of $\langle a, b \rangle(s, t)$ using basis terms identified in [17].
- Look for relations amongst various $(\mu_{d_1, d_2})_{a,b,c}(q, r, s)$ —primarily with $a = b = c = 0$.

We conclude by emphasising that our research agenda is driven as much by the desire to improve tools for computer-assisted discovery as it is by the precise needs of the current project.

ACKNOWLEDGEMENTS

Thanks are due to Andrew Mattingly, Victor Moll, and to Armin Straub for useful discussions. We also wish to thank an anonymous referee for particularly helpful comments; the manuscript is significantly better as a result. In our research, we employed computer equipment kindly provided for our use by Apple Computers and by the Lawrence Berkeley National Laboratory.

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LAWRENCE BERKELEY NATIONAL LAB (RETIRED), BERKELEY, CALIFORNIA 94720 – AND – DEPARTMENT OF COMPUTER SCIENCE, UNIVERSITY OF CALIFORNIA, DAVIS, DAVIS, CALIFORNIA 95616
E-mail address: david@davidhbailey.com

CARMA, UNIVERSITY OF NEWCASTLE, NSW 2303, AUSTRALIA
E-mail address: jon.borwein@gmail.com