Evaluations of Double L-values*

David Terhune

April 15, 2004

Department of Mathematics

The Pennsylvania State University

218 McAllister Bldg.

University Park, PA 16803

Ph. (814)865-5201

Fax (814)865-3735

Email: terhune@math.psu.edu

Proposed running header: Evaluations of Double L-values

*This article is initial research of the author done at The University of Texas at Austin under the direction of Fernando Rodriguez-Villegas.

Abstract

In this paper, a theorem of D. Zagier concerning double zeta evaluations is generalized to the double L-values. In addition, fast computation of the double L-values is demonstrated, extending the method of Crandall. The PARI commands are available electronically.

Keywords: Multiple L-values; Multiple polylogarithms.

MSC: 11M41, 33E20

1 Introduction

In this paper, we will denote by $\mathbb{Z}_+$ the set of positive integers, and by ϕ the Euler totient function.

The multiple zeta values of depth d of Euler-Riemann-Zagier are defined

$$\zeta(a_1, a_2, \ldots, a_d) = \sum_{0<n_1<n_2<\cdots<n_d} n_1^{-a_1} n_2^{-a_2} \cdots n_d^{-a_d}$$

where each $a_j \in \mathbb{Z}_+$, and $a_d > 1$. As mentioned in [2] and [5], these values have been related to such varied subjects as knot theory, cohomology of motives, and even quantum physics. By estimating the nested sums, it can be shown that the sum converges absolutely for

$$\Re(a_d) > 1, \qquad \Re(a_j) \geq 1, \quad j = 1, \ldots, d-1$$

In this paper, each a_j will assume only positive integer values.

For Dirichlet characters $\chi_1, \ldots, \chi_d$, we define the multiple L-values of depth d

$$L\binom{\chi_1, \ldots, \chi_d}{a_1, \ldots, a_d} = \lim_{N\to\infty} \sum_{0<n_1<\cdots<n_d\leq N} \frac{\chi_1(n_1)\cdots\chi_d(n_d)}{n_1^{a_1}\cdots n_d^{a_d}} \tag{1}$$

where each $a_j \in \mathbb{Z}_+$, if this limit exists. Note that our domain of absolute convergence for the multiple zetas applies trivially to these values also.

We define the multiple polylogarithm of depth d

$$Li_{a_1,\ldots,a_d}(x_1, \ldots, x_d) = \lim_{N\to\infty} \sum_{0<n_1<\cdots<n_d\leq N} \frac{x_1^{n_1}\cdots x_d^{n_d}}{n_1^{a_1}\cdots n_d^{a_d}} \tag{2}$$

for $a_j \in \mathbb{Z}_+$ and $x_j \in \mathbb{C}$, when this limit exists. For $d = 1$, this is the conventional polylogarithm $Li_a(x) = \sum_{n=1}^{\infty} x^n/n^a$. Note that if each x_j is a root of unity, then our multiple zeta domain of absolute convergence applies to these values also.

Many evaluations of multiple zeta values have been found (some of which were known to Euler). Some examples are:

$$\zeta(1,2) = \zeta(3) \qquad \zeta(1,3) = \frac{3}{2}\zeta(4) - \frac{1}{2}\zeta(2)^2$$

$$\zeta(1,4) = 2\zeta(5) - \zeta(2)\zeta(3) \qquad \zeta(1,1,2) = \zeta(4)$$

$$\zeta(2,3) = \zeta(1,2,2) = -\frac{11}{2}\zeta(5) + 3\zeta(2)\zeta(3)$$

$$\zeta(2,1,5) = \frac{157}{360}\zeta(8) + \frac{5}{2}\zeta(3)\zeta(5) - \frac{3}{2}\zeta(3)^2\zeta(2) + \frac{2}{5}\zeta(3,5)$$

We will give examples of similar evaluations for double L-values.

We make the following definition.

Definition 1. *For positive integers D and m, we denote by $R_{D,m}$ the ring generated by $\mathbb{Q}(\zeta_m)$ and the values of convergent polylogarithms at D-th roots of unity.*

We will use the notation $\chi \neq 1$ to indicate that χ is non-principal. D. Zagier[5] showed:

Let $a, b \in \mathbb{Z}_+$, with $b > 1$. If $a + b$ is odd, then $\zeta(a,b)$ lies in $R_{1,1}$.

In section 2 of this paper, the methods of [1] will be adapted to prove the main theorem, which generalizes Zagier's result to the double L-values.

Many of our evaluations arose initially from numerical computation, before proofs were found; in section 3, we will outline derivations of fast-converging series which were used in these computations. In section 4, we give an example of an actual PARI session confirming one of our evaluations. In the appendix, we list some evaluations which are special cases of our theorem, and which were numerically verified.

Throughout this paper, we will denote by ζ_D the Dth root of unity $e^{2\pi i/D}$, for $D \in \mathbb{Z}_+$. In our proof, we will use the finite Fourier expansion of a Dirichlet character χ of conductor D

$$\chi(n) = \sum_{k=1}^{D} c_k(\chi)\zeta_D^{nk} \tag{3}$$

where the $c_k(\chi)$ are complex numbers. We will use the fact that the $c_k(\chi)$, in fact, lie in the cyclotomic field obtained by adjoining ζ_D and the values of χ to

$\mathbb{Q}$. This is due to the fact that

$$c_k(\chi) = \frac{1}{D} \sum_{l=1}^{D} \chi(l) \zeta_D^{-kl} \tag{4}$$

which is easily verified. For example, it can be shown that if χ is primitive, $c_k(\chi) = \bar{\chi}(k)/G(\bar{\chi})$, where $G(\psi)$ denotes the Gauss sum of the character ψ. In this paper, we will use (3) and (4) to write multiple L-values in terms of values of multiple polylogarithms at roots of unity.

We make the following definition:

Definition 2. *Let $\chi_1, \ldots, \chi_d$ be Dirichlet characters, and $x_1, \ldots, x_d$ be roots of unity. We define the weight of*

$$\zeta(a_1, \ldots, a_d) \quad or \quad L\binom{\chi_1, \cdots, \chi_d}{a_1, \ldots, a_d} \quad or \quad Li_{a_1,\ldots,a_d}(x_1, \ldots, x_d)$$

to be $a_1 + \cdots + a_d$. Further, suppose $y_1, \ldots, y_k$ each have weight w, and z has weight v. Then we define the weight of $y_1 + \cdots + y_k$ to also be w and the weight of $y_1 z$ to be $v + w$.

The consistency of this definition is obviously still conjectural. Notice that all of our listed evaluations respect this notion of weight. In fact, so also do all known evaluations of multiple zeta values.

Concerning the conditional convergence of some of the multiple L-values, we find the following:

Proposition 1. *The sum defining either of the following converges:*

i) A multiple polylogarithm (2) at roots of unity with $x_d \neq 1$.

ii) A multiple L-value (1) with $\chi_d \neq 1$.

Proof. We first show that the defining sum for a number as in i converges. If $a_d > 1$, we are in Zhao's domain of absolute convergence; thus, we can assume $a_d = 1$. We will show the sequence of partial sums in the last index n_d is Cauchy.

We set

$$z(N) := \sum_{0<n_1<\cdots<n_{d-1}<N} \frac{x_1^{n_1}\cdots x_{d-1}^{n_{d-1}}}{n_1^{a_1}\cdots n_{d-1}^{a_{d-1}}}$$

and

$$c(n) := \sum_{m=1}^{n} x_d^m$$

Our assumptions guarantee that $c(n)$ is bounded. Consider for $N \in \mathbb{Z}_+$,

$$S_N = \sum_{n=1}^{N} z(n)\frac{x_d^n}{n} \tag{5}$$

We will show the sequence S_N is Cauchy in N. For $M, N \in \mathbb{Z}_+$, $M < N$,

$$\left|S_N - S_M\right| = \Big|\sum_{n=M+1}^{N} z(n)\frac{x_d^n}{n}\Big| \tag{6}$$

By Abel summation, this equals

$$\Big|\frac{z(N+1)c(N)}{N+1} + \sum_{n=M+1}^{N} c(n)\Big(\frac{z(n)}{n} - \frac{z(n+1)}{n+1}\Big)\Big| \tag{7}$$

The term in parentheses can be rewritten as

$$\sum_{0<n_1<\cdots<n_{d-1}<n} \frac{x_1\cdots x_{d-1}^{n_{d-1}}}{n_1^{a_1}\cdots n_{d-1}^{a_{d-1}}}\Big(\frac{1}{n} - \frac{1}{n+1}\Big) + \sum_{0<n_1<\cdots<n_{d-1}=n} \frac{x_1^{n_1}\cdots x_{d-1}^{n_{d-1}}}{n_1^{a_1}\cdots n_{d-1}^{a_{d-1}}(n+1)}$$

Hence, the second term in (7) can be majorized by a sum $y_1 + y_2$, where each y_j is a difference of two partial sums of a multiple zeta value with $a_d > 1$. Since the sequence of such partial sums is Cauchy, the second term in (7) approaches zero as $M, N \to \infty$.

To complete the proof that a sum as in i converges, it suffices to show $z(N)/N \to 0$ as $N \to \infty$. By inducting on d, and comparing $z(N)$ with an appropriate integral, one finds that $z(N)$ grows at most as a power of $\log(N)$.

To show that the defining sum for a number as in ii also converges, we define the partial sums

$$T_N = \sum_{0<n_1<\cdots<n_d\leq N} \frac{\chi_1(n_1)\cdots\chi_d(n_d)}{n_1^{a_1}\cdots n_{d-1}^{a_{d-1}} n_d}$$

We now use (3) and (4) to write this as a $\mathbb{C}$-linear combination of the quantities (5), each of which we have already shown to converge as $N \to \infty$. Terms with $x_d = 1$ cannot appear in this combination, since, in (3), for $\chi \neq 1$, $c_D(\chi) = 0$, where $D = \operatorname{cond}(\chi)$. Thus, the sequence $\{T_N\}$ also converges as $N \to \infty$. This finishes the proof of the proposition. $\square$

Therefore, we know the multiple L-values include the limits (1) for which $a_d > 1$, and also those for which $\chi_d \neq 1$ and $a_d = 1$.

2 Main Results

We will denote by μ_D the set of complex Dth roots of unity, for $D \in \mathbb{Z}_+$.

Let χ_D be the quadratic character defined by the Legendre symbol $\left(\frac{D}{\cdot}\right)$. Some evaluations of double L-values which can be found using the methods of this section are:

$$L\begin{pmatrix}\chi_{-3}, 1\\ 1, 3\end{pmatrix} = \frac{1}{2}(\log 3)L_{\chi_{-3}}(3) + \frac{13}{9}L_{\chi_{-3}}(1)\zeta(3) - \frac{1}{3}L_{\chi_{-3}}(2)\zeta(2) - L_{\chi_{-3}}(4) \quad (8)$$

$$L\begin{pmatrix}\chi_{-3}, 1\\ 2, 2\end{pmatrix} = L_{\chi_{-3}}(4) + \frac{4}{3}\zeta(2)L_{\chi_{-3}}(2) - \frac{26}{9}L_{\chi_{-3}}(1)\zeta(3) \quad (9)$$

$$L\begin{pmatrix}\chi_5, 1\\ 1, 2\end{pmatrix} = L_{\chi_5}(1)\zeta(2) - \frac{1}{12}(r_1 + 4r_2 + 7r_3)L_{\chi_5}(2)$$
$$- \frac{1}{4}\frac{\bar{G}_o}{G_e}(r_1 - ir_2 + ir_3 - r_4)L_{\chi_o}(2) + \frac{1}{4}\frac{G_o}{G_e}(r_1 + ir_2 - ir_3 - r_4)\bar{L}_{\chi_o}(2) \quad (10)$$

In the last expression, $r_j = \log(1 - \zeta^j)$, with $\zeta = \exp(2\pi i/5)$, G_e is the Gauss sum of χ_5, χ_o is the odd character of conductor 5 such that $\chi_o(2) = i$, and G_o its Gauss sum. This is also an example of an evaluation for which the coefficients do not lie in $\mathbb{Q}$. Note each of these evaluations is weight-preserving. At the end of this section, we will derive the identities (8) and (9). In addition, more evaluations of this type are listed in the appendix.

A partial fractions decomposition due to Markett[4] is

$$\frac{1}{m^a(m-n)^b} = \sum_{c+d=a+b} \{M^{a,b}_{c,d}\frac{1}{m^c n^d} + N^{a,b}_{c,d}\frac{1}{n^c(m-n)^d}\} \tag{11}$$

where c and d are restricted to the positive integers, and

$$M^{a,b}_{c,d} = (-1)^b\binom{d-1}{b-1} \qquad N^{a,b}_{c,d} = (-1)^{a+c}\binom{c-1}{a-1}$$

We will substitute (11) into the summands of double sums in order to find linear combinations of these double sums which equal a linear combination of products of single sums.

We define the following extension of binomial coefficients:

Definition 3. *For arbitrary integers a, b, we define the binomial coefficient*

$$\binom{a}{b} = \begin{cases} \frac{a(a-1)\cdots(b+1)}{(a-b)!}, & a \geq b \\ 0, & \textit{otherwise} \end{cases}$$

We will use the following to derive matrix identities in this proof.

Proposition 2. *For $a, b, c, d \in \mathbb{Z}$,*

$$\sum_{k=-\infty}^{\infty} (-1)^k \binom{a-k}{b}\binom{c}{d+k} = (-1)^d\binom{a+d-c}{b-c} \tag{12}$$

Proof. Note this is a finite sum for $a, b, c, d \geq 0$. We have for $e \in \mathbb{Z}$ and $f \in \mathbb{C}$ the power series expansions

$$\sum_{k=e}^{\infty}\binom{k}{e}x^k = \frac{x^e}{(1-x)^{e+1}} \qquad \sum_{k=0}^{f}(-1)^k\binom{f}{k}x^k = (1-x)^f \tag{13}$$

The second of these is the binomial series, and the first arises from differentiation of geometric series for $e \geq 0$. To show that the first holds for all $e \in \mathbb{Z}$, note that for $e < 0$,

$$\sum_{k=e}^{\infty}\binom{k}{e}x^k = \sum_{k=e}^{0}\binom{k}{e}x^k = \sum_{k=0}^{-e}\binom{-k}{e}x^{-k} \tag{14}$$

By our definition,

$$\binom{-k}{e} = \frac{-k(-k-1)\cdots(e+1)}{(-k-e)!}$$

for $0 \le k \le -e$. This equals

$$(-1)^{k+e}\frac{k(k+1)\cdots(-e-1)}{(-k-e)!} = (-1)^{k+e}\binom{-e-1}{k-1} \tag{15}$$

Substituting (15) into (14) gives

$$\sum_{k=0}^{-e}\binom{-k}{e}x^{-k} = \sum_{k=0}^{-e}(-1)^{k+e}\binom{-e-1}{k-1}x^{-k}$$
$$= \frac{(-1)^{e-1}}{x}\sum_{k=0}^{-e}\binom{-e-1}{k-1}(-x)^{-k+1} = \frac{(-1)^{e-1}}{x}\big(1-\frac{1}{x}\big)^{-e-1} = \frac{x^e}{(1-x)^{e+1}}$$

Thus, the first power series expansion in (13) does indeed hold for all integers e. Now, the desired sum (12) is $(-1)^d$ times the coefficient of x^{a+d} in the power series expansion of

$$\frac{x^b}{(1-x)^{b-c+1}} = x^c\frac{x^{b-c}}{(1-x)^{b-c+1}}$$

which is as stated, by the first formula in (13). □

Our main result is the following:

Theorem 1. *Let χ (resp. ψ) be a Dirichlet character of conductor D (resp. E), and $a, b \in \mathbb{Z}_+$ with $a + b \ge 3$. In addition, suppose $b > 1$ or $\psi \ne 1$. Set $m = \mathrm{lcm}(D, E, \phi(D), \phi(E))$ and $F = \mathrm{lcm}(D, E)$. If $\chi(-1)\psi(-1) = (-1)^{a+b-1}$, then*

$$L\binom{\chi, \psi}{a, b} \in R_{F,m}$$

.

Proof. We define for Dirichlet characters χ and ψ and positive integers a, b, N the partial sums

$$L_N\binom{\chi, \psi}{a, b} = \sum_{0<m<n\le N}\frac{\chi(m)\psi(n)}{m^a n^b} \qquad K_N\binom{\chi, \psi}{a, b} = \sum_{0<m<n\le N}\frac{\chi(m)\psi(n-m)}{m^a n^b}$$

$$L_N(\chi, a) = \sum_{n=1}^{N}\frac{\chi(n)}{n^a} \qquad Li_a^N(x) = \sum_{n=1}^{N}\frac{x^n}{n^a}$$

For $A, n, N \in \mathbb{Z}_+$, we will denote by $LC^N_{A,n}$ the set of $\mathbb{Q}(\zeta_n)$-linear combinations of products of terms $Li^N_a(\zeta)$ for $a \in \mathbb{Z}_+$ and $\zeta \in \mu_A$.

In deriving the identities promised by the theorem (including those listed both at the first of this section and in the appendix), we need the standard fact that

$$\lim_{N\to\infty} Li^N_1(x) = -\log(1-x) \tag{16}$$

holds for $|x| = 1$, $x \neq 1$, where $\log z$ denotes the principal branch of the logarithm

$$\frac{-i\pi}{2} < \text{Arg}\big(\log z\big) < \frac{i\pi}{2}$$

The corollary to theorem 1 requires the following, which is well known (see, e.g., [3]): For $\chi \neq 1$,

$$\lim_{N\to\infty} L_N(\chi, 1) = L(\chi, 1)$$

Our strategy in proving the theorem is as follows. We will use three techniques for finding $\mathbb{Z}$-linear combinations of L_N- and K_N-double sums which are equal to an element of $LC^N_{F,m}$, plus possibly some error terms. In lemma 1.2, it will be shown that the error terms approach zero as $N \to \infty$. The coefficients in these $\mathbb{Z}$-linear combinations will form a matrix, which will be shown to have full rank when the weight has the appropriate parity. Thus, in this case, we evaluate each L_N- and K_N-double sum as an element of $LC^N_{F,m}$, plus an expression which approaches zero as $N \to \infty$. At the end of the proof, we will resolve the issues concerning what happens as we let $N \to \infty$ in these evaluations.

The first of our three evaluation techniques consists of applications of the "shuffle" relation. This says that for $a, b \in \mathbb{Z}_+$,

$$L_N\begin{pmatrix}\chi, \psi\\ a, b\end{pmatrix} + L_N\begin{pmatrix}\psi, \chi\\ b, a\end{pmatrix} + \sum_{n=1}^{N} \frac{\chi(n)\psi(n)}{n^{a+b}} = L_N(\chi, a)L_N(\psi, b) \tag{17}$$

This follows by observing that both sides equal

$$\sum_{m,n=1}^{N} \frac{\chi(m)\psi(n)}{m^a n^b}$$

We use the finite Fourier expansion (3) and (4) to write the right-hand side and the last term on the left-hand side as an element of $LC_{F,m}^N$. Thus, we have $\mathbb{Z}$-linear combinations of L_N-double sums which equal linear combinations of products of single sums. Note that there are no error terms.

Remark: Letting $N \to \infty$ in (17), we also see

$$L\binom{\chi, \psi}{a, b} + L\binom{\psi, \chi}{b, a} + \sum_{n=1}^{\infty} \frac{\chi(n)\psi(n)}{n^{a+b}} = L(\chi, a)L(\psi, b)$$

when the sum defining each term converges.

In order to obtain our second evaluation technique, we write

$$L_N\binom{\chi, \psi}{a, b} = \sum_{n=1}^{N}\sum_{m=1}^{n-1} \frac{\chi(m)\psi(n)}{m^a n^b} = \sum_{n=1}^{N}\sum_{m=1}^{n-1} \frac{\chi(n-m)\psi(n)}{(n-m)^a n^b}$$

Using (11), this equals

$$\sum_{\substack{c+d=a+b \\ c,d>0}} \Big\{ M_{c,d}^{b,a} \sum_{n=1}^{N}\sum_{m=1}^{n-1} \frac{\chi(n-m)\psi(n)}{m^d n^c} + N_{c,d}^{b,a} \sum_{n=1}^{N}\sum_{m=1}^{n-1} \frac{\chi(n-m)\psi(n)}{m^c (n-m)^d} \Big\} \quad (18)$$

The first double sum in braces equals

$$\sum_{0<m<n\le N} \frac{\chi(n-m)\psi(n)}{m^d n^c} = \sum_{0<n<m\le N} \frac{\psi(m)\chi(m-n)}{m^c n^d}$$

$$= \chi(-1)\Big\{ \sum_{m,n=1}^{N} \frac{\psi(m)\chi(n-m)}{m^c n^d} - \delta_{\chi,1} L_N(\psi, c+d) - \sum_{0<m<n\le N} \frac{\psi(m)\chi(n-m)}{m^c n^d} \Big\}$$

$$= \chi(-1)\Big\{ \sum_{m,n=1}^{N} \frac{\psi(m)\chi(n-m)}{m^c n^d} - \delta_{\chi,1} L_N(\psi, c+d) - K_N\binom{\psi, \chi}{c, d} \Big\} \quad (19)$$

where we define for two Dirichlet characters χ and ψ

$$\delta_{\chi,\psi} = \begin{cases} 1, & \chi = \psi \\ 0, & \text{otherwise} \end{cases}$$

The first sum in braces in (19) can be written in terms of values of Li_a^N at roots of unity for various $a \in \mathbb{Z}_+$ by using (3) and (4). The second double sum in braces in (18) equals

$$\sum_{n=1}^{N}\sum_{m=1}^{N-n} \frac{\chi(m)\psi(m+n)}{m^d n^c} = \sum_{m,n=1}^{N} \frac{\chi(m)\psi(m+n)}{m^d n^c} - e_1^N \binom{\chi, \psi}{d, c} \tag{20}$$

where we have the error term

$$e_1^N \binom{\chi, \psi}{x, y} = \sum_{n=1}^{N} \sum_{m=N-n+1}^{N} \frac{\chi(m)\psi(m+n)}{m^x n^y} \tag{21}$$

The first sum on the RHS of (20) is also a linear combination of single sums. The error terms may be disregarded, as by lemma 1.2, they approach zero as $N \to \infty$. Thus, we express each $L_N(\chi, \psi; a, b)$ as a $\mathbb{Z}$-linear combination of the numbers $K_N(\psi, \chi; c, d)$ (where c, d range over the positive integers with $c + d = a + b$) plus an element of $LC_{F,m}^N$ (after using (3) and (4) to write single L_N-sums in terms of values of Li_a^N at roots of unity, for $a \in \mathbb{Z}_+$), plus an expression which approaches zero as $N \to \infty$.

In order to obtain our third and last evaluation technique, we apply a similar procedure to the K_N sums:

$$K_N \binom{\chi, \psi}{a, b} = \sum_{n=1}^{N}\sum_{m=1}^{n-1} \frac{\chi(m)\psi(n-m)}{m^a n^b} = \sum_{n=1}^{N}\sum_{m=1}^{n-1} \frac{\chi(n-m)\psi(m)}{(n-m)^a n^b}$$
$$= \sum_{\substack{c+d=a+b \\ c,d>0}} \Big\{ M_{c,d}^{b,a} \sum_{n=1}^{N}\sum_{m=1}^{n-1} \frac{\chi(n-m)\psi(m)}{m^d n^c} + N_{c,d}^{b,a} \sum_{m=1}^{N}\sum_{m=1}^{n-1} \frac{\chi(n-m)\psi(m)}{m^c (n-m)^d} \Big\}$$

The first double sum in braces equals

$$\sum_{0<m<n\le N} \frac{\chi(n-m)\psi(m)}{m^d n^c} = K_N \binom{\psi, \chi}{d, c}$$

while the second is

$$\sum_{n=1}^{N}\sum_{m=1}^{N-n} \frac{\psi(m)\chi(n)}{m^c n^d} = \sum_{m,n=1}^{N} \frac{\psi(m)\chi(n)}{m^c n^d} - e_2^N \binom{\psi, \chi}{c, d}$$
$$= L_N(\psi, c) L_N(\chi, d) - e_2^N \binom{\psi, \chi}{c, d}$$

where

$$e_2^N\binom{\chi,\psi}{x,y} = \sum_{n=1}^{N}\sum_{m=N+1-n}^{N}\frac{\chi(m)\psi(n)}{m^x n^y} \tag{22}$$

Thus, we express each value $K_N(\chi,\psi;a,b)$ as a $\mathbb{Z}$-linear combination of values $K_N(\psi,\chi;c,d)$ (where c,d range over the positive integers with $c+d=a+b$) plus an element of $LC^N_{F,m}$, plus some error terms.

Remark: By letting $N\to\infty$, we find linear combinations of L_N and K_N double sums which equal linear combinations of products of (single) polylogarithms evaluated at roots of unity, when each involved sum converges.

Set $w=a+b$ and $v=w-1$. We now have three methods of obtaining linear combinations of the $4v$ values

$$L_N\binom{\chi,\psi}{c,d},\quad L_N\binom{\psi,\chi}{c,d},\quad K_N\binom{\chi,\psi}{c,d},\quad K_N\binom{\psi,\chi}{c,d}$$

(where $c+d=a+b$, $c,d\in\mathbb{Z}_+$) which equal linear combinations of products of single sums, plus error terms.

For $j=1,\ldots,v$, set $p_j=(j,w-j)\in\mathbb{Z}_+\times\mathbb{Z}_+$. We now order the the double sums above as follows:

$$\begin{aligned}&L_N\binom{\chi,\psi}{p_1},\ldots,L_N\binom{\chi,\psi}{p_v},L_N\binom{\psi,\chi}{p_1},\ldots,L_N\binom{\psi,\chi}{p_v},\\&\qquad\ldots,K\binom{\chi,\psi}{p_1},\ldots,K_N\binom{\chi,\psi}{p_v},\ldots,K_N\binom{\psi,\chi}{p_1},\ldots,K_N\binom{\psi,\chi}{p_v}\end{aligned} \tag{23}$$

Our two partial fractions techniques give $4v$ linear relations among these numbers. We order these relations as follows. First, we list those relations resulting from applying our partial fractions technique to the first $2v$ numbers in (23) in the order listed there (as in our second evaluation rechnique). We list next the relations resulting from applying partial fractions to the last $2v$ numbers in (23) (as in the third evaluation technique). Finally, list the v relations coming from the shuffle relation (the first evaluation technique). We will assume these $5v$ relations are written as equations with all double-sum L_N and K_N values which appear written on the LHS, and all other terms on the RHS (error terms will be disregarded).

We will next construct a matrix of the coefficients appearing on the LHS's of these equations, and show that when w has a certain parity, this matrix has full rank. This implies that each of the numbers in (23) can be written in terms of the single sums appearing on the right-hand sides of these relations.

The square identity matrix of appropriate dimension will be denoted by I. We will denote by X_{ij} the ij-entry of a $D \times E$ matrix X, for $1 \leq i \leq D$ and $1 \leq j \leq E$. We define a $5v \times 4v$ matrix M by declaring M_{ij} to be the coefficient in the ith relation (listing the relations in the order given above) of the jth number in the list (23). The coefficients of the double sums on the LHS's of these relations form a matrix. In block matrix form, it is

$$M = \begin{pmatrix} I & & & \chi(-1)B \\ & I & \psi(-1)B & \\ & & I & A \\ & & A & I \\ I & P & & \end{pmatrix} \tag{24}$$

for some $v \times v$ matrices A and B, where P is the $v \times v$ permutation matrix with 1's along the anti-diagonal. Using previous computations to calculate A and B, we find

$$A_{ij} = -M^{b,a}_{c,d} = (-1)^{a-1}\binom{d-1}{a-1} = (-1)^{i-1}\binom{j-1}{i-1} \tag{25}$$

$$B_{ij} = M^{b,a}_{c,d} = (-1)^{a}\binom{d-1}{a-1} = (-1)^{i}\binom{w-j-1}{i-1} = (-AP)_{ij}$$

Hence,

$$M = \begin{pmatrix} I & & & -\chi(-1)AP \\ & I & -\psi(-1)AP & \\ & & I & A \\ & & A & I \\ I & P & & \end{pmatrix} \tag{26}$$

where A is defined by (25). Note

$$(A^2)_{ij} = (-1)^{i-1} \sum_{k=1}^{w-1} (-1)^{k-1} \binom{k-1}{i-1} \binom{j-1}{k-1}$$

$$= (-1)^{i-1} \sum_{k=0}^{w-2} (-1)^{k} \binom{k}{i-1} \binom{j-1}{j-k-1}$$

By proposition 2, this is

$$(-1)^{i+j} \binom{0}{i-j} = I_{ij}$$

Thus,

$$A^2 = I$$

It is elementary to see that $P^2 = I$. A crucial fact is

Lemma 1.1.

$$APA = (-1)^w PAP$$

Proof. We write

$$(AP)_{ij} = \sum_{k=1}^{w-1} (-1)^{i-1} \binom{k-1}{i-1} \delta_{k+j,w} = (-1)^{i-1} \binom{w-j-1}{i-1}$$

where for integers x, y,

$$\delta_{x,y} = \begin{cases} 1, & x = y \\ 0, & \text{otherwise} \end{cases}$$

Then

$$(APA)_{ij} = (-1)^{i-1} \sum_{k=1}^{w-1} (-1)^{k-1} \binom{w-k-1}{i-1} \binom{j-1}{k-1}$$

$$= (-1)^{i-1} \sum_{k=0}^{w-2} (-1)^{k} \binom{w-k-2}{i-1} \binom{j-1}{k}$$

while

$$(PAP)_{ij} = \sum_{k=1}^{w-1} \delta_{i+k,w} (-1)^{k-1} \binom{w-j-1}{k-1}$$

$$= (-1)^{w-i-1} \binom{w-j-1}{w-i-1} = (-1)^{w-i-1} \binom{w-j-1}{i-j}$$

Applying proposition 2 now gives the result. ∎

Our goal is to show the block matrix (26) has full rank when $\chi(-1)\psi(-1) = (-1)^{w-1} = (-1)^{a+b-1}$. Note that multiplying the fourth row on the left by A gives the third row; thus, the fourth row is redundant. Eliminating the fourth row, we define the remaining matrix

$$M_1 = \begin{pmatrix} I & & & -\chi(-1)AP \\ & I & -\psi(-1)AP & \\ & & I & A \\ I & P & & \end{pmatrix}$$

One can verify, using lemma 1.1, that M_1^{-1} equals

$$\frac{1}{2}\begin{pmatrix} I & -P & -\psi(-1)PAP & I \\ -P & I & \psi(-1)AP & P \\ -\psi(-1)PAP & -\psi(-1)PA & I & \psi(-1)PAP \\ -\chi(-1)PA & -\chi(-1)PAP & A & \chi(-1)PA \end{pmatrix}$$

when $\chi(-1)\psi(-1) = (-1)^{w-1}$. To finish the proof of the theorem, it remains to show that the error terms approach zero as $N \to \infty$, and, by analyzing the behavior of the sums appearing in our evaluations, to show that these evaluations really are correct.

Remark: The explicit form of M_1^{-1} above can be used to find formulas for the evaluations promised by the theorem. E.g., in the case of the double zeta values,

$$\begin{aligned} \zeta(k, w-k) = {} & \frac{1+(-1)^{k-1}}{2}\zeta(k)\zeta(w-k) \\ & - \frac{1}{2}\Big\{1 + (-1)^k\Big(\binom{w-1}{k} + \binom{w-1}{k-1}\Big)\Big\}\zeta(w) \\ & + (-1)^k \sum_{\substack{j=1 \\ j \text{ odd}}}^{w-1} \Big\{\binom{j-1}{k-1} + \binom{j-1}{w-k-1}\Big\}\zeta(j)\zeta(w-j) \end{aligned}$$

when $0 < k < w$ and w is odd. More generally, when $\chi(-1)\psi(-1) = (-1)^{w-1}$,

$$L\binom{\chi, \psi}{k, w-k} = \frac{1}{2}\Big\{(-1)^k \sum_{l=1}^{w-1} \Big\{\chi(-1)\binom{l-1}{k-1}\big(S^-_{w-l}(\psi, \chi) - \delta_{\chi,1} L_\psi(w)\big)$$
$$+ (-1)^{w+l}\binom{l-1}{w-k-1} S^+_{w-l}(\chi, \psi)\Big\} - (-1)^{w+k} T$$
$$+ \big(1 + \psi(-1)(-1)^{k+w}\big) L_\chi(k) L_\psi(w-k) - \sum_{n=1}^{\infty} \frac{\chi(n)\psi(n)}{n^w}\Big\}$$

where

$$T = \sum_{l=1}^{w-1} \Big\{\psi(-1)\binom{l-1}{w-k-1}\big(S^-_{w-l}(\chi, \psi)$$
$$- \delta_{\psi,1} L_\chi(w)\big) + (-1)^{w+l}\binom{l-1}{k-1} S^+_{w-l}(\psi, \chi)\Big\}$$

and we define for Dirichlet characters σ, τ, $w \in \mathbb{Z}$, $w \geq 3$,

$$S^-_j(\sigma, \tau) = \sum_{m,n=1}^{\infty} \frac{\sigma(m)\tau(n-m)}{m^j n^{w-j}}$$

$$S^+_j(\sigma, \tau) = \sum_{m,n=1}^{\infty} \frac{\sigma(m)\tau(m+n)}{m^j n^{w-j}}$$

We now proceed to evaluate the error terms.

Lemma 1.2. *Let e_1^N and e_2^N be as in (21) and (22). Then for any Dirichlet characters σ, τ,*

$$\lim_{N \to \infty} e_1 \binom{\sigma, \tau}{c, d} = \lim_{N \to \infty} e_2 \binom{\sigma, \tau}{c, d} = 0$$

where $c, d \in \mathbb{Z}_+$, $c + d \geq 3$.

Proof. In each case, we majorize by taking absolute values inside the summation. It is enough to consider the cases $c = 1$, $d = 2$, and $c = 2$, $d = 1$. By symmetry, we need only show that

$$\lim_{N \to \infty} \sum_{n=1}^{N} \sum_{m=N+1-n}^{N} \frac{1}{m^2 n} = 0$$

By estimating the inner sum, the above sum is

$$O\Big\{\frac{1}{N}\sum_{n=1}^{N}\frac{1}{n}+\sum_{n=1}^{N}\frac{1}{n(N+1-n)}\Big\}=O\Big\{\frac{\log N}{N}+\frac{1}{N+1}\sum_{n=1}^{N}\big(\frac{1}{n}+\frac{1}{N+1-n}\big)\Big\}$$

by applying partial fractions. Estimating the last sum, we obtain $O(\log N/N)$ for this sum also. Thus, the above limit is zero, as required. □

Hence, all error terms which appear approach zero as $N\to\infty$. To finish the proof of theorem 1, we now show that the evaluations obtained from our method actually are correct (i.e., that our manipulations of infinite sums are valid). Sums may appear in our evaluations which do not converge as $N\to\infty$. We will show that the summands in which these non-convergent sums appear approach zero as $N\to\infty$. We define

$$\zeta_N(1)=\sum_{n=1}^{N}\frac{1}{n}$$

Let S_N be one of the values in (23), which we know to converge. The verification may involve applying (3), (4), and proposition 1, if the convergence is conditional. We write the evaluation of S_N resulting from solving the system of equations from which M_1 was constructed (ignoring the error terms) in the form

$$S_N=\rho_0(N)+\rho_1(N)\zeta_N(1) \tag{27}$$

where for $j=1,2$, $\rho_j(N)$ is an element of $LC^N_{F,m}$, and each term $Li_a(x)$ which appears has either $a=1$ and $x\neq 1$, or $a>1$ (so that each term converges as $N\to\infty$). Since we only consider weights $w\geq 3$ in theorem 1, we do not here consider the term $\zeta_N(1)^2$, which could only result from evaluating a number of weight 2, since each of our evaluation techniques is weight-preserving. Now, dividing both sides of (27) by $\zeta_N(1)$ shows $\rho_1(N)\to 0$ as $N\to\infty$ (since the other terms do). In fact, our proof shows that $\rho_1(N)$ is a finite linear combination $\sum_j \alpha_j Li^N_c(x_j)$ where each $\alpha_j\in\mathbb{Q}(\zeta_m)$, $x_j\in\mu_F$, and $c=w-1$. Since $w\geq 3$, each summand of $\rho_1(N)$ has weight ≥ 2. Hence, $\rho_1(N)=O(1/N)$ at worst.

Since $\zeta_N(1) = O(\log N)$, $\lim_{N\to\infty} \rho_1(N)\zeta_N(1) = 0$. Thus, the contribution of the last term on the right side of (27) approaches zero as $N \to \infty$. This finishes the proof of theorem 1. □

In order to deduce the corollary, we will need the following proposition.

Proposition 3. *Let $a \in \mathbb{Z}$, $a > 1$, $D \in \mathbb{Z}_+$, and ζ be a complex Dth root of unity. Set $m = \mathrm{lcm}(D, \phi(D))$. Then $Li_a(\zeta)$ equals a finite linear combination*

$$\sum_{j=1}^{J} a_j L(a, \chi_j)$$

where each $a_j \in \mathbb{Q}(\zeta_m)$ and each χ_j is a Dirichlet character with conductor dividing D.

Proof. Set $\zeta = \zeta_D^k$, where $(k, D) = 1$. We write

$$\begin{aligned} Li_a(\zeta) = \sum_{l=1}^{D} \zeta_D^{kl} \sum_{\substack{n>0 \\ n\equiv l\ (D)}} \frac{1}{n^a} &= \sum_{l=1}^{D} \frac{\zeta_D^{kl}}{(l,D)^a} \sum_{\substack{n>0 \\ n\equiv l/(l,D)\ (D/(l,D))}} \frac{1}{n^a} \\ &= \sum_{l=1}^{D} \frac{\zeta_D^{kl}}{(l,D)^a} \phi\Big(\frac{D}{(l,D)}\Big)^{-1} \sum_{\chi} \bar{\chi}\Big(\frac{l}{(l,D)}\Big) L_\chi(a), \end{aligned}$$

where the last sum is over all characters χ of the form $\chi_0\psi$, with ψ a primitive character mod (l, D), and χ_0 the principal character modulo (l, D). □

Our proof of theorem 1 actually shows $L(\chi, \psi; a, b)$ can be written as a finite sum $\sum_j a_j l_j m_j$, where each $a_j \in \mathbb{Q}(\zeta_m)$, and each l_j and m_j are values of single polylogarithms at F-th roots of unity. Combining this fact with proposition 3, we have the following corollary.

Corollary 1.1. *With hypotheses as in theorem 1, $L(\chi, \psi; a, b)$ equals a finite sum $\sum a_j l_j m_j$, where each l_j and m_j is either an L-series value or a value of Li_1 at an F-th root of unity, and each $a_j \in \mathbb{Q}(\zeta_m)$.*

Remark: One hopes for the following extension of this result to the triple L-values:

Let χ be a Dirichlet character of conductor D, and $a, b, c \in \mathbb{Z}_+$, with $c > 1$. Suppose $\chi(-1) = (-1)^{a+b+c}$. Then

$$L\binom{\chi, 1, 1}{a, b, c}$$

lies in the ring generated by $\mathbb{Q}(\zeta_m)$ and the values of single and double polylogarithms at Dth roots of unity, where $m = \mathrm{lcm}(D, \phi(D))$.

The author has made some progress in this direction, for specific choices of χ; however, a proof for general χ remains elusive.

We will finish this section by deriving the identities (8) and (9). Let χ be the quadratic character $\left(\frac{-3}{\cdot}\right)$. We will here find evaluations for

$$L\binom{1, \chi}{3, 1}, \qquad L\binom{\chi, 1}{1, 3}, \quad \text{and} \quad L\binom{\chi, 1}{2, 2}$$

in terms of single L-values and values of Li_1 at cube roots of unity. We will need the following partial fractions expansion (which is a special case of (11)):

$$\frac{1}{n(n-m)^3} = -\frac{1}{m^3 n} + \frac{1}{m(n-m)^3} - \frac{1}{m^2(n-m)^2} + \frac{1}{m^3(n-m)} \tag{28}$$

Set $\omega = \exp(2\pi i/3)$. We will make use of the formulas

$$Li_1(\omega) = -\frac{1}{2}\log 3 + \frac{i\pi}{6} \qquad Li_a(\omega) = \frac{\sqrt{-3}}{2} L_\chi(a) - \frac{3^{a-1} - 1}{2 \cdot 3^{a-1}}\zeta(a) \tag{29}$$

where $a \in \mathbb{Z}$, $a > 1$. We find

$$L_N\binom{1, \chi}{3, 1} = \sum_{n=1}^{N}\sum_{m=1}^{n-1} \frac{\chi(n)}{m^3 n} = \sum_{n=1}^{N}\sum_{m=1}^{n-1} \frac{\chi(n)}{(n-m)^3 n}$$

Applying the partial fractions expansion (28) to the last double sum, we obtain

$$\sum_{n=1}^{N}\sum_{m=1}^{n-1} \chi(n)\Big\{\frac{-1}{m^3 n} + \frac{1}{m(n-m)^3} - \frac{1}{m^2(n-m)^2} + \frac{1}{m^3(n-m)}\Big\}$$

$$= -L_N\binom{1, \chi}{3, 1} + \sum_{m,n=1}^{N} \frac{\chi(m+n)}{mn^3} - \sum_{m,n=1}^{N} \frac{\chi(m+n)}{m^2 n^2} + \sum_{m,n=1}^{N} \frac{\chi(m+n)}{m^3 n}$$

plus some error terms which approach zero as $N \to \infty$, by lemma 1.2 of theorem 1 . By noting that the second and last terms on the right-hand side of this expression are equal, we obtain

$$L_N\binom{1,\chi}{3,1} = \sum_{m,n=1}^{N} \frac{\chi(m+n)}{mn^3} - \frac{1}{2}\sum_{m,n=1}^{N} \frac{\chi(m+n)}{m^2n^2}$$

plus error terms. Using the finite Fourier expansion $\chi(n) = (\omega^n - \omega^{-n})/\sqrt{-3}$, the right-hand side of the last expression is

$$\frac{1}{\sqrt{-3}}\Big(Li_3^N(\omega)Li_1^N(\omega) - Li_3^N(\omega^{-1})Li_1^N(\omega^{-1}) - \frac{1}{2}Li_2^N(\omega)^2 + \frac{1}{2}Li_2^N(\omega^{-1})^2\Big)$$
$$= \frac{1}{\sqrt{-3}}\Big(2i\,\Im\left(Li_1^N(\omega)Li_3^N(\omega)\right) - i\,\Im\left(Li_2^N(\omega)^2\right)\Big)$$

Letting $N \to \infty$ and applying (29), we see this equals

$$\frac{1}{\sqrt{-3}}\Big\{2i\,\Im\Big((-\frac{1}{2}\log 3 + \frac{i\pi}{6})(\frac{\sqrt{-3}}{2}L_\chi(3) - \frac{4}{9}\zeta(3))\Big)$$
$$- i\,\Im\Big((\frac{\sqrt{-3}}{2}L_\chi(2) - \frac{1}{3}\zeta(2))^2\Big)\Big\}$$
$$= \frac{1}{\sqrt{-3}}\Big\{2i(-\frac{\sqrt{-3}}{4}\log 3L_\chi(3) - \frac{2}{27}\pi\zeta(3)) - i(-\frac{1}{\sqrt{3}}L_\chi(2)\zeta(2))\Big\}$$
$$= -\frac{1}{2}\log 3L_\chi(3) - \frac{4\pi}{\sqrt{3}}\zeta(3) + \frac{1}{3}L_\chi(2)\zeta(2)$$
$$= -\frac{1}{2}\log 3L_\chi(3) - \frac{4}{9}L_\chi(1)\zeta(3) + \frac{1}{3}L_\chi(2)\zeta(2)$$

since $L_\chi(1) = \pi/3\sqrt{3}$. Thus,

$$L\binom{1,\chi}{3,1} = -\frac{1}{2}\log 3L_\chi(3) - \frac{4}{9}L_\chi(1)\zeta(3) + \frac{1}{3}L_\chi(2)\zeta(2)$$

Now, we can use the shuffle relation

$$L\binom{\chi,1}{1,3} + L\binom{1,\chi}{3,1} + L_\chi(4) = L_\chi(1)\zeta(3)$$

since each term of this expression converges. This proves the evaluation

$$L\binom{\chi,1}{1,3} = \frac{1}{2}\log 3L_\chi(3) + \frac{13}{9}L_\chi(1)\zeta(3) - \frac{1}{3}L_\chi(2)\zeta(2) - L_\chi(4)$$

verifying (8).

Similar methods show

$$K\binom{1,\chi}{1,3} = L\binom{1,\chi}{1,3} - L\binom{\chi,1}{2,2} - L\binom{\chi,1}{1,3} + L_\chi(4) \tag{30}$$

$$K\binom{1,\chi}{3,1} = L\binom{1,\chi}{1,3} + L_\chi(4) + L_\chi(1)\zeta(3) - L_\chi(2)\zeta(2) \tag{31}$$

where $K = \lim_{N\to\infty} K_N$. Next, we do a calculation:

$$\begin{aligned}\sum_{m,n=1}^{N} \frac{\chi(n-m)}{m^3 n} &= \sum_{0<m<n\le N} \frac{\chi(n-m)}{m^3 n} + \sum_{0<n<m\le N} \frac{\chi(n-m)}{m^3 n} \\ &= K_N\binom{1,\chi}{3,1} + \sum_{0<m<n\le N} \frac{\chi(m-n)}{mn^3} \\ &= K_N\binom{1,\chi}{3,1} - \sum_{0<m<n\le N} \frac{\chi(n-m)}{mn^3} \\ &= K_N\binom{1,\chi}{3,1} - K_N\binom{1,\chi}{1,3}\end{aligned}$$

By letting $N \to \infty$, we obtain

$$K\binom{1,\chi}{3,1} - K\binom{1,\chi}{1,3} = \sum_{m,n=1}^{\infty} \frac{\chi(n-m)}{m^3 n}$$

Subtracting (30) from (31) and solving for $L(\chi, 1; 2, 2)$, we obtain

$$L\binom{\chi,1}{2,2} = L_\chi(2)\zeta(2) - L_\chi(1)\zeta(3) - L\binom{\chi,1}{1,3} + \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \frac{\chi(n-m)}{m^3 n} \tag{32}$$

We can calculate the last term as before, obtaining

$$\sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \frac{\chi(n-m)}{m^3 n} = \frac{1}{2}\log 3 L_\chi(3) - \frac{4}{9} L_\chi(1)\zeta(3)$$

Plugging this back into (32), we get

$$L\binom{\chi,1}{2,2} = L_\chi(4) + \frac{4}{3}L_\chi(2)\zeta(2) - \frac{26}{9}L_\chi(1)\zeta(3)$$

deriving (9).

3 Series for Calculation

In this section, we derive some examples of series which were used to numerically verify evaluations of double L-values. In order to simplify our formulas, we redefine the Bernoulli numbers β_n

$$\sum_{n=1}^{\infty} e^{-nt} = \sum_{n=-1}^{\infty} \beta_n t^n, \qquad \Re(t) > 0, \quad |t| < 2\pi$$

and the Bernoulli numbers $\beta_{n,\chi}$ associated to a character χ

$$\sum_{n=1}^{\infty} \chi(n) e^{-nt} = \sum_{n=0}^{\infty} \beta_{n,\chi} t^n, \qquad \Re(t) > 0, \quad |t| < \frac{2\pi}{D}$$

where D is the conductor of χ. Expanding in residue classes gives the formula

$$\beta_{n,\chi} = \sum_{a=1}^{D-1} \chi(a) \sum_{m=0}^{n+1} \frac{(D-a)^m}{m!} D^{n-m} \beta_{n-m}$$

Using the method of Crandall[2], we derived the following fast-converging series for numerical calculation at positive integer arguments within the domain of (not necessarily absolute) convergence:

$$\zeta(s) = \frac{1}{(s-1)!} \Big\{ \sum_{n=-1}^{\infty} \beta_n \frac{1}{s+n} + \sum_{j=0}^{s-1} \sum_{n=1}^{\infty} \frac{(s-1)!}{j!} \frac{e^{-n}}{n^{s-j}} \Big\}$$

$$L_\chi(s) = \frac{1}{(s-1)!} \Big\{ \sum_{n=0}^{\infty} \beta_{n,\chi} g^{n+s} (n+s) + \sum_{n=1}^{\infty} \chi(n) \sum_{j=0}^{s-1} \frac{(s-1)!}{j!} g^j \frac{e^{-gn}}{n^{s-j}} \Big\}$$

Here, and in the following formulas we choose $g \in (0, 2\pi/D)$. In particular, if $D \le 4$, it suffices to use $g = 1$.

We will illustrate Crandall's method in finding a series for $L(\chi, 1; a, b)$ where χ has conductor D, $a, b \in \mathbb{Z}_+$, $b > 1$. We first multiply by $\Gamma(a)\Gamma(b)$ to obtain

$$\sum_{0<m<n} \frac{\chi(m)}{m^a n^b} \int_0^\infty \int_0^\infty t^{a-1} u^{b-1} e^{-t} e^{-u} \, dt \, du$$

Since the sum is absolutely convergent, we can write this as

$$\sum_{m,n=1}^{\infty} \frac{\chi(m)}{m^a (m+n)^b} \int_0^\infty \int_0^\infty t^{a-1} u^{b-1} e^{-t} e^{-u} \, dt \, du$$

By a standard change of variables, this is

$$\sum_{m,n=1}^{\infty} \chi(m) \int_0^\infty \int_0^\infty t^{a-1} u^{b-1} e^{-mt} e^{-(m+n)u} \, dt \, du$$

$$= \sum_{m,n=1}^{\infty} \chi(m) \int_0^{\infty} \int_0^{\infty} t^{a-1} u^{b-1} e^{-m(t+u)} e^{-nu} \, dt \, du$$

We now make the change of variables $v = u$, $w = t + u$. Since the Jacobian is 1, this is

$$\sum_{m,n=1}^{\infty} \chi(m) \int_{0<v<w} (w-v)^{a-1} v^{b-1} e^{-mw} e^{-nv} \, dv \, dw$$

$$= \sum_{k=0}^{a-1} (-1)^k \binom{a-1}{k} S_k$$

where

$$S_k = \sum_{m,n=1}^{\infty} \int_0^{\infty} \int_0^{w} v^{b+k-1} w^{a-k-1} e^{-mw} e^{-nv} \, dv \, dw$$

We now split up the domain of integration into three regions. Define

$$A = \{(v,w) | 0 < v < w < g\}$$

$$B = \{(v,w) | 0 < v < g < w\}$$

$$C = \{(v,w) | g < v < w\}$$

where g is chosen such that $0 < g < 2\pi/D$. Now $\int_A S_k$ equals

$$\sum_{m,n=1}^{\infty} \chi(m) \int_0^{g} \int_0^{w} v^{b+k-1} w^{a-k-1} e^{-mw} e^{-nv} \, dv \, dw$$

Making use of Bernoulli numbers, this is

$$\sum_{\substack{m=0 \\ n=-1}}^{\infty} \beta_{m,\chi} \beta_n \int_0^{g} \int_0^{w} v^{b+k+n-1} w^{a-k+m-1} \, dv \, dw$$

The straightforward integration then gives

$$\int_A S_k = \sum_{\substack{m=0 \\ n=-1}}^{\infty} \frac{\beta_{m,\chi} \beta_n}{(a+b+m+n)(b+k+n)} g^{a+b+m+n}$$

Next, $\int_B S_k$ equals

$$\sum_{m,n=1}^{\infty} \chi(m) \int_g^{\infty} \int_0^{g} v^{b+k-1} w^{a-k-1} e^{-mw} e^{-nv} \, dv \, dw$$

Again using Bernoulli numbers, this equals

$$\sum_{m=1}^{\infty} \chi(m) \int_1^{\infty} w^{a-k-1} e^{-mw}\, dw \cdot \sum_{n=-1}^{\infty} \beta_n \int_0^1 v^{b+k+n-1}\, dv$$

We evaluate the simple integral on the right, and evaluate the integral on the left by making use of the integration formula

$$\int t^l e^{-ct}\, dt = -e^{-ct} \sum_{k=0}^{l} \frac{l!}{k!} \frac{t^k}{c^{l-k+1}} \tag{33}$$

to obtain

$$\int_B S_k = \sum_{m=1}^{\infty} \chi(m) \sum_{j=0}^{a-k-1} \frac{(a-k-1)!}{j!} \frac{g^k e^{-mg}}{m^{a-k-j}} \cdot \sum_{n=-1}^{\infty} \frac{\beta_n}{b+k+n}$$

To find $\int_C S_k$, we use the integration formula (33) repeatedly:

$$\begin{aligned}
\int_C S_k &= \sum_{m,n=1}^{\infty} \int_g^{\infty} \int_g^{w} v^{b+k-1} w^{a-k-1} e^{-mw} e^{-nv}\, dv\, dw \\
&= \sum_{m,n=1}^{\infty} \chi(m) \int_g^{\infty} w^{a-k-1} e^{-mw} \sum_{j_1=0}^{b+k-1} \frac{(b+k-1)!}{j_1!} (-e^{-nv}) \frac{v^{j_1}}{n^{b+k-j_1}} \Big|_{v=g}^{w} dw \\
&= \sum_{m,n=1}^{\infty} \chi(m) \sum_{j_1=0}^{b+k-1} \frac{(b+k-1)!}{j_1!} \int_g^{\infty} w^{a-k-1} e^{-mw} \Big\{ \frac{g^{j_1} e^{-ng}}{n^{b+k-j_1}} - \frac{w^{j_1} e^{-nw}}{n^{b+k-j_1}} \Big\}\, dw \\
&= \sum_{m,n=1}^{\infty} \chi(m) \sum_{j_1=0}^{b+k-1} \frac{(b+k-1)!}{j_1!} \Big\{ \frac{g^{j_1} e^{-ng}}{n^{b+k-j_1}} \int_g^{\infty} w^{a-k-1} e^{-mw}\, dw \\
&\qquad - \frac{1}{n^{b+k-j_1}} \int_g^{\infty} w^{a-k+j_1-1} e^{-(m+n)w}\, dw \Big\} \\
&= \sum_{m,n=1}^{\infty} \chi(m) \sum_{j_1=0}^{b+k-1} \frac{(b+k-1)!}{j_1!} \frac{1}{n^{b+k-j_1}} \Big\{ g^{j_1} e^{-ng} \sum_{j_2=0}^{a-k-1} \frac{(a-k-1)!}{j_2!} \cdot \\
&\qquad \frac{g^{j_2} e^{-mg}}{m^{a-k-j_2}} - \sum_{j_3=0}^{a-k+j_1-1} \frac{(a-k+j_1-1)!}{j_3!} \frac{g^{j_3} e^{-(m+n)g}}{(m+n)^{a-k+j_1-j_3}} \Big\}
\end{aligned}$$

$$= \sum_{m,n=1}^{\infty} \chi(m) e^{-(m+n)g} \sum_{j_1=0}^{b+k-1} \frac{(b+k-1)!}{j_1!} \frac{1}{n^{b+k-1}} \Bigg\{ \sum_{j_2=0}^{a-k-1} \frac{(a-k-1)!}{j_2!} \cdot \frac{g^{j_1+j_2}}{m^{a-k-j_2}} - \sum_{j_3=0}^{a-k+j_1-1} \frac{(a-k+j_1-1)!}{j_3!} \frac{g^{j_3}}{(m+n)^{a-k+j_1-j_3}} \Bigg\}$$

Adding up $\sum_{k=0}^{a-1}(-1)^k\binom{a-1}{k}\int S_k$ over each of the three pieces, we obtain the resulting series for $L(\chi,1;a,b)$.

In order to calculate numerically a conditionally convergent sum, e.g., $Li_{1,1}(\zeta^{-1},\zeta)$, for $\zeta \neq 1$ a root of unity, a somewhat different method is necessary. By integrating geometric series, we get the integral representation

$$\int_0^{\zeta}\int_0^{\zeta^{-1}} \frac{u}{(1-u)(1-tu)}\,dt\,du$$

Making the change of variables $t=\zeta^{-1}t'$, $u=\zeta u'$, this is

$$\int_0^1\int_0^1 \frac{\zeta u}{(1-\zeta u)(1-tu)}\,dt\,du$$

Now we make another change of variables $t=e^{-t'}$, $u=e^{u'}$. We obtain

$$\zeta\int_0^{\infty}\int_0^{\infty} \frac{e^{-t-2u}}{(1-\zeta e^{-u})(1-e^{-t-u})}\,dt\,du$$

A last change of variables $w_1=u$, $w_2=t+u$ gives

$$\zeta\int_{0<w_1<w_2} \frac{e^{-w_1-w_2}}{(1-\zeta e^{-w_1})(1-e^{-w_2})}\,dw$$

We can expand the integrand in geometric series and use Crandall's method to evaluate this integral also, giving the series

$$Li_{1,1}(\zeta^{-1},\zeta) = \sum_{\substack{m=1\\n=0}}^{\infty} \frac{\alpha_{m-1}(\zeta^{-1})\beta_{n-1}}{m(m+n)} g^{m+n} + \sum_{n=1}^{\infty}\frac{e^{-ng}}{n}\cdot\sum_{m=1}^{\infty}\alpha_{m-1}(\zeta^{-1})\frac{g^m}{m} + \sum_{m,n=1}^{\infty}\zeta^n\frac{e^{-(m+n)g}}{m(m+n)}$$

where

$$\alpha_m(\sigma) = \sum_{k=1}^{D}\sigma^k\sum_{n=0}^{m+1}\frac{(D-k)^n}{n!}\beta_{m-n}D^{m-n} \quad \text{and} \quad 0<g<\frac{2\pi}{D}$$

with σ a generator of μ_D.

Another example of a value whose defining sum converges only conditionally, and which lends itself to a similar series is $Li_{s,1}(1,\zeta)$, for $s>1$ and ζ a root of unity. We find

$$\Gamma(s)Li_{s,1}(1,\zeta)=\sum_{m,n=1}^{\infty}\zeta^{m+n}\int_{0<w_1<w_2}(w_2-w_1)^{s-1}e^{-mw_2}e^{-nw_1}\,dw$$

Using methods similar to the above, we obtain the series

$$\begin{aligned}Li_{s,1}(1,\zeta)=\frac{1}{(s-1)!}\sum_{k=0}^{s-1}(-1)^k\binom{s-1}{k}\Bigg\{\sum_{m,n=0}^{\infty}\frac{\alpha_m(\zeta)\alpha_n(\zeta)g^{m+n}}{(s+m+n+1)(k+n+1)}\\ +\sum_{n=0}^{\infty}\frac{\alpha_n(\zeta)g^n}{k+n+1}\sum_{m=1}^{\infty}\sum_{j=0}^{s-k-1}\frac{(s-k-1)!}{j!}\frac{g^j(\zeta e^{-g})^m}{m^{s-k-j}}+\sum_{m,n=1}^{\infty}(\zeta e^{-g})^{m+n}\\ \sum_{j_1=0}^{k}\frac{k!}{j_1!}\frac{1}{n^{k+1-j_1}}\Bigg\{\sum_{j_2=0}^{s-k-1}\frac{(s-k-1)!}{j_2!}\frac{g^{j_1+j_2}}{m^{s-k-j_2}}\\ -\sum_{j_3=0}^{s-k+j_1-1}\frac{(s-k+j_1-1)!}{j_3!}\frac{g^{j_3}}{(m+n)^{s-k+j_1-j_3}}\Bigg\}\Bigg\}\end{aligned}$$

with $\alpha_m(\zeta)$ defined as before.

Using the Nth partial sum to approximate each infinite series, Crandall gives error bounds $(g/2\pi)^N$ on the pieces in which Bernoulli numbers are used (which come from the integrals over bounded regions), and e^{-N} for the other pieces (which come from integrals over the infinite regions). In practice, we used stabilization of the computed numbers as the criterion for accuracy.

We used the PARI command `lindep` to find evaluations numerically from numbers computed using Crandall's method. It should be mentioned that the output of this command is not necessarily the simplest integer relation among the input numbers; all that is guaranteed is a relation involving integers that are 'not too large.' Hence, the 'nicest' identity which we can derive may not be the one produced.

4 A Sample Computational Session

In this section, we give an example of a numerical verification of an explicit evaluation. Here is the code for a series for numerically computing $L(\chi, 1; s_1, s_2)$ for χ a Dirichlet character, $s_1, s_2 \in \mathbb{Z}_+$, and $s_2 > 1$:

```
{bernnew(n)=bernreal(n+1)/(n+1)!}

{k(D,n)=kronecker(D,n)}

{bernchar(D,n)=sum(a1=1,abs(D)-1,k(D,a1)*sum(m=0,n+1,
(abs(D)-a1)**m/m!*abs(D)**(n-m)*bernnew(n-m)))}

{g(D)=Pi/abs(D)}

{sumdbl(x,y,A,B,N,sum1,sum2)=sum1=0.;sum2=0.;
for(q1=1,N,
   sum2=sum2+x**q1/q1**A;
   sum1=sum1+y**(q1+1)/(q1+1)**B*sum2);
sum1}

{dbllseries(s1,s2,D,N1,N2,m,n,j,k1,k2,G)=
Gausssum=sum(k2=1,abs(D)-1,k(D,k2)*a(D)**k2);
v=vector(N1+2,x,bernnew(x-2));
vc=vector(N1+1,x,bernchar(D,x-1));
sum(j=0,s1-1,(-1)**j(s1-1)!/j!/(s1-j-1)!*
   (sum(m=0,N1,
      sum(n=-1,N1,vc[m+1]*v[n+2]*g(D)**(s1+s2+m+n)/(s1
      +s2+m+n)/(s2+j+n)))
   +sum(n=-1,N1,v[n+2]*g(D)**(s2+n+j)/(s2+n+j))*
      sum(j1=0,s1-j-1,(s1-j-1)!/j1!*g(D)**j1*
         sum(m=1,N2,k(D,m)*exp(-g(D)*m)/m**(s1-j-j1)))
   +sum(j1=0,s2+j-1,(s2+j-1)!/j1!*(sum(j2=0,s1-j-1,(s1-j-1)
      !/j2!*g(D)**(j1+j2)*
```

```
      sum(m=1,N2,k(D,m)*exp(-g(D)*m)/m**(s1-j-j2))*
         sum(n=1,N2,exp(-g(D)*n)/n**(s2+j-j1)))
   -sum(j3=0,s1-j+j1-1,(s1-j+j1-1)!/j3!*g(D)**j3*
      sum(k1=1,abs(D)-1,k(D,k1)*
         sumdbl(q(D)**(-k1),q(D)**k1*
            exp(-g(D)),s2+j-j1,s1-j+j1-j3,N2))/Gausssum)))))
/(s1-1)!/(s2-1)!}
```

Here, the command `bernnew` redefines the Bernoulli numbers to our definition; the command `bernchar` does the same for the Bernoulli numbers of a character. The command `sumdbl` is a subroutine facilitating the Bailey acceleration exposited in [2]. The `dbllseries` command computes the double L-value with upper limits $N1$ and $N2$, using the method of Crandall.

In conclusion, we give a session verifying the evaluation (9).

```
?  default(realprecision,80)
realprecision=86 significant digits (80 digits displayed)
?  dbllseries(2,2,-3,200,400)
%1 0.55407505801043974564948372602624184425169050810190 1
72268205722443573672465879 7 - 6.70254894 E-88*I
?  z2=Pi**2/6
%2 1.6449340668482264364724151666460251862189499012067 98
4377355582293700074704032008
?  z3=rzeta(3,200,400)
%3 1.2020569031595942853997381615114499907649862923404 98
8817922715553418382057863130
?  l1=lser(1,-3,200,400)
%4 0.6045997880780726168646927525473852440946887493642 46
8585232949788173774072197286 1
?  l2=lser(2,-3,200,400)
```

```
%5 0.781302412896486296867187429624092356365134336545285
42022210006333647205086362996
?  l3=lser(3,-3,200,400)
%6 0.884023811750079856743057916871011807747946186117658
93478258741494168416628016992
?  l4=lser(4,-3,200,400)
%7 0.940025680877123768691069445070885991643800309660335
012024137217271135803965594510
?  lindep([%1,l4,z2*l2,z3*l1],50)
%18 = [-9,9,12,-26]
```

Here, `rzeta` and `lser` are commands which compute values of the Riemann zeta function and L-series using the method of Crandall (for which the series were given in section 3). We used upper limits $N1 = 200$ for the Bernoulli number series and $N2 = 400$ for the exponential series. The reason for this was to counteract the lesser accuracy of the latter; we also could have adjusted the choice of g to balance the two. Observing the stabilization of the numbers, the apparent accuracy is 70 to 80 decimal places. We can see that the result of the `lindep` command in the last line verifies (9). A text file containing PARI code for these commands and similar ones can be downloaded from the website:

`http://www.math.psu.edu/terhune/`

5 Appendix: Further Examples of Evaluations

Each of these evaluations was calculated symbolically from a system of equations, and also verified numerically.

$$L\binom{\chi_{-3},1}{1,5} = \frac{1}{2}(\log 3)L_{\chi_{-3}}(5) + \frac{121}{81}L_{\chi_{-3}}(1)\zeta(5) - \frac{13}{27}L_{\chi_{-3}}(2)\zeta(4) + \frac{4}{9}L_{\chi_{-3}}(3)\zeta(3) - \frac{27}{81}L_{\chi_{-3}}(4)\zeta(2) - L_{\chi_{-3}}(6)$$

$$L\binom{\chi_{-3},1}{2,4} = 2L_{\chi_{-3}}(6) - \frac{484}{81}L_{\chi_{-3}}(1)\zeta(5) + \frac{40}{27}L_{\chi_{-3}}(2)\zeta(4) - \frac{8}{9}L_{\chi_{-3}}(3)\zeta(3) + L_{\chi_{-3}}(4)\zeta(2)$$

$$L\binom{\chi_{-3},1}{3,3} = -\frac{11}{2}L_{\chi_{-3}}(6) - \zeta(2)L_{\chi_{-3}}(4) + \frac{13}{9}\zeta(3)L_{\chi_{-3}}(3) + \frac{242}{27}L_{\chi_{-3}}(1)\zeta(5)$$

$$L\binom{\chi_{-3},1}{4,2} = \frac{9}{2}L_{\chi_{-3}}(6) - \frac{484}{81}L_{\chi_{-3}}(1)\zeta(5) - 2L_{\chi_{-3}}(3)\zeta(3) + \frac{4}{3}L_{\chi_{-3}}(4)\zeta(2)$$

$$L\binom{\chi_{-4},1}{1,3} = \frac{1}{2}(\log 2)L_{\chi_{-4}}(3) + \frac{35}{32}L_{\chi_{-4}}(1)\zeta(3) - \frac{1}{8}L_{\chi_{-4}}(2)\zeta(2) - L_{\chi_{-4}}(4)$$

$$L\binom{\chi_{-4},1}{2,2} = L_{\chi_{-4}}(4) + \frac{9}{8}L_{\chi_{-4}}(2)\zeta(2) - \frac{35}{16}L_{\chi_{-4}}(1)\zeta(3)$$

$$L\binom{\chi_{-4},1}{1,5} = \frac{1}{2}(\log 2)L_{\chi_{-4}}(5) + \frac{3}{32}L_{\chi_{-4}}(3)\zeta(3) + \frac{527}{512}L_{\chi_{-4}}(1)\zeta(5) - \frac{1}{8}L_{\chi_{-4}}(4)\zeta(2) - \frac{7}{128}L_{\chi_{-4}}(2)\zeta(4) - L_{\chi_{-4}}(6)$$

$$L\binom{\chi_{-4},1}{2,4} = 2L_{\chi_{-4}}(6) + \frac{3}{8}L_{\chi_{-4}}(4)\zeta(2) + \frac{135}{128}L_{\chi_{-4}}(2)\zeta(4) - \frac{3}{16}L_{\chi_{-4}}(3)\zeta(3) - \frac{527}{128}L_{\chi_{-4}}(1)\zeta(5)$$

$$L\binom{\chi_{-4},1}{3,3} = \frac{1581}{256}L_{\chi_{-4}}(1)\zeta(5) + \frac{35}{32}L_{\chi_{-4}}(3)\zeta(3) - \frac{3}{8}L_{\chi_{-4}}(4)\zeta(2) - \frac{11}{2}L_{\chi_{-4}}(6)$$

$$L\binom{\chi_{-4},1}{4,2} = \frac{9}{2}L_{\chi_{-4}}(6) + \frac{9}{8}L_{\chi_{-4}}(4)\zeta(2) - 2L_{\chi_{-4}}(3)\zeta(3) - \frac{527}{128}L_{\chi_{-4}}(1)\zeta(5)$$

References

[1] J. Borwein and R. Girgensohn, Evaluation of Triple Euler Sums, *Electr. J. Combin.* 3 (1996), no. 1, rsch. paper 23, 27 pp.

[2] R. E. Crandall, Fast Evaluation of Multiple Zeta Sums, *Math. Comp.* 67 (1998), 1163-1172.

[3] H. Davenport, Multiplicative Number Theory, Springer Verlag, Graduate Texts in Mathematics, New York, 1980.

[4] C. Markett, Triple Sums and the Riemann Zeta Function, *J. Number Theory* 48 (1994), 113-132.

[5] D. Zagier, Values of Zeta Functions and their Applications, *in* "Proceedings of the First European Congress of Mathematics", ed. by A. Joseph, et al., Vol. II, 497-512, Paris, 1994.