## Euler Sums and Contour Integral Representations

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## CONTENTS

1. Introduction
2. General summations
3. Linear Euler sums
4. Quadratic Euler sums
5. Cubic and higher order Euler sums
6. Models of Euler sum identities
7. Alternating Euler sums
8. Exotic sums

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## References

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This paper develops an approach to the evaluation of Euler sums that involve harmonic numbers, either linearly or nonlinearly. We give explicit formulæ for several classes of Euler sums in terms of Riemann zeta values. The approach is based on simple contour integral representations and residue computations.

## 1. INTRODUCTION

Harmonic numbers and their generalizations are classically defined by

$$
H_{n} \equiv H_{n}^{(1)}:=\sum_{j=1}^{n} \frac{1}{j}, \quad H_{n}^{(r)}:=\sum_{j=1}^{n} \frac{1}{j^{r}}
$$

The subject of this paper is Euler sums, which are the infinite sums whose general term is a product of harmonic numbers of index $n$ and a power of $n^{-1}$. It has been discovered in the course of the years that many Euler sums admit expressions involving finitely the "zeta values", that is to say values of the Riemann zeta function,

$$
\zeta(s):=\sum_{j=1}^{\infty} \frac{1}{j^{s}}
$$

at the positive integers. Typical evaluations to be discussed here are shown at the top of the next page.

Euler started this line of investigation in the course of a correspondence with Goldbach beginning in 1742 (see [Berndt 1989, p. 253] for a discussion) and he was the first to consider the linear sums,

$$
\begin{equation*}
S_{p, q}:=\sum_{n=1}^{\infty} \frac{H_{n}^{(p)}}{n^{q}} \tag{1-1}
\end{equation*}
$$

(a) $\quad \sum_{n \geq 1} \frac{H_{n}}{n^{2}}=2 \zeta(3), \quad \sum_{n \geq 1} \frac{H_{n}}{n^{3}}=\frac{5}{4} \zeta(4), \quad \sum_{n \geq 1} \frac{H_{n}}{n^{4}}=3 \zeta(5)-\zeta(2) \zeta(3)$
(b) $\sum_{n \geq 1} \frac{H_{n}^{(2)}}{n^{4}}=\zeta(3)^{2}-\frac{1}{3} \zeta(6)$
(c) $\sum_{n \geq 1} \frac{H_{n}^{(2)}}{n^{5}}=5 \zeta(2) \zeta(5)+2 \zeta(3) \zeta(4)-10 \zeta(7)$
(d) $\sum_{n \geq 1} \frac{\left(H_{n}\right)^{2}}{n^{5}}=6 \zeta(7)-\zeta(2) \zeta(5)-\frac{5}{2} \zeta(3) \zeta(4)$
(e) $\sum_{n \geq 1} \frac{\left(H_{n}\right)^{3}}{n^{4}}=\frac{231}{16} \zeta(7)-\frac{51}{4} \zeta(3) \zeta(4)+2 \zeta(2) \zeta(5)$
(f) $\quad \sum_{n \geq 1} \frac{\left(H_{n}\right)^{4}}{(n+1)^{3}}=\frac{185}{8} \zeta(7)-\frac{43}{2} \zeta(3) \zeta(4)+5 \zeta(2) \zeta(5)$
(g) $\sum_{n \geq 1} \frac{\left(H_{n}\right)^{3}}{n^{5}}-\frac{11}{4} \sum_{n \geq 1} \frac{H_{n}^{(2)}}{n^{6}}=\frac{469}{32} \zeta(8)-16 \zeta(3) \zeta(5)+\frac{3}{2} \zeta(2) \zeta(3)^{2}$.

Typical evaluations of Euler sums.

Euler, whose investigations were to be later completed by Nielsen [1906], discovered that the linear sums have evaluations in terms of zeta values in the following cases: $p=1 ; p=q ; p+q$ odd; $p+q$ even but with the pair $(p, q)$ being restricted to a finite set of so-called "exceptional" configurations $\{(2,4),(4,2)\}$. Of these cases, the one corresponding to $p=q$ is obvious given the symmetry relations

$$
\begin{equation*}
S_{p, q}+S_{q, p}=\zeta(p) \zeta(q)+\zeta(p+q) \tag{1-2}
\end{equation*}
$$

while the other ones correspond to essentially nontrivial identities, of which examples (a), (b), (c) at the top of page 16 are typical. Rather extensive numerical search for linear relations between linear Euler sums and polynomials in zeta values [Bailey et al. 1994] strongly suggest that Euler found all the possible evaluations of linear sums.

The next objects of interest are the nonlinear sums, involving products of at least two harmonic numbers. Let $\pi=\left(\pi_{1}, \ldots, \pi_{k}\right)$ be a partition of integer $p$ into $k$ summands, so that $p=\pi_{1}+\cdots+\pi_{k}$
and $\pi_{1} \leq \pi_{2} \leq \ldots \leq \pi_{k}$. The Euler sum of index $\pi, q$ is defined by

$$
S_{\pi, q}=\sum_{n=1}^{\infty} \frac{H_{n}^{\left(\pi_{1}\right)} H_{n}^{\left(\pi_{2}\right)} \cdots H_{n}^{\left(\pi_{k}\right)}}{n^{q}}
$$

the quantity $q+\pi_{1}+\cdots+\pi_{k}$ being called the weight and the quantity $k$ being the degree. As usual, repeated summands in partitions are indicated by powers, so that for instance

$$
S_{1^{2} 2^{3} 5, q}=S_{112225, q}=\sum_{n=1}^{\infty} \frac{\left(H_{n}\right)^{2}\left(H_{n}^{(2)}\right)^{3} H_{n}^{(5)}}{n^{q}}
$$

In the past, a few basic nonlinear sums have been evaluated thanks to their relations to the Eulerian beta integrals or to polylogarithms [de Doelder 1991]. Recently, a detailed numerical search conducted by Bailey, Borwein, and Girgensohn [Bailey et al. 1994] has revealed the existence of many surprising evaluations like examples (e) and (f) at the top of page 16. Some of these have since received
a due proof and for instance the paper [Borwein et al. 1995] gives explicit formulæ for

$$
S_{1^{2}, q}=\sum_{n=1}^{\infty} \frac{\left(H_{n}\right)^{2}}{n^{q}}
$$

whenever the weight $q+2$ is odd (see example (d) at the top of page 16), and an explicit reduction to $S_{2, q}$ when the weight is even.

The situation regarding explicit evaluations of Euler sums is at first sight rather puzzling. Some evaluations appear to generalize and form an infinite class-like $S_{1^{2}, q}$ above-while others seem to vanish mysteriously as soon as the weight exceeds a certain threshold. For instance, no finite formula in terms of zeta values is likely to exist for the cubic sums $S_{1^{3}, q}$ or the quartic sums $S_{1^{4}, q}$ of an odd weight exceeding 10 , while $S_{1^{3}, 4}, S_{1^{4}, 3}$ (examples (e) and (f) at the top of page 16) or even the septic $S_{1^{7}, 2}$ do reduce to zeta values [Bailey et al. 1994]. This suggests the existence of both "general" classes of evaluations and "exceptional" evaluations.
A recent approach, exemplified by [Hoffman 1992; Zagier 1994] sheds a new light on these phenomena. It is based on considering the multiple zeta functions defined by

$$
\zeta\left(a_{1}, a_{2}, \ldots, a_{l}\right):=\sum_{n_{1}<n_{2}<\cdots<n_{l}} \frac{1}{n_{1}^{a_{1}} n_{2}^{a_{2}} \cdots n_{l}^{a_{l}}},
$$

where $a_{1}+\cdots+a_{l}$ is called the weight and $l$ is the multiplicity. (We follow here the conventions of [Zagier 1994; Crandall and Buhler 1994] while other references, such as [Borwein et al. 1995], define multiple zetas using the opposite convention,

$$
n_{1}>n_{2}>\cdots>n_{l}
$$

in summations. The two presentations are trivial variants of each other, obtained one from the other by changing the order of the arguments.) Every Euler sum of weight $w$ and degree $k$ is clearly a $\mathbb{Q}$ linear combination of multiple zeta values (that is, values of multiple zeta functions at integer arguments) of weight $w$ and multiplicity at most $k+1$.

In other words, multiple zeta values are "atomic" quantities into which Euler sums decompose. Consequently, a complete model for the linear relations involving the multiple zeta values would yield a full decision procedure for determining whether any particular Euler sum admits a complete evaluation in terms of (single) zeta values.

A conjecture of Zagier, discussed later, states that the dimension $d_{w}$ of the $\mathbb{Q}$-linear space generated by the $2^{w-2}$ multiple zeta values of weight $w$ increases roughly like $1.32^{w}$. In contrast the number $\mu_{w}$ of weight-homogeneous monomials in zeta values of weight $w$ is much smaller asymptotically, being only $e^{O(\sqrt{w})}$. Thus, a priori, only a small fraction of quantities expressible in terms of multiple zetas should reduce to polynomials in (single) zeta values. However, initially, the difference $d_{w}-\mu_{w}$ is small and even equal to 0 for some of the low weights, $\{3,4,5,6,7,9\}$. As a consequence, any Euler sum of odd weight at most 9 must reduce to zeta values. The multiple zeta model therefore explains well the presence of exceptional evaluations of Euler sums that appear in this perspective to be unavoidable artefacts of low weight.
A characteristic aspect of the multiple zeta model is that it may predict relations but does not in general provide explicit formulce. This is where we fit in. Our approach is based on contour integral representations. It is directed at Euler sums that are particular "nonatomic" combinations of multiple zeta values, having almost complete symmetry. When applicable, this approach does not require inverting collections of linear relations, which may be rather difficult to do for a whole class of sums as exemplified by [Borwein et al. 1995; Borwein and Girgensohn 1996].

Euler sums and multiple zetas have connections with many branches of mathematics; see especially [Zagier 1994]. Broadhurst (see [Borwein and Girgensohn 1996]) encountered them in relation with Feynman diagrams and associated knots in perturbative quantum field theory. They also surface occasionally in combinatorial mathematics: evaluation (a) at the top of page 16 serves to analyze the
distribution of node degrees in quadtrees [Flajolet et al. 1995; Labelle and Laforest 1995] while alternating Euler sums make an appearance in the analysis of lattice reduction algorithms [Daudé et al. 1997].

The basic techniques of this paper, beyond the Cauchy-Lindelöf contour integrals of Lemma 2.1, have been worked out in an experimental manner using the computer algebra system Maple. This system "knows" the expansions of all the special functions needed here, and it has been used thoroughly in order to extract minimal kernels and summation formulæ, of which those shown in the box on page 24 are typical. Certainly, the intensive computations required by Section 6 (see Theorem 6.1 and Table 2) could not have been carried out manually, in view of the number of equations involved. In return, the summation formulæ of this paper (like those on page 24) could very well be encapsulated as templates in a general purpose summation package. Section 8 points in this direction and lists several types of sums that can now be computed mechanically using the approach of this paper.

## 2. GENERAL SUMMATIONS

Contour integration is a classical technique for evaluating infinite sums by reducing them to a finite number of residue computations. For instance, the easy identity

$$
2 \sum_{n=1}^{\infty} \frac{(-1)^{n}}{n^{2}+1}=\frac{2 \pi}{e^{\pi}-e^{-\pi}}-1
$$

can be derived transparently from a residue computation of the integral

$$
\frac{1}{2 i \pi} \int \frac{\pi}{\sin \pi s} \frac{d s}{s^{2}+1}
$$

over a circle centred at the origin and whose radius is taken arbitrarily large. The residues at the poles $s= \pm n$ with $n \neq 0$ generate the left-hand side of the equality, while the poles at $s=0, \pm i$ yield the explicit form appearing on the right. (Of course,
many other techniques can be employed to derive this identity, including Poisson's summation formula or Mittag-Leffler expansions of trigonometric functions.)

This summation mechanism is formalized by a lemma that goes back to Cauchy and is nicely developed throughout [Lindelöf 1905]. We define a kernel function $\xi(s)$ by the two requirements: $\xi(s)$ is meromorphic in the whole complex plane; $\xi(s)$ satisfies $\xi(s)=o(s)$ over an infinite collection of circles $|z|=\rho_{k}$ with $\rho_{k} \rightarrow+\infty$.

Lemma 2.1 (Cauchy, Lindelöf). Let $\xi(s)$ be a kernel function and let $r(s)$ be a rational function which is $O\left(s^{-2}\right)$ at infinity. Then

$$
\begin{equation*}
\sum_{\alpha \in O} \operatorname{Res}(r(s) \xi(s))_{s=\alpha}=-\sum_{\beta \in S} \operatorname{Res}(r(s) \xi(s))_{s=\beta} \tag{2-1}
\end{equation*}
$$

where $S$ is the set of poles of $r(s)$ and $O$ is the set of poles of $\xi(s)$ that are not poles of $r(s)$. Here $\operatorname{Res}(h(s))_{s=\lambda}$ denotes the residue of $h(s)$ at $s=\lambda$.

Proof. It suffices to apply the residue theorem to

$$
\frac{1}{2 i \pi} \int_{(\infty)} r(s) \xi(s) d s
$$

where $\int_{(\infty)}$ denotes integration along large circles, that is, the limit of integrals $\int_{|s|=\rho_{k}}$. See also the discussion in [Henrici 1974, § 4.9], where a kernel function is called a summatory function.

This formula does have the character of a summatory formula since the set $O$ of poles of an irrational kernel $\xi(s)$ (called the "ordinary poles") is infinite, while the set $S$ of poles of a rational function $r(s)$ (the "special poles") is necessarily finite. We also define the special residue sum to be the finite sum

$$
\mathcal{R}[\xi(s) r(s)]:=\sum_{\alpha \in S \cup\{0\}} \operatorname{Res}(\xi(s) r(s))_{s=\alpha} .
$$

The amalgamation of 0 to the special poles is just a notational convenience dictated by the fre-
quent need to isolate 0 in summatory formulæ. Then (2-1) is rephrased as

$$
\sum_{\alpha \in O \backslash\{0\}} \operatorname{Res}(r(s) \xi(s))_{s=\alpha}=-\mathcal{R}[\xi(s) r(s)] .
$$

Let $\left[(s-\lambda)^{r}\right] h(s)$ denote the coefficient of the $(s-\lambda)^{r}$ term in the Laurent expansion of $h(s)$ at $s=\lambda$. Residues are Laurent coefficients, and as such they are computable like Taylor coefficients, since

$$
\begin{aligned}
\operatorname{Res}(h(s))_{s=\lambda} & =\left[(s-\lambda)^{-1}\right] h(s) \\
& =\left[(s-\lambda)^{r-1}\right](s-\lambda)^{r} h(s),
\end{aligned}
$$

if $r$ is the order of the pole of $h(s)$ at $s=\lambda$. In other words, the special residue sum is always determined by a few Taylor series expansions taken at a finite collection of points.

We make here an essential use of kernels involving the $\psi$ function. The $\psi$ function [Whittaker and Watson 1927] is the logarithmic derivative of the Gamma function,

$$
\begin{equation*}
\psi(s)=\frac{d}{d s} \log \Gamma(s)=-\gamma-\frac{1}{s}+\sum_{n=1}^{\infty}\left(\frac{1}{n}-\frac{1}{n+s}\right) \tag{2-2}
\end{equation*}
$$

and it satisfies the complement formula

$$
\psi(s)-\psi(-s)=-\frac{1}{s}-\pi \cot \pi s
$$

as well as an expansion at $s=0$ that involves the zeta values:

$$
\begin{equation*}
\psi(s)+\gamma=-\frac{1}{s}+\zeta(2) s-\zeta(3) s^{2}+\cdots . \tag{2-3}
\end{equation*}
$$

From classical expansions and the properties just recalled of the $\psi$ function, one has at an integer $n$ the expressions listed on the top of the next page. Each of these functions, or any of its derivatives, is $O\left(|s|^{\varepsilon}\right)$ on circles of radius $n+\frac{1}{2}$ (with $n$ a positive integer) centred at the origin. Consequently, any polynomial form in

$$
\begin{equation*}
\pi \cot \pi s, \quad \frac{\pi}{\sin \pi s}, \quad \psi^{(j)}( \pm s) \tag{2-4}
\end{equation*}
$$

is itself a kernel function with poles at a subset of the integers. The purpose of this paper is precisely to investigate the power of such kernels in connection with summatory formulæ and Euler sums.

We shall impose throughout two conditions on the rational function $r(s)$ :

$$
\begin{align*}
\text { (i) } & r(s) \text { is } O\left(s^{-2}\right) \text { at infinity, } \\
\text { (ii) } & r(s) \text { has no pole in } \mathbb{Z} \backslash\{0\} . \tag{2-5}
\end{align*}
$$

Condition (i) is necessary for absolute convergence of the sums; condition (ii) is only a minor technical requirement. A direct use of the kernels of (2-4) then yields the summatory formulæ

$$
\begin{align*}
& \sum_{n=1}^{\infty} r(n)=-\mathcal{R}[r(s)(\psi(-s)+\gamma)],  \tag{2-6}\\
& \sum_{n=1}^{\infty}(r(n)+r(-n))=-\mathcal{R}[r(s) \pi \cot \pi s],  \tag{2-7}\\
& \sum_{n=1}^{\infty}(-1)^{n}(r(n)+r(-n))=-\mathcal{R}\left[r(s) \frac{\pi}{\sin \pi s}\right], \tag{2-8}
\end{align*}
$$

of which the last two are classical [Henrici 1974, $\S 4.9]$. The kernels are $\psi(-s)+\gamma, \pi \cot \pi s$, and $\pi / \sin \pi s$, as is apparent from the argument of the special residue sum. Clearly, equalities (2-7) and (2-8) become trivial if the rational function $r(s)$ is odd, and such parity phenomena surface recurrently in Euler sums evaluation.

A more interesting kernel is $(\psi(-s)+\gamma)^{2}$, whose residues at the positive integers generate harmonic numbers since

$$
(\psi(-s)+\gamma)^{2} \underset{s \rightarrow n}{\sim} \frac{1}{(s-n)^{2}}+2 H_{n} \frac{1}{s-n}+\cdots .
$$

In that case, under the conditions of (2-5), we find

$$
\begin{align*}
2 \sum_{n=1}^{\infty} r(n) H_{n}+\sum_{n=1}^{\infty} & r^{\prime}(n) \\
& =-\mathcal{R}\left[r(s)(\psi(-s)+\gamma)^{2}\right] \tag{2-9}
\end{align*}
$$

as results directly from the singular expansion of the kernel (see box at the top of page 20). Thus,

$$
\begin{array}{cl}
\pi \cot \pi s \underset{s \rightarrow n}{=} \frac{1}{s-n}-2 \sum_{k=1}^{\infty} \zeta(2 k)(s-n)^{2 k-1} & \\
\frac{\pi}{\sin \pi s} \underset{s \rightarrow n}{=}(-1)^{n}\left(\frac{1}{(s-n)}+2 \sum_{k=1}^{\infty}\left(1-2^{1-2 k}\right) \zeta(2 k)(s-n)^{2 k-1}\right) & \\
\psi(-s)+\gamma \underset{s \rightarrow n}{=} \frac{1}{s-n}+H_{n}+\sum_{k=1}^{\infty}\left((-1)^{k} H_{n}^{(k+1)}-\zeta(k+1)\right)(s-n)^{k}, & \text { if } n \geq 0 \\
\psi(-s)+\gamma \underset{s \rightarrow-n}{=} H_{n-1}+\sum_{k=1}^{\infty}\left(H_{n-1}^{(k+1)}-\zeta(k+1)\right)(s+n)^{k} & \text { if } n>0 \\
\frac{\psi^{(p-1)}(-s)}{(p-1)!} \underset{s \rightarrow n}{=} \frac{1}{(s-n)^{p}}\left(1+(-1)^{p} \sum_{i \geq p}\binom{i-1}{p-1}\left(\zeta(i)+(-1)^{i} H_{n}^{(i)}\right)(s-n)^{i}\right) & \text { if } n \geq 0, p>1 \\
\frac{\psi^{(p-1)}(-s)}{(p-1)!} \underset{s \rightarrow-n}{=}(-1)^{p} \sum_{i \geq 0}\binom{p-1+i}{p-1}\left(\zeta(p+i)-H_{n-1}^{(p+i)}\right)(s+n)^{i} & \text { if } n>0, p>1 \\
\frac{1}{s^{q}} \underset{\substack{=\\
s \rightarrow n}}{\sum_{j \geq 0}(-1)^{j}\binom{q+j-1}{q-1} \frac{(s-n)^{j}}{n^{q+j}}} & \text { if } n \neq 0, q \in \mathbb{Z}_{+}
\end{array}
$$

## Local expansions of basic kernels.

by $(2-6)-(2-8)$ and $(2-9)$, any sum whose general term is the product of the harmonic number $H_{n}$ and a rational function $r(n)$ reduces to a finite combination of values of the $\psi$ function and its derivatives taken at a finite set of points. Instantiating this treatment to the class of functions $r(s)=s^{-q}$, with $q$ an integer $\geq 2$, produces a formula already known to Euler.

Theorem 2.2 (Euler). For integer $q \geq 2$,

$$
\begin{aligned}
S_{1, q} & \equiv \sum_{n=1}^{\infty} \frac{H_{n}}{n^{q}} \\
& =\left(1+\frac{q}{2}\right) \zeta(q+1)-\frac{1}{2} \sum_{k=1}^{q-2} \zeta(k+1) \zeta(q-k) .
\end{aligned}
$$

Proof. A direct consequence of the summatory formula (2-9) and the expansion (2-3).

Special values are given in example (a) at the top of page 16 .

The treatment just developed of the simplest Euler sums is typical. For the case when $r(s)=s^{-q}$, only one residue needs to be determined, and the residue computation is strictly equivalent to a coefficient extraction. Given that the kernels employed throughout this paper are polynomials in $\psi$ and related trigonometric functions, the expressions obtained are invariably weight-homogeneous convolutions of zeta values. In addition, the degree of the kernel employed (that is itself suggested by the nature of each Euler sum considered) dictates the multiplicity of the convolution formulæ that are obtained by this process.

## Alternative Approaches

Following a suggestion by a referee, we briefly discuss some of the many approaches that have been developed regarding Euler sums. Partial fraction expansions of the Euler-Nielsen-Markett type (see [Nielsen 1906; Markett 1994; Borwein and Girgen-
sohn 1996]) are instrumental is providing relations. Identities of low weight can sometimes be proved by special integral representations and functional properties of polylogarithms [de Doelder 1991].

Amongst more general methods, we mention orthogonality and summatory formulæ. A recent paper [Crandall and Buhler 1994] derives the linear relations of Theorems 2.2 and 3.1 using orthogonality on the unit circle and the polylogarithmic series $\sum_{n} e^{2 i \pi n x} / n^{\alpha}$. This technique is reminiscent of the Poisson summation formula, but the extension to Euler sums of higher degree might be difficult given the scarcity of explicit Fourier transforms involving nonlinear forms in the $\psi$-function. A different type of orthogonality was suggested by a referee who proposed a Mellin-Perron type of formula,

$$
\begin{aligned}
\sum_{n>m} \frac{1}{n^{a} m^{b}} & =\frac{1}{2} \zeta(a+b) \\
& =\frac{1}{2 i \pi} \int_{c-i \infty}^{c+i \infty} \zeta(a-s) \zeta(b+s) \frac{d s}{s}
\end{aligned}
$$

(for some suitable $c$ ). Its possible use is however still unclear to us since the integrand has only 3 poles at $s=0, a-1,1-b$, while evaluations of Euler sums generally involve more than three terms.

Our paper is on the other hand very close to the Euler-Maclaurin summation formula, especially its complex version due to Abel and Plana [Henrici 1974, p. 274]:

$$
\begin{aligned}
\sum_{n=0}^{\infty} f(n)=\frac{1}{2} f(0)+\int_{0}^{\infty} & f(x) d x \\
& +i \int_{0}^{\infty} \frac{f(i y)-f(-i y)}{e^{2 \pi y}-1} d y
\end{aligned}
$$

This formula is proved [Henrici 1974; Lindelöf 1905] using the trigonometric kernel $\pi \cot \pi s$ in the style of Lemma 2.1. The goal of this paper is precisely to illustrate the versatility of nonlinear $\psi$-kernels that do not seem to have surfaced in the literature despite their simplicity and their power as regards nonlinear Euler sums. An instance of this fact is the solution of the cubic conjectures of [Bailey et al.

1994] given by Corollary 5.2. Also, in Theorems 4.1 and 5.1 and in the box on page 24 , such kernels are needed since purely trigonometric kernels only give access to a small subset of Euler sums, a fact confirmed by parity considerations as well as by the classification of kernels given in Section 6.

## 3. LINEAR EULER SUMS

Nielsen [1906], elaborating on Euler's work, proved by a method based on partial fraction expansions that every linear sum $S_{p, q}$ whose weight $p+q$ is odd is expressible as a polynomial in zeta values. To give an idea of the method [Nielsen 1906, p. 50], we show that $S_{1,2}=2 \zeta(3)$, an equality expressed in terms of double zetas as $\zeta(1,2)=\zeta(3)$. We have

$$
\begin{aligned}
\zeta(1,2)= & \sum_{0<a<n} \frac{1}{a n^{2}}=\sum_{0<a<n} \frac{1}{(n-a) n^{2}} \\
= & \sum_{0<a<n}-\frac{1}{a n^{2}}+\left(\frac{1}{a^{2}(n-a)}-\frac{1}{a^{2} n}\right) \\
= & -\zeta(1,2) \\
& +\sum_{0<a} \frac{1}{a^{2}}\left(\left(\frac{1}{1}-\frac{1}{a+1}\right)+\left(\frac{1}{2}-\frac{1}{a+2}\right)+\cdots\right),
\end{aligned}
$$

where the second line results from a partial fraction expansion and the last equality from series rearrangements. The last sum telescopes and yields

$$
\zeta(1,2)=-\zeta(1,2)+(\zeta(1,2)+\zeta(3)) .
$$

This example is typical. In general the method provides linear relations between the $S_{p, q}$ of the same weight and quadratic forms in zeta functions, from which a constructive (but not clearly explicit) reduction to zeta values can be derived. D. and J. Borwein and R. Girgensohn [Borwein et al. 1995] have succeeded in "inverting" the Euler-Nielsen relations by means of combinatorial matrix decompositions. We show here how to rederive directly the explicit evaluations of that paper.

Theorem 3.1 [Borwein et al. 1995]. For an odd weight $m=p+q$, the linear sums are reducible to zeta values,

$$
\begin{aligned}
& \sum_{n=1}^{\infty} \frac{H^{(p)}(n)}{n^{q}} \\
&= \zeta(m)\left(\frac{1}{2}-\frac{(-1)^{p}}{2}\binom{m-1}{p}-\frac{(-1)^{p}}{2}\binom{m-1}{q}\right) \\
&+\frac{1-(-1)^{p}}{2} \zeta(p) \zeta(q) \\
&+(-1)^{p} \sum_{k=1}^{\lfloor p / 2\rfloor}\binom{m-2 k-1}{q-1} \zeta(2 k) \zeta(m-2 k) \\
&+(-1)^{p} \sum_{k=1}^{\lfloor q / 2\rfloor}\binom{m-2 k-1}{p-1} \zeta(2 k) \zeta(m-2 k),
\end{aligned}
$$

where $\zeta(1)$ should be interpreted as 0 wherever it occurs.

Proof. In the context of this paper, the theorem results from applying the kernel

$$
\frac{1}{2} \pi \cot (\pi s) \frac{\psi^{(p-1)}(-s)}{(p-1)!}
$$

to the base function $r(s)=s^{-q}$. The only singularities are poles at the integers. At a negative integer $-n$ the pole is simple and the residue is

$$
\frac{(-1)^{m}}{2 n^{q}}\left(\zeta(p)-H_{n}^{(p)}+\frac{1}{n^{p}}\right)
$$

At a positive integer $n$, the pole has order $p+1$ and the residue is

$$
\begin{aligned}
& \frac{1}{2 n^{q}}\left(H_{n}^{(p)}-\zeta(p)\right)+(-1)^{p}\binom{m-1}{p} \frac{1}{2 n^{m}} \\
& \quad+\frac{1+(-1)^{p}}{2 n^{q}} \zeta(p)-(-1)^{p} \sum_{k=1}^{\lfloor p / 2\rfloor}\binom{m-2 k-1}{p-2 k} \frac{\zeta(2 k)}{n^{m-2 k}} .
\end{aligned}
$$

Finally the residue of the pole of order $m+1$ at 0 is found to be

$$
\begin{aligned}
& \frac{(-1)^{p}}{2}\binom{m-1}{q} \zeta(m) \\
& \quad+(-1)^{p+1} \sum_{k=1}^{\lfloor q / 2\rfloor}\binom{m-2 k-1}{p-1} \zeta(2 k) \zeta(m-2 k)
\end{aligned}
$$

Summing these three contributions yields the statement of the theorem.

For even weights, a modified form of the identity holds, but without any linear Euler sum occurring. This gives back well-known nonlinear relations between zeta values at even arguments. In this case of even weight $w$, there also exist relations between linear sums. The kernels

$$
\begin{equation*}
\xi_{j}(s)=\left(\psi^{(j)}(-s)\right)^{2} \tag{3-1}
\end{equation*}
$$

applied to $s^{-q}$ yield further relations. (For $j=1,2$, the general summation formulæ are given in $\left(S_{4}\right)$ and ( $S_{5}$ ) of the box on page 24.) When specialized to $r(s)=s^{-q}$, the kernel $\xi_{j}$ yields linear relations between

$$
\begin{equation*}
S_{2 j+1, q}, S_{2 j, q+1}, \ldots, S_{j+1, q+j} \tag{3-2}
\end{equation*}
$$

and polynomials in zeta values that are of a shape similar to the Euler-Nielsen relations. This gives the reductions

$$
\begin{aligned}
S_{3, q} & \mapsto S_{2, q+1} \\
S_{5, q} & \mapsto\left\{S_{2, q+3}, S_{4, q+1}\right\} \\
S_{7, q} & \mapsto\left\{S_{2, q+5}, S_{4, q+3}, S_{6, q+1}\right\}
\end{aligned}
$$

and so on. Such relations are to be complemented by the symmetry relations ( $1-1$ ).

Identity (c) in the box of page 16 is an evaluation that is typical of odd weight identities. For the exceptional even weights $\{4,6\}$, the symmetry
relations give $S_{2,2}$ and $S_{3,3}$, whence, by $\left(S_{4}\right),\left(S_{5}\right)$ of page 24 , all linear sums,

$$
\begin{aligned}
& \sum_{n=1}^{\infty} \frac{H_{n}^{(2)}}{n^{2}}=\frac{7}{4} \zeta(4), \\
& \sum_{n=1}^{\infty} \frac{H_{n}^{(3)}}{n^{3}}=\frac{1}{2} \zeta^{2}(3)+\frac{1}{2} \zeta(6), \\
& \sum_{n=1}^{\infty} \frac{H_{n}^{(2)}}{n^{4}}=\zeta(3)^{2}-\frac{1}{3} \zeta(6) .
\end{aligned}
$$

For the next even weights, we obtain relations from which it results, again in conjunction with the symmetry relations, that the sets

$$
\left\{S_{2,6}\right\}, \quad\left\{S_{2,8}\right\}, \quad\left\{S_{2,10}\right\}, \quad\left\{S_{2,12}, S_{4,10}\right\}
$$

are sufficient to express linearly all linear sums of weights $8,10,12,14$ (modulo zeta values). For instance, we have the relations

$$
\begin{aligned}
5 \sum_{n=1}^{\infty} \frac{H_{n}^{(2)}}{n^{6}}+2 \sum_{n=1}^{\infty} \frac{H_{n}^{(3)}}{n^{5}}= & -\frac{21}{4} \zeta(8)+10 \zeta(3) \zeta(5), \\
7 \sum_{n=1}^{\infty} \frac{H_{n}^{(2)}}{n^{8}}+2 \sum_{n=1}^{\infty} \frac{H_{n}^{(3)}}{n^{7}}= & -\frac{33}{2} \zeta(10) \\
& +14 \zeta(3) \zeta(7)+8 \zeta(5)^{2}, \\
7 \sum_{n=1}^{\infty} \frac{H_{n}^{(2)}}{n^{8}}-2 \sum_{n=1}^{\infty} \frac{H_{n}^{(4)}}{n^{6}}= & -\frac{227}{10} \zeta(10) \\
& +14 \zeta(3) \zeta(7)+10 \zeta(5)^{2} .
\end{aligned}
$$

Zagier [1994], by means of an analogy with the theory of modular forms, and Borwein et al. [1995], by exploiting directly the Euler-Nielsen relations, have shown that the linear relations of even weight determine all but $\lfloor(w-2) / 6\rfloor$ of the linear Euler sums that are thus considered to be "new" constants.

Note on the choice of kernels. The kernels are rather directly related to the quantities subject to summation. As we have seen, the residues of $(\psi(-s)+$ $\gamma)^{2}$ generate the harmonic numbers, so that sums involving $H_{n}$ should be represented by integrals involving this kernel, in accordance with ( $S_{3}$ ) of page 24 . The kernel $\psi^{\prime}(-s)^{2}$ similarly introduces
$H_{n}^{(2)}$ and $H_{n}^{(3)}$ and thus generates relation $\left(S_{4}\right)$ that involves two types of harmonic numbers. Furthermore, by combining formulæ for $r(s)$ and $r(-s)$, the terms involving $H_{n}^{(3)}$ disappear when $r(s)$ is an odd function; the use of $\pi \cot \pi s$ as replacement for one factor of $\psi^{\prime}(-s)$ precisely has the effect of achieving such a combination. Thus a sum like $\sum H_{n}^{(2)} r(n)$ becomes reducible when $r(s)$ is an odd function. Similar observations dictate the choice of kernels throughout this paper as is illustrated by the boxes on pages 24 and 26 .

## 4. QUADRATIC EULER SUMS

Starting from an observation of E. Au-Yeung that

$$
S_{1^{2}, 2}=\sum_{n=1}^{\infty} \frac{\left(H_{n}\right)^{2}}{n^{2}}=\frac{17}{4} \zeta(4),
$$

Borwein et al. [1995] have given a general reduction of the quadratic sums $S_{1^{2}, q}$ to double sums, which in turn entails a complete evaluation in terms of single zeta values for odd weight. These sums are closely related to derivatives of the Eulerian beta integral. We show here a direct derivation of the reductions by means of $\psi$ kernels that provides in passing general summatory formulæ for sums involving $\left(H_{n}\right)^{2}$. (See also the box on page 24 and Section 8.)

Theorem 4.1 [Borwein et al. 1995]. For all weights, the quadratic sums $S_{1^{2}, q}$ reduce to linear sums and polynomials in zeta values:
$S_{1^{2}, q}-S_{2, q}=q S_{1, q+1}-\frac{q(q+1)}{6} \zeta(q+2)+\zeta(2) \zeta(q)$.
Proof. The proof is based on the cubic kernel

$$
\xi(s)=(\psi(-s)+\gamma)^{3}
$$

and the usual residue computation. When applied to an arbitrary rational function $r(s)$ satisfying (2-5), it yields the summatory formula $\left(S_{7}\right)$ in the box on page 24. The specialization to $r(s)=s^{-q}$ gives the statement.
( $S_{1}$ ) $\quad \sum_{n=1}^{\infty} r(n)$

$$
=-\mathcal{R}[r(s)(\psi(-s)+\gamma)]
$$

( $S_{2}$ ) $\quad 2 \sum_{n=1}^{\infty} r_{0}(n)$

$$
=-\mathcal{R}\left[r_{0}(s) \pi \cot \pi s\right]
$$

$$
\begin{equation*}
2 \sum_{n=1}^{\infty} r(n) H_{n}+\sum_{n=1}^{\infty} r^{\prime}(n) \tag{3}
\end{equation*}
$$

$$
=-\mathcal{R}\left[r(s)(\psi(-s)+\gamma)^{2}\right]
$$

$\left(S_{4}\right)-4 \sum_{n=1}^{\infty} H_{n}^{(3)} r(n)+2 \sum_{n=1}^{\infty} H_{n}^{(2)} r^{\prime}(n)+\sum_{n=1}^{\infty}\left(4 \zeta(3) r(n)+2 \zeta(2) r^{\prime}(n)+\frac{1}{6} r^{\prime \prime \prime}(n)\right)$ $=-\mathcal{R}\left[r(s)\left(\psi^{\prime}(-s)\right)^{2}\right]$
$\left(S_{5}\right)$
(5) $48 \sum_{n=1}^{\infty} H_{n}^{(5)} r(n)-24 \sum_{n=1}^{\infty} H_{n}^{(4)} r^{\prime}(n)+4 \sum_{n=1}^{\infty} H_{n}^{(3)} r^{\prime \prime}(n)$

$$
+\sum_{n=1}^{\infty}\left(-48 \zeta(5) r(n)-24 \zeta(4) r^{\prime}(n)-4 \zeta(3) r^{\prime \prime}(n)+\frac{1}{30} r^{(v)}(n)\right)=-\mathcal{R}\left[r(s)\left(\psi^{\prime \prime}(-s)\right)^{2}\right]
$$

$$
\begin{align*}
& 2 \sum_{n=1}^{\infty} H_{n}^{(2)} r_{1}(n)+\sum_{n=1}^{\infty}\left(\frac{1}{2} r_{1}^{\prime \prime}(n)-2 \zeta(2) r_{1}(n)-\frac{r_{1}(n)}{n^{2}}\right)=-\mathcal{R}\left[r_{1}(s) \psi^{\prime}(-s) \pi \cot (\pi s)\right]  \tag{6}\\
& 3 \sum_{n=1}^{\infty} r(n)\left(H_{n}\right)^{2}-3 \sum_{n=1}^{\infty} r(n) H_{n}^{(2)}+3 \sum_{n=1}^{\infty} H_{n} r^{\prime}(n)+\sum_{n=1}^{\infty}\left(\frac{1}{2} r^{\prime \prime}(n)-3 r(n) \zeta(2)\right)  \tag{7}\\
&=-\mathcal{R}\left[r(s)(\psi(-s)+\gamma)^{3}\right]
\end{align*}
$$

General summatory formulæ resulting from kernels (last column) that are polynomial forms in $\psi$ functions. Here $r(s), r_{0}(s)$, and $r_{1}(s)$ denote rational functions that satisfy the conditions or (2-5), with additionally $r_{0}(s)$ even and $r_{1}(s)$ odd. Cubic formulæ are given in the proof of Theorem 5.1.

In Theorem 4.1, for even weights $\geq 8$, only $S_{1, q+1}$ reduces to zeta values. For odd weights, both $S_{1, q+1}$ and $S_{2, q}$ reduce to zeta values, hence a complete evaluation. We have, for small odd weight,

$$
\begin{aligned}
& \sum_{n=1}^{\infty} \frac{\left(H_{n}\right)^{2}}{n^{3}}=\frac{7}{2} \zeta(5)-\zeta(2) \zeta(3) \\
& \sum_{n=1}^{\infty} \frac{\left(H_{n}\right)^{2}}{n^{5}}=6 \zeta(7)-\zeta(2) \zeta(5)-\frac{5}{2} \zeta(3) \zeta(4) \\
& \sum_{n=1}^{\infty} \frac{\left(H_{n}\right)^{2}}{n^{7}}=\frac{55}{6} \zeta(9)-\zeta(2) \zeta(7) \\
& \quad-\frac{7}{2} \zeta(3) \zeta(6)-\frac{5}{2} \zeta(4) \zeta(5)+\frac{1}{3} \zeta(3)^{3}
\end{aligned}
$$

and for small even weight,

$$
\begin{array}{r}
\sum_{n=1}^{\infty} \frac{H_{n}^{2}}{n^{6}}-\sum_{n=1}^{\infty} \frac{H_{n}^{(2)}}{n^{6}}=\frac{91}{12} \zeta(8)-8 \zeta(3) \zeta(5)+\zeta(2) \zeta(3)^{2} \\
\sum_{n=1}^{\infty} \frac{H_{n}^{2}}{n^{8}}-\sum_{n=1}^{\infty} \frac{H_{n}^{(2)}}{n^{8}}=\frac{473}{40} \zeta(10)-10 \zeta(3) \zeta(7)-5 \zeta(5)^{2} \\
+\zeta(4) \zeta(3)^{2}+2 \zeta(2) \zeta(3) \zeta(5)
\end{array}
$$

with the following exceptional evaluations for the weights $\{4,6\}$ :

$$
\begin{align*}
& \sum_{n=1}^{\infty} \frac{\left(H_{n}\right)^{2}}{n^{2}}=\frac{17}{4} \zeta(4),  \tag{4-1}\\
& \sum_{n=1}^{\infty} \frac{\left(H_{n}\right)^{2}}{n^{4}}=\frac{97}{24} \zeta(6)-2 \zeta(3)^{2} .
\end{align*}
$$

$$
\begin{align*}
& A=(-1)^{p_{1}+p_{2}} \zeta\left(p_{1}\right) \zeta\left(p_{2}\right) \zeta(q)+(-1)^{p_{1}} \zeta\left(p_{1}\right) S_{p_{2}, q}+(-1)^{p_{2}} \zeta\left(p_{2}\right) S_{p_{1}, q} \\
& B= \sum_{i+j+2 k=p_{1}}(-1)^{j}\binom{j+q-1}{q-1}\binom{p_{2}+i-1}{p_{2}-1}\left((-1)^{p_{2}+i} S_{p_{2}+i, q+j}+\zeta\left(p_{2}+i\right) \zeta(q+j)\right) \zeta(2 k) \\
& C= \sum_{i+j+2 k=p_{2}}(-1)^{j}\binom{j+q-1}{q-1}\binom{p_{1}+i-1}{p_{1}-1}\left((-1)^{p_{1}+i} S_{p_{1}+i, q+j}+\zeta\left(p_{1}+i\right) \zeta(q+j)\right) \zeta(2 k)  \tag{2k}\\
& D= \sum_{j+2 k=p_{1}+p_{2}}(-1)^{j}\binom{j+q-1}{q-1} \zeta(2 k) \zeta(q+j) \\
& E=(-1)^{p_{1}+p_{2}+q}\left(-S_{p_{1}, p_{2}+q}-S_{p_{2}, p_{1}+q}-\zeta\left(p_{1}\right) S_{p_{2}, q}-\zeta\left(p_{2}\right) S_{p_{1}, q}\right. \\
&\left.\quad+\zeta\left(p_{1}+p_{2}+q\right)+\zeta\left(p_{1}+q\right) \zeta\left(p_{2}\right)+\zeta\left(p_{2}+q\right) \zeta\left(p_{1}\right)+\zeta\left(p_{1}\right) \zeta\left(p_{2}\right) \zeta(q)\right) \\
& F= \zeta\left(p_{1}+p_{2}+q\right)+(-1)^{p_{2}} \sum_{\sum_{i+2 k=p_{1}+q}\binom{p_{2}+i-1}{p_{2}-1} \zeta\left(p_{2}+i\right) \zeta(2 k)} \begin{array}{l}
\quad+(-1)^{p_{1}} \sum_{i+2 k=p_{2}+q}\binom{p_{1}+i-1}{p_{1}-1} \zeta\left(p_{1}+i\right) \zeta(2 k) \\
\\
\quad+(-1)^{p_{1}+p_{2}} \sum_{i_{1}+i_{2}+2 k=q}\binom{p_{1}+i_{1}-1}{p_{1}-1}\binom{p_{2}+i_{2}-1}{p_{2}-1} \zeta\left(p_{1}+i_{1}\right) \zeta\left(p_{2}+i_{2}\right) \zeta(2 k) .
\end{array}
\end{align*}
$$

The summands in the evaluation of Theorem 4.2.

The sum $S_{1^{2}, q}$ is also related to the triple zeta function $\zeta(1,1, q)$ since

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

as shown by an elementary computation. Thus, the statement is equivalent to a reduction of $\zeta(1,1, q)$ to double zetas.

## General quadratic sums

A more general reduction results from the kernel

$$
\begin{equation*}
\frac{\psi^{\left(p_{1}-1\right)}(-s)}{\left(p_{1}-1\right)!} \frac{\psi^{\left(p_{2}-1\right)}(-s)}{\left(p_{2}-1\right)!} \pi \cot \pi s \tag{4-2}
\end{equation*}
$$

but it involves a parity restriction on the weight because of its trigonometric factor.

Theorem 4.2. If $p_{1}+p_{2}+q$ is even, and $p_{1}>1$, $p_{2}>1, q>1$, the quadratic sums

$$
S_{p_{1} p_{2}, q}=\sum_{n \geq 1} \frac{H_{n}^{\left(p_{1}\right)} H_{n}^{\left(p_{2}\right)}}{n^{q}}
$$

are reducible to linear sums. We have

$$
\begin{aligned}
& \left((-1)^{p_{1}+p_{2}+q}+1\right) S_{p_{1} p_{2}, q} \\
& \quad=-A+2(-1)^{p_{2}} B+2(-1)^{p_{1}} C+2 D-E+2 F,
\end{aligned}
$$

where the quantities $A, B, C, D, E, F$ are defined in the box above and the sums are over all indices $\geq 0$. The value $\zeta(0)=-\frac{1}{2}$ should be used and $\zeta(1)$ should be replaced by 0 whenever it occurs.

Proof. Use the kernel of (4-2). The quantity $F$ represents

$$
-\mathcal{R}\left[s^{-q} \frac{\psi^{\left(p_{1}-1\right)}(-s)}{\left(p_{1}-1\right)!} \frac{\psi^{\left(p_{2}-1\right)}(-s)}{\left(p_{2}-1\right)!} \pi \cot \pi s\right],
$$

that is estimated as a Taylor coefficient. The other quantities represent combined contributions of the poles at $s= \pm n$.

A similar, and slightly simpler, expression holds when either $i=1$ or $j=1$, in which case one should replace $\psi^{(0)}(-s)$ by $\psi(-s)+\gamma$.

| Kernel | Reduction | Order |  |
| :--- | :--- | :---: | :--- |
| $(\psi(-s)+\gamma)^{2}$ | $S_{1, r}$ | 1 | Reduction, all $r$ (Thm. 2.2) |
| $\psi^{(p-1)}(-s) \pi \cot \pi s$ | $S_{p, q}$ | 1 | Reduction, odd weight $p+q$ (Thm. 3.1) |
| $\left(\psi^{(j)}(-s)\right)^{2}$ | $S_{2 j+1, q}, \ldots, S_{j+1, q+j}$ | 1 | Relations, even weight (Eqs. (3-1), (3-2)) |
| $(\psi(-s)+\gamma)^{3}$ | $S_{1^{2}, q}-S_{2, q}$ | 2 | Reduction, any weight |
| $\psi^{(i-1)}(-s) \psi^{(j-1)}(-s) \pi \cot \pi s$ | $S_{i j, k} \mapsto\left\{S_{a, b}\right\}$ | 2 | Reduction of order, even weight (Thm. 4.2) |
| $(\psi(-s)+\gamma)^{4}$ | $S_{1^{3}, q}-3 S_{12, q}$ | 3 | Reduction, any weight (Thm. 5.1) |

TABLE 1. A summary of kernels and the corresponding reductions.

As is well known, the multiple zeta functions satisfy shuffle relations that generalize the symmetry relation (1-2). For instance,

$$
\begin{align*}
\zeta(a) \zeta(b, c)=\zeta(a, b, c) & +\zeta(a+b, c)+\zeta(b, a, c) \\
& +\zeta(b, a+c)+\zeta(b, c, a) \tag{4-3}
\end{align*}
$$

for $a>1$ and $c>1$, as seen by considering all ways of interlacing the vector arguments (a) and $(b, c)$. The conjunction of the theorem and shuffle relations, provides a simple proof of "half" of the main result of [Borwein and Girgensohn 1996], according to which all triple zeta values of even weight are reducible to double zeta values. The reductions obtained are in addition explicit double convolutions of simple and double zeta values.

Corollary 4.3 [Borwein and Girgensohn 1996]. For $c>1$, triple zeta values $\zeta(a, b, c)$ whose weight $a+$ $b+c$ is even are reducible to double zeta values or equivalently to linear Euler sums.

Proof. It suffices to consider the trivially modified quadratic sums

$$
\begin{aligned}
T(i, j, k) & :=\sum_{n=1}^{\infty} H_{n-1}^{(i)} H_{n-1}^{(j)} \frac{1}{n^{k}} \\
& =S_{i j, k}-S_{j, k+i}-S_{i, k+j}+\zeta(i+j+k) \\
& =\zeta(i, j, k)+S_{i+j, k}+\zeta(j, i, k) .
\end{aligned}
$$

Assume first that $j>1 ; k>1$ is granted. Then, from the shuffle relations with $a=k, b=i$, and $c=j$, we find

$$
\begin{aligned}
\zeta(i, j, k)= & \zeta(k) \zeta(i, j)-\zeta(k+i, j)-\zeta(i, k+j) \\
& -(\zeta(k, i, j)+\zeta(i, k, j)) \\
= & \zeta(k) \zeta(i, j)-\zeta(k+i, j)-\zeta(i, k+j) \\
& -(T(i, j, k)-\zeta(i+j, k)-\zeta(i+j+k))
\end{aligned}
$$

The dual case when $i>1$ is treated by the substitutions $a=k, b=j$, and $c=i$. If both $i$ and $j$ equal 1 , then the reduction is attained by the computation of $S_{1^{2}, k}$.

It is believed that no reduction holds in general for triple zetas of odd weights [Borwein and Girgensohn 1996]. Actually, starting at (odd) weight 11, it seems that $\zeta(5,3,3)$ is independent of single zeta values. (Such properties can be approached heuristically by means of linear integer dependency algorithms based on lattice reduction or related techniques.) However, for the exceptional odd weights $\{5,7,9\}$, all triple zeta values are now known to be reducible to polynomials in single zetas: this is the other "half" of the main result of [Borwein and Girgensohn 1996] already referred to that we extend a little bit further in Section 6. An indirect consequence to be discussed in the next section is the reduction of the cubic sums $S_{1^{3}, q}$ corresponding to special quadruple zeta values.

## 5. CUBIC AND HIGHER ORDER EULER SUMS

For higher degree sums, like the cubic

$$
S_{1^{3}, q}:=\sum_{n=1}^{\infty} \frac{\left(H_{n}\right)^{3}}{n^{q}},
$$

it is natural to consider the kernels $(\psi(-s)+\gamma)^{4}$ and $(\psi(-s)+\gamma)^{3} \pi \cot \pi s$. Cross products start to proliferate but the relations obtained at the previous steps help reduce many of the sums.

Theorem 5.1. (i) For odd weights, the cubic combination $S_{1^{3}, q}-3 S_{12, q}$ is expressible in terms of zeta values.
(ii) For even weights, both $S_{1^{3}, q}$ and $S_{12, q}$ are reducible to $S_{2, q+1}$ and to polynomials in zeta values.

Proof. Let $r(s), r_{1}(s)$ satisfy the conditions of (2-5), and suppose additionally that $r_{1}(s)$ is odd. Then a direct residue computation gives

$$
\begin{aligned}
-\mathcal{R} & {\left[(\psi(-s)+\gamma)^{4} r(s)\right] } \\
= & 4 \sum_{n=1}^{\infty} r(n)\left(\left(H_{n}\right)^{3}-3 H_{n} H_{n}^{(2)}\right)+6 \sum_{n=1}^{\infty} r^{\prime}(n)\left(H_{n}\right)^{2} \\
& +\sum_{n=1}^{\infty} 4\left(H_{n}^{(3)}-3 \zeta(2) H_{n}-\zeta(3)\right) r(n) \\
& -4 \sum_{n=1}^{\infty}\left(H_{n}^{(2)}+\zeta(2)\right) r^{\prime}(n)+2 H_{n} r^{\prime \prime}(n)+\frac{r^{\prime \prime \prime}(n)}{6}
\end{aligned}
$$

and

$$
\begin{aligned}
-\mathcal{R} & {\left[(\psi(-s)+\gamma)^{3} \pi \cot (\pi s) r_{1}(s)\right] } \\
= & -6 \sum_{n=1}^{\infty} r_{1}(n) H_{n} H_{n}^{(2)}+3 \sum_{n=1}^{\infty}\left(H_{n}\right)^{2}\left(\frac{r_{1}(n)}{n}+r_{1}^{\prime}(n)\right) \\
& +3 \sum_{n=1}^{\infty}\left(H_{n}^{(3)}-\left(4 \zeta(2)+\frac{1}{n^{2}}\right) H_{n}-\zeta(3)+\frac{1}{3 n^{3}}\right) r_{1}(n) \\
& -\sum_{n=1}^{\infty}\left(3 H_{n}^{(2)}+5 \zeta(2)\right) r_{1}^{\prime}(n)+\frac{3}{2} H_{n} r_{1}^{\prime \prime}(n)+\frac{r_{1}^{\prime \prime \prime}(n)}{6}
\end{aligned}
$$

These formulæ complement the ones in the box on page 24 .

Instantiating the first identity to $r(s)=s^{-q}$ with even $q$ and appealing to relations $\left(S_{4}\right),\left(S_{6}\right)$ and $\left(S_{7}\right)$ of page 24 yields the first part of the theorem. The second identity is an explicit version of the quadratic reductions discussed in the previous section; it permits to dispose of the sum $S_{12, q}$ that
reduces to the linear sums $S_{2, q+1}$ for even weight. Instantiating it to $r(s)=s^{-q}$ with odd $q$ yields the second part of the theorem.
For even weight, we thus have an infinite collection of explicit reductions, including some that were presented as conjectural in Table 4 of [Bailey et al. 1994]:

$$
\begin{aligned}
& \begin{array}{l}
\sum_{n=1}^{\infty} \frac{\left(H_{n}\right)^{3}}{n^{5}}-\frac{11}{4} \sum_{n=1}^{\infty} \frac{H_{n}^{(2)}}{n^{6}}=\frac{469}{32} \zeta(8)-16 \zeta(3) \zeta(5) \\
\\
\quad+\frac{3}{2} \zeta(2) \zeta(3)^{2},
\end{array} \\
& \begin{array}{r}
\sum_{n=1}^{\infty} \frac{\left(H_{n}\right)^{3}}{n^{7}}-\frac{13}{4} \sum_{n=1}^{\infty} \frac{H_{n}^{(2)}}{n^{8}}=\frac{561}{20} \zeta(10)-\frac{47}{4} \zeta(5)^{2} \\
\quad-\frac{49}{2} \zeta(7) \zeta(3)+3 \zeta(2) \zeta(3) \zeta(5)+\frac{15}{4} \zeta(3)^{2} \zeta(4), \\
\sum_{n=1}^{\infty} \frac{\left(H_{n}\right)^{3}}{n^{9}}-\frac{15}{4} \sum_{n=1}^{\infty} \frac{H_{n}^{(2)}}{n^{10}}=\frac{1060345}{22112} \zeta(12) \\
-33 \zeta(5) \zeta(7)-35 \zeta(3) \zeta(9)-\frac{1}{4} \zeta(3)^{4}+\frac{3}{2} \zeta(2) \zeta(5)^{2} \\
\quad+\frac{21}{4} \zeta(3)^{2} \zeta(6)+\frac{15}{2} \zeta(3) \zeta(4) \zeta(5)+3 \zeta(2) \zeta(3) \zeta(7) .
\end{array}
\end{aligned}
$$

Corollary 5.2. The cubic sums $S_{1^{3}, q}$ of weights $\{5,6$, $7,9\}$ are reducible to zeta values:

$$
\begin{aligned}
& \sum_{n=1}^{\infty} \frac{\left(H_{n}\right)^{3}}{(n+1)^{2}}=\frac{15}{2} \zeta(5)+\zeta(2) \zeta(3) \\
& \sum_{n=1}^{\infty} \frac{\left(H_{n}\right)^{3}}{(n+1)^{3}}=-\frac{33}{16} \zeta(6)+2 \zeta(3)^{2} \\
& \sum_{n=1}^{\infty} \frac{\left(H_{n}\right)^{3}}{(n+1)^{4}}=\frac{119}{16} \zeta(7)-\frac{33}{4} \zeta(3) \zeta(4)+2 \zeta(2) \zeta(5) \\
& \sum_{n=1}^{\infty} \frac{\left(H_{n}\right)^{3}}{(n+1)^{6}}=\frac{197}{24} \zeta(9)-\frac{33}{4} \zeta(4) \zeta(5) \\
& \quad \quad-\frac{37}{8} \zeta(3) \zeta(6)+\zeta(3)^{3}+3 \zeta(2) \zeta(7)
\end{aligned}
$$

(The forms given are those of [Bailey et al. 1994].)
Proof. We only indicate briefly the chain of reductions. For weight 6 , this results from the evaluation of $S_{2,4}$ in (4-1). For weight 5 , the evaluation follows from Hoffman's [Hoffman 1992] complete reduction of multiple zetas in the case of all weights $\leq 6$. For the odd weights $\{7,9\}$, the reduction follows from
the Borwein-Girgensohn result after which triple zetas are reducible to double and single zetas for all weights $\leq 10$. Alternatively, one may use reduction by any maximal system of relations presented in Section 6.

## Higher Degree Euler Sums

Linear Euler sums reduce to zeta values in the case of an odd weight, while quadratic Euler sums reduce to linear sums (double zeta values) in the case of an even weight. We prove here a result to the effect that such reductions of order are general.

Theorem 5.3. (i) For odd weight $w=i+j+k+l$, all cubic sums $S_{i j k, l}$ reduce to combinations of Euler sums of order at most 2.
(ii) More generally, a nonlinear Euler sum

$$
S_{i_{1} i_{2} \cdots i_{r}, q}
$$

reduces to a combination of sums of lower orders whenever the weight $i_{1}+i_{2}+\cdots+i_{r}+q$ and the order $r$ are of the same parity.

Proof. We start with the case of cubic sums and adopt the kernel

$$
\begin{aligned}
\xi_{i, j, k}= & \frac{1}{(i-1)!(j-1)!(k-1)!} \\
& \times \psi^{(i-1)}(-s) \psi^{(j-1)}(-s) \psi^{(k-1)}(-s) \pi \cot \pi s,
\end{aligned}
$$

which is applied to $r(s)=s^{-l}$. The expansion at $s=m$,
$\frac{1}{(i-1)!} \psi^{(i-1)}(-s)=\frac{1}{(s-m)^{i}}+H_{m}^{(i)}+(-1)^{i} \zeta(i)+\cdots$,
implies that the sum of residues at positive integers is of the form $S_{i j k, l}+T$, where $T$ is a combination of quadratic sums. The expansion at $s=-m$,

$$
\frac{1}{(i-1)!} \psi^{(i-1)}(-s)=(-1)^{i-1}\left(H_{m-1}^{(i)}-\zeta(i)\right)+\cdots,
$$

implies that the sum of residues at negative integers is of the form $(-1)^{i+j+k+l-3} S_{i j k, l}+U$, where $U$ is a combination of quadratic sums. We thus have a reduction of order whenever the weight is odd.

The general case follows along the very same lines.

Broadhurst has made a conjecture (see [Borwein and Girgensohn 1996]) of a shape similar to our statement but concerning multiple zeta values instead. In the case of quadratic sums, we have at least seen that the shuffle relations entail a corresponding reduction for all triple zeta values. It does not seem that Broadhurst's conjecture can be deduced, even partially, from our theorem.

## 6. MODELS OF EULER SUM IDENTITIES

Various approaches have been developed for Euler sums evaluations. We discuss here general methods and leave aside methods based on definite integrals and polylogarithms of which De Doelder's paper [1991] is typical. Our purpose here is to obtain complete models for low weights and at the same time examine the power of various frameworks proposed, including the residue method.

## Shuffle Relations

These are relations that generalize the symmetry relation (shuffle of order 2) of (1-2) and the particular shuffle of order 3 of ( $4-3$ ). Consideration of the product of two multiple zeta functions $\zeta(\boldsymbol{u}), \zeta(\boldsymbol{v})$, with $\boldsymbol{u}, \boldsymbol{v}$ denoting arbitrary vectors of integers, gives the relation

$$
\begin{equation*}
\zeta(\boldsymbol{u}) \cdot \zeta(\boldsymbol{v})=\sum_{\boldsymbol{w} \in \boldsymbol{u} w v} \zeta(\boldsymbol{w}) \tag{6-1}
\end{equation*}
$$

where $(\boldsymbol{u} \boldsymbol{w} \boldsymbol{v})$ is the shuffle of vectors $\boldsymbol{u}, \boldsymbol{v}$, that is, the set of vectors defined recursively by

$$
\begin{aligned}
& (a \cdot \boldsymbol{u}) \boldsymbol{\text { w }}(b \cdot \boldsymbol{v}) \\
& =a \cdot(\boldsymbol{u} \boldsymbol{w}(b \cdot \boldsymbol{v})) \cup b \cdot((a \cdot \boldsymbol{u}) \boldsymbol{w} \boldsymbol{v}) \cup(a+b) \cdot(\boldsymbol{u} \boldsymbol{v})
\end{aligned}
$$

Here the dot operation is the concatenation of vectors (extended to sets in the usual way) and all operations are taken in the sense of multisets so as to preserve multiplicities.

Equation (6-1) simply expresses all possible interlacings of indices when a product is expanded by
distributivity. The shuffle relations are similar to symmetric function identities studied by Hoffman [1992] and, as noted by Zagier [1994], they imply that the linear space spanned by the multiple zeta values forms a ring.

We denote by $\Sigma$ the set of linear relations that arise from shuffles.

## Duality

Duality is a surprising property first conjectured in [Hoffman 1992] and proved in [Zagier 1994] upon a suggestion of Kontsevich. It is expressed by means of an encoding by binary vectors of multiple zeta values: given a vector $\boldsymbol{u}=\left(u_{1}, \ldots, u_{k}\right)$, its encoding is

$$
\beta\left(u_{1}, u_{2}, \ldots, u_{k}\right):=10^{u_{1}-1} 10^{u_{2}-1} \cdots 10^{u_{k}-1}
$$

where $0^{k}$ means 0 repeated $k$ times. We then introduce the quantities

$$
H(U):=\zeta\left(\beta^{(-1)} U\right)
$$

that are defined for all binary vectors starting with a 1 and ending with a 0 . Define the reverse-complement of a binary vector $U=\varepsilon_{1} \varepsilon_{2} \cdots \varepsilon_{l}$ as $U^{\star}=$ $\bar{\varepsilon}_{l} \bar{\varepsilon}_{l-1} \cdots \bar{\varepsilon}_{1}$, where $\bar{\varepsilon}=1-\varepsilon$. Then Hoffman's duality principle states that

$$
\begin{equation*}
H(U)=H\left(U^{\star}\right) \tag{6-2}
\end{equation*}
$$

This relation groups the multiple zetas into equal pairs and, for instance, implies that

$$
\begin{aligned}
\zeta(2,3,4) & =H(101001000)=H(111011010) \\
& =\zeta(1,1,2,1,2,2)
\end{aligned}
$$

The proof sketched in [Zagier 1994] is based on the multiple integral representation

$$
\begin{gathered}
H\left(\varepsilon_{1}, \ldots, \varepsilon_{k}\right)=\int_{0<t_{1}<\cdots<t_{k}<1} \cdots \int_{\varepsilon_{1}} t_{1} \cdots d_{\varepsilon_{k}} t_{k} \\
d_{0} t=\frac{d t}{t}, \quad d_{1} t=\frac{d t}{1-t}
\end{gathered}
$$

and on the change of variables $u_{j}=1-t_{j}$.

We denote by $\Delta$ the set of linear relations that arise from duality.

## Partial Fraction Expansions

The Euler-Nielsen method, of which an idea was given at the beginning of Section 3, applies to double zetas [Nielsen 1906], and, as established by Markett [1994] and by Borwein and Girgensohn [1996], it can be extended to triple zetas. We let $\Pi_{2}$ and $\Pi_{3}$ denote the linear relations that arise from this mechanism in the case of zetas of multiplicities 2 and 3.

## Residue Relations

We have designed a program in system Maple that computes relations on Euler sums that result from any kernel that is a polynomial form in $\psi$ functions and their derivatives. We denote by $R$ the set of relations that arise from such kernels applied to $1 / s^{q}$; see Section 2 and the box on page 20 .

Our program allows the exhaustive investigation of the relations deriving from the residue method applied to Euler sums of a fixed given weight. We have examined the dimension of the spaces of linear relations that result from any combination of the rules $\Sigma, \Delta, \Pi_{2}, \Pi_{3}, R$ for all weights up to 10 . This can be viewed as a supplement to Hoffman's investigations who obtained a complete basis of relations between multiple zetas for weights $\leq 6$.

First, the linear relations implied by the rules $\Sigma, \Delta, \Pi_{2}, \Pi_{3}, R$ take place a priori in the space of products of multiple zetas with total weight $w$. The shuffle relations reduce these products into linear combinations of multiple zetas of weight $w$, forming a space whose dimension is $2^{w-2}$. There are $E_{w}$ distinct Euler sums, where

$$
\begin{aligned}
\sum_{w=2}^{\infty} E_{w} z^{w}= & \frac{z^{2}}{1-z} \prod_{j=1}^{\infty} \frac{1}{1-z^{j}} \\
= & z^{2}+2 z^{3}+4 z^{4}+7 z^{5}+12 z^{6}+19 z^{7} \\
& \quad+30 z^{8}+45 z^{9}+67 z^{10}+97 z^{11}+\cdots
\end{aligned}
$$

and standard estimates on the number of partitions imply that $E_{w}=e^{O(\sqrt{w})}$.

We seek reductions of Euler sums into linear combinations of monomials in single zeta values whose number $\mu_{w}$ satisfies

$$
\begin{aligned}
\sum_{w=0}^{\infty} \mu_{w} z^{w}= & \frac{1}{1-z^{2}} \prod_{j=1}^{\infty} \frac{1}{1-z^{2 j+1}} \\
= & 1+z^{2}+z^{3}+z^{4}+2 z^{5}+2 z^{6}+3 z^{7} \\
& +3 z^{8}+5 z^{9}+5 z^{10}+7 z^{11}+8 z^{12}+\cdots
\end{aligned}
$$

The growth order of $\mu_{w}$ is again $e^{O(\sqrt{w})}$, though with a smaller exponential rate than $E_{w}$. These $\mu_{w}$ (presumably $\mathbb{Q}$-linearly independent) monomials span the space of "closed-form" expressions.

Thus, the numbers of multiple zeta forms, Euler sums, and polyzeta forms satisfy

$$
2^{w-2} \gg E_{w} \gg \mu_{w}
$$

Therefore, one should not expect on these grounds all multiple zetas nor even all Euler sums to reduce to combinations of zeta monomials. In other words, closed form is exceptional for an Euler sum.

Zagier has conducted extensive numerical computations of multiple zeta values of all weights up to 12 and has examined the apparent $\mathbb{Q}$-linear dependencies that result. Based on these computations and other algebraic arguments, he conjectures that the dimension $d_{w}$ is given by the recurrence $d_{w}=d_{w-2}+d_{w-3}, \quad d_{2}=d_{3}=d_{4}=1$, so

$$
\begin{aligned}
\sum_{w=2}^{\infty} d_{w} z^{w}= & \frac{1}{1-z^{2}-z^{3}} \\
= & 1+z^{2}+z^{3}+z^{4}+2 z^{5}+2 z^{6}+3 z^{7} \\
& +4 z^{8}+5 z^{9}+7 z^{10}+9 z^{11}+12 z^{12}+\cdots
\end{aligned}
$$

The growth of $d_{w}$ is of the approximate form $d_{w} \approx$ $1.32471^{w}$.

Thus, modulo Zagier's conjecture, the dimension of the $\mathbb{Q}$-linear space of multiple zeta values lies somewhere in between the (large) number $2^{w-2}$ of multiple zetas and the (small) number $\mu_{w}$ of closed-
form monomials. What is remarkable, however, is that there is almost coincidence of $d_{w}$ and $\mu_{w}$ for weights $<10$, the difference $d_{8}-\mu_{8}=1$ being accounted for by the occurrence of the (probably) irreducible $S_{2,6}$. Based on our program, we have verified the reductions implied by Zagier's conjecture for all weights up to 9 . (We do not claim much originality for the next result: it is largely a verification based on techniques introduced by Hoffman, Zagier, Markett, Borwein and Girgensohn.)

Theorem 6.1. All multiple zetas of weight $\leq 9$ are reducible to $\mathbb{Q}$-linear combinations of single zeta monomials with the addition of $\left\{S_{2,6}\right\}$ for weight 8.

Proof. Solve the linear systems deriving from the shuffle relations $\Sigma$, duality $\Delta$, partial fractions $\Pi_{2}$ and $\Pi_{3}$, and residues $R$.

Corollary 6.2. All Euler sums of the form $S_{1^{p}, q}$ for weights $p+q \in\{3,4,5,6,7,9\}$ are expressible polynomially in terms of zeta values. For weight 8, all such sums are the sum of a polynomial in zeta values and a rational multiple of $S_{2,6}$.

This corollary provides a justification of identities discovered experimentally by Bailey et al. [1994].

In passing, the computations underlying Theorem 6.1 allow one to delineate the power of various reduction principles. First, duality reduces by about a half the number of independent multiple zetas to be considered since it provides a number $\delta_{w}$ of nontrivial linear equalities that satisfies $\delta_{w}=2^{w-3}$ when $w$ is odd and $\delta_{w}=2^{w-3}-2^{w / 2-2}$ when $w$ is even. Next, the shuffle relations reduce all the products of multiple zetas to linear combinations of multiple zetas. Besides, the shuffle relations induce linear relations on multiple zetas. For instance, since $\zeta(1,2)=\zeta(3)$, the products of these by $\zeta(2)$ once expanded by the shuffle relations yield
$\zeta(2,1,2)+2 \zeta(1,2,2)+\zeta(1,4)-\zeta(2,3)-\zeta(5)=0$.
The Nielsen relations $\Pi_{2}$ appear to provide $\lfloor w / 2\rfloor$ independent linear relations of weight $w$, which is not much. Also, for odd weight, these relations are implied by the residue relations $R$ as expressed

| weight $w$ | $\Sigma$ | $\Delta$ | $\Pi_{2}$ | $\Pi_{3}$ | $R$ | total | $2^{w-2}-d_{w}$ |  |
| :---: | ---: | ---: | :---: | :---: | :---: | :---: | :--- | :--- |
| 3 | 0 | 1 | 1 | 0 | 1 | 1 | 1 | $\left(\Pi_{2}\right),(\Delta),(R)$ |
| 4 | 0 | 1 | 2 | 1 | 2 | 3 | 3 | $\left(\Pi_{2}, \Delta\right),\left(\Pi_{2}, \Pi_{3}\right),\left(\Pi_{2}, R\right),\left(\Pi_{3}, R\right)$ |
| 5 | 1 | 4 | 2 | 3 | 5 | 6 | 6 | $\left(\Pi_{2}, \Delta\right),\left(\Pi_{3}, \Delta\right),(R, \Delta),\left(\Pi_{3}, R\right)$ |
| 6 | 5 | 6 | 3 | 6 | 10 | 14 | 14 | $\left(\Pi_{2}, \Delta\right),\left(\Pi_{3}, \Delta\right),(R, \Delta)$ |
| 7 | 12 | 16 | 3 | 10 | 17 | 29 | 29 | $\left(\Pi_{3}, \Delta\right)$ |
| 8 | 31 | 28 | 4 | 15 | 31 | 60 | 60 | $\left(\Pi_{3}, \Delta\right),(R, \Delta)$ |
| 9 | 68 | 64 | 4 | 21 | 45 | 123 | 123 | $\left(\Pi_{3}, \Delta, R\right)$ |
| 10 | 151 | 120 | 5 | 27 | 75 | 248 | 249 | $\left(\Pi_{3}, \Delta\right),(R, \Delta)$ |

TABLE 2. Rank of relations versus weight. Each set of relations generates a vector space of linear relations on the multiple zetas. For each weight, we indicate the dimension of this space, which gives a measure of the power of the relations.
by Theorem 3.1. The Markett relations $\Pi_{3}$ seem to induce $O\left(w^{2}\right)$ independent linear relations of weight $w$. In Table 2, we give the dimension of the vector space of linear relations induced by the rule $\Sigma$; we also give the dimension of the linear relations induced by $\Pi_{2}, \Pi_{3}, \Delta$, and $R$ once linearized by the shuffle relations. The total dimension of the space of relations we get is indicated in the next column. It is to be compared with the value $2^{w-2}-d_{w}$ implied by Zagier's conjecture. In the last column we indicate which minimal combinations of relations make it possible to generate all the known relations (in conjunction with $\Sigma$ ).
An interesting aspect of the proof of Theorem 6.1 is that residue relations contribute new relations to the arsenal of currently known methods and permit to attain the limit described by Zagier's conjecture for weights up to 9 inclusive. This is demonstrated in the last column of Table 2, where it appears that all 4 relations are necessary to get 123 independent linear relations of weight 9 (since the weight is odd $\Pi_{2}$ is implied by $R$ ). For instance, the kernel $(\psi(s)+\gamma)^{3} \psi^{\prime}(-s)$ applied to the base function $1 / s^{5}$ induces a relation that is not a consequence of the linear relations induced by the partial fraction relations together with duality and the shuffle relations. For weight 10, the last line of Table 2 indicates that the relations $\Sigma, \Delta, \Pi_{2}, \Pi_{3}, R$ are no longer sufficient to generate all the linear relations implied by Zagier's conjecture.

There are two computationally intensive steps in this verification, the generation of all the residue relations and the elimination process. Elimination is required to obtain the dimension of the space of linear relations generated by the nonlinear shuffle relations; it has been performed by a Gröbner basis computation.

## 7. ALTERNATING EULER SUMS

We now turn to the evaluation of alternating Euler sums by means of contour integrals. Let
$\bar{H}_{n}^{(r)}:=\sum_{j=1}^{n} \frac{(-1)^{j-1}}{j^{r}}, \quad \bar{H}_{n}:=H_{n}^{(1)}=\sum_{j=1}^{n} \frac{(-1)^{j-1}}{j}$ denote the alternating harmonic numbers. There are altogether four types of linear sums:

$$
\begin{array}{ll}
S_{p, q}^{++}=\sum_{n=1}^{\infty} \frac{H_{n}^{(p)}}{n^{q}}, & S_{p, q}^{+-}=\sum_{n=1}^{\infty}(-1)^{n-1} \frac{H_{n}^{(p)}}{n^{q}}, \\
S_{p, q}^{-+}=\sum_{n=1}^{\infty} \frac{\bar{H}_{n}^{(p)}}{n^{q}}, & S_{p, q}^{--}=\sum_{n=1}^{\infty}(-1)^{n-1} \frac{\bar{H}_{n}^{(p)}}{n^{q}} .
\end{array}
$$

Clearly the $S_{p, q}^{++}$are the standard Euler sums defined earlier. Such numbers have been considered by Euler, Nielsen and many others.

A natural kernel for the sums of type $S^{+-}$is a combination of $\psi$ functions and $\pi / \sin \pi s$, since the latter introduces sign alternation. Some parity constraints must however intervene since poles
occur at positive and negative integers. The other results are best stated in terms of the alternating zeta function,

$$
\bar{\zeta}(s):=\sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n^{s}}=\left(1-2^{1-s}\right) \zeta(s),
$$

with $\bar{\zeta}(1)=\log 2$. Alternating harmonic numbers are introduced by the modified $\psi$ function,

$$
\begin{aligned}
\bar{\psi}(s) & :=\sum_{k=0}^{\infty} \frac{(-1)^{k}}{s+k}=\frac{1}{2} \psi\left(\frac{s+1}{2}\right)-\frac{1}{2} \psi\left(\frac{s}{2}\right) \\
& =\frac{1}{s}-\log 2+\bar{\zeta}(2) s-\bar{\zeta}(3) s^{2}+\bar{\zeta}(4) s^{3}-\cdots
\end{aligned}
$$

This is also known as Nielsen's $\beta$ function; it satisfies

$$
\begin{aligned}
& \bar{\psi}(n)=(-1)^{n}\left(\bar{H}_{n-1}-\log 2\right), \\
& \bar{\psi}(s)_{s \rightarrow-n}=(-1)^{n}\left(\frac{1}{s+n}+\left(\bar{H}_{n}-\log 2\right)+\cdots\right),
\end{aligned}
$$

where $n$ is a positive integer.
The following evaluations are all found in [Sitaramachandra Rao 1987], which contains an exhaustive discussion of sums $S_{1, r}^{ \pm \pm}$together with a thorough bibliography. Here the identities come out as simple consequences of the process employed earlier for standard Euler sums.

Theorem 7.1 [Sitaramachandra Rao 1987].
(i) For any weight $1+q$,

$$
\begin{aligned}
2 S_{1, q}^{-+}=2 \zeta(q) \log 2-q \zeta(q+1) & +2 \bar{\zeta}(q+1) \\
& +\sum_{k=1}^{q} \bar{\zeta}(k) \bar{\zeta}(q-k+1) .
\end{aligned}
$$

(ii) In the case of a weight $1+q$ that is odd,

$$
\begin{aligned}
& 2 S_{1, q}^{+-}=(q+1) \bar{\zeta}(q+1)-\zeta(q+1) \\
&-2 \sum_{k=1}^{q / 2-1} \bar{\zeta}(2 k) \zeta(q+1-2 k),
\end{aligned}
$$

$$
2 S_{1, q}^{--}=2(\zeta(q)+\bar{\zeta}(q)) \log 2-(q+1) \bar{\zeta}(q+1)+\zeta(q+1)
$$

$$
+2 \sum_{k=1}^{q / 2-1} \zeta(2 k) \bar{\zeta}(q+1-2 k) .
$$

Proof. The result falls as a ripe fruit when we use respectively the kernels

$$
\bar{\psi}(s)^{2}, \quad \frac{\pi}{\sin \pi s}(\psi(-s)+\gamma), \quad \bar{\psi}(s) \pi \cot \pi s
$$

In the first case, the sign alternation of the general term disappears because of the squaring of $\bar{\psi}(s)$, so that we get directly $S_{1, q}^{-+}$. In the other cases, two almost identical sums result from the residues at the positive and negative integers, and the combination involves a coefficient of $\left(1+(-1)^{q}\right)$, so that estimates are restricted to the case of $q$ odd. Notice finally that the use of the kernel

$$
\bar{\psi}(s)(\psi(-s)+\gamma)
$$

allows one to relate $S_{1, q}^{+-}$and $S_{1, q}^{--}$irrespective of the parity of the weights:

$$
\begin{aligned}
& S_{1, q}^{--}+(-1)^{q} S_{1, q}^{+-} \\
& \quad=\bar{\zeta}(q) \log 2-\sum_{i=1}^{q-1}(-1)^{i} \bar{\zeta}(i) \zeta(q+1-i) .
\end{aligned}
$$

In other words, there is a new variety of constants defined by

$$
\mu_{q}=S_{1,2 q+1}^{+-}=\sum_{n=1}^{\infty}(-1)^{n-1} \frac{H_{n}}{n^{2 q+1}},
$$

where

$$
\mu_{q}=\frac{1}{(2 q)!} \int_{0}^{1} \frac{\log ^{2 q}(z) \log (1+z)}{z(1+z)} d z .
$$

We have from [de Doelder 1991; Sitaramachandra Rao 1987]

$$
\begin{aligned}
& \mu_{0}=\frac{1}{2} \zeta(2)-\frac{1}{2} \log ^{2} 2, \\
& \mu_{1}=-2 \operatorname{Li}_{4}\left(\frac{1}{2}\right)+\frac{11}{4} \zeta(4)+\frac{1}{2} \zeta(2) \log ^{2} 2 \\
& -\frac{1}{12} \log ^{4} 2-\frac{7}{4} \zeta(3) \log 2,
\end{aligned}
$$

where $\operatorname{Li}_{q}(z)=\sum_{n=1}^{\infty} z^{n} n^{-q}$ is the polylogarithm. The constant $\mu_{1}$ is related to several of Ramanujan's evaluations as well as to the analysis of lattice reduction [Daudé et al. 1997] mentioned in the introduction. Higher order $\mu$ 's are not known to be related to classical constants.

Nielsen, following Euler, proved relations suggesting that alternating sums of odd weight should reduce to polynomials in zeta values augmented with $L=\bar{\zeta}(1)=\log 2$. This approach is developed in [Borwein et al. 1995], where it is shown that the Euler-Nielsen relations can be inverted (though explicit formulæ are not given).

Shuffle relations analogous to (1-1),

$$
\begin{aligned}
& \bar{\zeta}(p) \zeta(q)+\bar{\zeta}(p+q)=S_{p, q}^{-+}+S_{q, p}^{+-}, \\
& \bar{\zeta}(p) \bar{\zeta}(q)+\zeta(p+q)=S_{p, q}^{--}+S_{q, p}^{--},
\end{aligned}
$$

reduce the number of quantities to be investigated. However, since our interest is in general summatory formulæ, we prefer to develop an approach from scratch.

Theorem 7.2. Let $w=p+q$ be an odd weight. Then:
(i) $\left((-1)^{q}-(-1)^{p}\right) S_{p, q}^{-+}$is given by

$$
\begin{aligned}
& (-1)^{p} \bar{\zeta}(p+q)+\left((-1)^{p}-1\right) \bar{\zeta}(p) \zeta(q) \\
& \quad+2 \sum_{j+2 k=p}\binom{q+j-1}{q-1} \zeta(q+j) \bar{\zeta}(2 k) \\
& \quad+2(-1)^{p} \sum_{i+2 k=q}\binom{p+i-1}{p-1}(-1)^{i} \bar{\zeta}(p+i) \bar{\zeta}(2 k) .
\end{aligned}
$$

(ii) $2 S_{p, q}^{+-}$is given by

$$
\left(1-(-1)^{p}\right) \zeta(p) \bar{\zeta}(q)+\bar{\zeta}(p+q)
$$

$$
\begin{aligned}
& +2 \sum_{j+2 k=p}\binom{q+j-1}{q-1}(-1)^{j+1} \bar{\zeta}(q+j) \bar{\zeta}(2 k) \\
& +2(-1)^{p} \sum_{i+2 k=q}\binom{p+i-1}{p-1} \zeta(p+i) \bar{\zeta}(2 k) .
\end{aligned}
$$

(iii) $\left((-1)^{p}-(-1)^{q}\right) S_{p, q}^{--}$is given by

$$
(-1)^{p+1} \zeta(p+q)+\left(1-(-1)^{p}\right) \bar{\zeta}(p) \bar{\zeta}(q)
$$

$$
+2 \sum_{j+2 k=p}\binom{q+j-1}{q-1} \bar{\zeta}(q+j) \zeta(2 k)
$$

$$
-2(-1)^{p} \sum_{i+2 k=q}\binom{p+i-1}{p-1}(-1)^{i} \bar{\zeta}(p+i) \zeta(2 k) .
$$

Proof. Just use the kernels $\frac{1}{(p-1)!} \bar{\psi}^{(p-1)}(s) \frac{\pi}{\sin \pi s}$,
$\frac{1}{(p-1)!} \psi^{(p-1)}(s) \frac{\pi}{\sin \pi s}, \frac{1}{(p-1)!} \bar{\psi}^{(p-1)}(s) \pi \cot \pi s$.

## 8. EXOTIC SUMS

The use of kernels involving $\psi$ and its relatives is not just restricted to Euler sums. We have chosen here a random sample of four types of "exotic" summatory formulæ pointing the way to extensions of the method and possibly to a new functionality in computer algebra systems regarding several classes of infinite summations.

$$
\begin{array}{ll}
\left(\begin{array}{ll}
\left(T_{1}\right) & 2 \sum_{n=1}^{\infty}(-1)^{n} r_{0}(n)
\end{array}\right. & =-\mathcal{R}\left[r_{0}(s) \frac{\pi}{\sin \pi s}\right] \\
\left(\begin{array}{l}
T_{2}
\end{array} \quad 2 \sum_{n=1}^{\infty} \bar{H}_{n} r(n)-\sum_{n=1}^{\infty}\left(2 \log 2 r(n)+r^{\prime}(n)\right)\right. & =\mathcal{R}\left[\bar{\psi}^{2}(-s) r(s)\right] \\
\left(T_{3}\right) & 2 \sum_{n=1}^{\infty}(-1)^{n} H_{n} r_{0}(n)+\sum_{n=1}^{\infty}(-1)^{n}\left(r_{0}^{\prime}(n)-\frac{r_{0}(n)}{n}\right) \\
& =-\mathcal{R}\left((\psi(-s)+\gamma) \frac{\pi}{\sin \pi s} r_{0}(s)\right) \\
\left(T_{4}\right) & 2 \sum_{n=1}^{\infty}(-1)^{n} \bar{H}_{n} r_{0}(n)-\sum_{n=1}^{\infty}(-1)^{n}\left(r_{0}^{\prime}(n)+2 \log 2 r_{0}(n)\right)-\frac{r_{0}(n)}{n} \\
& =-\mathcal{R}\left(\bar{\psi}(s) \pi \cot \pi s r_{0}(s)\right)
\end{array}
$$

General summatory formulæ for alternating sums. Here $r(s), r_{0}(s)$ denote rational functions that satisfy the conditions of (2-5), with additionally $r_{0}(s)$ even.

1. Consider the family of sums

$$
A_{q}:=\sum_{n=1}^{\infty} \frac{\left(H_{n}\right)^{2}}{((2 n-1)(2 n)(2 n+1))^{q}} .
$$

We claim that $A_{q}$ reduces to a polynomial in zeta values and $\log 2$ whenever $q$ is odd.

Set $r(n)=((2 n-1)(2 n)(2 n+1))^{-q}$ and take $q$ odd. By Equation $\left(S_{7}\right)$ on page 24, we have a first reduction (modulo values of $\psi$ functions at $\pm \frac{1}{2}$ ) to $\sum H_{n} r^{\prime}(n)$ and $\sum H_{n}^{(2)} r(n)$. The first sum reduces in all cases; the second sum reduces again since $r(s)$ is assumed to be odd. An instance is then

$$
\begin{aligned}
& A_{3}=(1)^{2} \frac{1}{(123)^{3}}+\left(1+\frac{1}{2}\right)^{2} \frac{1}{(345)^{3}} \\
&+\left(1+\frac{1}{2}+\frac{1}{3}\right)^{2} \frac{1}{(567)^{3}}+\cdots \\
&=4 \ln ^{3} 2+\left(\frac{7}{8} \zeta(3)-\frac{35}{4}\right) \ln ^{2} 2 \\
& \quad-\left(\frac{45}{32} \zeta(4)+\frac{7}{8} \zeta(3)-\frac{9}{8} \zeta(2)-12\right) \ln 2+\frac{45}{64} \zeta(4) \\
& \quad-\frac{1}{4} \zeta(2)-\frac{3}{32} \zeta(2) \zeta(3)-\frac{41}{8} \zeta(3)+\frac{17}{32} \zeta(5) .
\end{aligned}
$$

Several related, but simpler, identities appear in Chapter 9 of Ramanujan's notebooks; see [Berndt 1989].
2. Sums related to Catalan's constant have been discovered by Ramanujan [Berndt 1989] and further explored by Sitaramachandra Rao [1987]. We offer here the evaluations

$$
\begin{aligned}
\sum_{n=1}^{\infty}(-1)^{n} \frac{H_{n}}{2 n+1} & =\sum_{n=0}^{\infty} \frac{(-1)^{n}}{(2 n+1)^{2}}-\frac{1}{2} \pi \log 2, \\
\sum_{n=0}^{\infty}(-1)^{n} \frac{H_{n}}{(2 n+1)^{3}} & =3 \sum_{n=0}^{\infty} \frac{(-1)^{n}}{(2 n+1)^{4}}-\frac{7}{16} \pi \zeta(3) \\
& -\frac{1}{16} \pi^{3} \log 2,
\end{aligned}
$$

and the well-known
$\sum_{n=0}^{\infty} \frac{(-1)^{n}}{(2 n+1)^{3}}=\frac{1}{32} \pi^{3}, \quad \sum_{n=0}^{\infty} \frac{(-1)^{n}}{(2 n+1)^{5}}=\frac{5}{1536} \pi^{5}$,
which derive from the kernel $(\psi(-s)+\gamma) \frac{\pi}{\sin \pi s}$.
3. The use of kernels involving $i=\sqrt{-1}$ in arguments of $\psi$ functions leads to yet another class
of summation formulæ. For instance, one has the highly symmetrical formulas

$$
\begin{aligned}
\sum_{m, n \geq 1} \frac{1}{m^{2}\left(m^{2}+n^{2}\right)} & =\frac{1}{2} \zeta(2)^{2}, \\
\sum_{m, n \geq 1} \frac{1}{m^{6}\left(m^{2}+n^{2}\right)} & =\zeta(2) \zeta(6)-\frac{1}{2} \zeta(4)^{2} \\
\sum_{m, n \geq 1} \frac{1}{m n^{3}\left(m^{2}+n^{2}\right)} & =\frac{1}{2} \zeta(3)^{2} \\
\sum_{m, n \geq 1} \frac{1}{m n^{7}\left(m^{2}+n^{2}\right)} & =\zeta(3) \zeta(7)-\frac{1}{2} \zeta(5)^{2}
\end{aligned}
$$

(with a periodicity of exponents modulo 4) from the kernel $(\psi(1+i s)+\gamma)(\psi(-s)+\gamma)$. Zagier [1994] has studied a related but "harder" class of sums.
4. Lastly, the summation process exemplified by the formulas in the boxes of pages 24 and 34 extends to irrational meromorphic functions provided they remain small on circles (or other large contours) on which the kernel is itself small. In that case, one has a relation between two types of infinite sums. For instance, the kernel ( $\pi \cot \pi s$ ) applied to the functions $(\pi \operatorname{coth} \pi s) / s^{q}$ yields identities like

$$
\sum_{n=1}^{\infty} \frac{\operatorname{coth} \pi k}{k^{3}}=\frac{7}{180} \pi^{3}, \quad \sum_{n=1}^{\infty} \frac{\operatorname{coth} \pi k}{k^{7}}=\frac{19}{56700} \pi^{7}
$$

which were discovered by Ramanujan [Berndt 1985].

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