On the double zeta values

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Introduction

In a very important recent paper [1], F. Brown solved long standing conjectures about multiple zeta values (here abbreviated as MZV). In particular, he showed that any such series

$$\zeta(n_1, \ldots, n_r) = \sum_{0<k_1<\ldots<k_r} \frac{1}{k_1^{n_1} \ldots k_r^{n_r}} \tag{1}$$

(with integers $n_1 \geq 1, \ldots, n_{r-1} \geq 1, n_r \geq 2$) can be expressed as *a linear combination with rational coefficients of special values* $\zeta(m_1, \ldots, m_s)$ *where each* m_i *is* 2 *or* 3. The uniqueness of such a linear combination is beyond reach for the moment, but F. Brown [1], after A.B. Goncharov [2] has promoted the MZV's to *motivic multizeta values* $\zeta^{\mathfrak{m}}(n_1, \ldots, n_r)$, and shown that the $\zeta^{\mathfrak{m}}(m_1, \ldots, m_s)$'s with m_i in $\{2, 3\}$ form a rational basis of the space of the motivic MZV's.

In the course of his proof, he needs an identity of the form

$$H(a, b) = \sum_{i=1}^{k} \alpha_i^{a,b} \, \zeta(2i+1) \, H(k-i) \tag{2}$$

with $k = a + b + 1$ and[1]

$$H(m) := \zeta(\underbrace{2, \ldots, 2}_{m}), \quad H(a, b) := \zeta(\underbrace{2, \ldots, 2}_{a}, 3, \underbrace{2, \ldots, 2}_{b}). \tag{3}$$

[1] We use the convention $H(0) = 1$.

F. Brown was not able to give an explicit formula for the rational coefficients $\alpha_i^{a,b}$, but this was supplied by D. Zagier [5], thus completing the proof by F. Brown. It is known since Euler that, for a given integer $m \geq 1$, the numbers $H(m)/\pi^{2m}$, $\zeta(2m)/\pi^{2m}$ and $\zeta(2)^m/\pi^{2m}$ are all rational, and $\zeta(0) = -\frac{1}{2}$. So in the statement of formula (2), one could replace $H(k-i)$ by $\zeta(2k-2i)$ or by $\zeta(2)^{k-i}$, without loosing the rationality of the coefficients $\alpha_i^{a,b}$.

Let us remind the definition of the *weight*

$$w = n_1 + \ldots + n_r$$

of the MZV $\zeta(n_1, \ldots, n_r)$. In particular $\zeta(n)$ is of weight n. From his result, D. Zagier deduces that, *for a given odd weight* $w = 2k+1$ (with $k \geq 1$), the following two families of k real numbers

$$(B_1) \qquad H(a,b) \quad \text{for} \quad a \geq 0, \quad b \geq 0\,, \quad a+b = k-1$$

$$(B_2) \qquad \zeta(2k+1)\,, \quad \zeta(2i+1)\,\zeta(2k-2i) \quad \text{for} \quad 1 \leq i \leq k-1$$

generate the same vector subspace D_w of $\mathbb{R}$ over the rational numbers. D. Zagier has announced that the same space is generated by another family of k numbers, namely

$$(B_3) \qquad \zeta(2k+1)\,, \quad \zeta(2i, 2k-2i+1) \quad \text{for} \quad 1 \leq i \leq k-1\,.$$

In this paper, we shall first prove a slightly weaker statement namely that, *modulo the simple zetas* $\zeta(n)$*, the products of two simple zetas and the double zetas generate the same vector space over* $\mathbb{Q}$ *in* $\mathbb{R}$*.* On the one hand, the following formula

$$\zeta(m)\,\zeta(n) = \zeta(m,n) + \zeta(n,m) + \zeta(m+n) \tag{4}$$

(a particular case of the so-called "stuffle formula") enables us to express the product of two simple zetas in terms of double zetas. We shall prove the converse formula

$$\begin{aligned} \zeta(m,n) \;=\; & \frac{1}{2}\,(1+(-1)^n)\,\zeta(m)\,\zeta(n) \\ +\; & \frac{1}{2}\left[(-1)^n \binom{m+n}{m} - 1\right]\zeta(m+n) \\ -\; & (-1)^n \sum_{i=1}^{(m+n-3)/2} \left[\binom{m+n-2i-1}{m-1} + \binom{m+n-2i-1}{n-1}\right] \\ & \zeta(2i)\,\zeta(m+n-2i) \end{aligned} \tag{5}$$

for $m \geq 1$, $n \geq 1$ and $m+n$ odd. Once this is proved, a simple arithmetic proof, used already by F. Brown and D. Zagier, enables to conclude that the *families* (B_2) *and* (B_3) *generate the same vector space over* $\mathbb{Q}$.

Our proof is purely algebraic and rests on the use of the stuffle formula (4), *the shuffle formula* (59) *and Hoffman's derivation formula* (62), in conjonction with the *manipulation of suitable generating series.* It is generally expected that the three families (B_1), (B_2) and (B_3) of k real numbers are linearly independent over the field $\mathbb{Q}$ of rational numbers. That is, the vector space D_{2k+1} is of dimension k over $\mathbb{Q}$. For the time being, using results of A.B. Goncharov [2] and F. Brown [1], one can promote the double zetas $\zeta(m,n)$ to motivic ones $\zeta^{\mathfrak{m}}(m,n)$ and show that the motivic families $(B_1^{\mathfrak{m}})$, $(B_2^{\mathfrak{m}})$ and $(B_3^{\mathfrak{m}})$ form three basis of the motivic space $D_{2k+1}^{\mathfrak{m}}$. Since our proof rests on the regularized double shuffle relations only, and since the motivic versions of these formulas are known (see I. Soudères [4]), *our proof of formula* (5) *extends litterally to the motivic case.*

1 Review of the stuffle relation

Let us repeat this relation

$$\zeta(m)\,\zeta(n) = \zeta(m,n) + \zeta(n,m) + \zeta(m+n) \quad (\text{for } m \geq 2,\ n \geq 2)\,, \tag{6}$$

and the definitions of the numbers occuring in it

$$\zeta(m) = \sum_{k>0} \frac{1}{k^m}\,, \qquad \zeta(m,n) = \sum_{0<k<\ell} \frac{1}{k^m\,\ell^n}\,. \tag{7}$$

The standard proof is simple: write $\zeta(m)\,\zeta(n)$ as a double series $\sum_{\substack{k>0\\ \ell>0}} \frac{1}{k^m\,\ell^n}$ extended over the domain of pairs of integers $k>0$, $\ell>0$. Then split this summation as the sum of three subsummations

$$\sum_{k>0,\,\ell>0} = \sum_{0<k<\ell} + \sum_{0<\ell<k} + \sum_{0<k=\ell} \tag{8}$$

and (6) follows immediately.

We give another proof which is based on an integral representation for the simple and double zetas. For $\zeta(m)$ with $m \geq 2$, here is the calculation

$$\begin{aligned}
\zeta(m) &= \sum_{k\geq 1} \frac{1}{k^m} = \sum_{k\geq 1} \left[\int_0^1 x^{k-1}\,dx\right]^m \\
&= \sum_{k\geq 1} \int_{C_m} (x_1 \ldots x_m)^{k-1}\,dx_1 \ldots dx_m \\
&= \int_{C_m} \sum_{k\geq 1} (x_1 \ldots x_m)^{k-1}\,dx_1 \ldots dx_m \\
&= \int_{C_m} \frac{dx_1 \ldots dx_m}{1 - x_1 \ldots x_m}\,.
\end{aligned}$$

Hence

$$\zeta(m) = \int_{C_m} \frac{dx_1 \ldots dx_m}{1 - x_1 \ldots x_m}\,, \tag{9}$$

where C_m is the unit cube defined by $0 \leq x_1 \leq 1, \ldots, 0 \leq x_m \leq 1$ in $\mathbb{R}^m$. A similar calculation yields

$$\zeta(m,n) = \int_{C_{m+n}} \frac{y_2}{(1 - y_1\,y_2)(1 - y_2)}\,dx_1 \ldots dx_{m+n} \tag{10}$$

with $y_1 = x_1 \ldots x_m$ and $y_2 = x_{m+1} \ldots x_{m+n}$. All terms in formula (6) are integrals over the cube C_{m+n} of rational functions of $x_1, \ldots, x_{m+n}$ and the proof follows from the following identity for the integrands

$$\begin{aligned}
\frac{1}{(1-y_1)(1-y_2)} &= \frac{y_2}{(1 - y_1\,y_2)(1 - y_2)} + \frac{y_1}{(1 - y_1\,y_2)(1 - y_1)} \\
&+ \frac{1}{1 - y_1\,y_2}\,,
\end{aligned} \tag{11}$$

that is

$$1 - y_1\,y_2 = y_2(1 - y_1) + y_1(1 - y_2) + (1 - y_1)(1 - y_2)\,. \tag{12}$$

We shall now *reformulate the stuffle relation using generating series.* It is convenient to introduce a symbol $\zeta(1)$ to be interpreted as 0. Hence we define

$$Z[u] = \sum_{m\geq 1} \zeta(m)\,u^{m-1} \tag{13}$$

and from $\zeta(1) = 0$, one deduces that $Z[0] = 0$ and the summation can be restricted to $m \geq 2$. Similarly, let us remark that $\zeta(m, n)$ is defined for $m \geq 1$ and $n \geq 2$. We extend this definition to the case $n = 1$ by the conventions

$$\zeta(1, 1) = 0\,, \tag{14}$$

$$\zeta(m, 1) = -\zeta(m+1) - \zeta(1, m) \qquad (\text{for } m \geq 2)\,. \tag{15}$$

With this convention, the *stuffle formula* (6) *is valid for* $m \geq 1$*,* $n \geq 1$ *and* $m + n \geq 3$*.* But for $m = n = 1$, one obtains

$$\zeta(1)\,\zeta(1) = 2\,\zeta(1, 1) \tag{16}$$

without the term $\zeta(2)$. This being understood, we define the generating series

$$Z[u, v] = \sum_{m \geq 1,\, n \geq 1} \zeta(m, n)\, u^{m-1}\, v^{n-1}\,. \tag{17}$$

The stuffle formula can be reformulated as

$$Z[u]\, Z[v] = Z[u, v] + Z[v, u] + L[u, v] \tag{18}$$

with

$$L[u, v] := \sum_{k \geq 3} \sum_{m+n=k} \zeta(m+n)\, u^{m-1}\, v^{n-1}\,. \tag{19}$$

Notice that, with our conventions, one has $Z[0] = Z[0, 0] = 0$. To be valid, identity (18) requires $L[0, 0] = 0$, hence the special form of the summation for $L[u, v]$, restricted to $m \geq 1$, $n \geq 1$, $m + n \geq 3$.

The relation

$$\sum_{m+n=k} u^{m-1}\, v^{n-1} = \frac{u^{k-1} - v^{k-1}}{u - v} \qquad (\text{for } k \geq 2) \tag{20}$$

enables one to conclude

$$L[u, v] = \frac{Z[u] - Z[v]}{u - v} - \zeta(2)\,. \tag{21}$$

For later purposes, we need to split the series $Z[u]$ and $Z[u, v]$ into even and odd parts, as follows:

$$Z[u] = Z_+[u] + Z_-[u] \quad \text{where} \quad Z_\pm[-u] = \pm\, Z_\pm[u]\,,$$

$$Z[u,v] = Z_+[u,v] + Z_-[u,v] \quad \text{where} \quad Z_\pm[-u,-v] = \pm\, Z_\pm[u,v]\,.$$

We are interested in $Z_-[u,v]$ *which is the generating series for the double zetas whose weight* $w = m+n$ *is odd.* From (18) and (21), one obtains the final result:

$$\begin{cases} Z_+[u]\, Z_-[v] + Z_+[v]\, Z_-[u] &= Z_-[u,v] + Z_-[v,u] + L_-[u,v] \\ L_-[u,v] &= \dfrac{Z_+[u] - Z_+[v]}{u-v}\,, \end{cases} \tag{22}$$

where the annoying constant $-\zeta(2)$ in (21) has disappeared.

2 Some integration formulas: the simple zetas

Let us define the functions

$$S_k(u) = \sum_{m \geq 2} k^{-m}\, u^{m-1} \tag{23}$$

for $k \geq 1$. One derives immediately the following expressions

$$S_k(u) = \frac{u}{k(k-u)}\,, \tag{24}$$

$$S_k(u) = \frac{1}{k-u} - \frac{1}{k}\,, \tag{25}$$

$$S_k(u) = \int_0^1 (x^{-u} - 1)\, x^{k-1}\, dx\,. \tag{26}$$

Since $\zeta(m)$ is equal to $\sum\limits_{k \geq 1} k^{-m}$ for $m \geq 2$, and since by convention $\zeta(1) = 0$, we can rewrite $Z[u] = \sum\limits_{m \geq 2} \zeta(m)\, u^{m-1}$ as $\sum\limits_{k \geq 1} S_k(u)$; the series is absolutely convergent (for any complex number u distinct from any integer $k \geq 1$) since (24) gives the estimate $S_k(u) = O\big(\frac{1}{k^2}\big)$ for fixed u. Hence $Z[u]$ *is a meromorphic function of* u*, with single poles of residue* -1 *for* u *equal to* $1, 2, 3, \ldots$ From (25) and (26) we derive two important representations of $Z[u]$, namely

$$Z[u] = \sum_{k \geq 1} \left(\frac{1}{k-u} - \frac{1}{k} \right)\,, \tag{27}$$

$$Z[u] = \int_0^1 \frac{x^{-u} - 1}{1 - x}\, dx\,. \tag{28}$$

From this integral formula, one derives immediately

$$Z[u+1] = Z[u] - \frac{1}{w}\,. \tag{29}$$

Introducing the *classical psi function*

$$\psi(s) = \frac{d}{ds} \log \Gamma(s)\,, \tag{30}$$

one can translate the relation (27) as[2]

$$Z[u] = \psi(1) - \psi(1-u)\,. \tag{31}$$

Thus the formulas (28) and (29) correspond to well-known properties of the psi function.

The integral (28) is convergent in the neighborhood of $x = 0$ when the real part $\mathrm{Re}(u)$ of u satisfies $\mathrm{Re}(u) < 1$. By well-known properties of Mellin transforms, $Z[u]$ is holomorphic in the half-plane $\mathrm{Re}\, u < 1$ and extends as a meromorphic function to the complex plane $\mathbb{C}$. The correction -1 to x^{-u} ensures that the integral is convergent in the neighborhood of $x = 1$. We shall meet similar, but more complicated, phenomena for the double integrals representing the double zetas, which are regularized Mellin transforms. In a later study of multiple zeta values, we shall have to develop systematic regularization procedures which are inspired by the well-known methods in quantum field theories.

3 Some integration formulas: the double zetas

We shall give another proof of the stuffle formula in the form (18). For this purpose, we need suitable double Mellin transforms, namely

$$L[u,v] = \int_0^1 \int_0^1 \frac{x^{-u}\, y^{-v} - 1}{1 - xy}\, dx\, dy \tag{32}$$

$$Z[u,v] = \int_0^1 \int_0^1 y\, \frac{x^{-u}\, y^{-v} - x^{-u} - y^{-u} + 1}{(1-y)(1-xy)}\, dx\, dy - L[u,0]\,. \tag{33}$$

[2]Let us recall that $-\psi(1)$ is the *Euler constant* γ_E.

(A) *Proof of formula* (32):

Recall that the constant term of $L[u,v]$, as defined by formula (19), is 0. We modify this by putting $\overline{L}[u,v] = L[u,v] + \zeta(2)$, that is

$$\overline{L}[u,v] = \sum_{\substack{m\geq 1\\ n\geq 1}} \zeta(m+n)\, u^{m-1}\, v^{n-1}\,. \tag{34}$$

Since $\zeta(2)$ is equal to $\int_0^1\int_0^1 \frac{dx\,dy}{1-xy}$ as we saw in Section 1, formula (9), we have to prove the following relation

$$\overline{L}[u,v] = \int_0^1\int_0^1 \frac{x^{-u}\,y^{-v}}{1-xy}\,dx\,dy\,. \tag{35}$$

Using the definition of $\zeta(m+n)$ as $\sum\limits_{k\geq 1} k^{-m}\cdot k^{-n}$, inserting this in (34), and rearranging the triple series, we obtain

$$\overline{L}[u,v] = \sum_{k\geq 1} \frac{1}{k-u}\cdot\frac{1}{k-v}\,. \tag{36}$$

On the other hand, in the integral (35) develop $\frac{1}{1-xy}$ as a geometric series $\sum\limits_{k\geq 1} x^{k-1}\,y^{k-1}$ and integrate term by term. We obtain the same series as in (36). Q.E.D.

An immediate corollary of (32) is the following:

$$L[u,v] - L[u,0] - L[0,v] = \int_0^1\int_0^1 \frac{(x^{-u}-1)(y^{-v}-1)}{1-xy}\,dx\,dy\,. \tag{37}$$

Let us give now two new proofs of formula (21), that is

$$\overline{L}[u,v] = \frac{Z[u]-Z[v]}{u-v}\,. \tag{38}$$

The first one uses series, that is (36) for $\overline{L}[u,v]$ and (27) for $Z[u]$. Then our relation reduces to the obvious relation

$$\frac{1}{k-u}\cdot\frac{1}{k-v} = \frac{1}{u-v}\cdot\left[\left(\frac{1}{k-u}-\frac{1}{k}\right)-\left(\frac{1}{k-v}-\frac{1}{k}\right)\right]. \tag{39}$$

For the second proof, use the integral representation (35) for $\overline{L}[u,v]$ and the general integration formula

$$\int_0^1\int_0^1 f(x,y)\,dx\,dy = \int_0^1 dz \int_z^1 f\Big(x,\frac{z}{x}\Big)\,\frac{dx}{x}\,, \tag{40}$$

to get

$$\begin{aligned}
\overline{L}[u,v] &= \int_0^1 \frac{z^{-v}\,dz}{1-z}\int_z^1 x^{v-u-1}\,dx \\
&= \int_0^1 \frac{z^{-v}\,dz}{1-z}\cdot\frac{1-z^{v-u}}{v-u} \\
&= \int_0^1 \frac{z^{-v}-z^{-u}}{(1-z)(v-u)}\,dz \\
&= \frac{1}{v-u}\int_0^1 \frac{z^{-v}-1}{1-z}\,dz - \frac{1}{v-u}\int_0^1 \frac{z^{-u}-1}{1-z}\,dz
\end{aligned}$$

and we conclude by (28).

(B) *Proof of formula* (33):

Using the definition (17) of $Z[u,v]$ and the convention $\zeta(1,1)=0$, we split the summation into two subseries, that is $Z[u,v]=A+B$ with

$$A = \sum_{m\geq 1,\, n\geq 2} \zeta(m,n)\,u^{m-1}\,v^{n-1}\,, \tag{41}$$

$$B = \sum_{m\geq 2} \zeta(m,1)\,u^{m-1}\,. \tag{42}$$

To compute A, replace $\zeta(m,n)$ by its definition $\sum_{0<k<\ell} k^{-m}\,\ell^{-n}$, interchange the summations $\sum_{m,n}$ with $\sum_{k,\ell}$ and perform the easy summations over m and n. We get therefore

$$A = \sum_{0<k<\ell} \frac{1}{k-u}\left[\frac{1}{\ell-v}-\frac{1}{\ell}\right]. \tag{43}$$

We introduce now the integral representations

$$\frac{1}{k-u} = \int_0^1 x^{-u}\,x^{k-1}\,dx\,, \tag{44}$$

$$\frac{1}{\ell - v} - \frac{1}{\ell} = \int_0^1 (y^{-v} - 1)\, y^{\ell-1}\, dy \tag{45}$$

and interchange integration and summation. Using the series expansion

$$\sum_{0<k<\ell} x^{k-1}\, y^{\ell-1} = \frac{y}{(1-y)(1-xy)}\,, \tag{46}$$

we conclude

$$A = \int_0^1 \int_0^1 y\, \frac{x^{-u}(y^{-v}-1)}{(1-y)(1-xy)}\, dx\, dy\,. \tag{47}$$

To evaluate B, let us go back to the definition

$$\zeta(m,1) = -\zeta(m+1) - \zeta(1,m)\,. \tag{48}$$

By definition, the series $-\sum_{m\geq 2} \zeta(m+1)\, u^{m-1}$ is equal to $-L[u,0]$ (see formula (19)). It remains to sum the series

$$C = \sum_{m\geq 2} \zeta(1,m)\, u^{m-1}\,. \tag{49}$$

Returning to the definition $\zeta(1,m) = \sum_{0<k<\ell} k^{-1}\, \ell^{-m}$, a simple manipulation of series yields $C = \sum_{0<k<\ell} k^{-1}\, S_\ell(u)$. By using the integral representations

$$k^{-1} = \int_0^1 x^{k-1}\, dx\,, \quad S_\ell(u) = \int_0^1 (y^{-u} - 1)\, y^{\ell-1}\, dy\,, \tag{50}$$

and interchanging integration and summation, we end up with

$$C = \int_0^1 \int_0^1 y\, \frac{y^{-u}-1}{(1-y)(1-xy)}\, dx\, dy\,. \tag{51}$$

We have therefore

$$Z[u,v] = A + B = A - C - L[u,0]$$

and we conclude by using formulas (47) and (51). Q.E.D.

(C) *Proof of the stuffle formula:*

Putting

$$\overline{Z}[u,v] := Z[u,v] + L[u,0]\,, \tag{52}$$

the stuffle formula amounts to

$$\overline{Z}[u,v] + \overline{Z}[v,u] = Z[u]\,Z[v] - L[u,v] + L[u,0] + L[0,v]\,. \tag{53}$$

Using (28) and (37), we evaluate the right-hand side of this relation as the integral

$$B(u,v) = \int_0^1 \int_0^1 (x^{-u}-1)(y^{-v}-1)\left[\frac{1}{(1-x)(1-y)} - \frac{1}{1-xy}\right] dx\,dy\,. \tag{54}$$

On the other hand, while symmetrizing $Z[u,v] + Z[v,u]$ we can replace in the integral (33) the term $-y^{-u}$ by $-y^{-v}$, hence $\overline{Z}[u,v] + \overline{Z}[v,u]$ is the sum of the two integrals $A[u,v]$ and $A[v,u]$, where

$$A[u,v] := \int_0^1 \int_0^1 (x^{-u}-1)(y^{-v}-1)\,\frac{y}{(1-y)(1-xy)}\,dx\,dy\,. \tag{55}$$

We calculate $A[v,u]$ by exchanging the integration variables x, y, hence

$$A[v,u] = \int_0^1 \int_0^1 (x^{-u}-1)(y^{-v}-1)\,\frac{x}{(1-x)(1-xy)}\,dx\,dy\,. \tag{56}$$

From all these relations, it follows that the stuffle formula (53) is equivalent to $A[u,v] + A[v,u] = B[u,v]$. This follows immediately from the relation

$$\frac{1}{(1-x)(1-y)} = \frac{1}{1-xy} + \frac{y}{(1-y)(1-xy)} + \frac{x}{(1-x)(1-xy)}\,. \tag{57}$$

This is an identity among rational functions that we met already in Section 1, formula (11). Q.E.D.

Remarks. a) In this section, u and v are complex variables. If we assume $|u| < 1$, $|v| < 1$, all series are absolutely convergent. Exchanging summation and integration rests on the general principle

$$\int_T \sum_i f_i(t)\,dt = \sum_i \int_T f_i(t)\,dt \tag{58}$$

which is guaranteed by the assumption

$$\sum_i \int_T |f_i(t)|\, dt < +\infty\,.$$

Then we can proceed through analytic continuation for general values of u and v. Notice that $Z[u,v]$ is a meromorphic function with poles located at $u = k$ or $v = k$ for $k = 1, 2, \ldots$.

b) Using geometric series, the right-hand side $R(x,y)$ of formula (57) can be written as

$$R(x,y) = \sum_{0\leq k=\ell} x^k\, y^\ell + \sum_{0\leq k<\ell} x^k\, y^\ell + \sum_{0\leq \ell<k} x^k\, y^\ell\,.$$

Using once again the *splitting principle for double series*, we get

$$R(x,y) = \sum_{k\geq 0,\, \ell\geq 0} x^k\, y^\ell = \frac{1}{1-x}\cdot\frac{1}{1-y}\,.$$

This is formula (57)!

4 Review of the shuffle formula

We shall use the following special case of the *shuffle formula*

$$\begin{aligned}\zeta(m)\,\zeta(n) &= \sum_{i=1}^{n} \binom{m+n-i-1}{m-1} \zeta(i, m+n-i) \\ &+ \sum_{i=1}^{m} \binom{m+n-i-1}{n-1} \zeta(i, m+n-i)\,. \qquad (59)\end{aligned}$$

When $m \geq 2$ and $n \geq 2$, all zeta values occuring there are defined by convergent series and integrals[3], and our proof shall be via integral representations. We want to extend the validity of formula (59) to the exceptional cases where m or n is equal to 1. For instance, for $m = 1$, we obtain the specialization

$$0 = 2\,\zeta(1,n) + \sum_{i=2}^{n-1} \zeta(i, n+1-i) + \zeta(n,1) \qquad (60)$$

[3]We call them *convergent* zeta values!

for $n \geq 2$, according to our convention $\zeta(1) = 0$. Recall that $\zeta(n,1)$ is defined in terms of convergent zeta values by the relation

$$\zeta(n,1) = -\zeta(1,n) - \zeta(n+1)\,. \tag{61}$$

Hence (60) reduces to

$$\zeta(n+1) = \sum_{i=1}^{n-1} \zeta(i, n+1-i) \qquad (\text{for } n \geq 2)\,. \tag{62}$$

This is a special case of *Hoffman's relation* [3].

(A) *Proof of the shuffle formula:*

We introduce the abbreviation

$$Y_m(x) = \frac{x^{m-1}}{(m-1)!}\,. \tag{63}$$

To calculate the integral

$$I_m := \int_0^\infty Y_m(x)\, \frac{dx}{e^x - 1}\,, \tag{64}$$

use the series expansion

$$\frac{1}{e^x - 1} = \sum_{k \geq 1} e^{-kx}\,, \tag{65}$$

integrate term by term using the well-known relation

$$\int_0^\infty Y_m(x)\, e^{-kx}\, dx = k^{-m}\,, \tag{66}$$

hence $I_m = \sum_{k \geq 1} k^{-m} = \zeta(m)$. We conclude[4]

$$\int_0^\infty Y_m(x)\, \frac{dx}{e^x - 1} = \zeta(m)\,. \tag{67}$$

A similar calculation yields

$$\int_0^\infty \int_0^\infty Y_m(x)\, Y_n(y)\, \frac{dx\, dy}{(e^{x+y} - 1)(e^y - 1)} = \zeta(m,n)\,. \tag{68}$$

[4]This is a special case of the well-known integral representation of Riemann's zeta function!

For $m \geq 2$, $Y_m(x)$ is divisible by x, and since $\frac{x}{e^x-1}$ is continuous up to $x = 0$, the integral (67) converges up to $x = 0$ (the convergence for $x = \infty$ is guaranteed since the integrand is $O(e^{-x/2})$). Similarly, the integral (68) converges for $m \geq 1$ and $n \geq 2$.

We need a *general integration formula.* In the plane with coordinates u, v let us consider the domain D defined by $u > 0$, $v > 0$. Up to a set of measure 0, it splits as $D = D_1 \cup D_2$ where

$$D_1 = \{0 < u < v\}\,, \qquad D_2 = \{0 < v < u\}\,.$$

The changes of coordinates $u = y$, $v = x + y$ for D_1 and $u = x + y$, $v = y$ for D_2 reduce these inequalities to $x > 0$, $y > 0$, hence the relation

$$\begin{aligned} \int_0^\infty \int_0^\infty f(x,y)\,dx\,dy &= \int_0^\infty \int_0^\infty f(y, x+y)\,dx\,dy \\ &+ \int_0^\infty \int_0^\infty f(x+y, y)\,dx\,dy\,. \end{aligned} \tag{69}$$

From (67), we obtain by multiplication

$$\zeta(m)\,\zeta(n) = \int_0^\infty \int_0^\infty Y_m(x)\,Y_n(y)\,\frac{dx\,dy}{(e^x-1)(e^y-1)} \tag{70}$$

for $m \geq 2$, $n \geq 2$. Using the integration formula (69), this transforms as $\zeta(m)\,\zeta(n) = I_{m,n} + I_{n,m}$ where

$$I_{m,n} := \int_0^\infty \int_0^\infty Y_m(y)\,Y_n(x+y)\,\frac{dx\,dy}{(e^{x+y}-1)(e^y-1)}\,. \tag{71}$$

A simple calculation using the binomial formula yields the following algebraic identity

$$Y_m(y)\,Y_n(x+y) = \sum_{i=1}^{n} \binom{m+n-i-1}{m-1} Y_i(x)\,Y_{m+n-i}(y)\,. \tag{72}$$

Inserting this into the integral (71) and using (68) gives the result

$$I_{m,n} = \sum_{i=1}^{n} \binom{m+n-i-1}{m-1} \zeta(i, m+n-i)\,. \tag{73}$$

We conclude the proof of formula (59) using $\zeta(m)\,\zeta(n) = I_{m,n} + I_{n,m}$. Q.E.D.

(B) *Proof of Hoffman's relation:*

We have to show that the sum

$$S_n := \sum_{i=1}^{n-1} \zeta(i, n+1-i) = \zeta(1,n) + \zeta(2,n-1) + \ldots + \zeta(n-1,2) \tag{74}$$

is equal to $\zeta(n+1)$ for $n \geq 2$. An equivalent form of the binomial theorem is the formula

$$Y_n(x+y) = \sum_{i=1}^{n} Y_i(x)\, Y_{n+1-i}(y)\,, \tag{75}$$

hence by subtraction

$$\sum_{i=1}^{n-1} Y_i(x)\, Y_{n+1-i}(y) = Y_n(x+y) - Y_n(x)\,. \tag{76}$$

Using formula (68), we obtain

$$\zeta(i, n+1-i) = \int_0^\infty \int_0^\infty Y_i(x)\, Y_{n+1-i}(y)\, \frac{dx\, dy}{(e^{x+y}-1)(e^y-1)}\,. \tag{77}$$

Summing and using (76), we conclude

$$S_n = \int_0^\infty \int_0^\infty [Y_n(x+y) - Y_n(x)] \cdot \frac{dx\, dy}{(e^{x+y}-1)(e^y-1)}\,. \tag{78}$$

Here is a slight difficulty: we cannot split this integral as a difference of two integrals since the integral $\int_0^A \frac{dy}{e^y-1}$ diverges like $\int_0^A \frac{dy}{y}$. We put a regularization factor[5] by replacing dy by $y^\varepsilon dy$ for a small $\varepsilon > 0$.

Let us introduce therefore

$$S_{n,\varepsilon} := \int_0^\infty \int_0^\infty [Y_n(x+y) - Y_n(x)]\, \frac{y^\varepsilon\, dx\, dy}{(e^{x+y}-1)(e^y-1)}\,. \tag{79}$$

It is now legitimate to split this integral as a difference of two integrals. The first one is

$$\int_0^\infty \int_0^\infty \frac{Y_n(x+y)}{e^{x+y}-1} \cdot \frac{y^\varepsilon}{e^y-1}\, dx\, dy$$

[5] All known proofs of Hoffman's relation seem to need some kind of limiting process!

which is transformed, according to (69) into[6]

$$\int_0^\infty \int_0^\infty \frac{Y_n(x)}{e^x - 1} \cdot \frac{y^\varepsilon}{e^y - 1}\, dx\, dy - \int_0^\infty \int_0^\infty \frac{Y_n(x)}{e^x - 1} \cdot \frac{(x+y)^\varepsilon}{e^{x+y} - 1}\, dx\, dy\,.$$

Inserting this into (79) yields

$$S_{n,\varepsilon} = \int_0^\infty \int_0^\infty Y_n(x)\, F_\varepsilon(x,y)\, dx\, dy\,, \tag{80}$$

with the definition

$$F_\varepsilon(x,y) = \frac{y^\varepsilon}{(e^x - 1)(e^y - 1)} - \frac{(x+y)^\varepsilon}{(e^{x+y} - 1)(e^x - 1)} - \frac{y^\varepsilon}{(e^{x+y} - 1)(e^y - 1)}\,. \tag{81}$$

It is now legitimate to go to the limit $\varepsilon \to 0$. According to (78) and (79), one has $S_n = \lim_{\varepsilon \to 0} S_{n,\varepsilon}$, hence

$$S_n = \int_0^\infty \int_0^\infty Y_n(x)\, F(x,y)\, dx\, dy \tag{82}$$

where $F(x,y)$ is the limit of $F_\varepsilon(x,y)$ for $\varepsilon \to 0$. From (81) one observes that $F(x,y)$ is of the form $H(e^x, e^y)$ with

$$H(a,b) := \frac{1}{(a-1)(b-1)} - \frac{1}{(ab-1)(a-1)} - \frac{1}{(ab-1)(b-1)}\,. \tag{83}$$

We are back to our old friend expressed in formulas (11) and (57). It is immediate that $H(a,b)$ is equal to $\frac{1}{ab-1}$, hence by (82), we obtain

$$S_n = \int_0^\infty \int_0^\infty Y_n(x)\, \frac{dx\, dy}{e^{x+y} - 1}\,. \tag{84}$$

This last integral is easy to evaluate: develop $\frac{1}{e^{x+y}-1}$ as $\sum_{k \geq 1} e^{-kx} \cdot e^{-ky}$ according to (65), then use formula (66) to derive

[6] Since in general, one has $\iint g(x,y)\, dx\, dy = \iint g(y,x)\, dx\, dy$, we can rewrite $\int_0^\infty \int_0^\infty f(y, x+y)\, dx\, dy$ as $\int_0^\infty \int_0^\infty f(x, x+y)\, dx\, dy$ in formula (69).

$$S_n = \sum_{k\geq 1} k^{-n} \cdot k^{-1} = \zeta(n+1)\,. \tag{85}$$

Q.E.D.

(C) *Generating series:*

We remind the reader of the definitions

$$\begin{aligned} Z[u] &= \sum_{m\geq 2} \zeta(m)\, u^{m-1} \\ L[u,v] &= \sum_{\substack{m\geq 1,\, n\geq 1 \\ m+n\geq 3}} \zeta(m+n)\, u^{m-1}\, v^{n-1} \\ Z[u,v] &= \sum_{m\geq 1,\, n\geq 1} \zeta(m,n)\, u^{m-1}\, v^{n-1} \end{aligned}$$

and of the convention $\zeta(1,1) = 0$. One has

$$Z[u, u+v] = \sum_{m\geq 1,\, n\geq 1} \zeta(m,n)\, u^{m-1} (u+v)^{n-1}\,, \tag{86}$$

hence expanding via the binomial theorem, one obtains

$$Z[u, u+v] = \sum_{m\geq 1,\, n\geq 1} u^{m-1}\, v^{n-1} \sum_{i=1}^{m} \binom{m+n-i-1}{n-1} \zeta(i, m+n-i)\,. \tag{87}$$

Treating $Z[v, u+v]$ in a similar way, we conclude that the shuffle relation (59) is therefore equivalent to

$$Z[u]\, Z[v] = Z[u, u+v] + Z[v, u+v]\,. \tag{88}$$

Hoffman's relation (62) takes the equivalent form[7]

$$Z[u,u] = Z[u,0] + L[u,0]\,. \tag{89}$$

We leave it as an exercise to the reader to prove these two relations using the integral representations for these generating series (see formulas (32) and (33)).

[7]This relation obtains immediately by putting $v = 0$ in the relations (18) and (88). Hence it is not a new relation.

5 The main formulas

Using generating series, and keeping only the odd part, we reformulate the stuffle and the shuffle relations respectively as

$$Z_-[u,v] + Z_-[v,u] = A[u,v] \tag{90}$$

$$Z_-[u,u+v] + Z_-[v,u+v] = B[u,v] \tag{91}$$

using the definitions

$$A[u,v] := Z_+[u]\,Z_-[v] + Z_+[v]\,Z_-[u] - \frac{Z_+[u] - Z_+[v]}{u-v} \tag{92}$$

$$B[u,v] := Z_+[u]\,Z_-[v] + Z_+[v]\,Z_-[u]\,. \tag{93}$$

We introduce two other functions

$$C[u,v] := A[u,v] + A[u-v,u] - A[v-u,v] \tag{94}$$

$$D[u,v] := B[-u,v] + B[v-u,u] - B[u-v,v]\,. \tag{95}$$

Using the stuffle relation (90), we calculate

$$\begin{aligned} C[u,v] &= Z_-[u,v] + Z_-[v,u] + Z_-[u-v,u] - Z_-[v-u,v] \\ &- Z_-[v,v-u] + Z_-[u,u-v]\,. \end{aligned} \tag{96}$$

Similarly, using the shuffle relation, we obtain

$$\begin{aligned} D[u,v] &= Z_-[u,v] - Z_-[v,u] - Z_-[u-v,u] + Z_-[v-u,v] \\ &+ Z_-[v,v-u] + Z_-[-u,v-u]\,. \end{aligned} \tag{97}$$

By adding, this yields

$$C[u,v] + D[u,v] = 2\,Z_-[u,v] + Z_-[u,u-v] + Z_-[-u,v-u]\,. \tag{98}$$

Since the function $Z_-[u,v]$ is odd, the last two terms cancel, and therefore

$$2\,Z_-[u,v] = C[u,v] + D[u,v]\,. \tag{99}$$

We can refer to the definitions (92) to (95) of the functions $A[u,v]$ to $D[u,v]$ to derive an explicit form for $Z_-[u,v]$. Here is the final result:

$$\begin{aligned} &Z_-[u,v] = Z_+[u]\,Z_-[v] + Z_+[u-v]\,Z_-[u] - Z_+[u-v]\,Z_-[v] \qquad (100) \\ &+ \frac{1}{2}\left[-\frac{Z_+[u]-Z_+[v]}{u-v} + \frac{Z_+[u-v]-Z_+[u]}{v} - \frac{Z_+[v-u]-Z_+[v]}{u}\right]. \end{aligned}$$

Another proof is as follows: check that the function $Z_-[u,v]$ defined by this formula is odd (which is obvious) and verify that it satisfies the stuffle equation (90) as well as the shuffle equation (91). The reasoning leading to equation (99) shows that there exists a unique function satisfying these conditions.

Let us introduce now the *antisymmetric double zetas*

$$\eta(m,n) := \zeta(m,n) - \zeta(n,m) \tag{101}$$

and their generating series[8]

$$H[u,v] = Z[u,v] - Z[v,u]\,. \tag{102}$$

We split it into an even part $H_+[u,v]$ and an odd part $H_-[u,v]$. From formula (100), one derives

$$\begin{aligned} H_-[u,v] &= Z_-[u,v] - Z_-[v,u] \\ &= Z_+[u]\,Z_-[v] - Z_+[v]\,Z_-[u] \\ &+ 2\,Z_+[u-v]\,(Z_-[u] - Z_-[v]) \\ &+ \frac{Z_+[u-v] - Z_+[u]}{v} - \frac{Z_+[v-u] - Z_+[v]}{u}\,. \end{aligned} \tag{103}$$

It is more convenient to slightly modify this generating series by introducing the new series

$$H_-[-u,v] = -H_-[u,-v] = \sum_{\substack{m\geq 1\\ n\geq 1}} (-1)^n\,\eta(m,n)\,u^{m-1}\,v^{n-1}\,. \tag{104}$$

We have the following variant of formula (100)

$$\begin{aligned} H_-[-u,v] &= Z_+[u]\,Z_-[v] + Z_+[v]\,Z_-[u] \\ &- 2\,Z_+[u+v]\,(Z_-[u] + Z_-[v]) \\ &+ \frac{(u+v)\,Z_+[u+v] - u\,Z_+[u] - v\,Z_+[v]}{uv}\,. \end{aligned} \tag{105}$$

Noticing that the first term $Z_+[u]\,Z_-[v] + Z_+[v]\,Z_-[u]$ is simply the odd part of the product

$$Z[u]\,Z[v] = \sum_{\substack{m\geq 1\\ n\geq 1}} \zeta(m)\,\zeta(n)\,u^{m-1}\,v^{n-1}$$

[8] Read $H[u,v]$ as "eta" and $Z[u,v]$ as "zeta" using the upper case greek letters!

and that $u\,Z_+[u]$ is equal to $\sum_{k\geq 1}\zeta(2k+1)\,u^{2k+1}$, we transform the relation (105) into[9]

$$\begin{aligned}(-1)^n\,\eta(m,n) &= \zeta(m)\,\zeta(n)+\binom{m+n}{m}\zeta(m+n)\\ &- 2\sum_{i=1}^{\lfloor n/2\rfloor}\binom{m+n-2i-1}{m-1}\zeta(2i)\,\zeta(m+n-2i)\\ &- 2\sum_{i=1}^{\lfloor m/2\rfloor}\binom{m+n-2i-1}{n-1}\zeta(2i)\,\zeta(m+n-2i) \quad (106)\end{aligned}$$

in the case of a *odd weight* $m+n=2k+1$ with $k\geq 1$.

From the stuffle relation (6) and definition (101) of $\eta(m,n)$, one derives

$$\zeta(m,n)=\frac{1}{2}\left[\eta(m,n)+\zeta(m)\,\zeta(n)-\zeta(m+n)\right]. \quad (107)$$

This proves the final formula announced as (5) in the introduction

$$\begin{aligned}\zeta(m,n) &= \frac{1}{2}\left(1+(-1)^n\right)\zeta(m)\,\zeta(n)\\ &+ \frac{1}{2}\left[(-1)^n\binom{m+n}{m}-1\right]\zeta(m+n)\\ &- (-1)^n\sum_{i=1}^{(m+n-3)/2}\left[\binom{m+n-2i-1}{m-1}+\binom{m+n-2i-1}{n-1}\right]\\ &\quad \zeta(2i)\,\zeta(m+n-2i) \quad (108)\end{aligned}$$

in the case of an *odd weight* $m+n=2k+1$.

We urge the reader to check the formula (106) against the numerical data given in tables I and II.

[9]As usual we denote by $\lfloor x\rfloor$ the *integer part* of a number x, that is $x=\lfloor x\rfloor+\theta$ with $0\leq\theta<1$.

Appendix A. Examples and Tables

Weight 3:

With our convention $\zeta(1) = 0$, the stuffle formula takes the form

$$0 = \zeta(1)\,\zeta(2) = \zeta(1,2) + \zeta(2,1) + \zeta(3) \tag{109}$$

while the shuffle formula takes the form

$$0 = \zeta(1)\,\zeta(2) = 2\,\zeta(1,2) + \zeta(2,1)\,. \tag{110}$$

One derives

$$\begin{cases} \zeta(1,2) & = & \zeta(3) \\ \zeta(2,1) & = & -\,2\,\zeta(3)\,. \end{cases} \tag{111}$$

The formula $\zeta(1,2) = \zeta(3)$, that is explicitely

$$\sum_{\substack{k\geq 1\\ j\geq 1}} \frac{1}{k(k+j)^2} = \sum_{k\geq 1} \frac{1}{k^3} \tag{112}$$

is a famous result of Euler. For the antisymmetric double zetas $\eta(m,n) = \zeta(m,n) - \zeta(n,m)$, one derives

$$\begin{cases} \eta(1,2) & = & +\,3\,\zeta(3) \\ \eta(2,1) & = & -\,3\,\zeta(3)\,. \end{cases} \tag{113}$$

Weight 5:

Stuffle relations:

$$\begin{aligned} \zeta(1)\,\zeta(4) &= \zeta(1,4) + \zeta(4,1) + \zeta(5) = 0 \\ \zeta(2)\,\zeta(3) &= \zeta(2,3) + \zeta(3,2) + \zeta(5)\,. \end{aligned}$$

Shuffle relations:

$$\begin{aligned} \zeta(1)\,\zeta(4) &= 2\,\zeta(1,4) + \zeta(2,3) + \zeta(3,2) + \zeta(4,1) = 0 \\ \zeta(2)\,\zeta(3) &= 3\,\zeta(1,4) + 2\,\zeta(2,3) + \zeta(3,2) \\ &+ 3\,\zeta(1,4) + \zeta(2,3) \\ &= 6\,\zeta(1,4) + 3\,\zeta(2,3) + \zeta(3,2)\,. \end{aligned}$$

We have 4 linear relations for 4 unknown quantities $\zeta(1,4)$, $\zeta(2,3)$, $\zeta(3,2)$, $\zeta(4,1)$. Here is the solution

$$\begin{aligned}\zeta(1,4) &= 2\,\zeta(5) - \zeta(2)\,\zeta(3)\\ \zeta(2,3) &= -\frac{11}{2}\,\zeta(5) + 3\,\zeta(2)\,\zeta(3)\\ \zeta(3,2) &= \frac{9}{2}\,\zeta(5) - 2\,\zeta(2)\,\zeta(3)\\ \zeta(4,1) &= -\,3\,\zeta(5) + \zeta(2)\,\zeta(3)\,.\end{aligned}$$

In matrix form, this is written as

	$\zeta(5)$	$\zeta(2)\,\zeta(3)$
$\zeta(1,4)$	2	$-\,1$
$\zeta(2,3)$	$-\,11/2$	3
$\zeta(3,2)$	$9/2$	$-\,2$
$\zeta(4,1)$	$-\,3$	1

From this we derive

$$\begin{aligned}\eta(1,4) &= -\,\eta(4,1) = 5\,\zeta(5) - 2\,\zeta(2)\,\zeta(3)\\ \eta(2,3) &= -\,\eta(3,2) = -\,10\,\zeta(5) + 5\,\zeta(2)\,\zeta(3)\,.\end{aligned}$$

The case of weight 7 can be treated similarly. In table I, I give in matrix form the results for the weights 3, 5, 7. To make use of this table, recall the relations

$$\zeta(m,n) = \frac{1}{2}\left[\eta(m,n) + \zeta(m)\,\zeta(n) - \zeta(m+n)\right] \quad (114)$$

$$\text{for} \quad m \geq 1\,,\ n \geq 1$$

$$\eta(1,2k) = (2k+1)\,\zeta(2k+1) - 2\sum_{i=1}^{k-1} \zeta(2i)\,\zeta(2k-2i+1) \quad (115)$$

hence

$$\zeta(1,2k) = k\,\zeta(2k+1) - \sum_{i=1}^{k-1} \zeta(2i)\,\zeta(2k-2i+1)\,. \quad (116)$$

If we solve the linear stuffle and shuffle relations without imposing $\zeta(1) = 0$, we get an extra term $-\zeta(2k)\,\zeta(1)$ in $\eta(1,2k)$, hence a correction $-\frac{1}{2}\,\zeta(2k)\,\zeta(1)$ for $\zeta(1,2k)$ and $\zeta(2k,1)$. This explains the last column in our tables.

Table I

Antisymmetric double zetas in weight 3, 5, 7[10]

Weight 3

	$\zeta(3)$	$\zeta(2)\,\zeta(1)$
$\eta(1,2)$	3	-1
$\eta(2,1)$	-3	1

Weight 5

	$\zeta(5)$	$\zeta(2)\,\zeta(3)$	$\zeta(4)\,\zeta(1)$
$\eta(1,4)$	5	-2	-1
$\eta(2,3)$	-10	5	0
$\eta(3,2)$	10	-5	0
$\eta(4,1)$	-5	2	1

Weight 7

	$\zeta(7)$	$\zeta(2)\,\zeta(5)$	$\zeta(4)\,\zeta(3)$	$\zeta(6)\,\zeta(1)$
$\eta(1,6)$	7	-2	-2	-1
$\eta(2,5)$	-21	9	4	0
$\eta(3,4)$	35	-20	-1	0
$\eta(4,3)$	-35	20	1	0
$\eta(5,2)$	21	-9	-4	0
$\eta(6,1)$	-7	2	2	1

[10]Calculated directly by the author.

Table II

Antisymmetric double zetas in weight 9, 11[11]

Weight 9

	$\zeta(9)$	$\zeta(2)\,\zeta(7)$	$\zeta(4)\,\zeta(5)$	$\zeta(6)\,\zeta(3)$	$\zeta(8)\,\zeta(1)$
$\eta(1,8)$	9	-2	-2	-2	-1
$\eta(2,7)$	-36	13	8	4	0
$\eta(3,6)$	84	-42	-12	-1	0
$\eta(4,5)$	-126	70	9	0	0
$\eta(5,4)$	126	-70	-9	0	0
$\eta(6,3)$	-84	42	12	1	0
$\eta(7,2)$	36	-13	-8	-4	0
$\eta(8,1)$	-9	2	2	2	1

Weight 11

	$\zeta(11)$	$\zeta(2)\,\zeta(9)$	$\zeta(4)\,\zeta(7)$	$\zeta(6)\,\zeta(5)$	$\zeta(8)\,\zeta(3)$	$\zeta(10)\,\zeta(1)$
$\eta(1,10)$	11	-2	-2	-2	-2	-1
$\eta(2,9)$	-55	17	12	8	4	0
$\eta(3,8)$	165	-72	-30	-12	-1	0
$\eta(4,7)$	-330	168	41	8	0	0
$\eta(5,6)$	462	-252	-42	-1	0	0
$\eta(6,5)$	-462	252	42	1	0	0
$\eta(7,4)$	330	-168	-41	-8	0	0
$\eta(8,3)$	-165	72	30	12	1	0
$\eta(9,2)$	55	-17	-12	-8	-4	0
$\eta(10,1)$	-11	2	2	2	2	1

[11] Calculated by the author using tables of Minh *et al.*

Appendix B. A compendium of useful formulas

B.1. Simple zetas

$$
\begin{aligned}
\zeta(m) &= \sum_{k\geq 1} k^{-m} \\
&= \int_0^\infty \frac{x^{m-1}}{(m-1)!}\,\frac{dx}{e^x-1} \\
&= \int_{C_m} \frac{dx_1\dots dx_m}{1-x_1\dots x_m}\,.
\end{aligned}
$$

Here $m \geq 2$, and C_m is the unit cube in the space $\mathbb{R}^m$, defined by the inequalities $0 \leq x_1 \leq 1, \dots, 0 \leq x_m \leq 1$. To be supplemented by $\zeta(1) = 0$.

B.2. Generating series for simple zetas

$$
\begin{aligned}
Z[u] &= \sum_{m\geq 1} \zeta(m)\,u^{m-1} \qquad\qquad (\text{notice} \quad \zeta(1)=0) \\
&= \sum_{k\geq 1} \left[\frac{1}{k-u} - \frac{1}{k}\right] \\
&= \int_0^1 \frac{x^{-u}-1}{1-x}\,dx \\
&= \int_0^\infty \frac{e^{ux}-1}{e^x-1}\,dx \\
L[u] &= \sum_{m\geq 2} \zeta(m+1)\,u^{m-1} \\
&= \sum_{k\geq 1} \frac{u}{k^2(k-u)} \\
&= \int_0^1\int_0^1 \frac{x^{-u}-1}{1-xy}\,dx\,dy \\
&= \int_0^\infty\int_0^\infty \frac{e^{ux}-1}{e^{x+y}-1}\,dx\,dy \\
Z[u] &= u(L[u]+\zeta(2))\,.
\end{aligned}
$$

B.3. Double zetas

$$\begin{aligned}\zeta(m,n) &= \sum_{0<k<\ell} k^{-m}\,\ell^{-n}\\ &= \int_0^\infty\int_0^\infty \frac{x^{m-1}}{(m-1)!}\,\frac{y^{n-1}}{(n-1)!}\,\frac{dx\,dy}{(e^{x+y}-1)(e^y-1)}\\ &= \int_{C_{m+n}} \frac{x_{m+1}\dots x_{m+n}\,dx_1\dots dx_{m+n}}{(1-x_1\dots x_{m+n})(1-x_{m+1}\dots x_{m+n})}\,.\end{aligned}$$

Here $m \geq 1$ and $n \geq 2$. To be supplemented by

$$\zeta(1,1)=0\,,\quad \zeta(m,1)=-\zeta(m+1)-\zeta(1,m)\qquad \text{for}\quad m\geq 2\,.$$

B.4. Generating series for double zetas

$$\begin{aligned}Z[u,v] &= \sum_{m\geq 1,\,n\geq 1}\zeta(m,n)\,u^{m-1}\,v^{n-1}\\ &= \sum_{0<k<\ell}\left(\frac{1}{k-u}\cdot\frac{1}{\ell-v}-\frac{1}{k-u}\cdot\frac{1}{\ell}-\frac{1}{k}\cdot\frac{1}{\ell-u}+\frac{1}{k\ell}\right)-L[u]\\ &= \int_0^1\int_0^1 y\,\frac{x^{-u}\,y^{-v}-x^{-u}-y^{-u}+1}{(1-xy)(1-y)}\,dx\,dy-L[u]\\ &= \int_0^\infty\int_0^\infty \frac{(e^{ux+vy}-e^{ux}-e^{uy}+1)}{(e^{x+y}-1)(e^y-1)}\,dx\,dy-L[u]\,.\end{aligned}$$

B.5. Rational functions

$$\begin{aligned}\sum_{0<k=\ell} x^{k-1}\,y^{\ell-1} &= \frac{1}{1-xy}\\ \sum_{0<k<\ell} x^{k-1}\,y^{\ell-1} &= \frac{y}{(1-y)(1-xy)}\\ \sum_{0<\ell<k} x^{k-1}\,y^{\ell-1} &= \frac{x}{(1-x)(1-xy)}\end{aligned}$$

$$\frac{1}{1-x}\cdot\frac{1}{1-y}=\frac{1}{1-xy}+\frac{y}{(1-y)(1-xy)}+\frac{x}{(1-x)(1-xy)}\,.$$

B.6. Stuffle relation

$$\zeta(m)\,\zeta(n)=\zeta(m,n)+\zeta(n,m)+\zeta(m+n)$$

for $m\geq 1,\ n\geq 1,$ *except* $m=n=1$

$$\begin{cases} Z[u]\,Z[v] &=& Z[u,v]+Z[v,u]+L[u,v]\\ L[u,v] &=& \dfrac{Z[u]-Z[v]}{u-v}-\zeta(2)\,. \end{cases}$$

B.7. Other expressions for $L[u,v]$

$$\begin{aligned} L[u,v] &= \sum_{\substack{m\geq 1,\,n\geq 1\\ m+n\geq 3}}\zeta(m+n)\,u^{m-1}\,v^{n-1}\\ &= \sum_{k\geq 1}\left(\frac{1}{k-u}\cdot\frac{1}{k-v}-\frac{1}{k^2}\right)\\ &= \int_0^1\int_0^1\frac{x^{-u}\,y^{-v}-1}{1-xy}\,dx\,dy\\ &= \int_0^\infty\int_0^\infty\frac{e^{ux+vy}-1}{e^{x+y}-1}\,dx\,dy\\ L[u] &= L[u,0]=L[0,u]\\ L[u,v]-L[u]-L[v] &= \int_0^1\int_0^1\frac{(x^{-u}-1)(y^{-v}-1)}{1-xy}\,dx\,dy\\ &= \int_0^\infty\int_0^\infty\frac{(e^{ux}-1)(e^{vy}-1)}{e^{x+y}-1}\,dx\,dy\,. \end{aligned}$$

B.8. Shuffle formula and Hoffman's relation

$$\begin{aligned}
\zeta(m)\,\zeta(n) &= \sum_{i=1}^{n} \binom{m+n-i-1}{m-1} \zeta(i, m+n-i) \\
&+ \sum_{i=1}^{m} \binom{m+n-i-1}{n-1} \zeta(i, m+n-i) \\
\zeta(n+1) &= \sum_{i=1}^{n-1} \zeta(i, n+1-i) \\
Z[u]\,Z[v] &= Z[u, u+v] + Z[v, u+v] \\
L[u] &= Z[u,u] - Z[u,0]\,.
\end{aligned}$$

B.9. Structure of double zetas

$$\begin{aligned}
&\zeta(m,n) + \zeta(n,m) = \zeta(m)\,\zeta(n) - \zeta(m+n) \\
&\zeta(m,n) - \zeta(n,m) = \eta(m,n) \\
&\zeta(m,n) = \frac{1}{2}\left(\eta(m,n) + \zeta(m)\,\zeta(n) - \zeta(m+n)\right)
\end{aligned}$$

$$\begin{aligned}
&\zeta(1,2k) = k\,\zeta(2k+1) - \sum_{i=2}^{k-1} \zeta(2i)\,\zeta(2k-2i+1) \\
&\zeta(2k,1) = -(k+1)\,\zeta(2k+1) + \sum_{i=1}^{k-1} \zeta(2i)\,\zeta(2k-2i+1) + \zeta(2k)\,\zeta(1) \\
&\eta(1,2k) = -\eta(2k,1) = (2k+1)\,\zeta(2k+1) \\
&\qquad\qquad -2\sum_{i=1}^{k-1} \zeta(2i)\,\zeta(2k-2i+1) - \zeta(2k)\,\zeta(1)\,.
\end{aligned}$$

Notice that $\zeta(1) = 0$ according to our conventions! In all these formulas $m \geq 1$, $n \geq 1$ and $k \geq 1$. The case $m = n = 1$ is to be omitted.

B.10. The main formulas

$$
\begin{aligned}
(-1)^n \, \eta(m,n) &= \zeta(m)\,\zeta(n) + \binom{m+n}{m} \zeta(m+n) \\
&- 2 \sum_{i=1}^{\lfloor n/2 \rfloor} \binom{m+n-2i-1}{m-1} \zeta(2i)\,\zeta(m+n-2i) \\
&- 2 \sum_{i=1}^{\lfloor m/2 \rfloor} \binom{m+n-2i-1}{n-1} \zeta(2i)\,\zeta(m+n-2i)
\end{aligned}
$$

$$
\begin{aligned}
\zeta(m,n) &= \frac{1}{2}\,(1+(-1)^n)\,\zeta(m)\,\zeta(n) \\
&+ \frac{1}{2} \left[(-1)^n \binom{m+n}{m} - 1 \right] \zeta(m+n) \\
&- (-1)^n \sum_{i=1}^{(m+n-3)/2} \left[\binom{m+n-2i-1}{m-1} + \binom{m+n-2i-1}{n-1} \right] \\
&\quad \zeta(2i)\,\zeta(m+n-2i)
\end{aligned}
$$

In these formulas $m \geq 1$, $n \geq 1$ and $m+n$ is odd, $m+n \geq 3$.

B.11. Generating series

$$
\begin{aligned}
& Z_-[u,v] = Z_+[u]\,Z_-[v] + Z_+[u-v]\,Z_-[u] - Z_+[u-v]\,Z_-[v] \\
+ \; & \frac{1}{2} \left[-\frac{Z_+[u]-Z_+[v]}{u-v} + \frac{Z_+[u-v]-Z_+[u]}{v} - \frac{Z_+[v-u]-Z_+[v]}{u} \right].
\end{aligned}
$$

$$
H[u,v] = Z[u,v] - Z[v,u]\,.
$$

$$
\begin{aligned}
H_-[u,v] &= Z_-[u,v] - Z_-[v,u] \\
&= Z_+[u]\,Z_-[v] - Z_+[v]\,Z_-[u] \\
&+ 2\,Z_+[u-v]\,(Z_-[u] - Z_-[v]) \\
&+ \frac{Z_+[u-v]-Z_+[u]}{v} - \frac{Z_+[v-u]-Z_+[v]}{u}\,.
\end{aligned}
$$

$$
\begin{aligned}
H_-[-u,v] &= Z_+[u]\,Z_-[v] + Z_+[v]\,Z_-[u] \\
&- 2\,Z_+[u+v]\,(Z_-[u] + Z_-[v]) \\
&+ \frac{(u+v)\,Z_+[u+v] - u\,Z_+[u] + v\,Z_+[v]}{uv}\,.
\end{aligned}
$$

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$$\eta(m,n) = \zeta(m,n) - \zeta(n,m)\,.$$

From our tables and by similarity with D. Zagier's tables, it was easy to guess the patterns and to discover the formulas with binomial coefficients.

Added in proof (April 2011). I just received the final version of Zagier's paper [5]. Our main formula (5) is stated there, and its proof is very similar to our proof. The fact that the families (B_2) and (B_3) generate the same vector space over $\mathbb{Q}$ is also proved, and the proof rests on the arithmetical method of Brown and Zagier mentioned in the introduction. What is not in Zagier's paper are the antisymmetric double zetas, the motivic version and the integral formulas for the generating series.

References

[1] F.C.S. Brown, Mixed Tate motives over $\mathbb{Z}$ (to appear).

[2] A.B. Goncharov, Galois symmetries of fundamental groupoids and noncommutative geometry, *Duke Math. J.*, **128** (2005), pp. 209-284.

[3] M.E. Hoffman, The algebra of multiple harmonic sums, *Journ. of Algebra*, **194** (1997), pp. 477-495.

[4] I. Soudères, Motivic double shuffle, *Int. J. Number Theory*, **6** (2010), pp. 339-370.

[5] D.B. Zagier, Evaluation of the multiple zeta values $\zeta(2,\ldots,2,3,2,\ldots,2)$ (to appear).