EVALUATION OF THE MULTIPLE ZETA VALUES $\zeta(2,\ldots,2,3,2,\ldots,2)$

D. Zagier

Abstract. A formula is given for the special multiple zeta values occurring in the title as rational linear combinations of products $\zeta(m)\pi^{2n}$ with m odd. The existence of such a formula had been proved using motivic arguments by Francis Brown, but the explicit formula (more precisely, certain 2-adic properties of its coefficients) were needed for his proof in [1] of the conjecture that all periods of mixed Tate motives over $\mathbb{Z}$ are $\mathbb{Q}[(2\pi i)^{\pm 1}]$-linear combinations of multiple zeta values. The formula is proved indirectly, by computing the generating functions of both sides in closed form (one as the product of a sine function and a ${}_3F_2$-hypergeometric function, and one as a sum of 14 products of sine functions and digamma functions) and then showing that both are entire functions of exponential growth and that they agree at sufficiently many points to force their equality. We also show that the space spanned by the multiple zeta values in question coincides with the space of double zeta values of odd weight and find a relation between this space and the space of cusp forms on the full modular group.

1. Introduction and statement of results

Multiple zeta values are real numbers, originally defined by Euler, that have been much studied in recent years because of their many surprising properties and the many places they appear in mathematics and mathematical physics, ranging from periods of mixed Tate motives to values of Feynman integrals in perturbative quantum field theory. There are many conjectures concerning the values of these numbers. Two of the most interesting were proved very recently by Francis Brown [1] (see also [2]), but for the proofs he needed to have explicit formulas expressing the specific multiple zeta values indicated in the title in terms of values of the Riemann zeta function. It is the purpose of this note to give these formulas and their proof.

We first give the definition and formulations of some of the main conjectures concerning multiple zeta values (henceforth usually abbreviated MZV's), and then indicate the statements of the results that we will prove. For positive integers $k_1,\ldots,k_n$ with $k_n \ge 2$ we define the MZV $\zeta(k_1,\ldots,k_n)$ as the iterated multiple sum

$$\zeta(k_1,\ldots,k_n) \;=\; \sum_{0<m_1<\cdots<m_n} \frac{1}{m_1^{k_1}\cdots m_n^{k_n}}\,. \tag{1}$$

(Many papers use the opposite convention, with the m_i's ordered by $m_1 > \cdots > m_n > 0$, but (1) will be more convenient for us.) These series usually converge quite slowly, but they can be rewritten in several different ways that allow their rapid calculation to high precision. I performed such computations a number of years ago (they were later extended much further) and found that the MZV's of a given weight $k = k_1+\cdots+k_n$ satisfy many numerical linear relations over $\mathbb{Q}$, e.g. of the $2^{10} = 1024$ MZV's of weight 12, only 12 were linearly independent. The numerical data suggested the conjecture that the dimension of the $\mathbb{Q}$-vector space $\mathfrak{Z}_k$ spanned by all MZV's of weight k is given by

$$\dim \mathfrak{Z}_k \;\stackrel{?}{=}\; d_k\,, \tag{2}$$

where d_k is defined as the coefficient of x^k in the power series expansion of $\frac{1}{1-x^2-x^3}$ (or equivalently by the recursion $d_k = d_{k-2}+d_{k-3}$ with the initial conditions $d_0 = 1$ and $d_k = 0$ for $k<0$). Proving this conjecture is hopeless at the present time; indeed, there is not a single value of k for which it is known that $\dim \mathfrak{Z}_k > 1$. (In particular, the irrationality of $\zeta(k_1, \ldots, k_n)/\pi^{k_1+\cdots+k_n}$ is not known for a single value of the vector $(k_1, \ldots, k_n)$. Nor is it known—although it is surely true—that the different subspaces $\mathfrak{Z}_k$ of $\mathbb{R}$ are disjoint, so that the sum $\mathfrak{Z} = \sum_k \mathfrak{Z}_k$ is direct.) However, the true MZV's in $\mathbb{R}$ are the images under a $\mathbb{Q}$-linear map of certain "motivic" MZV's which are defined purely algebraically, and it was proved (independently) by Terasoma [10] and Goncharov [6, 3] that the upper bound implied by the conjectural dimension formula held for these, implying in particular the inequality

$$\dim \mathfrak{Z}_k \;\le\; d_k\,. \tag{3}$$

Now it is clear that d_k can also be defined as the number of MZV's of weight k all of whose arguments are 2's and 3's, and M. Hoffman [7] made the conjecture that these special MZV's span $\mathfrak{Z}_k$. This statement refines (3), and also implies, if one believes the conjecture (2), that the MZV's in question form a $\mathbb{Q}$-basis of $\mathfrak{Z}_k$ for all k.

In a different direction, Terasoma and Goncharov established (3) by showing that all MZV's are periods of mixed Tate motives that are unramified over $\mathbb{Z}$, and another well-known conjecture in the area states the converse, i.e., that all periods of mixed Tate motives over $\mathbb{Z}$ can be expressed as linear combinations (over $\mathbb{Q}[(2\pi i)^{\pm 1}]$) of MZV's. Equivalently, this says that the dimension of the space of motivic MZV's of weight k is equal to d_k.

The result obtained by Francis Brown was a proof of both of these two conjectures, assuming certain quite specific properties of certain coefficients occurring in the relations over $\mathbb{Q}$ of some special MZV's. Specifically, he showed that the special MZV's

$$H(a,b) \;:=\; \zeta(\underbrace{2,\ldots,2}_{a},3,\underbrace{2,\ldots,2}_{b}) \qquad (a,\,b\,\ge\,0), \tag{4}$$

which are part of Hoffman's conjectural basis, are $\mathbb{Q}$-linear combinations of products $\pi^{2m}\,\zeta(2n+1)$ with $m+n = a+b+1$. His proof, which used motivic ideas, did not yield an explicit formula for these linear combinations, but numerical evidence suggested several properties satisfied by their coefficients (and in particular of the coefficient of $\zeta(2a+2b+3)$) which he could show were sufficient to imply the truth of both Hoffman's conjecture and the statement about motivic periods. In this paper we will state and prove an explicit formula expressing the numbers (4) in terms of Riemann zeta values and confirming the numerical properties that were required for Brown's proof.

Before giving the formula for the numbers $H(a,b)$, we first recall the much easier formula

$$H(n) \;:=\; \zeta(\underbrace{2,\ldots,2}_{n}) \;=\; \frac{\pi^{2n}}{(2n+1)!} \qquad (n\,\ge\,0), \tag{5}$$

for the simplest of the Hoffman basis elements. The proof of (5) is well known, but we give it anyway, both for completeness and because similar ideas will be used below: one simply forms the generating function $\sum_{n=0}^{\infty}(-1)^n H(n)\, x^{2n+1}$ and then, directly from the definition of $H(n)$, finds

$$\sum_{n=0}^{\infty}(-1)^n\, H(n)\, x^{2n+1} \;=\; x\prod_{m=1}^{\infty}\Bigl(1\,-\,\frac{x^2}{m^2}\Bigr) \;=\; \frac{\sin \pi x}{\pi} \;=\; \sum_{n=0}^{\infty}(-1)^n\,\frac{\pi^{2n}\,x^{2n+1}}{(2n+1)!}\;, \tag{6}$$

the last two equalities both being due to Euler. Using (5), one can reformulate the above statement about the expression of the numbers $H(a,b)$ in terms of powers of π^2 and values of the Riemann zeta function at odd arguments by saying that each $H(a,b)$ is a rational linear combination of products $H(m)\,\zeta(2n+1)$ with $m+n = a+b+1$. (It is in fact in this form that the above-mentioned non-explicit formula was proved by Brown.) It turns out that the coefficients in this new expression are simpler than those in terms of either the products $\pi^{2m}\zeta(2n+1)$ or $\zeta(2m)\zeta(2n+1)$. These coefficients were first guessed on the basis of numerical data for weights up to 13, obtained using the numerical algorithms mentioned above. We give this data (initially only known to be true numerically, but to very high precision) and then state the general formula which it suggests:

$$\begin{pmatrix} \zeta(3,2) \\ \zeta(2,3) \end{pmatrix} = \begin{pmatrix} \frac{9}{2} & -2 \\ -\frac{11}{2} & 3 \end{pmatrix} \begin{pmatrix} \zeta(5) \\ \zeta(2)\,\zeta(3) \end{pmatrix},$$

$$\begin{pmatrix} \zeta(3,2,2) \\ \zeta(2,3,2) \\ \zeta(2,2,3) \end{pmatrix} = \begin{pmatrix} -\frac{291}{16} & 12 & -2 \\ \frac{75}{8} & -\frac{11}{2} & 0 \\ \frac{157}{16} & -\frac{15}{2} & 3 \end{pmatrix} \begin{pmatrix} \zeta(7) \\ \zeta(2)\,\zeta(5) \\ \zeta(2,2)\,\zeta(3) \end{pmatrix},$$

$$\begin{pmatrix} \zeta(3,2,2,2) \\ \zeta(2,3,2,2) \\ \zeta(2,2,3,2) \\ \zeta(2,2,2,3) \end{pmatrix} = \begin{pmatrix} \frac{641}{16} & -30 & 12 & -2 \\ \frac{455}{16} & -\frac{291}{16} & 2 & 0 \\ -\frac{889}{16} & \frac{299}{8} & -\frac{15}{2} & 0 \\ -\frac{223}{16} & \frac{189}{16} & -\frac{15}{2} & 3 \end{pmatrix} \begin{pmatrix} \zeta(9) \\ \zeta(2)\,\zeta(7) \\ \zeta(2,2)\,\zeta(5) \\ \zeta(2,2,2)\,\zeta(3) \end{pmatrix},$$

$$\begin{pmatrix} \zeta(3,2,2,2,2) \\ \zeta(2,3,2,2,2) \\ \zeta(2,2,3,2,2) \\ \zeta(2,2,2,3,2) \\ \zeta(2,2,2,2,3) \end{pmatrix} = \begin{pmatrix} -\frac{17925}{256} & 56 & -30 & 12 & -2 \\ -\frac{11535}{64} & \frac{1985}{16} & -30 & 2 & 0 \\ \frac{10689}{128} & -\frac{889}{16} & \frac{157}{16} & 0 & 0 \\ \frac{9585}{64} & -\frac{1753}{16} & \frac{315}{8} & -\frac{15}{2} & 0 \\ \frac{4603}{256} & -\frac{255}{16} & \frac{189}{16} & -\frac{15}{2} & 3 \end{pmatrix} \begin{pmatrix} \zeta(11) \\ \zeta(2)\,\zeta(9) \\ \zeta(2,2)\,\zeta(7) \\ \zeta(2,2,2),\zeta(5) \\ \zeta(2,2,2,2)\,\zeta(3) \end{pmatrix},$$

$$\begin{pmatrix} \zeta(3,2,2,2,2,2) \\ \zeta(2,3,2,2,2,2) \\ \zeta(2,2,3,2,2,2) \\ \zeta(2,2,2,3,2,2) \\ \zeta(2,2,2,2,3,2) \\ \zeta(2,2,2,2,2,3) \end{pmatrix} = \begin{pmatrix} \frac{55299}{512} & -90 & 56 & -30 & 12 & -2 \\ \frac{281655}{512} & -\frac{102405}{256} & 140 & -30 & 2 & 0 \\ \frac{67683}{256} & -\frac{11535}{64} & \frac{641}{16} & -2 & 0 & 0 \\ -\frac{151965}{256} & \frac{52929}{128} & -\frac{1753}{16} & \frac{189}{16} & 0 & 0 \\ -\frac{157641}{512} & \frac{15217}{64} & -\frac{1785}{16} & \frac{315}{8} & -\frac{15}{2} & 0 \\ -\frac{11261}{512} & \frac{5115}{256} & -\frac{255}{16} & \frac{189}{16} & -\frac{15}{2} & 3 \end{pmatrix} \begin{pmatrix} \zeta(13) \\ \zeta(2)\,\zeta(11) \\ \zeta(2,2)\,\zeta(9) \\ \zeta(2,2,2)\,\zeta(7) \\ \zeta(2,2,2,2)\,\zeta(5) \\ \zeta(2,2,2,2,2)\,\zeta(3) \end{pmatrix}.$$

In these formulas one immediately sees certain patterns—all denominators are powers of 2, many of the entries are zero, the northeast and southeast corners of the matrices stabilize, etc.—and looking sufficiently carefully at the coefficients one is finally led to guess the complete formula given in the following theorem:

Theorem 1. *For all integers a, $b \geq 0$ we have*

$$H(a,b) \;=\; 2\sum_{r=1}^{a+b+1} (-1)^r \left[\binom{2r}{2a+2} - \left(1-\frac{1}{2^{2r}}\right)\binom{2r}{2b+1}\right] H(a+b-r+1)\,\zeta(2r+1)\,, \qquad (7)$$

where the value of $H(a+b-r+1)$ is given by (5). *Conversely, each product $H(m)\zeta(k-2m)$ of odd weight k is a rational linear combination of numbers $H(a,b)$ with $a+b=(k-3)/2$.*

Remark. The coefficients in the expressions for the products $H(m)\zeta(k-2m)$ as linear combinations of the numbers $H(a,b)$ do not seem to be given by any simple formula. For example, the inverse of the 5×5 matrix given above expressing the vector $\{\,H(a,b) \mid a+b=4\,\}$ in terms of the vector $\{\,\zeta(2a+3)H(b) \mid a+b=4\,\}$ is

$$\frac{1}{2555171}\begin{pmatrix} 450607872 & 750355968 & 819546624 & 620662272 & 300405248 \\ 742409280 & 1236102000 & 1349936640 & 1022542528 & 494939520 \\ 369002592 & 613537008 & 669540272 & 508012288 & 246001728 \\ 89977320 & 147349978 & 160083660 & 122931470 & 59984880 \\ 15331307 & 22114173 & 23488575 & 19354609 & 11072595 \end{pmatrix},$$

in which no simple pattern can be discerned and in which even the denominator (here prime) cannot be recognized. This shows that the Hoffman basis, although it works over $\mathbb{Q}$, is very far from giving a basis over $\mathbb{Z}$ of the $\mathbb{Z}$-lattice of MZV's, and suggests the question of finding better basis elements.

Theorem 1 (together with the identity (5)) tells us that for each odd weight $k = 2K+1$ the numbers $H(a, K-1-a)$ $(0 \le a \le K-1)$ and $\zeta(2r+1)\pi^{2K-2r}$ $(1 \le r \le K)$ span the same vector space over $\mathbb{Q}$ (and hence presumably each give a basis for this space, since the numbers $\zeta(2r+1)/\pi^{2r+1}$ are believed to be linearly independent over $\mathbb{Q}$). This same space has yet another description as the space spanned by the double zeta values $\zeta(m,n)$ with $m+n=k$, as was essentially proved by Euler. The number of these double zeta values, together with $\zeta(k)$ itself (which is known to be the sum of all of them) equals $2K$, so these numbers cannot form a basis, but this set of numbers splits up naturally into two subsets of K elements each:

(a) $\quad \zeta(k)$ and $\zeta(2r, k-2r) \qquad (r = 1, \ldots, K-1)$,
(b) $\quad \zeta(2r+1, k-2r-1) \qquad (r = 0, \ldots, K-1)$,

and we can ask whether each of these sets already spans (and therefore is a conjectural base of) the space in question. The answer is given in the following two theorems, which will be proved in §5 and §6, respectively.

Theorem 2. *For each odd integer $k = 2K+1 \ge 3$, the K numbers (a) span the same space as the K numbers $\{H(a,b) \mid a+b = K-1\}$ or $\{\pi^{2r}\zeta(k-2r) \mid 0 \le r \le K-1\}$.*

Theorem 3. *For each odd integer $k = 2K+1 \ge 5$, the numbers (b) satisfy $[(K-5)/3]$ relations over $\mathbb{Q}$.*

The number $[(K-5)/3] = [(k-11)/6]$ in this theorem actually arises as $\dim S_{k-1} + \dim S_{k+1}$, where S_h denotes the space of cusp forms of weight h on the full modular group $SL(2,\mathbb{Z})$. (More precisely, it arises as the sum of the dimensions of the space of odd period polynomials of weight $k-1$ and even period polynomials of weight $k+1$, but it is well-known that these spaces of period polynomials are isomorphic to the space of cusp forms on $SL(2,\mathbb{Z})$.) This connection is interesting both in itself and because of the relation to the results of [5], in which various relations were made between double zeta values $\zeta(a,b)$ of *even* weight $a+b=k$ and cusp forms (resp. even or odd period polynomials) of the same weight.

Finally, in §7 of the paper we prove the analogue of Theorem 1 for the Hoffman "star" elements $H^*(a,b)$ (defined like $H(a,b)$ but using "multiple zeta-star values," i.e., by allowing equality among the m_i's in (1)), by showing that their generating function is a simple multiple of the generating function of the $H(a,b)$'s. As a corollary, we obtain a recent result of Ihara, Kajikawa, Ohno and Okuda [8] showing that all odd zeta values $\zeta(2K+1)$ are very simple linear combinations of the numbers $H^*(a, K-1-a)$, unlike the situation for the usual Hoffman elements, where, as we just saw, the corresponding coefficients can apparently not be given in closed form.

2. The generating functions of $H(a,b)$ and $\widehat{H}(a,b)$

Our strategy to prove the theorem is to study the two generating functions

$$F(x,y) \;=\; \sum_{a,\,b\ge 0} (-1)^{a+b+1} H(a,b)\, x^{2a+2}\, y^{2b+1}\,, \tag{8}$$

$$\widehat{F}(x,y) \;=\; \sum_{a,\,b\ge 0} (-1)^{a+b+1} \widehat{H}(a,b)\, x^{2a+2} y^{2b+1}\,, \tag{9}$$

where $\widehat{H}(a,b)$ denotes the expression occurring on the right-hand side of (7). In this section we will compute each of these generating functions in terms of classical special functions (Propositions 1 and 2). If the two expressions obtained were the same, we would be done, but in fact they are completely different, one involving a higher hypergeometric function and the other a complicated linear combination of digamma functions. We therefore have to proceed indirectly, showing that both F and $\widehat{F}$ are entire functions of order 1 in x and y and that they agree whenever $x = y$ or x or y is an integer. This will imply the equality $F = \widehat{F}$ and hence $H = \widehat{H}$.

We begin with $F(x,y)$. Recall that the hypergeometric function ${}_pF_{p-1}\Big(\begin{matrix} a_1,\dots,a_p \\ b_1,\dots,b_{p-1}\end{matrix}\Big|\, x\Big)$ is defined as $\sum_{m=0}^{\infty} \frac{(a_1)_m \cdots (a_p)_m}{(b_1)_m \cdots (b_{p-1})_m} \frac{x^m}{m!}$, where $(a)_m = a(a+1)\cdots(a+m-1)$ denotes the ascending Pochhammer symbol.

Proposition 1. *The generating function $F(x,y)$ can be expressed as the product of a sine function and a hypergeometric function:*

$$F(x,y) \;=\; \frac{\sin \pi y}{\pi}\; {}_3F_2'\Big(\begin{matrix} x, \; -x, \; 0 \\ 1+y, \; 1-y \end{matrix}\Big|\, 1\Big), \tag{10}$$

where the second factor on the right is the z-derivative at $z = 0$ of ${}_3F_2\Big(\begin{matrix} x, \; -x, \; z \\ 1+y, \; 1-y \end{matrix}\Big|\, 1\Big)$.

Proof. The proof is similar to that in (6). From the definition of multiple zeta values we have

$$F(x,y) \;=\; -x^2\, y \sum_{m=1}^{\infty} \prod_{0<k<m} \Big(1 - \frac{x^2}{k^2}\Big) \cdot \frac{1}{m^3} \cdot \prod_{l>m} \Big(1 - \frac{y^2}{l^2}\Big) \tag{11}$$

$$= \; \frac{\sin \pi y}{\pi} \sum_{m=1}^{\infty} \frac{1}{m} \frac{(-x)_m\, (x)_m}{(1-y)_m (1+y)_m}\,, \tag{12}$$

and this formula is easily seen to be equivalent to the one given in the proposition. ∎

Next, we calculate $\widehat{F}(x,y)$. Here the answer involves the digamma function $\psi(x) = \Gamma'(x)/\Gamma(x)$ (logarithmic derivative of the gamma function).

Proposition 2. *The generating function $\widehat{F}(x,y)$ is an integral linear combination of fourteen functions of the form $\psi\big(1 + \frac{u}{2}\big) \frac{\sin \pi v}{2\pi}$ with $u \in \{\pm x \pm y, \, \pm 2x \pm 2y, \, \pm 2y\}$ and $v \in \{x, \, y\}$.*

Proof. From the definition of $\widehat{H}(a,b)$ and $\widehat{F}(x,y)$ we find

$$\begin{aligned}
\widehat{F}(x,y) \;=\; & 2 \sum_{\substack{r \ge 1 \\ s \ge 0}} \frac{(-1)^s \pi^{2s}}{(2s+1)!}\, \zeta(2r+1) \Bigg[\sum_{a=0}^{r-1} \binom{2r}{2a+2} x^{2a+2}\, y^{2r+2s-2a-1} \\
& \qquad - \big(1 - 2^{-2r}\big) \sum_{b=0}^{r-1} \binom{2r}{2b+1} x^{2r+2s-2b}\, y^{2b+1} \Bigg] \\
=\; & \frac{\sin \pi y}{\pi} \sum_{r=1}^{\infty} \zeta(2r+1) \left[(x+y)^{2r} + (x-y)^{2r} - 2y^{2r}\right] \\
& \qquad - \frac{\sin \pi x}{\pi} \sum_{r=1}^{\infty} (1 - 2^{-2r})\, \zeta(2r+1) \left[(x+y)^{2r} - (x-y)^{2r}\right] \\
=\; & \frac{\sin \pi y}{\pi} \left[A(x+y) + A(x-y) - 2A(y)\right] \;-\; \frac{\sin \pi x}{\pi} \left[B(x+y) - B(x-y)\right],
\end{aligned} \tag{13}$$

where $A(z)$ and $B(z)$ denote the power series

$$A(z) \;=\; \sum_{r=1}^{\infty} \zeta(2r+1)\, z^{2r}\,, \qquad B(z) \;=\; \sum_{r=1}^{\infty} (1-2^{-2r})\, \zeta(2r+1)\, z^{2r}\,. \tag{14}$$

These series converge only for $|z|<1$, but if we rewrite them as

$$A(z) \;=\; \sum_{n=1}^{\infty} \frac{z^2}{n\,(n^2-z^2)}\,, \qquad B(z) \;=\; \sum_{n=1}^{\infty} \frac{(-1)^{n-1} z^2}{n\,(n^2-z^2)} \tag{15}$$

then the new series converge for all z and define meromorphic functioms of z in the whole complex plane, with simple poles only at $z \in \mathbb{Z} \smallsetminus \{0\}$. We can also write them in terms of the digamma function $\psi(x) = \Gamma'(x)/\Gamma(x)$ by the formulas

$$\begin{aligned} A(z) \;&=\; \frac{1}{2}\sum_{n=1}^{\infty}\Bigl(\frac{1}{n-z}+\frac{1}{n+z}-\frac{2}{n}\Bigr) \;=\; \psi(1) \;-\; \frac{1}{2}\bigl(\psi(1+z)\;+\;\psi(1-z)\bigr)\,, \\ B(z) \;&=\; \frac{1}{2}\sum_{n=1}^{\infty}(-1)^{n-1}\Bigl(\frac{1}{n-z}+\frac{1}{n+z}-\frac{2}{n}\Bigr) \;=\; A(z) \;-\; A(z/2)\,. \end{aligned} \tag{16}$$

Substituting (16) into (13) gives an expression for $\widehat{F}$ of the form stated in the proposition. ∎

As explained above, the expressions for F and $\widehat{F}$ in these two propositions are very different, and the proof of their equality will proceed in an indirect manner. For this purpose we will need the analytic properties of both functions given in the following proposition.

Proposition 3. *Both $F(x,y)$ and $\widehat{F}(x,y)$ are entire functions on $\mathbb{C}\times\mathbb{C}$ and are bounded by a constant multiple of $e^{\pi X}\log X$ as $X \to \infty$, where $X = \max\{|x|,\,|y|\}$, and also by a multiple (depending on x) of $e^{\pi|\Im(y)|}$ as $|y|\to\infty$ with $x \in \mathbb{C}$ fixed.*

Proof. For $F(x,y)$ the first two statements follow from the estimate

$$0 \;<\; H(a,b) \;<\; \frac{1}{a+1}\,H(n) \;=\; \frac{1}{a+1}\,\frac{\pi^{2n}}{(2n+1)!} \qquad (a+b+1=n),$$

which implies the convergence of the series in (8) for all x, $y \in \mathbb{C}$ and gives the majorization

$$\max_{|x|,\,|y|\le M} |F(x,y)| \;<\; \sum_{n=1}^{\infty}\Bigl(1+\frac{1}{2}+\cdots\frac{1}{n}\Bigr)\frac{\pi^{2n}M^{2n+1}}{(2n+1)!} \;=\; \mathrm{O}\bigl(e^{\pi M}\log M\bigr)\,. \tag{17}$$

For the third statement, we note that it suffices to prove the desired estimate

$$|F(x,y)| \;=\; \mathrm{O}_x\bigl(e^{\pi|\Im(y)|}\bigr)\,, \tag{18}$$

for (say) $|\Im(y)| \ge 2$, because then the Phragmén-Lindelöf theorem together with the fact that $F(x,y)$ is a function of order 1 with respect to y (by the estimate (17)) imply the same estimate within the strip. But if $|\Im(y)| \ge 2$ then an easy estimate gives $|(1-y)_m(1+y)_m| > m!^2$ for all $m \ge 1$, and since $(-x)_m(x)_m = \mathrm{O}_x((m-1)!^2)$ this means that the sum in (12) is majorized by a multiple (depending on x) of the convergent sum $\sum_m m^{-3}$, establishing the desired estimate (18).

For $\widehat{F}(x,y)$ the holomorphy follows from (13) and (15) or (16): the latter equations show that the only singularities of $A(z)$ and $B(z)$ are simple poles at $z \in \mathbb{Z}$ with residues given by

$$\mathrm{Res}_{z=n} A(z) \;=\; -\frac{\mathrm{sgn}\, n}{2}\,, \qquad \mathrm{Res}_{z=n} B(z) \;=\; (-1)^n \frac{\mathrm{sgn}\, n}{2} \qquad\qquad (n \in \mathbb{Z}), \tag{19}$$

so the potential poles in (13) when $y \in \mathbb{Z}$ are canceled by the zeros of $\sin \pi y$ and the potential poles when $x \pm y = n \in \mathbb{Z}$ cancel because the residues of $A(x \pm y)$ and $\pm B(x \pm y)$ differ by a factor $\mp(-1)^n$ and the coefficients $\dfrac{\sin \pi x}{\pi}$ and $\dfrac{\sin \pi y}{\pi}$ differ by the same factor. Finally, both majorizations

$$\max_{|x|,\,|y| \le M} |\widehat{F}(x,y)| \;=\; \mathrm{O}\big(e^{\pi M} \log M\big) \tag{20}$$

and

$$|\widehat{F}(x,y)| \;=\; \mathrm{O}_x\big(e^{\pi |\Im(y)|}\big) \tag{21}$$

follows from the easy estimate[1] $\psi(x) = \mathrm{O}(\log x) + \mathrm{O}(1/\mathrm{dist}(x,\mathbb{Z}))$. ■

3. Special values of $F(x,y)$ and $\widehat{F}(x,y)$

In the next three propositions we verify the equality of the two functions F and $\widehat{F}$ for various special values of their arguments.

Proposition 4. *For $x \in \mathbb{C}$ we have*

$$F(x,x) \;=\; -\frac{\sin \pi x}{\pi} A(x) \;=\; \widehat{F}(x,x)\,, \tag{22}$$

where $A(z)$ is the meromorphic function defined by equation (14), (15) *or* (16)*.*

Corollary. *For $n \ge 1$ we have the identity*

$$\sum_{a+b+1=n} H(a,b) \;=\; \sum_{a+b+1=n} \widehat{H}(a,b) \;=\; \sum_{r=1}^{n} (-1)^{r-1} \frac{\pi^{2n-2r}}{(2n-2r+1)!}\, \zeta(2r+1)\;. \tag{23}$$

Proof. From (12) and (15) we immediately find

$$F(x,x) \;=\; \frac{\sin \pi x}{\pi} \sum_{m=1}^{\infty} \frac{1}{m} \cdot \frac{-x}{-x+m} \cdot \frac{x}{x+m} \;=\; -\frac{\sin \pi x}{\pi} A(x)\,,$$

while from (13) and (16) we find (using $A(0) = B(0) = 0$)

$$\widehat{F}(x,x) \;=\; \frac{\sin \pi x}{\pi} \big[A(2x) \,-\, 2A(x) \,-\, B(2x)\big] \;=\; -\frac{\sin \pi x}{\pi} A(x)\,.$$

This proves (41), and the corollary follows directly by substituting (14) for $A(x)$. ■

We observe that both (5) and (23) (for $H(a,b)$) are special cases of the main result of [9], which gave an explicit formula in terms of a generating function of the numbers $G_0(k,n,s)$ defined as the sum of all MZV's of weight (= sum of the arguments) k, depth (= number of arguments) n and height (= number of arguments greater than 1) s, because we have $H(n) = G_0(2n,n,n)$ and $\sum_{a=0}^{n-1} H(a, n-1-a) = G_0(2n+1,n,n)$. But the verification that the formula given in [9] specializes to (23) in the special case of $G_0(2n+1,n,n)$ is just as long as the derivation of (23) from the formulas (12) and (15), so we have given only the latter.

[1] Use the standard estimate $\psi(x) = \log(x) + \mathrm{O}(1/x)$ in the half-plane $\Re(x) \ge 0$ and the functional equation $\psi(x) - \psi(1-x) = \pi \cot \pi x = \mathrm{O}(1) + \mathrm{O}(1/\mathrm{dist}(x,\mathbb{Z}))$ for x in the half-plane $\Re(x) \le 0$.

Proposition 5. *For all $n \in \mathbb{N}$ and $y \in \mathbb{C}$ we have*

$$F(n,y) \;=\; \frac{\sin \pi y}{\pi} \sideset{}{^*}\sum_{|k|\le n} \frac{\operatorname{sgn} k}{y-k} \;=\; \widehat{F}(n,y)\,, \tag{24}$$

where the asterisk on the summation sign means that the terms $k=\pm n$ are to be weighted with a factor $1/2$.

Proof. We compute $\widehat{F}(n,y)$ first. From (16) we obtain the functional equation

$$A(z+1) \,-\, A(z) \;=\; -\frac{1}{2}\Bigl(\frac{1}{z+1} \,+\, \frac{1}{z}\Bigr) \tag{25}$$

for the function $A(z)$, so (13) gives

$$\widehat{F}(n,y) \;=\; \frac{\sin \pi y}{\pi}\,\bigl(A(y+n) \,-\, 2A(y) \,+\, A(y-n)\bigr) \;=\; -\frac{\sin \pi y}{\pi} \sideset{}{^*}\sum_{k=0}^{n} \Bigl(\frac{1}{k+y} \,+\, \frac{1}{k-y}\Bigr)\,,$$

proving the second equation in (24). On the other hand, the series in (12) for $x=n$ terminates at the $m=n$ term, and using the partial fraction expansion

$$\frac{(-x)_m\,(x)_m}{(1-y)_m(1+y)_m} \;=\; -x\sum_{k=1}^{m}(-1)^{m-k}\,\frac{k\,(x-m+1)_{2m-1}}{(m+k)!(m-k)!}\Bigl(\frac{1}{k+y} \,+\, \frac{1}{k-y}\Bigr)\,, \tag{26}$$

which is proved easily by comparing the residues at the simple poles $y=\pm 1,\ldots,\pm m$, we find

$$F(n,y) \;=\; -\frac{\sin \pi y}{2\pi}\sum_{k=1}^{n} c(n,k)\Bigl(\frac{1}{k+y} \,+\, \frac{1}{k-y}\Bigr) \tag{27}$$

with rational coefficients $c(m,k)$ defined by

$$c(n,k) \;=\; \sum_{m=k}^{n}(-1)^{m-k}\,\frac{nk}{m^2}\binom{m+n-1}{2m-1}\binom{2m}{m-k}.$$

Comparing (27) with the desired formula for $F(n,y)$ we find that it suffices to prove that

$$c(n,k) = 1 \,+\, \operatorname{sgn}(n-k) \qquad (n,\,k \in \mathbb{N})\,. \tag{28}$$

This can be done in several ways. Here is one. From the binomial theorem we have for each $m \in \mathbb{N}$

$$\sum_{|k|\le m}(-1)^{m-k}\,\frac{k}{m}\binom{2m}{m-k}x^k \;=\; -\frac{x}{m}\,\frac{d}{dx}\Bigl(\frac{(1-x)^{2m}}{x^n}\Bigr) \;=\; -\frac{(1+x)(1-x)^{2m-1}}{x^m}\,, \tag{29}$$

$$\sum_{n\ge m}\frac{n}{m}\binom{m+n-1}{2m-1}y^n \;=\; \frac{y}{m}\,\frac{d}{dy}\Bigl(\frac{y^m}{(1-y)^{2m}}\Bigr) \;=\; \frac{(1+y)\,y^m}{(1-y)^{2m+1}}\,. \tag{30}$$

Replacing y by xy in equation (30), multiplying with (29), and summing over all $m \ge 1$ gives

$$\begin{aligned}\sum_{n,\,k\ge 1}^{\infty} c(n,k)\,x^{n+k}y^n \;&=\; -\frac{(1+x)(1+xy)}{(1-x)(1-xy)}\sum_{m=1}^{\infty}\Bigl(\frac{(1-x)^2y}{(1-xy)^2}\Bigr)^m \\ &=\; -\frac{(1-x^2)y(1+xy)}{(1-y)(1-xy)(1-x^2y)} \;=\; -\frac{1+x}{1-x}\Bigl(\frac{1}{1-y} - \frac{2}{1-xy} + \frac{1}{1-x^2y}\Bigr)\,,\end{aligned}$$

and developing the expression on the right in a power series in x and y gives (28). ∎

Proposition 6. *For all $k \in \mathbb{N}$ and $x \in \mathbb{C}$ we have*

$$F(x,k) \;=\; (-1)^k \;+\; \frac{\sin \pi x}{\pi} \sideset{}{^*}\sum_{|j|\le k} \frac{(-1)^{k-j}}{j-x} = \widehat{F}(x,k)\,, \tag{31}$$

where the asterisk on the summation sign has the same meaning as in Proposition 5.

Proof. Again we start with $\widehat{F}$. From (16) and (25) we find the functional equation

$$\begin{aligned} B(x+1) \,-\, B(x-1) \;&=\; A(x+1) \,-\, A(x-1) \,-\, \Big[A\big(\tfrac{x+1}{2}\big) \,-\, A\big(\tfrac{x-1}{2}\big)\Big] \\ &=\; -\frac{1}{2}\Big(\frac{1}{x+1} + \frac{2}{x} + \frac{1}{x-1}\Big) + \frac{1}{2}\Big(\frac{2}{x+1} + \frac{2}{x-1}\Big) \;=\; \frac{1}{2}\Big(\frac{1}{x+1} - \frac{2}{x} + \frac{1}{x-1}\Big) \end{aligned}$$

and hence

$$B(x+k) \,-\, B(x-k) \;=\; \frac{1}{2}\Big(\frac{1}{x+k} - \frac{2}{x+k-1} + \frac{2}{x+k-2} - \cdots - \frac{2}{x-k+1} + \frac{1}{x-k}\Big)\,,$$

and substituting this into (13) immediately gives the second equality in (31). (The term $(-1)^k$ comes from the pole of $A(y)$ in (13), using (19).) On the other hand, formula (12) expresses $F(x,y)$ as the product of a function vanishing at $y=k$ and a function with a simple pole at $y=k$, so we get

$$(-1)^k\, F(x,k) \;=\; \sum_{m=1}^{\infty} \operatorname{Res}_{y=k}\Big(\frac{1}{m}\,\frac{(-x)_m\,(x)_m}{(1-y)_m(1+y)_m}\Big) \;=\; kx \sum_{m=k}^{\infty} \frac{(-1)^{m-k}}{m}\,\frac{(x+m-1)_{2m-1}}{(m+k)!(m-k)!}\,,$$

where for the second equality we have used (26). We can rewrite the right-hand side of this as $\frac{1}{2}\big(f_k(x) \,+\, f_k(x-1)\big)$ with $f_k(x)$ defined by the infinite series

$$f_k(x) \;=\; \sum_{m=k}^{\infty} (-1)^{m-k}\,\frac{k}{m}\binom{m+x}{2m}\binom{2m}{m-k}\,. \tag{32}$$

The first equality in (31) is therefore an immediate consequence of the following lemma.

Lemma 1. *For $k \in \mathbb{N}$ and $x \in \mathbb{C}$ the function $f_k(x)$ defined by (32) is given by*

$$f_k(x) \;=\; 1 + \frac{\sin \pi x}{\pi} \sum_{j=1-k}^{k} \frac{(-1)^j}{x-j}\,.$$

Proof. We use the method of telescoping series. For $(m,j) \in \mathbb{N} \times \mathbb{Z}$ we define polynomials in x by

$$a_{m,j} \;=\; \binom{x+m}{m+j}\binom{m-x-1}{m-j-1}, \qquad b_{m,j} = \frac{(-1)^{m-j-1}}{2}\Big(\frac{j}{m} + \frac{2x+1}{2m+1}\Big)\binom{m+x}{2m}\binom{2m}{m-j}\,,$$

with the convention that $\binom{x}{m} = 0$ for $m < 0$ (so that $a_{m,j}$ is non-zero only for $-m \le j < m$ and $b_{m,j}$ only for $-m \le j \le m$). A direct computation shows that

$$a_{m+1,j} \,-\, a_{m,j} \;=\; b_{m,j+1} \,-\, b_{m,j}\,.$$

Summing this over $(m,j) \in [1, M-1] \times [-k, k-1]$ for $M > k > 0$, we find

$$\sum_{j=-k}^{k-1} a_{M,j} \;=\; \sum_{j=-k}^{k-1} a_{1,j} \;+\; \sum_{m=1}^{M-1} \bigl(b_{m,k} - b_{m,-k}\bigr)$$
$$=\; 1 \;-\; \sum_{m=k}^{M-1} (-1)^{m-k} \, \frac{k}{m} \binom{m+x}{2m} \binom{2m}{m-k}.$$

On the other hand, writing

$$a_{M,j} \;=\; \frac{(-1)^{j-1}}{x-j} \cdot x \Bigl(1 - \frac{x^2}{1^2}\Bigr) \cdot \Bigl(1 - \frac{x^2}{(M-1)^2}\Bigr)\Bigl(1 - \frac{x}{M}\Bigr) \cdot \frac{M!\,(M-1)!}{(M+j)!\,(M-j-1)!}\,,$$

we see that $\lim_{M\to\infty} a_{M,j} = \dfrac{(-1)^{j-1}}{x-j} \, \dfrac{\sin \pi x}{\pi}$. This proves the lemma (including the convergence of the infinite sum defining $f_k(x)$) and completes the proof of Proposition 6. ■

4. Proof of Theorem 1

We can now complete the proof of the main equality (7) as follows. We have shown that $F(x,y)$ and $\widehat{F}(x,y)$ are entire functions of x and y satisfying the estimates (17), (18), (20) and (21), and that they agree whenever $x = y$ or either x or y is an integer. (The latter fact follows from Propositions 5 and 6 and the fact that both $F(x,y)$ and $\widehat{F}(x,y)$ are even functions of x and odd functions of y and vanish when $x = 0$.) It follows that for fixed x the function $f(y) = F(x,y) - \widehat{F}(x,y)$ is an entire function of order 1 which vanishes at all integers and satisfies $f(y) = \mathrm{O}(e^{\pi|\Im(y)|})$, so by the following lemma it is a multiple of $\sin \pi y$ and hence (since it also vanishes at $y = x$) vanishes identically. It follows that $F(x,y) = \widehat{F}(x,y)$ and hence that $H(a,b) = \widehat{H}(a,b)$ for all a, b.

Lemma 2. *An entire function $f : \mathbb{C} \to \mathbb{C}$ that vanishes at all integers and satisfies $f(z) = O(e^{\pi|\Im(z)|})$ is a constant multiple of* $\sin(\pi z)$.

Proof. The estimate implies that $f(z)$ has order 1. Therefore the quotient $g(z) = f(z)/\sin(\pi z)$, which by the assumption $f|_{\mathbb{Z}} = 0$ is an entire function, also has order 1 (for instance, because both $f(z)$ and $\sin(\pi z)$, and hence also $g(z)$, have Hadamard products of the form $e^{az+b}\prod(1-z/\alpha_j)e^{z/\alpha_j}$). The growth assumption on f implies that g is bounded outside a strip of finite width around the real axis, and the Phragmén-Lindelöf theorem implies (since it has finite order) that it is bounded also inside this strip, so g is constant by Liouville's theorem. ■

Remark. In this proof we used only Propositions 3, 4 and 6. We could have used the (easier) Proposition 5 instead of Proposition 6 if in Proposition 3 we had proved the analogues of the estimates (18) and (21) with the roles of x and y interchanged. These are in fact true, although we omit the proof. Alternatively, we could use either Proposition 5 or Proposition 6 together with just the easier estimates (17) and (20) by using a strengthening of the above lemma in which the estimate $\mathrm{O}(e^{\pi|\Im(z)|})$ is replaced by $\mathrm{O}(e^{\pi|z|})$. This stronger lemma is in fact true and consultations with friends led to two proofs (one, after discussions with David Wigner and Anton Mellit, using the theory of analytic functionals and the approximability of holomorphic functions by polynomials on domains of certain shapes, and the other, communicated to me by Michael Sodin, using a convexity property of the Phragmén-Lindelöf indicator function), but since both of them need fairly sophisticated techniques from complex function theory it seemed preferable to simply prove the strengthened estimates (18) and (21) and use only the simpler lemma above. Subsequently, I was informed by

François Gramain that the lemma is in fact known: it was proved by both Polya (L'Ens. Math. **22**, 1922) and Valiron (Bulletin des Sciences Math. **49**, 1925) and is quoted in the book *Entire Functions* by R.P. Boas, Corollary 9.4.2. I nevertheless have retained the more elementary proof in order to keep this paper self-contained.

For the second statement of the theorem, we have to show that the matrix M with coefficients

$$M_{br} \;=\; \frac{1}{2r}\left(2^{2r}\binom{2r}{2K-2b} \;-\; \left(2^{2r}-1\right)\binom{2r}{2b+1}\right) \qquad (0 \le b \le K-1, \quad 1 \le r \le K)$$

is invertible. (Here we have changed the coefficients occurring in (7) by a factor $(-1)^r 2^{2r-2}/r$ depending only on r, which clearly does not affect the invertibility of the matrix.) As mentioned at the end of the introduction, we do not know how to write down the inverse of this matrix explicitly, but its existence is proved easily by a 2-adic argument: the estimate $v_2(2r) < 2r$ and the identity $\frac{1}{2r}\binom{2r}{2b+1} = \frac{1}{2b+1}\binom{2r-1}{2b}$ imply that M_{br} is 2-integral for all b and r, is odd (i.e., has 2-adic valuation 0) for $r = b+1$, and is even (i.e., has positive 2-adic valuation) for $r \le b$, and from this it follows that the determinant of M is a 2-adic unit and hence is not equal to zero.

5. Double zeta values and products of single zeta values

In this section we fix an odd number $k = 2K+1 \ge 3$ and discuss the relationship between the double zeta values $\zeta(m,n)$ and the zeta products $\zeta(a)\zeta(b)$ of weight $m+n = a+b = k$.

As mentioned in the introduction, it was already found by Euler [4] (explicitly for k up to 13) that all double zeta values of odd weight are rational linear combinations of products of "Riemann" zeta values. A simple derivation of this fact was sketched in [5], but without giving an explicit formula. Since we will need such a formula, we will reproduce the argument from [5] in a more concrete form.

Proposition 7. *The double zeta value $\zeta(m,n)$ $(m \ge 1,\ n \ge 2)$ of weight $m+n = k = 2K+1$ is given in terms of products $\zeta(2s)\,\zeta(k-2s)$ $\quad(0 \le s \le K-1)$ by*

$$\zeta(m,n) \;=\; (-1)^m \sum_{s=0}^{K-1}\left[\binom{k-2s-1}{m-1} + \binom{k-2s-1}{n-1} - \delta_{n,2s} + (-1)^m\delta_{s,0}\right]\zeta(2s)\zeta(k-2s)\,. \qquad (33)$$

Proof. We start with the "double shuffle relations," which express in two different ways products of Riemann zeta values as linear combinations of double zeta values:

$$\zeta(r)\,\zeta(s) \;=\; \zeta(r,s) \,+\, \zeta(s,r) \,+\, \zeta(k) \qquad (r+s=k;\ r,s \ge 2)\,, \qquad (34)$$

$$\zeta(r)\,\zeta(s) \;=\; \sum_{n=2}^{k-1}\left[\binom{n-1}{r-1} \,+\, \binom{n-1}{s-1}\right]\zeta(k-n,n) \qquad (r+s=k;\ r,s \ge 2)\,. \qquad (35)$$

Both are valid as they stand only in the domain stated, and in both cases we could suppose without any loss of information that $r \le s$, since both sides of the equations are symmetric in r and s. Thus we have only $2(K-1)$ equations for the $2K-1$ unknowns $\zeta(m,k-m)$ $(1 \le m \le k-2)$. However, both (34) and (35) remain true if we fix any value T for the divergent zeta value $\zeta(1)$ (here 0 or γ, Euler's constant, would be natural choices but we can also simply take T to be an indeterminate) and use (34) to define the divergent double zeta value $\zeta(k-1,1)$, so this gives $2K-1$ equations in $2K-1$ unknowns. To solve them, we introduce the generating functions

$$\mathcal{P}(X,Y) \;=\; \sum_{\substack{r,\,s\ge 1\\ r+s=k}} \zeta(r)\,\zeta(s)\,X^{r-1}\,Y^{s-1}\,, \qquad \mathcal{D}(X,Y) \;=\; \sum_{\substack{m,\,n\ge 1\\ m+n=k}} \zeta(m,n)\,X^{m-1}\,Y^{n-1}$$

(where we are using our new conventions $\zeta(1)=T$, $\zeta(k-1,1)=\zeta(k-1)T-\zeta(k)-\zeta(1,k-1)$). Then (34) and (35) translate into the equations

$$\mathcal{P}(X,\,Y) \;=\; \mathcal{D}(X,\,Y)+\mathcal{D}(Y,\,X)+\mathcal{Z}(X,\,Y) \;=\; \mathcal{D}(X,\,X+Y)+\mathcal{D}(Y,\,X+Y)\,,$$

where $\mathcal{Z}(X,\,Y)=\zeta(k)\,\frac{X^{k-1}-Y^{k-1}}{X-Y}$. Applying these two equations alternately a total of six times and considering $\mathcal{P}$ and $\mathcal{Z}$ as known gives

$$\mathcal{D}(X,Y) \;\equiv\; -\mathcal{D}(Y,X) \;\equiv\; \mathcal{D}(X-Y,X) \;\equiv\; \cdots \;\equiv\; \mathcal{D}(-X,-Y)$$

modulo known quantities and hence, since $\mathcal{D}(-X,-Y)=-\mathcal{D}(X,Y)$ for k odd, lets us solve for $\mathcal{D}$. The result can be written as $\mathcal{D}(X,Y)=\mathcal{Q}(X,Y)+\mathcal{Q}(X-Y,-Y)+\mathcal{Q}(X-Y,X)$, where $\mathcal{Q}(X,\,Y)=(\mathcal{P}(X,Y)+\mathcal{P}(-X,Y)-\mathcal{Z}(X,Y))/2$, and this is equivalent (using $\zeta(0)=-\frac{1}{2}$) to (33). ■

Either of the double shuffle relations (34) or (35) permits us to express the single zeta products $\zeta(2r)\zeta(k-2r)$ in terms of all double zeta values of weight k, but we would like to do this using (a) only the "even-odd" values $\zeta(2r,k-2r)$ or (b) only the "odd-even" double zeta values $\zeta(2r+1,k-2r-1)$, where in the former case we must also include $\zeta(k)$ to have the right number of values. This turns out to be possible only in the former case, as we now show. The odd-even case and its relation to modular forms will be the subject of §6.

Since in case (a) we have taken $\zeta(k)$ as one of the basis elements, we can omit it from the basis and work modulo $\zeta(k)$ in the right-hand side of (33), which simplifies to

$$\zeta(2r,k-2r) \;\equiv\; \sum_{s=1}^{K-1}\left[\binom{2K-2s}{2r-1}+\binom{2K-2s}{2K-2r}\right]\zeta(2s)\,\zeta(k-2s) \qquad (1\le r\le K-1) \tag{36}$$

in this case, where the congruence is modulo $\mathbb{Q}\,\zeta(k)$. Let $\mathcal{A}=\mathcal{A}_K$ be the $(K-1)\times(K-1)$ matrix whose (r,s)-entry is the expression in square brackets in (36). Theorem 1 is then a consequence of (36) and the following lemma. I would like to thank David Wigner for suggesting the simple proof of this lemma, which despite its similarity with the corresponding proof in §4 I had overlooked.

Lemma 3. *The determinant of the matrix $\mathcal{A}_K$ is non-zero.*

Proof. Any binomial coefficient $\binom{m}{n}$ with m even and n odd is even (because it is equal to m/n times $\binom{m-1}{n-1}$), so the matrix $\mathcal{A}_K$ is congruent modulo 2 to a unipotent triangular matrix and hence has odd determinant. ■

Although Lemma 3 suffices to prove the result stated in the introduction, I nevertheless mention three more precise statements that I found experimentally. The first is the conjectural formula

$$\det\mathcal{A} \;\stackrel{?}{=}\; \pm(k-2)!! \tag{37}$$

for the determinant of $\mathcal{A}$, where $(k-2)!!$ denotes the "double factorial" $1\times3\times5\times\cdots\times(k-2)$ and where the sign is -1 if $K\equiv3 \pmod 4$ and $+1$ otherwise. The other two are explicit identities, one giving a decomposition of $\mathcal{A}$ into triangular matrices which would imply (37) and one giving a formula for the inverse of $\mathcal{A}$ in terms of Bernoulli numbers. All three identities have been verified up to $K=50$ but not proved (although this could presumably be done if necessary using standard techniques for finite hypergeometric sums, or even mechanically using the Wilf-Zeilberger algorithm), but they both seem worth mentioning since they may give further information about the space of double zeta values of odd weight k. The factorization formula is

$$\mathcal{L}\,\mathcal{A} \stackrel{?}{=} \mathcal{U} \tag{38}$$

where $\mathcal{L}$ and $\mathcal{U}$ are the lower and upper triangular $(K-1)\times(K-1)$ matrices given by

$$\mathcal{L}_{pr} \;=\; \frac{2r-K-\frac12}{2p-K-\frac12}\binom{K-\frac12}{K-p}\binom{K-\frac12}{K-r}^{-1}\binom{2p-K-\frac12}{p-r} \qquad (1\le p,\,r\le K-1)$$

and

$$\mathcal{U}_{ps} \;=\; (-1)^{p-1}\,4^{2p-s}\left(s-\tfrac12\right)\binom{K-\frac12}{2p-1}\binom{K-\frac12}{s-1}^{-1} Q_{s-p}(s,s-K) \qquad (1\le p,\,s\le K-1)$$

respectively, where Q_n is the polynomial

$$Q_n(x,y) \;=\; \begin{cases} 0 & \text{if } n<0,\\ 1 & \text{if } n=0,\\ \displaystyle\sum_{m=1}^{n}\frac{(-4)^m}{(2m+1)!}\,\frac{m}{n}\cdot\binom{2n}{n+m}(x)_m\,(y)_m & \text{if } n\ge 1.\end{cases}$$

(Here $(x)_m$ is the Pochhammer symbol as defined in §2.) Formula (38), or even the weaker form of it in which the formula for U_{ps} when $s>p$ is not specified, implies formula (37), as was already mentioned. More interesting, it provides an alternative set of generators (and presumably basis) of the $\mathbb{Q}$-vector space we are looking at (or rather, of the quotient of this space by the 1-dimensional subspace spanned by $\zeta(k)$) which is related to both the even-odd double zeta value basis and to the product basis by triangular matrices, suggesting the existence of possibly interesting filtrations on the double zeta space. However, no further properties of these new basis elements were found. In particular, a numerical check showed that in general they are not rationally proportional, even modulo the 1-dimensional space $\mathbb{Q}\,\zeta(k)$, to any of the 2^{k-2} convergent MZV's of weight k.

The final formula, or pair of formulas, says that the inverse of the matrix $\mathcal{A}$ is given by either of the two expressions

$$\begin{aligned}\left(\mathcal{A}^{-1}\right)_{s,r} &\overset{?}{=} \frac{-2}{2s-1}\sum_{n=0}^{k-2s}\binom{k-2r-1}{k-2s-n}\binom{n+2s-2}{n}B_n\\ &\overset{?}{=} \frac{2}{2s-1}\sum_{n=0}^{k-2s}\binom{2r-1}{k-2s-n}\binom{n+2s-2}{n}B_n \qquad (1\le s,\,r\le K-1)\,,\end{aligned}$$

where B_n denotes the nth Bernoulli number. In particular,

$$\left(\mathcal{A}^{-1}\right)_{s,1} \overset{?}{=} -\frac{1}{2}\left(\mathcal{A}^{-1}\right)_{s,K-1} \overset{?}{=} 2\binom{2K-2}{2s-1}\frac{B_{2K-2s}}{2K-2s} \qquad (1\le s\le K-2)\,,$$

i.e., the first and the last columns of $\mathcal{A}^{-1}$ consist of simple multiples of Bernoulli numbers.

6. Double zeta values of odd weight and modular forms

We now turn to the case of odd-even double zeta values. Here (33) says

$$\zeta(2m+1,\,k-2m-1) \;=\; \sum_{n=1}^{K}\left[\delta_{n,m}+\delta_{n,K}-\binom{2n}{2m}-\binom{2n}{2K-2m-1}\right]\zeta(2n+1)\zeta(k-2n-1)\,. \quad (39)$$

However, unlike the case for $\mathcal{A}$, the matrix $\mathcal{B} = \mathcal{B}_K = (\mathcal{B}_{m,n})_{0\le m\le K-1,\,1\le n\le K}$, where $\mathcal{B}_{m,n}$ denotes the expression in square brackets in (39), is singular for all $K \ge 5$. In this section we relate the kernel of $\mathcal{B}$ to cusp forms of weight $k \pm 1$ on $SL(2,\mathbb{Z})$.

The connection will in fact not be directly with cusp forms, but with their period polynomials. Recall that for each even integer $h > 2$ the space $\mathbf{W}_h$ of weight h period polynomials is the space of polynomials $P(X)$ satisfying the functional equations

$$P(X) + X^{h-2}P\big(\frac{-1}{X}\big) = 0\,, \qquad P(X) + X^{h-2}P\big(1-\frac{1}{X}\big) + (X-1)^{h-2}P\big(\frac{-1}{X-1}\big) = 0\,,$$

corresponding to the conditions on 1-cocycles for $PSL(2,\mathbb{Z})$ imposed by the relations in that group. It splits as the direct sum of $\mathbf{W}_h^+$ and $\mathbf{W}_h^-$, the symmetric and antisymmetric polynomials with respect to $P(X) \mapsto X^{h-2}P(1/X)$. The elements of $\mathbf{W}_h^+$ are odd polynomials, those of $\mathbf{W}_h^-$, even ones. There is also a characterization of each space $\mathbf{W}_h^\pm$ by a single functional equation:

$$\mathbf{W}_h^\pm = \big\{P(X) \in \mathbb{C}[X] \mid P(X) = P(X+1) \pm X^{h-2}P(1+1/X)\big\} \tag{40}$$

(Lewis functional equation). The space $\mathbf{W}_h^-$ contains an "uninteresting" 1-dimensional subspace spanned by the polynomial $X^{h-2}-1$ (corresponding to the coboundaries, or from another point of view to the Eisenstein series). If we either divide by it or—as we will do—restrict to the subspace of polynomials with no constant term, then both spaces of period polynomials have the same dimension as the space S_h of cusp forms of weight h on $SL(2,\mathbb{Z})$, and are in fact canonically isomorphic to it by a well-known mapping (Eichler-Shimura-Manin theory of periods). For example, for $h = 12$, $h = 16$ and $h = 18$, we have $\dim S_h = 1$ and hence (up to a constant factor, and with the condition $P(0) = 0$) precisely one symmetric and one antisymmetric period polynomial, as follows:

$$\begin{aligned}
s_{12}(x) &= 4\,X^9 - 25\,X^7 + 42\,X^5 - 25\,X^3 + 4\,X\,,\\
s_{16}(x) &= 36\,X^{13} - 245\,X^{11} + 539\,X^9 - 660\,X^7 + 539\,X^5 - 245\,X^3 + 36\,X\,,\\
s_{18}(x) &= 24\,X^{15} - 154\,X^{13} + 273\,X^{11} - 143\,X^9 - 143\,X^7 + 273\,X^5 - 154\,X^3 + 24\,X\,,\\
a_{12}(x) &= X^8 - 3\,X^6 + 3\,X^4 - X^2\,,\\
a_{16}(x) &= 2\,X^{12} - 7\,X^{10} + 11\,X^8 - 11\,X^6 + 7\,X^4 - 2\,X^2\,,\\
a_{18}(x) &= 8\,X^{14} - 25\,X^{12} + 26\,X^{10} - 26\,X^6 + 25\,X^4 - 8\,X^2\,,
\end{aligned}$$

On the other hand, the kernels of the matrix $\mathcal{B}_K$ for $K = 5$, 6, 7 and 8 are given by

$$\mathbb{C}\cdot\begin{pmatrix}4\\-9\\6\\-1\\0\end{pmatrix}, \quad \mathbb{C}\cdot\begin{pmatrix}4\\-25\\42\\-25\\4\\0\end{pmatrix}, \quad \mathbb{C}\cdot\begin{pmatrix}12\\-35\\44\\-33\\14\\-2\\0\end{pmatrix}, \quad \mathbb{C}\cdot\begin{pmatrix}36\\-245\\539\\-660\\539\\-245\\36\\0\end{pmatrix} \bigoplus \mathbb{C}\cdot\begin{pmatrix}56\\-150\\130\\0\\-78\\50\\-8\\0\end{pmatrix},$$

where in the last case the basis of the 2-dimensional kernel has been chosen to make the structure more transparent. We see that the kernels for $K = 6$ and $K = 8$ contain vectors whose entries (apart from the final 0) are symmetric and that these entries coincide with the coefficients of the symmetric period polynomial $s_{2K}(X)$, while the remaining vectors in the kernel for $K = 5$, 7 and

8 have entries equal (up to a factor 1/2) to the coefficients of the *derivatives* of the antisymmetric period polynomials $a_{2K+2}(X)$:

$$\begin{aligned} a'_{12}(x)/2 &= 4X^7 - 9\,X^5 + 6\,X^3 - X\,, \\ a'_{16}(x)/2 &= 12\,X^{11} - 35\,X^9 + 44\,X^7 - 33\,X^5 + 14\,X^3 - 2\,X\,, \\ a'_{18}(x)/2 &= 56\,X^{13} - 150\,X^{11} + 130\,X^9 - 78\,X^5 + 50\,X^3 - 8\,X\,. \end{aligned}$$

The proof that these relations hold, i.e., that there is an injective mapping

$$\mathbf{W}^+_{2K} \bigoplus \mathbf{W}^-_{2K+2} \quad\longrightarrow\quad \mathrm{Ker}(\mathcal{B}_K) \tag{41}$$

as just described, is not too difficult, but I have not been able to show that this map is an isomorphism, i.e., that there are no other relations. (And in any case this statement would not permit one to replace "$[(K-5)/3]$ relations" by "precisely $[(K-5)/3]$ relations" in Theorem 3, since the linear independence over $\mathbb{Q}$ of the numbers $\zeta(2s+1)/\pi^{2s+1}$ is not known.) We indicate the proof briefly.

The first step is to show that all elements in the kernel have last component equal to 0 (as one can see in the examples given above). This is of interest since it is equivalent to the statement that there is a vector $\lambda = (\lambda_0, \ldots, \lambda_{K-1})$ whose image under $\mathcal{B}^t$ is the vector $(0, \ldots, 0, 1)$, and that in turn implies an explicit formula $\zeta(k) \;=\; -2\sum_{m=0}^{K-1} \lambda_m \zeta(2m+1, k-2m)$ for odd zeta values in terms of odd-even double zeta values. We content ourselves here with giving the formula for λ, leaving the routine verification of its defining property to the reader:

$$\lambda_m \;=\; \frac{1}{3(K-1)} \cdot \begin{cases} 2\,(2K-1) & \text{if } m=0\,, \\ 2K-4m-1 & \text{if } 1 \le m \le K-2\,, \\ -(2K-1) & \text{if } m = K-1\,. \end{cases}$$

We then observe that the statement that $c = (c_1, \ldots, c_{K-1}, 0)^t$ is in the kernel of $\mathcal{B}$ is equivalent to the statement that the polynomial $C(X) := \sum_{n=1}^{K-1} c_n X^{2n}$ satisfies the functional equation

$$C(X) \;-\; C(X+1) \;-\; X^{2K-1}\,C(1+1/X) \;=\; (\text{odd polynomial in } X)\,. \tag{42}$$

(This is a direct consequence of the definition of the coefficients of $\mathcal{B}$ in (39), in which the "$\delta_{n,K}$" term can now be omitted since we know that $c_K = 0$.) If we denote by $\mathbf{C}_K$ the space of even polynomials satisfying (42), then the map $\mathbf{W}^+_{2K} \oplus \mathbf{W}^-_{2K+2} \to \mathbf{C}_K$ whose existence and injectivity we want to prove sends a polynomial $P \in \mathbf{W}^+_{2K}$ to $C(X) = XP(X)$ and a polynomial $P \in \mathbf{W}^-_{2K+2}$ to $C(X) = X^{2K-1}P'(1/X)$. (The injectivity of each of these maps separately is then obvious, and their combined injectivity almost equally so, since the images have incompatible symmetry properties $c_n = c_{K-n}$ and $nc_n = -(K-n)c_{K-n}$. Note also that $\mathbf{C}_K$ has an uninteresting one-dimensional subspace, consisting of constants, that we are not allowing, but which corresponds under the map just given to the uninteresting subspace $\langle X^{2K}-1\rangle$ of $\mathbf{W}^-_{2K+2}$ that we excluded by our normalization condition.) Denote the left-hand side of (42) by L. Then if $C(X) = XP(X)$ with $P \in W^+_{2K}$ we find

$$L \;=\; (X+1)\left[P(X) - P(X+1) - X^{2K-2}P(1+1/X)\right] \;-\; P(X) \;=\; -\,P(X) \;=\; (\text{odd})$$

by virtue of (40), and if $C(X) \;=\; X^{2K-1}P'(1/X)$ with $P \;\in\; \mathbf{W}^-_{2K+2}$ then using (40) and the symmetry properties $P(X) = P(-X) = -X^{2K}P(1/X)$ we find

$$L \;=\; (X+1)^{2K+1}\,\frac{d}{dx}\left[P\Big(\frac{-1}{X+1}\Big) - P\Big(\frac{X}{X+1}\Big) + (X+1)^{-2K}P(-X)\right] \;-\; P'(X) \;=\; -P'(X)\,,$$

which is again odd. This concludes the proof of Theorem 3.

It is perhaps worth remarking that we have given a simple description of the kernel of $\mathcal{B}_K$, but not of the relations among the odd-even double zeta values themselves, which correspond to the kernel of the transpose, e.g., the kernel of $\mathcal{B}^t_5$ is generated by $(-6, 17, 13, -27, 3)$ and we have $-6\,\zeta(1,10) + 17\,\zeta(3,8) + 13\,\zeta(5,6) - 27\,\zeta(7,4) + 3\,\zeta(9,2) \;=\; 0$. I was not able to find an explicit description of the elements of the kernel of $\mathcal{B}^t_K$.

7. Multiple zeta-star values and Hoffman star elements

The "multiple zeta-star values" $\zeta^*(k_1,\ldots,k_n)$ are defined (again for $k_i \ge 1$, $k_n \ge 2$) by

$$\zeta^*(k_1,\ldots,k_n) \;=\; \sum_{1\le m_1\le\cdots\le m_n} \frac{1}{m_1^{k_1}\cdots m_n^{k_n}}\,. \tag{41}$$

They span the same $\mathbb{Q}$-vector space as the usual MZV's and one again has the conjecture that the "Hoffman star elements"

$$H^*(a_0,\ldots,a_r) \;:=\; \zeta^*(\underbrace{2,\ldots,2}_{a_0},3,\underbrace{2,\ldots,2}_{a_1},\ldots,3,\underbrace{2,\ldots,2}_{a_r}) \qquad (a_0\,\ldots,a_r \,\ge\, 0) \tag{42}$$

form a $\mathbb{Q}$-basis of this space. The simple Hoffman star elements are given by the formula

$$H^*(n) \;:=\; \zeta^*(\underbrace{2,\ldots,2}_{n}) \;=\; 2\,(1-2^{1-2n})\,\zeta(2n) \qquad (n\,\ge\,0), \tag{43}$$

as one sees immediately from the generating function

$$\sum_{n=0}^{\infty} H^*(n)\,x^{2n} \;=\; \prod_{m=1}^{\infty}\frac{1}{1\,-\,x^2/m^2} \;=\; \frac{\pi x}{\sin\pi x}\,. \tag{44}$$

The double Hoffman star elements were studied in a recent preprint of Ihara, Kajikawa, Ohno and Okuda [8], who showed that odd zeta values can be expressed very simply as rational linear combinations of them. In this section we give a closed formula for the double Hoffman star elements and a new proof of this identity.

Recall that Theorem 1 gave the formula

$$H(a,b) \;=\; 2\sum_{r=1}^{K}(-1)^r\left[\binom{2r}{2a+2} \,-\, \Bigl(1-\frac{1}{2^{2r}}\Bigr)\binom{2r}{2b+1}\right] H(K-r)\,\zeta(2r+1)$$

for the usual double Hoffman elements, where $a,\, b\ge 0$ and $K=a+b+1$. The formula in the star case is very similar.

Theorem 4. *For $a,\, b\ge 0$ we have*

$$H^*(a,b) \;=\; -2\sum_{r=1}^{K}\left[\binom{2r}{2a} \,-\, \delta_{r,a} \,-\, \Bigl(1-\frac{1}{2^{2r}}\Bigr)\binom{2r}{2b+1}\right] H^*(K-r)\,\zeta(2r+1) \tag{45}$$

where $K=a+b+1$ and $H^*(n)$ is given by (43).

Corollary (= Theorem 2 of [8]**).** *For $K\ge 1$ we have*

$$2K(1\,-\,2^{-2K})\,\zeta(2K+1) \;=\; \sum_{a=0}^{K-1}\Bigl(1\,+\,\frac{1}{2}\,\delta_{a,0}\Bigr)\,H^*(a,K-1-a)\,. \tag{46}$$

Proof. Just as in the simple Hoffman star case (44), we work with generating functions. We have

$$\begin{aligned}\sum_{a,\,b\ge0} H^*(a,b)\,x^{2a}\,y^{2b} \;&=\; \sum_{m=1}^{\infty}\left(\prod_{k=1}^{m}\frac{1}{1\,-\,x^2/k^2}\right)\cdot\frac{1}{m^3}\cdot\left(\prod_{l=m}^{\infty}\frac{1}{1\,-\,y^2/l^2}\right)\\ &=\; \frac{\pi x}{\sin\pi x}\cdot\frac{\pi y}{\sin\pi y}\cdot\sum_{m=1}^{\infty}\prod_{k=m+1}^{\infty}\Bigl(1\,-\,\frac{x^2}{k^2}\Bigr)\cdot\frac{1}{m^3}\cdot\prod_{l=1}^{m-1}\Bigl(1\,-\,\frac{y^2}{l^2}\Bigr)\\ &=\; \frac{\pi x}{\sin\pi x}\cdot\frac{\pi y}{\sin\pi y}\cdot\frac{-F(y,x)}{xy^2}\,,\end{aligned}$$

where the last equality comes from eq. (11). Now by formula (13) and the equality $F = \widehat{F}$, together with the generating function (44), the right-hand side of this expression can be rewritten as

$$
\begin{aligned}
-\ \frac{\pi y}{\sin \pi y} \cdot \frac{A(y+x) + A(y-x) - 2A(x)}{y^2} &+ \frac{\pi x}{\sin \pi x} \cdot \frac{B(y+x) - B(y-x)}{xy} \\
= -\sum_{n=0}^{\infty} H^*(n)\, y^{2n} \cdot \sum_{r=1}^{\infty} \zeta(2r+1)\, &\frac{(x+y)^{2r} + (x-y)^{2r} - 2x^{2r}}{y^2} \\
+ \sum_{n=0}^{\infty} H^*(n)\, y^{2n} \cdot \sum_{r=1}^{\infty} (1 - 2^{-2r})\zeta(2r+1)\, &\frac{(x+y)^{2r} - (x-y)^{2r}}{xy}\,,
\end{aligned}
$$

and equation (45) follows by comparing coefficients on both sides. The corollary is an immediate consequence, since for $1 \le r \le K$ we have

$$
\begin{aligned}
&-2 \sum_{a+b=K-1} \Bigl(1 + \frac{1}{2}\,\delta_{r,a}\Bigr) \left[\binom{2r}{2a} - \delta_{r,a} - \Bigl(1 - \frac{1}{2^{2r}}\Bigr)\binom{2r}{2b+1}\right] \\
&\quad = -(2^{2r} - 1) + 2\bigl(1 - 2^{-2r}\bigr)\left(2^{2r} + \frac{1}{2}\binom{2r}{2K-1}\right) = 2K\bigl(1 - 2^{-2K}\bigr)\,\delta_{r,K}\,. \qquad \blacksquare
\end{aligned}
$$

Remarks. 1. The simplicity of (46) as opposed to the corresponding formula for $\zeta(2K+1)$ in terms of the original Hoffman elements $H(a,b)$ might give some hope that the Hoffman star elements are perhaps closer to being a $\mathbb{Z}$-basis of the $\mathbb{Z}$-lattice of MZV's. But in fact this is not the case: if one inverts the matrix occurring in (45) to write the products $H^*(n)\,\zeta(2r+1)$ as rational linear combinations of the numbers $H^*(a,b)$, then except in the case $n = 0$ one again finds large primes in the denominators and no apparent pattern in the numerators. Nevertheless, the numbers are not completely random. For instance, for $2 \le K \le 40$ the determinant of the matrix in question is always divisible by the numerator of $B_{2K+2}/(2K+2)$ and also by $(2^{2K} - 1)^{[K/6]+1}$. The former observation is related to similar experimental findings of Masanobu Kaneko that he communicated to me privately.

2. The proof we have given of Theorem 4 and its corollary is analytic, and works only for the multiple zeta-star values as real numbers, whereas the proof of Theorem 2 in [8] is algebraic and deduces the identity in question only from the double shuffle relations. If that proof can be extended to give a similarly algebraic proof of Theorem 4, then one also gets a new and purely algebraic proof of Theorem 1 (since the relationship between the generating functions of $H(a,b)$ and $H^*(a,b)$ can be used in either direction). This would be of especial interest because for the application to periods of mixed Tate motives in [1] Brown needs the truth of (7) in the context of motivic zeta values, not merely of real ones, and has to carry out a subtle inductive argument in order to deduce this statement from the statement over $\mathbb{R}$.

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