Second lecture: April 11, 2011

2 Zagier's contribution to Brown's proof

We explain the strategy of Zagier [14] for proving the relation which was needed and conjectured by F. Brown [5, 6] concerning the numbers

$$H(a,b) := \zeta(\{2\}_b 3\{2\}_a)$$

for $a \geq 0$ and $b \geq 0$. In particular $H(0,0) = \zeta(3)$. Beware that the normalization used by F. Brown and by D. Zagier is the opposite of ours, this is why a and b are in this reverse order here.

Set also (cf. Corollary 9)

$$H(n) = \zeta(\{2\}_n) = \frac{\pi^{2n}}{(2n+1)!}$$

for $n \geq 0$ with $H(0) = 1$.

Consider the alphabet $\{2,3\}$; give to the letter 2 the weight 2 and to the letter 3 the weight 3, so that the word $2^b \cdot 3 \cdot 2^a$ has weight $2a+2b+3$, while the word 2^n has weight $2n$. Give also the weight ℓ to $\zeta(\ell)$ for $\ell \geq 2$ (this is an abuse of langage). Looking at homogeneous relations, one considers on the one side the numbers $H(a,b)$ and on the other side the numbers $\zeta(\ell)H(m)$ with $\ell \geq 2$ and $m \geq 0$, restricted to the relation $2a+2b+3 = \ell + 2m$, hence $\ell = 2a+2b+3-2m$ is odd.

Theorem 10 (Zagier, 2011)**.** *Let a and b be non–negative integers. Set $k = 2a+2b+3$. Then there exist $a+b+1$ rational integers $c_{m,r,a,b}$ with $m \geq 0$, $r \geq 1$, $m+r = a+b+1$, such that*

$$H(a,b) = \sum_{m+r=a+b+1} c_{m,r,a,b} H(m)\zeta(2r+1).$$

Conversely, given two integers r and m with $r \geq 1$ and $m \geq 0$, there exist $m+r$ rational numbers $c'_{m,r,a,b}$ with $a \geq 0$, $b \geq 0$, $a+b = m+r-1$, such that

$$H(m)\zeta(2r+1) = \sum_{a+b=m+r-1} c'_{m,r,a,b} H(a,b).$$

The integers $c_{m,r,a,b}$ are explicitly given:

$$c_{m,r,a,b} = 2(-1)^r \left[\binom{2r}{2a+2} - \left(1 - \frac{1}{2^{2r}}\right)\binom{2r}{2b+1} \right]$$

The second part of Theorem 10 means that the square matrix $\bigl(c_{m,r,a,b}\bigr)$, of size $a+b+1$, has maximal rank.

We only give the sketch of proof of the first part of Theorem 10. Consider the generating series

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

and

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

where

$$\widehat{H}(a,b) = \sum_{m=0}^{a+b} c_{m,a,b}H(m)\zeta(k-2m).$$

The first step relates $F(x,y)$ to a hypergeometric series ${}_3F_2$, namely $F(x,y)$ is the product of $(1/\pi)\sin(\pi y)$ by the z–derivative at $z=0$ of the function

$${}_3F_2\left(\begin{matrix} x,\ -x,\ z \\ 1+y,\ 1-y \end{matrix}\middle| 1\right).$$

The second step relates $\widehat{F}(x,y)$ to the digamma function $\psi(x) = \Gamma'(x)/\Gamma(x)$ (logarithmic derivative of Γ), namely $\widehat{F}(x,y)$ is a linear combination of fourteen functions of the form

$$\psi\left(1+\frac{u}{2}\right)\frac{\sin(\pi v)}{2\pi} \quad \text{with} \quad u \in \{\pm x \pm y,\ \pm 2x \pm 2y,\ \pm 2y\} \quad \text{and} \quad v \in \{x,y\}.$$

The third step is the proof that F and $\widehat{F}$ are both entire function on $\mathbf{C}\times\mathbf{C}$, they are bounded by a constant multiple of $e^{\pi X}\log X$ when $X = \max\{|x|,|y|\}$ tends to infinity, and also by a constant multiple of $e^{\pi|\Im(y)|}$ when $|y|$ tends to infinity while $x \in \mathbf{C}$ is fixed.

The fourth step is about the diagonal: for $z \in \mathbf{C}$, we have

$$F(z,z) = \widehat{F}(z,z).$$

Several equivalent explicit formula for this function are given. Let

$$A(z) := -\frac{\pi}{\sin(\pi z)}F(z,z).$$

Then

$$A(z) = \sum_{r=1}^{\infty}\zeta(2r+1)z^{2r} = \sum_{n=1}^{\infty}\frac{z^2}{n(n^2-z^2)}$$

and

$$A(z) = \frac{1}{2}\sum_{n=1}^{\infty}\left(\frac{1}{n-z}+\frac{1}{n+z}-\frac{2}{n}\right) = \psi(1) - \frac{1}{2}\big(\psi(1+z)+\psi(1-z)\big).$$

The fifth step shows that $F(n,y)$ and $\widehat{F}(n,y)$ are equal when $n \in \mathbf{N}$ and $y \in \mathbf{C}$, an explicit formula is given.

The sixth step shows that $F(x,k)$ and $\widehat{F}(x,k)$ are equal when $k \in \mathbf{N}$ and $x \in \mathbf{C}$, an explicit formula is given.
Now comes the conclusion, which rests on the next lemma:

Lemma 11. *An entire function $f : \mathbf{C} \to \mathbf{C}$ that vanishes at all rational integers and satisfies*

$$f(z) = O\left(e^{\pi|\Im(z)|}\right)$$

is a constant multiple of $\sin(\pi z)$.

A proof of this lemma, using a Theorem of Phragmén–Lindelöf, is given by Zagier (Lemma 2 in [14]), but he also notices that other references have been given subsequently to him, in particular by F. Gramain who pointed out that this lemma is known since the work of Pólya and Valiron; a reference is in the book of Boas on entire functions.

3 Lyndon words: conjectural transcendence basis

D. Broadhurst considered the question of finding a transcendence basis for the algebra of MZV, he suggested that one should consider Lyndon words. We first give the definitions.

Here we use the alphabet alphabet $A = \{a, b\}$. The set of words on A is denoted by A^* (see §6.2). The elements of A^* can be written

$$a^{n_1}b^{m_1}\cdots a^{n_k}b^{m_k}$$

with $k \geq 0$, $n_1 \geq 0$, $m_k \geq 0$ and $m_i \geq 1$ for $1 \leq i < k$, and with $n_i \geq 1$ for $2 \leq i \leq k$. We endowed A^* with the lexicographic order with $a < b$. A *Lyndon word* is a non–empty word $w \in A^*$ such that, for each decomposition $w = uv$ with $u \neq e$ and $v \neq e$, the inequality $w < v$ holds. Denote by $\mathcal{L}$ the set of Lyndon words. Examples of Lyndon words are a, b, ab^k $(k \geq 0)$, $a^\ell b$ $(\ell \geq 0)$, a^2b^2, a^2bab. Let us check, for instance, that a^2bab is a Lyndon word: this follows from the observation that a^2bab is smaller than any of

$$abab,\ bab,\ ab,\ b.$$

But a^2ba^2b is not a Lyndon word since $a^2ba^2b > a^2b$.

Any Lyndon word other than b starts with a and any Lyndon word other than a ends with b.

Here are the 21 Lyndon words on the alphabet $\{a, b\}$ with weight ≤ 15 when a has weight 2 and b weight 3:

$$a < a^6b < a^5b < a^4b < a^4b^2 < a^3b < a^3bab < a^3b^2 < a^3b^3 < a^2b < a^2bab$$
$$< a^2bab^2 < a^2b^2 < a^2b^2ab < a^2b^3 < ab < abab^2 < ab^2 < ab^3 < ab^4 < b.$$

We list them according to their weight $p = 2, \ldots, 15$, we display their number $N(p)$ and the corresponding multiple zeta values where the word a^n is replaced by the tuple $\{2\}_n$ and b^n by $\{3\}_n$:

$p = 2$; $N(2) = 1$; a; $\zeta(2)$
$p = 3$; $N(3) = 1$; b; $\zeta(3)$
$p = 4$; $N(4) = 0$
$p = 5$; $N(5) = 1$; ab; $\zeta(2, 3)$
$p = 6$; $N(6) = 0$
$p = 7$; $N(7) = 1$; a^2b; $\zeta(2, 2, 3)$
$p = 8$; $N(8) = 1$; ab^2; $\zeta(2, 3, 3)$
$p = 9$; $N(9) = 1$; a^3b; $\zeta(2, 2, 2, 3)$
$p = 10$; $N(10) = 1$; a^2b^2; $\zeta(2, 2, 3, 3)$
$p = 11$; $N(11) = 2$; a^4b, ab^3; $\zeta(2, 2, 2, 2, 3)$, $\zeta(2, 3, 3, 3)$
$p = 12$; $N(12) = 2$; a^3b^2, a^2bab; $\zeta(2, 2, 2, 3, 3)$, $\zeta(2, 2, 3, 2, 3)$
$p = 13$; $N(13) = 3$; a^5b, a^2b^3, $abab^2$;
$\zeta(2, 2, 2, 2, 2, 3)$, $\zeta(2, 2, 3, 3, 3)$, $\zeta(2, 3, 2, 3, 3)$
$p = 14$; $N(14) = 3$; a^4b^2, a^3bab, ab^4;
$\zeta(2, 2, 2, 2, 3, 3)$, $\zeta(2, 2, 2, 3, 2, 3)$, $\zeta(2, 3, 3, 3, 3)$
$p = 15$; $N(15) = 4$; a^6b, a^3b^3, a^2bab^2, a^2b^2ab; ;
$\zeta(2, 2, 2, 2, 2, 2, 3)$, $\zeta(2, 2, 2, 3, 3, 3)$, $\zeta(2, 2, 3, 2, 3, 3)$, $\zeta(2, 2, 3, 3, 2, 3)$.

Conjecture 12. *The set of multiple zeta values $\zeta(s_1, \ldots, s_k)$, with $k \geq 1$ and $s_j \in \{2, 3\}$ for $1 \leq j \leq k$, such that $s_1 s_2 \cdots s_k$ is a Lyndon word on the alphabet $\{2, 3\}$, give a transcendence basis of $\mathfrak{Z}$.*

The number $N(p)$ of elements of weight p in a transcendence basis of $\mathfrak{Z}$ should not depend on the choice of the transcendence basis, and it should be the number of Lyndon words of weight p on the alphabet $\{2, 3\}$.

In the next section we shall see that for $p \geq 1$ we have

$$N(p) = \frac{1}{p} \sum_{\ell | p} \mu(p/\ell) P_\ell$$

where $(P_\ell)_{\ell \geq 1}$ is the linear recurrence sequence defined by

$$P_\ell = P_{\ell-2} + P_{\ell-3} \quad \text{for } \ell \geq 4$$

with the initial conditions

$$P_1 = 0, \quad P_2 = 2, \quad P_3 = 3.$$

If one forgets about the weight of the words, one may list the Lyndon words according to the number of letters (which correspond to the length for MZV with $s_j \in \{2, 3\}$), which yields a partial order on the words on the alphabet $\{a, b\}$ where there are 2^k words with k letters. Here are the Lyndon words with k letters on the alphabet $\{a, b)$ for the first values of k, with their numbers L_k:
$k = 1$, $L_1 = 2$; a, b.
$k = 2$, $L_2 = 1$; ab.

$k = 3, \quad L_3 = 2; \qquad a^2b,\ ab^2.$
$k = 4, \quad L_4 = 3, \qquad a^3b,\ a^2b^2,\ ab^3.$
$k = 5, \quad L_5 = 6, \qquad a^4b,\ a^3b^2,\ a^2bab,\ a^2b^3,\ abab^2,\ ab^4.$
$k = 6, \quad L_6 = 9, \qquad a^5b,\ a^4b^2,\ a^3bab,\ a^3b^3,\ a^2ba^2b,\ a^2bab^2,\ a^2b^2ab,\ abab^3,\ ab^5$

The sequence $(L_k)_{k\geq 1}$ starts with

$$2, 1, 2, 3, 6, 9, 18, 30, 56, 99, 186, 335, 630, 1161, 2182, 4080, 7710, 14532, 27594, \ldots$$

(See [3] `A001037`).