# Double zeta values and modular forms *

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The *double zeta value* is defined by the convergent series

$$\zeta(k_1,k_2)=\sum_{m_1>m_2>0}\frac{1}{m_1^{k_1}m_2^{k_2}},$$

where $k_1$ and $k_2$ are positive integers with $k_1>1$. This is a special case ("depth 2") of the *multiple zeta value*, which is defined by

$$\zeta(k_1,k_2,\ldots,k_n)=\sum_{m_1>m_2>\cdots>m_n>0}\frac{1}{m_1^{k_1}m_2^{k_2}\cdots m_n^{k_n}},$$

and was studied already back in 18th century by Euler. For the multiple zeta value $\zeta(k_1,k_2,\ldots,k_n)$, the number $k_1+k_2+\cdots+k_n$ is called *weight*, and $n$ *depth*. Hence, for the double zeta value $\zeta(k_1,k_2)$, the weight is $k_1+k_2$ and the depth is 2. For some technical reason, we shall look at the modified double zeta values $\widetilde{\zeta}(k_1,k_2)$ defined by

$$\widetilde{\zeta}(k_1,k_2):=(2\pi\sqrt{-1})^{-(k_1+k_2)}\zeta(k_1,k_2).$$

We are interested in the $\mathbb{Q}$-vector space spanned by the double zeta values of fixed weight.

**Definition.** *For $k\geq 3$, define the $\mathbb{Q}$-vector space $\mathcal{DZ}_k$ by*

$$\mathcal{DZ}_k=\sum_{i=2}^{k-1}\mathbb{Q}\widetilde{\zeta}(i,k-i).$$

Some ten years ago, Don Zagier conjectured

**Conjecture (Zagier).** *For $k\geq 3$, we have*

$$\begin{aligned}\dim_{\mathbb{Q}}\mathcal{DZ}_k &= \left[\frac{k+1}{2}\right]-1-\dim_{\mathbb{C}}S_k(SL_2(\mathbb{Z}))\\ &= \begin{cases}\dfrac{k}{2}-1-\dim_{\mathbb{C}}S_k(SL_2(\mathbb{Z})) & \text{if } k \text{ is even},\\ \dfrac{k-1}{2} & \text{if } k \text{ is odd}.\end{cases}\end{aligned}$$

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*Here, $S_k(SL_2(\mathbb{Z}))$ is the $\mathbb{C}$-vector space of cusp forms of weight $k$ for the modular group $SL_2(\mathbb{Z})$.*

In the following, we shall sketch a proof of the inequality

$$\dim_{\mathbb{Q}} \mathcal{DZ}_k \leq \left[\frac{k+1}{2}\right] - 1 - \dim_{\mathbb{C}} S_k(SL_2(\mathbb{Z})),$$

by studying the "*double Eisenstein series.*" This inequality was proved by Zagier himself and Goncharov in different methods. The stress here is the new approach using the double Eisenstein series. Note that the proof of the converse inequality "$\geq$", which together would establish the validity of the conjecture, seems to be out of reach. (Recall that we do not know for instance if $\dim_{\mathbb{Q}}\left(\mathbb{Q}\widetilde{\zeta}(2,4)+\mathbb{Q}\widetilde{\zeta}(3,3)\right) > 1$, nor any single example with $\dim_{\mathbb{Q}} \mathcal{DZ}_k > 1$.)

**Definition.** *For $\tau \in \mathfrak{H}$ := upper half-plane, an element $\lambda = m\tau + n \in \mathbb{Z}\tau + \mathbb{Z}$ is positive, denoted by $\lambda > 0$, if either $m > 0$ or $m = 0$, $n > 0$. For $\lambda$, $\mu \in \mathbb{Z}\tau + \mathbb{Z}$, we write $\lambda > \mu$ if $\lambda - \mu > 0$.*

We define the Eisenstein series $G_k(\tau)$ for $k \geq 3$ and the *double Eisenstein series* $G_{k,l}(\tau)$ for $k \geq 3$, $l \geq 2$ by

$$G_k(\tau) = \sum_{m\tau+n>0} \frac{1}{(m\tau+n)^k}$$

and

$$G_{k,l}(\tau) = \sum_{\substack{\lambda>\mu>0 \\ \lambda,\mu\in\mathbb{Z}\tau+\mathbb{Z}}} \frac{1}{\lambda^k \mu^l}.$$

If $k = 2$, the series defining $G_k(\tau)$ is not absolutely convergent and we define $G_2(\tau)$ by

$$G_2(\tau) = \zeta(k) + \sum_{m=1}^{\infty}\sum_{n\in\mathbb{Z}} \frac{1}{(m\tau+n)^k}.$$

As for $G_{k,l}(\tau)$, the situation is more subtle unless $k \geq 3$, $l \geq 2$. We shall define $G_{k,l}(\tau)$ in the non-absolutely convergent case by the $q$-series given below.

Put $\widetilde{G}_k(\tau) = (2\pi\sqrt{-1})^{-k} G_k(\tau)$ and $\widetilde{G}_{k,l}(\tau) = (2\pi\sqrt{-1})^{-k-l} G_{k,l}(\tau)$. We give Fourier expansions of $\widetilde{G}_k(\tau)$ and $\widetilde{G}_{k,l}(\tau)$.

The expansion of $\widetilde{G}_k(\tau)$ is standard and is given by

$$\widetilde{G}_k(\tau) = \widetilde{\zeta}(k) + \frac{(-1)^k}{(k-1)!}\sum_{n=1}^{\infty} \sigma_{k-1}(n) q^n,$$

where $\widetilde{\zeta}(k) = (2\pi\sqrt{-1})^{-k}\zeta(k)$, $\sigma_{k-1}(n) = \sum_{d|n} d^{k-1}$, $q = e^{2\pi\sqrt{-1}\tau}$. Note that the series has rational coefficients except the constant term for odd $k$, which is pure imaginary. Put $g_k = \frac{(-1)^k}{(k-1)!} \sum_{n=1}^{\infty} \sigma_{k-1}(n) q^n$ so that $\widetilde{G}_k(\tau) = \widetilde{\zeta}(k) + g_k$.

**Proposition 1.** *Let $k \geq 3$ and $1 \leq i \leq k-2$. A Fourier series of $\widetilde{G}_{k-i,i}(\tau)$ is given by*

$$\begin{aligned} \widetilde{G}_{k-i,i}(\tau) &= \widetilde{\zeta}(k-i,i) + \widetilde{\zeta}(i)\, g_{k-i} \\ &+ (-1)^i \sum_{j=2}^{k-2} \left\{ \binom{j-1}{i-1} + (-1)^{k+j} \binom{j-1}{k-i-1} \right\} \widetilde{\zeta}(j)\, g_{k-j} \\ &+ \frac{(-1)^k}{(i-1)!(k-i-1)!} \sum_{m>n>0} \left( \sum_{u>0} u^{k-i-1} q^{mu} \right) \left( \frac{1}{2}\delta_{i,1} + \sum_{v>0} v^{i-1} q^{nv} \right). \end{aligned}$$

*(We set $\widetilde{\zeta}(1) = 0$. The right-hand side is the definition of $\widetilde{G}_{k-i,i}(\tau)$ unless $k \geq 5$ and $i \geq 2$.)*

We note that the series belongs to $\sqrt{-1}^k \mathbb{R} + q\mathbb{Q}[[q]] + \sqrt{-1} q \mathbb{R}[[q]]$. Later we shall consider the "imaginary part" of $\widetilde{G}_{k-i,i}(\tau)$ when $k$ is even, which is a rational linear combination of $\widetilde{\zeta}(j) g_{k-j}$ for odd $j$.

**Proposition 2 (shuffle products).** *For $k \geq 3$ and $2 \leq i \leq k/2$, we have the following relations.*

*(i)* $\widetilde{G}_i(\tau)\, \widetilde{G}_{k-i}(\tau) = \widetilde{G}_{i,k-i}(\tau) + \widetilde{G}_{k-i,i}(\tau) + \widetilde{G}_k(\tau)$.

*(ii)* $\widetilde{G}_i(\tau)\, \widetilde{G}_{k-i}(\tau) = \sum_{j=2}^{k-1} \left\{ \binom{j-1}{i-1} + \binom{j-1}{k-i-1} \right\} \widetilde{G}_{j,k-j}(\tau)$.

*Proof.* Rather tedious computations involving binomial identities. The computation only uses the $q$-expansions to avoid manipulation of conditionally convergent series. □

**Corollary.** *For $k \geq 3$ and $2 \leq i \leq k/2$, we have the "double shuffle relation"*

$$\sum_{j=2}^{k-1} \left\{ \binom{j-1}{i-1} + \binom{j-1}{k-i-1} - \delta_{i,j} - \delta_{k-i,j} \right\} \widetilde{G}_{j,k-j}(\tau) - \widetilde{G}_k(\tau) = 0,$$

*($\delta_{i,j}$ = Kronecker's delta).*

Taking the constant term of the Fourier expansion of this expression, we obtain the double shuffle relation of double zeta values. If we formally put $i = 1$ in that relation, the divergent terms cancel out (formally) and we obtain the "sum formula"

$$\sum_{j=2}^{k-1} \widetilde{\zeta}(j, k-j) = \widetilde{\zeta}(k),$$

which is thought of as an example of the "regularized double shuffle relations." The next proposition "lifts" the sum formula for double zeta values, but involves one extra term of the derivative of the (single) Eisenstein series.

**Proposition 3.** *For $k \geq 3$, we have*

$$\sum_{j=2}^{k-1} \widetilde{G}_{j,k-j}(\tau) = \widetilde{G}_k(\tau) - \frac{\widetilde{G}'_{k-2}(\tau)}{2(k-2)}, \qquad ({}' = q\frac{d}{dq} = \frac{1}{2\pi\sqrt{-1}}\frac{d}{d\tau}).$$

*Proof.* Also a quite complicated calculation using $q$-series. We need a formula for the sum of powers of integers in terms of Bernoulli polynomials and the lemma below. □

**Lemma.** *Let $M$ and $N$ be positive integers. We have the following equality of disjoint unions of sets of integers.*

$$\coprod_{j=0}^{M-1} \{\textit{divisors of } N(M-j) \textit{ with } > j\} = \coprod_{j=1}^{M} \{\textit{divisors of } Nj \textit{ with } \geq j\}.$$

*In particular* $(N = 1)$,

$$\bigcup_{j=0}^{M-1} \{\textit{divisors of } M-j \textit{ with } > j\} = \{1, 2, \ldots, M\}.$$

Combining Proposition 3 with a formula of Ramanujan, we obtain a refinement of the sum formula.

**Corollary.**

(i)

$$\sum_{\substack{j=2 \\ j:even}}^{k-2} \widetilde{G}_{j,k-j}(\tau) = \frac{3}{4}\widetilde{G}_k(\tau) - \frac{\widetilde{G}'_{k-2}(\tau)}{2(k-2)}.$$

(ii)

$$\sum_{\substack{j=3 \\ j:odd}}^{k-1} \widetilde{G}_{j,k-j}(\tau) = \frac{1}{4}\widetilde{G}_k(\tau).$$

**Definition.** *For $k \geq 3$, put*

$$\mathcal{DE}_k = \sum_{i=2}^{k-1} \mathbb{Q}\, \widetilde{G}_{i,k-i}(\tau).$$

Assume $k$ is even $\geq 4$ (odd weight case is treated similarly but less interesting because of the absence of modular forms).

**Proposition 4.** *We have*

$$M_k^{\mathbb{Q}}(SL_2(\mathbb{Z})) \oplus \mathbb{Q}\,\widetilde{G}'_{k-2}(\tau) \subseteq \mathcal{DE}_k,$$

*where $M_k^{\mathbb{Q}}(SL_2(\mathbb{Z}))$ is the $\mathbb{Q}$-vector space of holomorphic modular forms of weight $k$ on $SL_2(\mathbb{Z})$ whose Fourier coefficients belong to $\mathbb{Q}$.*

*Proof.* We know $\mathcal{DE}_k \ni \widetilde{G}_k, \widetilde{G}'_{k-2}, \widetilde{G}_i \cdot \widetilde{G}_{k-i}$ $(4 \leq i \leq k/2)$ by the shuffle products (Proposition 2) and the sum formula (Proposition 3). In view of works of Rankin and Eichler-Shimura (do we really need all this?), the space $M_k^{\mathbb{Q}}(SL_2(\mathbb{Z}))$ is spanned by $\widetilde{G}_k$ and $\widetilde{G}_i \cdot \widetilde{G}_{k-i}$ $(4 \leq i \leq k/2)$, hence the result follows. □

**Proposition 5.** *The space $\mathcal{DE}_k$ is spanned by $\widetilde{G}_{i,k-i}(\tau)$ $(k/2+2 \leq i \leq k-1)$, $\widetilde{G}_k(\tau)$, and $\widetilde{G}'_{k-2}(\tau)$. In particular, we have $\dim_{\mathbb{Q}} \mathcal{DE}_k \leq k/2$.*

*Proof.* The double shuffle relations (Corollary to Proposition 2) and the sum formula (Proposition 3) give $k/2$ linear relations among $\widetilde{G}_k, \widetilde{G}'_{k-2}, \widetilde{G}_{k-i,i}$ $(1 \leq i \leq k-2)$. Looking at the coefficients, the proposition directly follows. □

Now we consider two projections $\pi_1: \mathcal{DE}_k \longrightarrow \mathcal{DZ}_k$ and $\pi_2: \mathcal{DE}_k \longrightarrow \Im\mathcal{DE}_k$, where, for $f \in \mathcal{DE}_k$, we define

$$\begin{aligned} \pi_1(f) &= \text{constant term of the Fourier series of } f, \\ \pi_2(f) &= \text{imaginary part (times } \sqrt{-1}) \text{ of the Fourier series of } f. \end{aligned}$$

The space $\Im\mathcal{DE}_k$ is the "imaginary part" of $\mathcal{DE}_k$, embedded into $\mathbb{C}[[q]]$ via Fourier series. By definition, we have the following two exact sequences

$$0 \longrightarrow \ker \pi_1 \longrightarrow \mathcal{DE}_k \xrightarrow{\pi_1} \mathcal{DZ}_k \longrightarrow 0$$

and

$$0 \longrightarrow \ker \pi_2 \longrightarrow \mathcal{DE}_k \xrightarrow{\pi_2} \Im\mathcal{DE}_k \longrightarrow 0.$$

**Theorem 1 (Goncharov, Zagier).** *For $k \geq 4$ even, we have*

$$\dim_{\mathbb{Q}} \mathcal{DZ}_k \leq \frac{k}{2} - 1 - \dim S_k(SL_2(\mathbb{Z})).$$

*Proof.* We know by Proposition 4 that $\ker \pi_1 \supseteq S_k^{\mathbb{Q}}(SL_2(\mathbb{Z})) \oplus \mathbb{Q}\,\widetilde{G}'_{k-2}(\tau)$. From this and Proposition 5, we obtain the theorem. □

The equality holds if and only if both $\dim \mathcal{DZ}_k = k/2$ and $\ker \pi_1 = S_k^{\mathbb{Q}}(SL_2(\mathbb{Z})) \oplus \mathbb{Q}\,\widetilde{G}'_{k-2}(\tau)$ hold true.

As for the second exact sequence, we see by Proposition 1 (Fourier series) that the map $\pi_2$ on the generators (abundant) $\widetilde{G}_{i,k-i}(\tau)$ $(2 \le i \le k-2)$ is given explicitly by

$$
\begin{aligned}
&{}^t(\pi_2(\widetilde{G}_{2,k-2}), \pi_2(\widetilde{G}_{3,k-3}), \dots, \pi_2(\widetilde{G}_{k-2,2})) \\
&\qquad = Q_k \cdot {}^t(\widetilde{\zeta}(3) g_{k-3}, \widetilde{\zeta}(5) g_{k-5}, \dots, \widetilde{\zeta}(k-3) g_3),
\end{aligned}
$$

with

$$
\begin{aligned}
Q_k &:= \left( \delta_{k-i,j} + (-1)^{i+j} \binom{j-1}{i-1} + (-1)^{k+i} \binom{j-1}{k-i-1} \right)_{\substack{2 \le i \le k-2 \\ 2 \le j \le k-2,\ j:odd}} \\
&= \left( \delta_{k-2-i,2j} + (-1)^{i} \binom{2j}{i} - (-1)^{i} \binom{2j}{k-2-i} \right)_{\substack{1 \le i \le k-3 \\ 1 \le j \le k/2-2}}.
\end{aligned}
$$

**Theorem 2.** $\operatorname{rank} Q_k = k/2 - 2 - \dim S_k(SL_2(\mathbb{Z}))$.

*Proof.* Use the theory of periods of $S_k(SL_2(\mathbb{Z}))$. □

Now we impose the hypothesis:

Hypothesis $(OZ)_k$: $\widetilde{\zeta}(3), \widetilde{\zeta}(5), \dots, \widetilde{\zeta}(k-3)$ are all linearly independent over $\mathbb{Q}$.

**Proposition 6.** *Under the hypothesis* $(OZ)_k$, *we have* $\dim \mathcal{DE}_k = k/2$, $\dim \Im\mathcal{DE}_k = k/2 - 1 - \dim M_k(SL_2(\mathbb{Z}))$, *and* $\ker \pi_2 = M_k^{\mathbb{Q}} \oplus \mathbb{Q}\widetilde{G}_{k-2}(\tau)$.

The matrix $Q_k$ is nice. It's kernel vectors on the right give even period polynomials, whereas those on the left give linear combinations of double Eisenstein series which become modular, so their constant terms give relations of double zeta values.

**Example** For $k = 12$, we have

$$
Q_{12} = \begin{pmatrix}
-2 & -4 & -6 & -8 \\
1 & 6 & 15 & 28 \\
0 & -4 & -20 & -48 \\
0 & 1 & 15 & 42 \\
0 & 0 & 0 & 0 \\
0 & 0 & -14 & -42 \\
0 & 4 & 20 & 48 \\
0 & -6 & -15 & -27 \\
2 & 4 & 6 & 8
\end{pmatrix}.
$$

The kernel vector

$$
Q_{12} \begin{pmatrix} 1 \\ -3 \\ 3 \\ -1 \end{pmatrix} = \mathbf{0}
$$

corresponds to the even period polynomial $X^8 - 3X^6 + 3X^4 - X^2$.

On the other hand, the kernel on the left of $Q_{12}$ is 6 $(= k/2 - 1 + \dim S_k)$ dimensional and spanned by

$$\begin{array}{ll} (1,0,0,0,0,0,0,0,1), & (0,0,7,28,0,20,0,0,0) \\ (0,0,1,0,0,0,1,0,0), & (15,30,6,0,0,0,0,16,0) \\ (0,0,0,0,1,0,0,0,0), & (5,10,12,8,0,0,0,0,0). \end{array}$$

The three vectors on the first column come from the product of ordinary Eisenstein series. For instance, $(1,0,0,0,0,0,0,0,1)$ corresponds to the fact that $\widetilde{G}_{2,10}(\tau) + \widetilde{G}_{10,2}(\tau)$ has $\mathbb{Q}$-rational coefficients, which is clear from the shuffle product identity

$$\widetilde{G}_{2,10}(\tau) + \widetilde{G}_{10,2}(\tau) = \widetilde{G}_2(\tau)\widetilde{G}_{10}(\tau) - \widetilde{G}_{12}(\tau).$$

As an other example, let us take $(0,0,7,28,0,20,0,0,0)$. Corresponding to this, we have the relation

$$7\widetilde{G}_{4,8}(\tau) + 28\widetilde{G}_{5,7}(\tau) + 20\widetilde{G}_{7,5}(\tau) = \frac{3\cdot 11\cdot 149}{2^2\cdot 691}\widetilde{G}_{12}(\tau) - \frac{1}{2^7\cdot 3^2\cdot 5\cdot 691}\Delta(\tau).$$

$(\Delta(\tau) = q\prod_{n=1}^{\infty}(1-q^n)^{24})$ and hence

$$\begin{aligned} \Delta(\tau) \;=\; & 2^5\cdot 3^3\cdot 5\cdot 11\cdot 149\,\widetilde{G}_{12}(\tau) - 2^7\cdot 3^2\cdot 5\cdot 7\cdot 691\,\widetilde{G}_{4,8}(\tau) \\ & -2^9\cdot 3^2\cdot 5\cdot 7\cdot 691\,\widetilde{G}_{5,7}(\tau) - 2^9\cdot 3^2\cdot 5^2\cdot 691\,\widetilde{G}_{7,5}(\tau). \end{aligned}$$

Comparing the Fouries coefficients on both sides, we obtain (apparently new) formula for $\tau(n)$, the $n$th Fourier coefficient of $\Delta(\tau)$:

$$\begin{aligned} \tau(n) \;=\; & \frac{149}{840}\sigma_{11}(n) - \frac{691}{180}\sigma_7(n) - \frac{11747}{126}\sigma_5(n) + \frac{173441}{360}\sigma_3(n) \\ & -\frac{3455}{9}\sigma_1(n) - \frac{2764}{3}\rho_{3,7}(n) - \frac{19348}{3}\rho_{4,6}(n) - \frac{13820}{3}\rho_{6,4}(n) \\ =\; & \frac{149}{2^3\cdot 3\cdot 5\cdot 7}\sigma_{11}(n) - \frac{691}{2^2\cdot 3^2\cdot 5}\sigma_7(n) - \frac{17\cdot 691}{2\cdot 3^2\cdot 7}\sigma_5(n) \\ & +\frac{251\cdot 691}{2^3\cdot 3^2\cdot 5}\sigma_3(n) - \frac{5\cdot 691}{3^2}\sigma_1(n) - \frac{2^2\cdot 691}{3}\rho_{3,7}(n) \\ & -\frac{2^2\cdot 7\cdot 691}{3}\rho_{4,6}(n) - \frac{2^2\cdot 5\cdot 691}{3}\rho_{6,4}(n), \end{aligned}$$

where

$$\rho_{k,l}(n) := \sum_{\substack{a+b=n \\ a,b>0}} \sum_{\substack{u|a,\, v|b \\ \frac{a}{u} > \frac{b}{v}}} u^k\, v^l.$$

Or if we take the simplest $(0,0,0,0,1,0,0,0,0)$, we have correspondingly (or from $\widetilde{G}_{6,6}(\tau) = (\widetilde{G}_6(\tau)^2 - \widetilde{G}_{12}(\tau))/2$)

$$\widetilde{G}_{6,6}(\tau) = \frac{2^2\cdot 3}{691}\widetilde{G}_{12}(\tau) - \frac{1}{2^7\cdot 3\cdot 5^2\cdot 691}\Delta(\tau),$$

and thus

$$\Delta(\tau) = 2^9 \cdot 3^2 \cdot 5^2 \, \widetilde{G}_{12}(\tau) - 2^7 \cdot 3 \cdot 5^2 \cdot 691 \, \widetilde{G}_{6,6}(\tau).$$

Comparing the coefficients, we obtain

$$\begin{aligned} \tau(n) &= \frac{2}{693}\sigma_{11}(n) + \frac{691}{2^2 \cdot 3^2 \cdot 7}\sigma_5(n) - \frac{691}{2^2 \cdot 3^2}\sigma_3(n) + \frac{5 \cdot 691}{2 \cdot 3^2 \cdot 11}\sigma_1(n) \\ &- \frac{2 \cdot 691}{3}\rho_{5,5}(n). \end{aligned}$$

Since $693 = 691 + 2$, it is transparent that we have the famous congruence of Ramanujan:

$$\tau(n) \equiv \sigma_{11}(n) \pmod{691}.$$

The other example $(5, 10, 12, 8, 0, 0, 0, 0, 0)$ gives

$$\begin{aligned} &5\widetilde{G}_{2,10}(\tau) + 10\widetilde{G}_{3,9}(\tau) + 12\widetilde{G}_{4,8}(\tau) + 8\widetilde{G}_{5,7}(\tau) \\ &\qquad = \frac{41 \cdot 1321}{2^2 \cdot 3 \cdot 691}\widetilde{G}_{12}(\tau) + \frac{1}{2^4 \cdot 3 \cdot 5 \cdot 7 \cdot 691}\Delta(\tau) - \frac{1}{4}\widetilde{G}'_{10}(\tau) \end{aligned}$$

and taking it's constant term

$$5\zeta(2, 10) + 10\zeta(3, 9) + 12\zeta(4, 8) + 8\zeta(5, 7) = \frac{41 \cdot 1321}{2^2 \cdot 3 \cdot 691}\zeta(12).$$

Also we have yet another formula for $\tau(n)$, etc.

# References


[1] D. Zagier, Periods of modular forms, trace of Hecke operators, and multiple zeta values, *RIMS Kokyuroku*, **843**, (1993), 162–170.

[2] D. Zagier, Values of zeta functions and their applications, in *First European Congress of Mathematics, Volume II*, *Progress in Math.*, **120**, (1994), 497-512.