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Multiple zeta values of fixed weight, depth, and height

by Yasuo Ohno* and Don Zagier

Department of Mathematics, Faculty of Science and Engineering, Kinki University, Higashi-Osaka, Osaka, 577-8502 Japan
e-mail: ohno@math.kindai.ac.jp
Max-Planck-Institut für Mathematik, Vivatsgasse 7, 53111 Bonn, Germany
e-mail: zagier@mpim-bonn.mpg.de

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ABSTRACT

We give a generating function for the sums of multiple zeta values of fixed weight, depth and height in terms of Riemann zeta values.

For any multi-index $\mathbf{k} = (k_1, k_2, \ldots, k_n)$ $(k_i \in \mathbf{Z}_{>0})$, the *weight*, *depth*, and *height* of $\mathbf{k}$ are by definition the integers $k = k_1 + k_2 + \cdots + k_n$, n, and $s = \#\{i \mid k_i > 1\}$, respectively. We denote by $I(k,n,s)$ the set of multi-indices $\mathbf{k}$ of weight k, depth n, and height s, and by $I_0(k,n,s)$ the subset of *admissible* indices, i.e., indices with the extra requirement that $k_n \geq 2$. For any admissible index $\mathbf{k} = (k_1, k_2, \ldots, k_n) \in I_0(k,n,s)$, the *multiple zeta value* $\zeta(\mathbf{k})$ is defined by

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

We denote by $G_0(k,n,s)$ the value of the sum

$$(1) \qquad G_0(k,n,s) = \sum_{\mathbf{k}\in I_0(k,n,s)} \zeta(\mathbf{k}).$$

Since the set $I_0(k,n,s)$ is non-empty only if the indices k, n and s satisfy the in-

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equalities $s \geq 1$, $n \geq s$, and $k \geq n+s$, we can collect all the numbers $G_0(k,n,s)$ into a single generating function

$$(2) \qquad \Phi_0(x,y,z) \;=\; \sum_{k,n,s} G_0(k,n,s)\, x^{k-n-s}\, y^{n-s}\, z^{s-1} \quad \in \mathbf{R}[[x,y,z]].$$

Our main result will then be

Theorem 1. *The power series* (2) *is given by*

$$(3) \qquad \Phi_0(x,y,z) \;=\; \frac{1}{xy-z}\left(1 - \exp\left(\sum_{n=2}^{\infty} \frac{\zeta(n)}{n}\, S_n(x,y,z)\right)\right),$$

where the polynomials $S_n(x,y,z) \in \mathbf{Z}[x,y,z]$ are defined by the formula

$$(4) \qquad S_n(x,y,z) \;=\; x^n + y^n - \alpha^n - \beta^n. \qquad \alpha,\beta \;=\; \frac{x+y \pm \sqrt{(x+y)^2 - 4z}}{2}$$

or alternatively by the identity

$$(5) \qquad \log\left(1 - \frac{xy-z}{(1-x)(1-y)}\right) \;=\; \sum_{n=2}^{\infty} \frac{S_n(x,y,z)}{n}$$

together with the requirement that $S_n(x,y,z^2)$ is a homogeneous polynomial of degree n. In particular, all of the coefficients $G_0(k,n,s)$ of $\Phi_0(x,y,z)$ can be expressed as polynomials in $\zeta(2)$, $\zeta(3)$, ... with rational coefficients.

In view of (5), we can also restate (3) in the alternative form

$$(6) \qquad 1 - (xy-z)\,\Phi_0(x,y,z) \;=\; \prod_{m=1}^{\infty}\left(1 - \frac{xy-z}{(m-x)(m-y)}\right),$$

which is simpler looking but does not directly give the coefficients of the power series as finite expressions in terms of Riemann zeta values.

Proof. A convenient approach to the multiple zeta value $\zeta(\mathbf{k})$ is to consider it as the limiting value at $t = 1$ of the function

$$L_{\mathbf{k}}(t) \;=\; L_{k_1,k_2,\ldots,k_n}(t) = \sum_{0<m_1<m_2<\cdots<m_n} \frac{t^{m_n}}{m_1{}^{k_1} m_2{}^{k_2} \cdots m_n{}^{k_n}} \qquad (|t|<1).$$

(Note that we consider $L_{\mathbf{k}}(t)$ not just for $\mathbf{k} \in I_0$ but for all $\mathbf{k} \in I$.) For $\mathbf{k}$ empty we define $L_{\mathbf{k}}(t)$ to be 1. For non-negative integers k, n and s set

$$G(k,n,s;t) \;=\; \sum_{\mathbf{k} \in I(k,n,s)} L_{\mathbf{k}}(t)$$

(so $G(0,0,0;t) = 1$ and $G(k,n,s;t) = 0$ unless $k \geq n+s$ and $n \geq s \geq 0$), and let $G_0(k,n,s;t)$ be the function defined by the same formula but with the summation restricted to $\mathbf{k} \in I_0(k,n,s)$. We denote by $\Phi = \Phi(x,y,z;t)$ and $\Phi_0 = \Phi_0(x,y,z;t)$ the corresponding generating functions

$$\Phi = \sum_{k,n,s\geq 0} G(k,n,s;t) x^{k-n-s} y^{n-s} z^s = 1 + L_1(t)y + L_{1,1}(t)y^2 + \cdots$$

and

$$\Phi_0 = \sum_{k,n,s\geq 0} G_0(k,n,s;t) x^{k-n-s} y^{n-s} z^{s-1} = L_2(t) + L_{1,2}(t)y + L_3(t)x + \cdots .$$

Our object is to express the generating function $\Phi_0(x,y,z) = \Phi_0(x,y,z;1)$ in terms of Riemann zeta values. Using the obvious formula

$$\frac{d}{dt} L_{k_1,\ldots,k_n}(t) = \begin{cases} t^{-1} L_{k_1,\ldots,k_{n-1},k_n-1}(t) & \text{if} \quad k_n \geq 2, \\ (1-t)^{-1} L_{k_1,\ldots,k_{n-1}}(t) & \text{if} \quad k_n = 1 \end{cases}$$

for the derivative of $L_{\mathbf{k}}(t)$, we obtain

$$\frac{d}{dt} G_0(k,n,s;t) = \frac{1}{t}\Big(G(k-1,n,s-1;t) - G_0(k-1,n,s-1;t) + G_0(k-1,n,s;t)\Big),$$

$$\frac{d}{dt}\Big(G(k,n,s;t) - G_0(k,n,s;t)\Big) = \frac{1}{1-t} G(k-1,n-1,s;t)$$

or, in terms of generating functions,

$$\frac{d\Phi_0}{dt} = \frac{1}{yt}\Big(\Phi - 1 - z\Phi_0\Big) + \frac{x}{t}\Phi_0. \qquad \frac{d}{dt}\Big(\Phi - z\Phi_0\Big) = \frac{y}{1-t}\Phi.$$

Eliminating Φ, we obtain the differential equation

$$t(1-t)\,\frac{d^2\Phi_0}{dt^2} + \Big((1-x)(1-t) - yt\Big)\,\frac{d\Phi_0}{dt} + (xy-z)\,\Phi_0 = 1$$

for the power series Φ_0. The unique solution of this vanishing at $t = 0$ is given by

$$\Phi_0(x,y,z;t) = \frac{1}{xy-z}\Big(1 - F(\alpha - x, \beta - x; 1 - x; t)\Big),$$

where $\alpha + \beta = x + y$, $\alpha\beta = z$ and $F(a,b;c;x)$ denotes the Gauss hypergeometric function. Specializing to $t = 1$ and using Gauss's formula for $F(a,b;c;1)$ gives

$$1 - (xy - z)\Phi_0(x,y,z;1) = F(\alpha - x, \beta - x; 1 - x; 1) = \frac{\Gamma(1-x)\Gamma(1-y)}{\Gamma(1-\alpha)\Gamma(1-\beta)},$$

and now using the expansion $\Gamma(1-x) = \exp\big(\gamma x + \sum_{n\geq 2} \zeta(n)\, x^n/n\big)$ yields equation (3).

We end by mentioning several special cases of the theorem which were previously known or are of special interest.

(1) Specializing (3) to $z = xy$ corresponds to dropping all information

about s, the number of indices k_i greater than 1, so the function $\Phi_0(x,y,xy)$ equals $\sum_{k>n>0} G_0(k,n)x^{k-n-1}y^{n-1}$ where $G_0(k,n) = \sum_s G_0(k,n,s)$ is the sum of all multiple zeta values of weight k and depth n. On the other hand, taking the limit as $z \to xy$ in (6), we find

$$\Phi_0(x,y,xy) = \sum_{m=2}^{\infty} \frac{1}{(m-x)(m-y)} = \sum_{k>n>0} \zeta(k)\, x^{k-n-1} y^{n-1},$$

so we obtain the sum formula $G_0(k,n) = \zeta(k)$ already proved in [1] and [6].

(2) If $s = 1$, then the only admissible multi-index of weight k and depth n is $(1,\dots,1,k-n)$ (with $n-1$ 1's), so $G(k,n,1) = \zeta(1,\dots,1,k-n)$. On the other hand, we have $S_n(x,y,0) = x^n + y^n - (x+y)^n$, so (3) for $z = 0$ reduces to

$$\sum_{a,b\geq 1} \zeta(\underbrace{1,\dots,1}_{a-1},b+1)\, x^a y^b = \Phi_0(x,y,0)$$
$$= \frac{1}{xy}\left(1 - \exp\left(\sum_{n=2}^{\infty} \zeta(n)\, \frac{x^n + y^n - (x+y)^n}{n}\right)\right),$$

a formula given also in [6].

(3) The well-known duality relation for multiple zeta values says that there is a bijection $\mathbf{k} \to \mathbf{k}'$ from $I_0(k,n,s)$ to $I_0(k,k-n,s)$ such that $\zeta(\mathbf{k}) = \zeta(\mathbf{k}')$ for all $\mathbf{k}$. In particular, $G_0(k,n,s) = G_0(k,k-n,s)$, so the generating function $\Phi_0(x,y,z)$ must be symmetric in x and y, a symmetry which is of course evident in the formula (3).

(4) Specializing (3) to $x = 0$ and $y = 0$ gives formulas for the sums of all multiple zeta values having all $k_i \geq 2$ or all $k_i \leq 2$, respectively. The simultaneous specialization to $x = y = 0$ corresponds to the unique zeta value $\zeta(2,\dots,2)$ (with $k = 2n = 2s$), so from (3) we get

$$\sum_{s=1}^{\infty} \zeta(\underbrace{2,\dots,2}_{s})\, z^{s-1} = \Phi_0(0,0,z) = -\frac{1}{z}\left(1 - \exp\left(-\sum_{n=1}^{\infty} \frac{\zeta(2n)}{n}\,(-z)^n\right)\right),$$
$$= \frac{1}{z}\left(\frac{\sinh \pi\sqrt{z}}{\pi\sqrt{z}} - 1\right) = \sum_{s=1}^{\infty} \frac{\pi^{2s}}{(2s+1)!}\, z^{s-1}$$

and hence

$$\zeta(\underbrace{2,\dots,2}_{s}) = \frac{\pi^{2s}}{(2s+1)!},$$

a formula also already given in [6].

(5) Finally, by specializing to $y = -x$ in Theorem 1, we obtain the formula

$$\sum_{s\leq n\leq 2k-s} (-1)^n\, G_0(2k,n,s) = \frac{(-1)^k\, \pi^{2k}}{(2k+1)!} \sum_{r=0}^{k-s} \binom{2k+1}{2r} (2-2^{2r})\, B_{2r} \quad (k \geq s \geq 1)$$

proved by Le and Murakami in [3]. Indeed, from equation (4) or equation (5) we have

$$S_n(x,-x,z) = \begin{cases} 2\left(x^{2m} - (-z)^m\right) & \text{if} \quad n = 2m, \\ 0 & \text{if} \quad n \equiv 1 \pmod 2, \end{cases}$$

so (3) and the standard Taylor expansion of $\log\bigl((x/2)/\sinh x/2\bigr)$ give

$$\begin{aligned}
\Phi_0(x,-x,z) &= \frac{1}{x^2+z}\left(\exp\left(\sum_{m=1}^{\infty} \frac{x^{2m} - (-z)^m}{m}\,\zeta(2m)\right) - 1\right) \\
&= \frac{1}{x^2+z}\left(\frac{\pi x}{\sin \pi x}\,\frac{\sinh \pi\sqrt{z}}{\pi\sqrt{z}} - 1\right) \\
&= \frac{\pi x}{\sin \pi x}\,\frac{(\sinh \pi\sqrt{z})/\pi\sqrt{z} - (\sin \pi x)/\pi x}{z + x^2} \\
&= \left(\sum_{r=0}^{\infty} (-1)^r \frac{B_{2r}}{(2r)!}\left(2 - 2^{2r}\right)\pi^{2r}x^{2r}\right) \times \\
&\qquad \times \left(\sum_{p \geq 0,\, s \geq 1} (-1)^p \frac{\pi^{2p+2s}\, x^{2p}\, z^{s-1}}{(2p+2s+1)!}\right).
\end{aligned}$$

The required identity now follows by comparing the coefficients of $x^{2k-2s}z^{s-1}$ on both sides.

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