ON MULTIPLE ZETA VALUES OF EXTREMAL HEIGHT

MASANOBU KANEKO and MIKA SAKATA™

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Abstract

We give three identities involving multiple zeta values of height one and of maximal height: an explicit formula for the height-one multiple zeta values, a regularised sum formula and a sum formula for the multiple zeta values of maximal height.

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1. Main results

The multiple zeta value (MZV) is a real number given by the nested series

$$\zeta(k_1, \dots, k_r) = \sum_{0 < m_1 < \dots < m_r} \frac{1}{m_1^{k_1} \cdots m_r^{k_r}}$$

for each index set $\mathbf{k} = (k_1, \dots, k_r)$ of positive integers k_i , with the last entry $k_r > 1$ for convergence. We introduce the parameters $\mathbf{w}(\mathbf{k}) := k_1 + \dots + k_r$, $\mathbf{d}(\mathbf{k}) := r$ and $\mathbf{h}(\mathbf{k}) := \#\{i \mid k_i > 1, 1 \le i \le r\}$, called respectively the weight, the depth and the height of the index set \mathbf{k} (or of the multiple zeta value $\zeta(\mathbf{k}) = \zeta(k_1, \dots, k_r)$).

In this paper, we present the following three identities which involve multiple zeta values of extremal height, that is, the MZVs of height one or of maximal height (all components of the index set are greater than one).

THEOREM 1.1 (Explicit formula for the MZV of height one). For any integers $r, k \ge 1$,

$$\zeta(\underbrace{1,\ldots,1}_{r-1},k+1) = \sum_{j=1}^{\min(r,k)} (-1)^{j-1} \sum_{\substack{\mathbf{w}(\mathbf{a})=k,\mathbf{w}(\mathbf{b})=r\\\mathbf{d}(\mathbf{a})=d(\mathbf{b})=j}} \zeta(\mathbf{a}+\mathbf{b}), \tag{1.1}$$

where, for two indices $\mathbf{a} = (a_1, \dots, a_j)$ and $\mathbf{b} = (b_1, \dots, b_j)$ of the same depth, $\zeta(\mathbf{a} + \mathbf{b})$ denotes $\zeta(a_1 + b_1, \dots, a_j + b_j)$.

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Note that the right-hand side of this formula is symmetric in r and k and thus the formula makes the duality $\zeta(\underbrace{1,\ldots,1}_{r-1},k+1)=\zeta(\underbrace{1,\ldots,1}_{k-1},r+1)$ visible. (Note that we

use the duality in our proof, so that we are not giving an alternative proof of the duality.) To our knowledge, no such symmetric explicit formula for the MZV of height one is known, except for the well-known symmetric generating function [1, 4]:

$$1 - \sum_{r,k \ge 1} \zeta(\underbrace{1, \dots, 1}_{r-1}, k+1) x^r y^k = \frac{\Gamma(1-x)\Gamma(1-y)}{\Gamma(1-x-y)} = \exp\left(\sum_{n=2}^{\infty} \zeta(n) \frac{x^n + y^n - (x+y)^n}{n}\right).$$

Also, we should remark that the right-hand side of the theorem is symmetric with respect to any permutations of the arguments, so that the theorem of Hoffman [5, Theorem 2.2] ensures that the right-hand side is a polynomial in the Riemann zeta values $\zeta(n)$. This fact can also be seen from the generating function above. Moreover, we note that all the MZVs appearing on the right-hand side are of maximal height.

As a final remark, the case of r = 2 gives nothing but the 'sum formula' for depth two (r = 1 gives the trivial identity $\zeta(k + 2) = \zeta(k + 2)$). It was Tsumura who first remarked that we could obtain the depth two sum formula if we looked at the behaviour at s = 0 of the identity (2.1) in the next section for r = 2.

Recall that the classical sum formula states that the sum of all MZVs of fixed weight and depth is equal to the Riemann zeta value of that weight. If we extend the sum to include nonconvergent MZVs with the shuffle regularisation, the result will be the MZV of height one (up to sign). We do not know if there exists any nice stuffle regularised sum formula.

THEOREM 1.2 (Shuffle regularised sum formula). For any integers $r, k \ge 1$,

$$\sum_{\substack{\mathbf{w}(\mathbf{k})=r+k\\\mathbf{d}(\mathbf{k})=r}} \zeta^{\mathrm{III}}(\mathbf{k}) = (-1)^{r-1} \zeta(\underbrace{1,\ldots,1}_{r-1},k+1),$$

where $\zeta^{\text{III}}(\mathbf{k})$ is the shuffle regularised value, which will be recalled in Section 2.

Finally, we give a kind of sum formula for the MZVs of maximal height in the form of a generating function. This is essentially known, but may be new in this form of presentation. Let T(k) be the sum of all multiple zeta values of weight k and of maximal height:

$$T(k) := \sum_{\substack{k_1 + \dots + k_r = k \\ r \ge 1, \forall k_i \ge 2}} \zeta(k_1, \dots, k_r).$$

Recall that the multiple zeta-star value $\zeta^*(k_1,\ldots,k_r)$ is given by the nonstrict nested sum

$$\zeta^{\star}(k_1,\ldots,k_r) = \sum_{0 < m_1 \le \cdots \le m_r} \frac{1}{m_1^{k_1} \cdots m_r^{k_r}}$$

THEOREM 1.3. We have the generating series identity

$$1 + \sum_{k=2}^{\infty} T(k)x^{k} = \left(1 + \sum_{n=1}^{\infty} \zeta^{*}(2, \dots, 2)x^{2n}\right) \left(1 + \sum_{n=1}^{\infty} \zeta(3, \dots, 3)x^{3n}\right).$$

After necessary preliminaries in the next section, we prove these results in Section 3.

2. Preliminaries

Recall the function introduced in [2],

$$\xi(k_1,\ldots,k_r;s) = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} \frac{\text{Li}_{k_1,\ldots,k_r}(1-e^{-t})}{e^t-1} dt,$$

where $Li_{k_1,...,k_r}(z)$ is the multiple polylogarithm function defined by

$$\operatorname{Li}_{k_1,\dots,k_r}(z) = \sum_{0 < m_1 < \dots < m_r} \frac{z^{m_r}}{m_1^{k_1} \cdots m_r^{k_r}}$$

When $k_r > 1$, the value at z = 1 of $\text{Li}_{k_1, \dots, k_r}(z)$ is nothing but the multiple zeta value $\zeta(k_1, \dots, k_r)$. The function $\xi(k_1, \dots, k_r; s)$ is analytically continued to an *entire* function in s. In the special case where $(k_1, \dots, k_r) = (1, \dots, 1, k)$, Arakawa and the first-named

author [2, Theorem 8] established the following identity (we interchange r and k and shift s to s+1), which is crucial in our proofs of Theorems 1.1 and 1.2:

$$\xi(\underbrace{1,\ldots,1}_{k-1},r;s+1) = (-1)^{r-1} \sum_{\substack{a_1+\cdots+a_r=k\\\forall a_p \geq 0}} \binom{s+a_r}{a_r} \zeta(a_1+1,\ldots,a_{r-1}+1,a_r+1+s) + \sum_{i=0}^{r-2} (-1)^i \zeta(\underbrace{1,\ldots,1}_{k-1},r-i) \zeta(\underbrace{1,\ldots,1}_{i},1+s)$$
(2.1)

for any $r, k \ge 1$. Here, we have introduced a complex variable s in the outer-most exponent of the MZV by setting

$$\zeta(k_1,\ldots,k_{r-1},k_r+s) := \sum_{0 < m_1 < \cdots < m_r} \frac{1}{m_1^{k_1} \cdots m_{r-1}^{k_{r-1}} m_r^{k_r+s}}.$$

As remarked in [7, Remark 3.7], (2.1) is equivalent to the connection formula of Euler's type of the multi-polylogarithm $\text{Li}_{1,\ldots,1,r}(z)$. It is shown in [2] that the function

 $\zeta(k_1, \ldots, k_{r-1}, k_r + s)$ can be meromorphically continued to the whole s-plane and has a pole at s = 0 if $k_r = 1$. We need the description of the principal part at s = 0 in terms of regularised polynomials, which we now explain.

For an index $\mathbf{k} = (k_1, \dots, k_r)$, we denote by $Z_{\mathbf{k}}^{\text{III}}(T)$ and $Z_{\mathbf{k}}^*(T)$ respectively the shuffle and the stuffle (harmonic) regularised polynomials associated to \mathbf{k} . These are the polynomials in $\mathbb{R}[T]$ uniquely characterised by the asymptotics

$$\operatorname{Li}_{k_1,\ldots,k_r}(z) = Z_{\mathbf{k}}^{\text{III}}(-\log(1-z)) + O((1-z)^{\varepsilon})$$
 as $z \to 1$ for some $\varepsilon > 0$

and

$$\sum_{0 < m_1 < \dots < m_r < M} \frac{1}{m_1^{k_1} \cdots m_r^{k_r}} = Z_{\mathbf{k}}^* (\log M + \gamma) + O(M^{-\varepsilon}) \quad \text{as } M \to \infty \text{ for some } \varepsilon > 0,$$

where γ is Euler's constant. We refer the reader to [6] for details about the regularisations. We denote the constant term $Z_{\mathbf{k}}^{\text{III}}(0)$ of the shuffle-regularised polynomial $Z_{\mathbf{k}}^{\text{III}}(T)$ by $\zeta^{\text{III}}(\mathbf{k})$ and call it the shuffle-regularised value of (possibly divergent) $\zeta(\mathbf{k})$. If \mathbf{k} is of the form $\mathbf{k} = (k_1, \dots, k_n, \underbrace{1, \dots, 1})$ with $k_n > 1, m \ge 0$,

then both $Z_{\mathbf{k}}^{\text{III}}(T)$ and $Z_{\mathbf{k}}^*(T)$ are of degree m and each coefficient of T^i is a linear combination of multiple zeta values of weight m-i. If m=0 (and so n=r), then $Z_{\mathbf{k}}^{\text{III}}(T)=Z_{\mathbf{k}}^*(T)=Z_{\mathbf{k}}^{\text{III}}(0)=Z_{\mathbf{k}}^*(0)=\zeta(k_1,\ldots,k_r)$. Now write

$$Z_{\mathbf{k}}^{\text{III}}(T) = \sum_{i=0}^{m} a_i(\mathbf{k}) \frac{T^i}{i!} \quad \text{and} \quad Z_{\mathbf{k}}^*(T) = \sum_{i=0}^{m} b_i(\mathbf{k}) \frac{(T-\gamma)^i}{i!}.$$

Then, as shown in [3], the principal parts at s = 0 of $\Gamma(s+1)\zeta(k_1, \ldots, k_{r-1}, k_r + s)$ and $\zeta(k_1, \ldots, k_{r-1}, k_r + s)$ are given respectively by

$$\Gamma(s+1)\zeta(k_1,\dots,k_{r-1},k_r+s) = \sum_{i=0}^m \frac{a_i(\mathbf{k})}{s^i} + O(s) \quad \text{as } s \to 0$$
 (2.2)

and

$$\zeta(k_1,\ldots,k_{r-1},k_r+s) = \sum_{i=0}^m \frac{b_i(\mathbf{k})}{s^i} + O(s) \text{ as } s \to 0.$$

We take this opportunity to point out a flaw in the proof in [3]. The integral in the sum on the right of the equation below (32) may not converge. But the argument can easily be modified by splitting the integral \int_0^∞ on the left as $\int_0^1 + \int_1^\infty$ and looking at the limits when $s \to 0$ separately.

3. Proofs

Proof of Theorem 1.1. Since we have the duality $\zeta(\underbrace{1,\ldots,1}_{r-1},k+1)=\zeta(\underbrace{1,\ldots,1}_{k-1},r+1)$

and the right-hand side of (1.1) is symmetric in r and k, it is enough to prove the theorem under the assumption that $k \ge r$. We proceed by induction on r. When r = 1, both sides become $\zeta(k+1)$ and the assertion is true for all $k \ge 1$. Suppose that $r \ge 2$ and the theorem is true when the depth on the left is less than r (and k is greater than or equal to the depth).

We look at the values at s = 0 of both sides of (2.1). The value on the left is

evaluated in [2, Theorem 9] as
$$\xi(\underbrace{1,\ldots,1}_{k-1},r;1) = \zeta(\underbrace{1,\ldots,1}_{r-1},k+1)$$
. Since the functions $\zeta(a_1+1,\ldots,a_{r-1}+1,a_r+1+s)$ with $a_r=0$ as well as $\zeta(\underbrace{1,\ldots,1}_{r-1},1+s)$ on the right

have poles at s = 0, we need to look at the constant term of the Laurent expansion of the right-hand side. (Because $\xi(1,\ldots,1,r;s+1)$ is entire, all the poles on the right actually cancel out.) In what follows within the proof of Theorem 1.1, we simply write

the constant term at s = 0 of $\zeta(k_1, \ldots, k_{r-1}, k_r + s)$ as $\zeta(k_1, \ldots, k_{r-1}, k_r)$ even when $k_r = 1$, which is equal to $Z_{k_1,\dots,k_r}^*(\gamma)$ as recalled in the previous section. Note that these values satisfy the stuffle (harmonic) product rule. With this convention,

$$\zeta(\underbrace{1,\ldots,1}_{r-1},k+1) = (-1)^{r-1} \sum_{\substack{a_1+\cdots+a_r=k\\\forall a_p \ge 0}} \zeta(a_1+1,\ldots,a_r+1) + \sum_{i=0}^{r-2} (-1)^i \zeta(\underbrace{1,\ldots,1}_{k-1},r-i) \cdot \zeta(\underbrace{1,\ldots,1}_{i+1}).$$

We apply the duality $\zeta(\underbrace{1,\ldots,1}_{k-1},r-i)=\zeta(\underbrace{1,\ldots,1}_{r-i-2},k+1)$ in the second sum on the right and use the induction hypothesis (since r-i-1 < r) to obtain

$$\zeta(\underbrace{1,\ldots,1}_{r-1},k+1) = (-1)^{r-1} \sum_{\substack{a_1+\cdots+a_r=k\\\forall a_p\geq 0}} \zeta(a_1+1,\ldots,a_r+1) \\
+ \sum_{i=0}^{r-2} (-1)^i \sum_{j=1}^{r-i-1} (-1)^{j-1} \sum_{\substack{\mathbf{w}(\mathbf{a})=k,\,\mathbf{w}(\mathbf{b})=r-i-1\\\mathbf{d}(\mathbf{a})=\mathbf{d}(\mathbf{b})=j}} \zeta(\mathbf{a}+\mathbf{b}) \cdot \zeta(\underbrace{1,\ldots,1}_{i+1}) \\
= (-1)^{r-1} \sum_{\substack{a_1+\cdots+a_r=k\\\forall a_p\geq 0}} \zeta(a_1+1,\ldots,a_r+1) \\
+ \sum_{j=1}^{r-1} (-1)^{j-1} \sum_{\substack{\mathbf{w}(\mathbf{a})=k\\\mathbf{d}(\mathbf{a})=j}} \sum_{i=0}^{r-j-1} (-1)^i \sum_{\substack{\mathbf{w}(\mathbf{b})=r-i-1\\\mathbf{d}(\mathbf{b})=j}} \zeta(\mathbf{a}+\mathbf{b}) \cdot \zeta(\underbrace{1,\ldots,1}_{i+1}).$$

Now we expand the product $\zeta(\mathbf{a} + \mathbf{b}) \cdot \zeta(\underbrace{1, \dots, 1}_{i+1})$ by using the stuffle product and rearrange the terms according to the number of ones to compute the inner sum

$$\sum_{i=0}^{r-j-1} (-1)^i \sum_{\substack{\mathbf{w}(\mathbf{b})=r-i-1\\\mathbf{d}(\mathbf{b})=j}} \zeta(\mathbf{a}+\mathbf{b}) \cdot \zeta(\underbrace{1,\ldots,1}_{i+1}).$$

For that purpose, we introduce more notation. For a fixed index $\mathbf{a} = (a_1, \dots, a_j)$ of depth j and integers $l, n \ge 0$, we set

$$S(\mathbf{a}, l, n) := \sum_{\substack{\mathbf{w}(\mathbf{b}) = r - l \\ \mathbf{d}(\mathbf{b}) = i, \mathbf{h}(\mathbf{b}) = n}} \zeta(a_1 + b_1, \dots, 1, \dots, a_s + b_s, \dots, 1, \dots, a_j + b_j),$$

summing over all $\mathbf{b} = (b_1, \dots, b_j)$ of weight r - l, depth j and height n, and over all possible positions of exactly l ones in the arguments. Then, by the stuffle product rule,

$$\sum_{\substack{\mathbf{w}(\mathbf{b})=r-i-1\\ \mathbf{d}(\mathbf{b})=j}} \zeta(\mathbf{a}+\mathbf{b}) \cdot \zeta(\underbrace{1,\ldots,1}_{i+1}) = \sum_{l=\max(0,i+1-j)}^{i+1} \sum_{n=i+1-l}^{j} \binom{n}{i+1-l} S(\mathbf{a},l,n).$$

We note that, when we expand $\zeta(\mathbf{a} + \mathbf{b})\zeta(\underbrace{1,\ldots,1}_{i+1})$ by the stuffle product, the number of

ones in each term should at least i+1-j when j < i+1. And, if the number of ones is l, then the height n on the right varies from i+1-l to j. A particular term in the sum $S(\mathbf{a}, l, n)$ on the right comes in exactly $\binom{n}{i+1-l}$ ways from the product $\zeta(\mathbf{a} + \mathbf{b})\zeta(\underbrace{1, \ldots, 1})$

on the left, because there are i + 1 - l out of n positions of the index $\mathbf{a} + \mathbf{b}$ on the left which produce that particular term on the right by colliding with i + 1 - l ones at those positions.

When we sum this up alternatingly for i = 0, ..., r - j - 1 with signs, all coefficients of $S(\mathbf{a}, l, n)$ with $n, l \ge 1$ vanish, because of the binomial identity $\sum_{i=l-1}^{n+l-1} (-1)^i \binom{n}{i+1-l} = 0$ if $n, l \ge 1$. Hence, using the identity $\sum_{i=0}^{n-1} (-1)^i \binom{n}{i+1} = 1$ if $n \ge 1$ (the case l = 0),

$$\sum_{i=0}^{r-j-1} (-1)^i \sum_{\substack{\mathbf{w}(\mathbf{b})=r-i-1\\ \mathbf{d}(\mathbf{b})=j}} \zeta(\mathbf{a}+\mathbf{b}) \cdot \zeta(\underbrace{1,\ldots,1}_{i+1}) = \sum_{n=1}^j S(\mathbf{a},0,n) + (-1)^{r-j-1} S(\mathbf{a},r-j,0).$$

When $j \le r - 1$, we have $\sum_{n=1}^{j} S(\mathbf{a}, 0, n) = \sum_{w(\mathbf{b}) = r, d(\mathbf{b}) = j} \zeta(\mathbf{a} + \mathbf{b})$ and this gives

$$\sum_{j=1}^{r-1} (-1)^{j-1} \sum_{\substack{\mathbf{w}(\mathbf{a})=k, \mathbf{w}(\mathbf{b})=r\\ \mathbf{d}(\mathbf{a})=\mathbf{d}(\mathbf{b})=j}} \zeta(\mathbf{a} + \mathbf{b}). \tag{3.1}$$

Finally,

$$\sum_{j=1}^{r-1} (-1)^{j-1} \sum_{\substack{\mathbf{w}(\mathbf{a})=k \\ \mathbf{d}(\mathbf{a})=j}} (-1)^{r-j-1} S(\mathbf{a}, r-j, 0) = (-1)^r \sum_{j=1}^{r-1} \sum_{\substack{\mathbf{w}(\mathbf{a})=k \\ \mathbf{d}(\mathbf{a})=j}} S(\mathbf{a}, r-j, 0)$$

$$= (-1)^r \sum_{\substack{a_1+\dots+a_r=k \\ a_p \geq 0, \text{ at least one } a_p = 0}} \zeta(a_1+1, \dots, a_r+1).$$

Hence, this and the terms in

$$(-1)^{r-1} \sum_{\substack{a_1 + \dots + a_r = k \\ \forall a_n \ge 0}} \zeta(a_1 + 1, \dots, a_r + 1)$$

with at least one $a_p = 0$ cancel out, thereby leaving the term

$$(-1)^{r-1} \sum_{\substack{\mathbf{w}(\mathbf{a})=k, \ \mathbf{w}(\mathbf{b})=r\\ \mathbf{d}(\mathbf{a})=d(\mathbf{b})=r}} \zeta(\mathbf{a}+\mathbf{b}). \tag{3.2}$$

The sum of (3.1) and (3.2) gives the right-hand side of the theorem.

PROOF OF THEOREM 1.2. We multiply by $\Gamma(s+1)$ on both sides of the identity (2.1) and look at the constant terms of the Laurent expansions at s = 0. The left-hand side is holomorphic at s = 0 and gives the value $\zeta(\underbrace{1, \dots, 1}_{r-1}, k+1)$, as we already saw

in the last subsection. The function $\binom{s+a_r}{a_r}\Gamma(s+1)\zeta(a_1+1,\ldots,a_{r-1}+1,a_r+1+s)$ on the right is holomorphic at s = 0 if $a_r > 1$ and in that case gives the value $\zeta(a_1 + 1, \dots, a_{r-1} + 1, a_r + 1)$. If $a_r = 0$, then

$$\binom{s+a_r}{a_r}\Gamma(s+1)\zeta(a_1+1,\ldots,a_{r-1}+1,a_r+1+s) = \Gamma(s+1)\zeta(a_1+1,\ldots,a_{r-1}+1,1+s)$$

has a pole at s = 0. The constant term of its Laurent expansion is $\zeta^{\text{III}}(a_1 + 1, \dots, a_r + 1)$

by (2.2). On the other hand, the function
$$\Gamma(s+1)\zeta(\underbrace{1,\ldots,1}_i,1+s)$$
 has no constant term at $s=0$ because $Z_{\underbrace{1,\ldots,1}}^{\text{III}}(T)=T^{i+1}/(i+1)!$. This concludes the proof.

We remark that we can prove the theorem alternatively by computing the left-hand side using the regularisation formula [6, (5.2)]. By Theorem 1.2 and [6, Corollary 5], we easily obtain the following sum formula for the shuffle-regularised polynomials:

$$\sum_{\substack{\mathbf{w}(\mathbf{k})=r+k\\ i\neq k}} \zeta^{\mathbf{III}}(\mathbf{k};T) = \sum_{i=0}^{r-1} (-1)^{r-1-i} \zeta(\underbrace{1,\ldots,1}_{r-1-i},k+1) \frac{T^i}{i!}$$

for any $r, k \ge 1$, where $\zeta^{\text{III}}(\mathbf{k}; T) = Z^{\text{III}}_{\mathbb{R}}(w)$ in the notation of [6] with w being a word corresponding to k.

PROOF OF THEOREM 1.3. This is almost obvious if we write $k_i \geq 2$ as $k_i = 2 + \cdots + 2$ (for k_i even) or $k_i = 3 + 2 + \cdots + 2$ (for k_i odd) and consider the stuffle product of $\zeta^*(2,\ldots,2)\zeta(3,\ldots,3)$ after writing $\zeta^*(2,\ldots,2)$ as sums of ordinary MZVs.

An alternative proof is given by using the main identity in [8]. As is already remarked there, if we specialise y = 0 and $z = x^2$ in [8, Equation 3],

$$1 + \sum_{k=2}^{\infty} T(k) x^k = \exp\left(\sum_{n=1}^{\infty} \frac{\zeta(2n)}{n} x^{2n}\right) \cdot \exp\left(\sum_{n=1}^{\infty} (-1)^{n-1} \frac{\zeta(3n)}{n} x^{3n}\right).$$

It is standard that

$$\exp\left(\sum_{n=1}^{\infty} \frac{\zeta(2n)}{n} x^{2n}\right) = \Gamma(1+x)\Gamma(1-x) = \prod_{m=1}^{\infty} \left(1 - \frac{x^2}{m^2}\right)^{-1} = 1 + \sum_{n=1}^{\infty} \zeta^{\star}(2, \dots, 2) x^{2n},$$

whereas the identity

$$\exp\left(\sum_{n=1}^{\infty} (-1)^{n-1} \frac{\zeta(3n)}{n} x^{3n}\right) = 1 + \sum_{n=1}^{\infty} \zeta(3, \dots, 3) x^{3n}$$

is a special case of [6, Corollary 2 of Proposition 4].

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MASANOBU KANEKO, Faculty of Mathematics, Kyushu University,

Motooka 744, Nishi-ku, Fukuoka 819-0395, Japan

e-mail: mkaneko@math.kyushu-u.ac.jp

MIKA SAKATA, Graduate School of Mathematics, Kyushu University,

Motooka 744, Nishi-ku, Fukuoka 819-0395, Japan

e-mail: m-sakata@math.kyushu-u.ac.jp