DEVELOPMENTS IN MATHEMATICS 14

ZETA FUNCTIONS, TOPOLOGY AND QUANTUM PHYSICS

Edited by
Takashi Aoki
Shigeru Kanemitsu
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Springer

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ZETA FUNCTIONS, TOPOLOGY AND QUANTUM PHYSICS

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Preface

This volume contains papers by invited speakers of the symposium "Zeta Functions, Topology and Quantum Physics" held at Kinki University in Osaka, Japan, during the period of March 3-6, 2003. The aims of this symposium were to establish mutual understanding and to exchange ideas among researchers working in various fields which have relation to zeta functions and zeta values.

We are very happy to add this volume to the series *Developments in Mathematics* from Springer. In this respect, Professor Krishnaswami Alladi helped us a lot by showing his keen and enthusiastic interest in publishing this volume and by contributing his paper with Alexander Berkovich.

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Osaka, October 2004

Takashi Aoki
Shigeru Kanemitsu
Mikio Nakahara
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Zeta Functions, Topology,
and
Quantum Physics

Kinki University, Osaka, Japan

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GÖLLNITZ-GORDON PARTITIONS WITH WEIGHTS AND PARITY CONDITIONS

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Abstract A Göllnitz-Gordon partition is one in which the parts differ by at least 2, and where the inequality is strict if a part is even. Let $Q_i(n)$ denote the number of partitions of n into distinct parts $\not\equiv i \pmod 4$. By attaching weights which are powers of 2 and imposing certain parity conditions on Göllnitz-Gordon partitions, we show that these are equinumerous with $Q_i(n)$ for $i = 0, 2$. These complement results of Göllnitz on $Q_i(n)$ for $i = 1, 3$, and of Alladi who provided a uniform treatment of all four $Q_i(n)$, $i = 0, 1, 2, 3$, in terms of weighted partitions into parts differing by ≥ 4. Our approach here provides a uniform treatment of all four $Q_i(n)$ in terms of certain double series representations. These double series identities are part of a new infinite hierarchy of multiple series identities.

Keywords: Göllnitz-Gordon partitions, weighted partitions, parity conditions, chain decomposition, double series representation, infinite hierarchy, Bailey lemma, q-trinomial identities

1. Introduction

For $i = 0, 1, 2, 3$, let $Q_i(n)$ denote the number of partitions of n into distinct parts $\not\equiv i \pmod 4$. The well known (Little) Theorem of Göllnitz [6] is:

Theorem 1. *For $i = 1, 3$, $Q_i(n)$ equals the number of partitions of n into parts differing by ≥ 2, where the inequality is strict if a part is odd, and the smallest part is $> \frac{(4-i)}{2}$.*

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The analytic representation of Theorem 1 is

$$\sum_{n=0}^{\infty} \frac{q^{n^2+n}(-q;q^2)_n}{(q^2;q^2)_n} = (-q^2;q^4)_\infty(-q^3;q^4)_\infty(-q^4;q^4)_\infty \tag{1.1}$$

when $i = 1$, and

$$\sum_{n=0}^{\infty} \frac{q^{n^2+n}(-q^{-1};q^2)_n}{(q^2;q^2)_n} = (-q;q^4)_\infty(-q^2;q^4)_\infty(-q^4;q^4)_\infty, \tag{1.2}$$

when $i = 3$. In (1.1), (1.2), and in what follows, we have used the standard notation

$$(a)_n = (a;q)_n = \prod_{j=0}^{n-1}(1 - aq^j)$$

for any complex number a, and

$$(a)_\infty = \lim_{n\to\infty}(a)_n = \prod_{j=0}^{\infty}(1 - aq^j),$$

for $|q| < 1$. The products on the right in (1.1), (1.2) are also equal to

$$\frac{1}{(q^2;q^8)_\infty(q^3;q^8)_\infty(q^7;q^8)_\infty}$$

and

$$\frac{1}{(q;q^8)_\infty(q^5;q^8)_\infty(q^6;q^8)_\infty},$$

respectively, which have obvious interpretations as generating functions of partitions into parts in certain residue classes (mod 8), repetition allowed. The equally well known Göllnitz-Gordon partition theorem is

Theorem 2. *For $i = 1, 3$, the number of partitions into parts $\equiv \pm i, 4$* (mod 8) *equals the number of partitions into parts differing by ≥ 2, where the inequality is strict if a part is even, and the smallest part is $\geq i$.*

The analytic representation of Theorem 2 is

$$\sum_{n=0}^{\infty} \frac{q^{n^2}(-q;q^2)_n}{(q^2;q^2)_n} = \frac{1}{(q;q^8)_\infty(q^4;q^8)_\infty(q^7;q^8)_\infty} \tag{1.3}$$

when $i = 1$, and

$$\sum_{n=0}^{\infty} \frac{q^{n^2+2n}(-q;q^2)_n}{(q^2;q^2)_n} = \frac{1}{(q^3;q^8)_\infty(q^4;q^8)_\infty(q^5;q^8)_\infty} \tag{1.4}$$

when $i = 3$. Actually (1.3) and (1.4) are equations (36) and (37) in Slater's famous list [9], but it was Göllnitz [6] and Gordon [7] who independently realized their combinatorial interpretation.

By a reformulation of the (Big) Theorem of Göllnitz [6] (not Theorem 1) using certain quartic transformations, Alladi [1] provided a uniform treatment of all four partition functions $Q_i(n)$, $i = 0, 1, 2, 3$ in terms of partitions into parts differing by ≥ 4, and with certain powers of 2 as weights attached. As a consequence, it was noticed in [1] that $Q_2(n)$ and $Q_0(n)$ possess certain more interesting properties than their well known counterparts $Q_1(n)$ and $Q_3(n)$. In particular, $Q_2(n)$ alone among the four functions satisfies the property that for every positive integer k, $Q_2(n)$ is a multiple of 2^k for almost all n which was proved by Gordon in an Appendix to [1].

Our goal is to prove Theorem 3 in §2 which shows that by attaching weights which are powers of 2 to the Göllnitz-Gordon partitions of n, and by imposing certain parity conditions, this is made equal to $Q_2(n)$. Here by a *Göllnitz-Gordon partition* we mean a partition into parts differing by ≥ 2, where the inequality is strict if a part is even. There is a similar result for $Q_0(n)$, and this is stated as Theorem 4 at the end of §2. Theorems 3 and 4 are nice complements to Theorem 1 and to results of Alladi [1].

A combinatorial proof of Theorem 3 is given in full in the next section. Theorem 4 is only stated, and its proof which is similar, is omitted.

In proving Theorem 3 we are able to cast it as an analytic identity (see (3.2) in §3) which equates a double series with the product which is the generating function of $Q_2(n)$. It turns out that there is a two parameter refinement of (3.2) (see (3.3) of §3) which leads to similar double series representations for all four products

$$\prod_{m>0, m \not\equiv i \pmod 4} (1 + q^m)$$

for $i = 0, 1, 2, 3$. It will be shown in §3 that only in the cases $i = 1, 3$ do these double series reduce to the single series in (1.1) and (1.2).

Actually, the double series identity (3.2) is the case $k = 2$ of a new infinite hierarchy of identities valid for every $k \geq 1$. In §4 we use a limiting case of Bailey's lemma to derive this hierarchy. We give a partition theoretic interpretation of the case $k = 1$ and state without proof a doubly bounded polynomial identity which yields our new hierarchy as a limiting case. This polynomial identity will be investigated in detail elsewhere.

2. A new weighted partition theorem

Normally, by the parity of an integer we mean its residue class (mod 2). Here by the parity of an odd (or even) integer we mean its residue class (mod 4).

Next, given a partition π into parts differing by ≥ 2, by a *chain* χ in π we mean a maximal string of parts differing by exactly 2. Thus every partition into parts differing by ≥ 2 can be decomposed into chains. Note that if one part of a chain is odd (resp. even), then all parts of the chain are odd (resp. even). Hence we may refer to a chain as an odd chain or an even chain. Also let $\lambda(\chi)$ denote the least part of a chain χ and $\lambda(\pi)$ the least part of π.

Note that in a Göllnitz-Gordon partition, since the gap between even parts is > 2, this is the same as saying that every even chain is of length 1, that is, it has only one element.

Finally, given part b of partition π, by $t(b;\pi) = t(b)$ we denote the number of odd parts of π that are $< b$. With this new statistic t we now have

Theorem 3. *Let $\mathcal{S}$ denote the set of all special Göllnitz-Gordon partitions, namely, Göllnitz-Gordon partitions π satisfying the parity condition that for every even part b of π*

$$b \equiv 2t(b) \pmod 4. \tag{2.1}$$

Decompose each $\pi \in \mathcal{S}$ into chains χ and define the weight $\omega(\chi)$ as

$$\omega(\chi) = \begin{cases} 2, & \text{if } \chi \text{ is an odd chain, } \lambda(\chi) \geq 5, \\ & \text{and } \lambda(\chi) \equiv 1 + 2t(\lambda(\chi)) \pmod 4, \\ 1, & \text{otherwise.} \end{cases} \tag{2.2}$$

The weight $\omega(\pi)$ of the partition π is defined multiplicatively as

$$\omega(\pi) = \prod_{\chi} \omega(\chi),$$

the product over all chains χ of π. We then have

$$Q_2(n) = \sum_{\pi\in\mathcal{S},\, \sigma(\pi)=n} \omega(\pi),$$

where $\sigma(\pi)$ is the sum of the parts of π.

Proof: Consider the partition $\pi : b_1 + b_2 + \cdots + b_N$, $\pi \in \mathcal{S}$, where contrary to the standard practice of writing parts in descending order, we now have $b_1 < b_2 < \cdots < b_N$. Subtract 0 from b_1, 2 from b_2, $\ldots$, $2N-2$

from b_N, to get a partition π^*. We call this process the *Euler subtraction.* Note that in π^* the even parts cannot repeat, but the odd parts can. Let the parts of π^* be $b_1^* \leq b_2^* \leq \cdots \leq b_N^*$.

Now identify the parts of π which are odd, and which are the smallest parts of chains and satisfy both the parity and low bound conditions in (2.2). Mark such parts with a *tilde* at the top. That is, if b_k is such a part, we write $b_k = \widetilde{b}_k$ for purposes of identification. Let $\widetilde{b}_k$ yield $\widetilde{b}_k^* = b_k^*$ after the Euler subtraction.

Next, split the parts of π^* into two piles π_1^* and π_2^*, with π_1^* consisting only of certain odd parts, and π_2^* containing the remaining parts. In this decomposition we adopt the following rule:

(a) the odd parts of π^* which are not identified as above are put in π_1^*.

(b) the odd parts of π^* which have been identified could be put in either π_1^* or π_2^*.

Thus we have two choices for each identified part.

Let us say, in a certain given situation, after making the choices, we have n_1 parts in π_1^* and n_2 parts in π_2^*. We now add 0 to the smallest part of π_2^*, 2 to the second smallest part of π_2^*, ..., $2n_2 - 2$ to the largest part of π_2^*, $2n_2$ to the smallest part of π_1^*, $2n_2 + 2$ to the second smallest part of π_1^*, ..., $2(n_1 + n_2) - 2 = 2N - 2$ to the largest part of π_1^*. We call this the *Bressoud redistribution* process. As a consequence of this redistribution, we have created two partitions π_1 (out of π_1^*) and π_2 (out of π_2^*) satisfying the following conditions:

(i) π_1 consists only of distinct odd parts, with each odd part being greater than twice the number of parts of π_2.

(ii) Since both the even and odd parts of π_2^* are distinct, the parts of π_2 differ by ≥ 4. Also since the odd parts of π_2^* are chosen from the smallest of parts of certain chains in π, the odd parts of π_2 actually differ by ≥ 6, and each such odd part is ≥ 5.

In transforming the original partition π into the pair (π_1, π_2), we need to see how the parity conditions of π given by (2.1) and (2.2) transform to parity conditions in π_1 and π_2.

First observe that since the parity conditions on π are imposed only on the even parts of π and the *identified* odd parts of π, the transformed parity conditions (to be determined below) will be imposed only on π_2 and not on π_1. Thus π_1 will satisfy only condition (i) above.

Suppose b_k is an even part of π and that $t(b_k; \pi) = t$, that is there are t odd parts of π which are less than b_k. Now b_k becomes

$$b_k^* = b_k - (2k - 2)$$

after the Euler subtraction. Notice that $t(b_k^*;\pi^*) = t(b_k;\pi) = t$. Now suppose that from among the t odd parts of π^* less than b_k^*, r of them are put in π_1^* and the remaining $t-r$ odd parts are put in π_2^*. Then b_k^* becomes the $(k-r)-th$ smallest part in π_2^*. So in the Bressoud redistribution process, $2(k-r)-2$ is added to b_k^* making it a new even part e_{k-r} in π_2. Thus

$$e_{k-r} = b_k^* + 2(k-r) - 2 = b_k - (2k-2) + 2(k-r) - 2 = b_k - 2r. \quad (2.3)$$

We see from (2.1) and (2.3) that

$$e_{k-r} \equiv 2t - 2r = 2(t-r) = 2t(e_{k-r};\pi_2) \pmod 4 \quad (2.4)$$

and so the parity condition (2.1) on the even parts does not change when going to π_2. Thus we may write (2.4) in short as

$$e \equiv 2t(e) \pmod 4 \quad (2.5)$$

for any even part in π_2.

Now we need to determine the parity conditions on the odd parts in π_2 which are derived from some of the identified odd parts of π. To this end suppose that $\widetilde{b}_k$ is an identified odd part of π which becomes $\widetilde{b}_k^* = \widetilde{b}_k - (2k-2)$ in π^* due to the Euler subtraction, and that $\widetilde{b}_k^*$ is placed in π_2^*. Let $t(\widetilde{b}_k;\pi) = t$. Notice that

$$t(\widetilde{b}_k;\pi) = t(\widetilde{b}_k^*;\pi^*) = t.$$

Suppose that from among the t odd parts of π^* which are $\widetilde{b}_k^*$, r of them are placed in π_1^* and the remaining $t-r$ are placed in π_2^*. Then $\widetilde{b}_k^*$ becomes the $(k-r)-th$ smallest part in π_2^*. Thus under the Bressoud redistribution, $2(k-r)-2$ is added to it to yield the part f_k given by

$$f_k = \widetilde{b}_k^* + 2(k-r) - 2 = \widetilde{b}_k - (2k-2) + (2(k-r)-2) = \widetilde{b}_k - 2r$$

as in (2.3). Therefore the parity condition (2.2) yields

$$f_k \equiv 1 + 2t - 2r = 1 + 2(t-r) \pmod 4.$$

But $t(f_k;\pi_2) = t - r$. So this could be expressed in short as

$$f \equiv 1 + 2t(f) \pmod 4 \quad (2.6)$$

for any odd part of π_2. Thus the pair of partitions (π_1,π_2) is determined by condition (i) on π_1, and conditions (ii) and the parity conditions (2.5) and (2.6) on π_2.

In going from π to the pair (π_1, π_2) we had a *choice* of deciding whether an *identified* part of π would end up in π_1 or π_2. This choice is precisely the weight $\omega(\chi) = 2$ associated with certain chains χ. The weight of the partition π is computed multiplicatively because these choices are *independent.* So what we have established up to now is:

Lemma 1. *The weighted count of the special Göllnitz-Gordon partitions of n equals the number of bipartitions (π_1, π_2) of n satisfying conditions (i), (ii),* (2.5) *and* (2.6).

Next, we discuss a bijective map

$$\pi_2 \mapsto (\pi_3, \pi_4), \tag{2.7}$$

where π_3 is a partition into distinct multiples of 4 and π_4 is a partition into distinct odd parts such that

$$\nu(\pi_2) = \nu(\pi_3) \tag{2.8}$$

and

$$2\nu(\pi_2) > \Lambda(\pi_4). \tag{2.9}$$

Here by $\nu(\pi)$ we mean the number of parts of a partition π and by $\Lambda(\pi)$ the largest part of π.

To describe the map (2.7) we represent π_2 as a Ferrers graph with weights $1, 2$ or 4, at each node. We construct the graph as follows:

1) With each odd (resp. even) part f (resp. e) of π_2 we associate a row of $\frac{3+f+2t(f)}{4}$ (resp. $\frac{e+2t(e)}{4}$) nodes.

2) We place a 1 at end of any row that represents an odd part of π_2.

3) Every node in the column directly above each 1 is given weight 2.

4) Each remaining node is given weight 4.

Every part of π_2 is given by the sum of weights in an associated row. It is clear from these weights, that the partition represented by this weighted Ferrers graph satisfies precisely the conditions (ii), (2.5) and (2.6) that characterize π_2.

$$\begin{array}{llllllllll}
\pi_2: & 4 & 2 & 4 & 4 & 2 & 4 & 4 & 4 & 1 \\
& 4 & 2 & 4 & 4 & 2 & 4 & 4 & & \\
& 4 & 2 & 4 & 4 & 1 & & & & \\
& 4 & 1 & & & & & & &
\end{array}$$

Next we extract from this weighted Ferrers graph all columns with a 1 at the bottom, and assemble these columns as rows to form a 2-modular Ferrers graph as shown below.

$$\pi_4: \quad \begin{array}{cccc} 2 & 2 & 2 & 1 \\ 2 & 2 & 1 & \\ 1 & & & \end{array}$$

Clearly this 2-modular graph represents a partition π_4 that satisfies condition (2.9).

After this extraction, the decorated graph of π_2 becomes a 4-modular graph (in this case a graph with weight 4 at every node). This graph π_3 clearly satisfies (2.8).

$$\pi_3: \quad \begin{array}{cccccc} 4 & 4 & 4 & 4 & 4 & 4 \\ 4 & 4 & 4 & 4 & 4 & \\ 4 & 4 & 4 & & & \\ 4 & & & & & \end{array}$$

It is easy to check that (2.7) is a bijection. Thus Lemma 1 can be recasted in the form

Lemma 2. *The weighted count of the special Göllnitz-Gordon partitions of n as in Theorem 3 is equal to the number of partitions of n in the form (π_1, π_3, π_4) where*

(iii) π_3 consists only of distinct multiples of 4,

(iv) π_4 has distinct odd parts and $\Lambda(\pi_4) < 2\nu(\pi_3)$,

(v) π_1 has distinct odd parts and $\lambda(\pi_1) > 2\nu(\pi_3)$,

Finally, observe that conditions (iv) and (v) above yield partitions into distinct odd parts (without any other conditions). This together with (iii) yields partitions counted by $Q_2(n)$, thereby completing the combinatorial proof of Theorem 3.

In a similar fashion, we can obtain the following representation for $Q_0(n)$ with weights and parity conditions imposed on the Göllnitz-Gordon partitions:

Theorem 4. *Let $\mathcal{S}^*$ denote the set of all special Göllnitz-Gordon partitions, namely, Göllnitz-Gordon partitions π satisfying the parity condition that for every even part b of π*

$$b \equiv 2(t(b) - 1) \pmod 4. \tag{2.10}$$

Decompose each $\pi \in \mathcal{S}^*$ into chains χ and define the weight $\omega(\chi)$ as

$$\omega(\chi) = \begin{cases} 2, & \textit{if } \chi \textit{ is an odd chain, } \lambda(\chi) \geq 3, \\ & \textit{and } \lambda(\chi) \equiv 2t(\lambda(\chi)) - 1 \pmod 4, \\ 1, & \textit{otherwise.} \end{cases} \tag{2.11}$$

The weight $\omega(\pi)$ of the partition π is defined multiplicatively as

$$\omega(\pi) = \prod_{\chi} \omega(\chi),$$

the product over all chains χ of π. We then have

$$Q_0(n) = \sum_{\pi \in \mathcal{S}^*,\, \sigma(\pi)=n} \omega(\pi),$$

where $\sigma(\pi)$ is the sum of the parts of π.

3. Series representations

If we let $\nu(\pi_1) = n_1$ and $\nu(\pi_2) = n_2$, then (2.7) and conditions (iii), (iv), and (v) of Lemma 2 imply that the generating function of all such triples of partitions (π_1, π_3, π_4) is

$$\frac{q^{n_1^2+2n_1n_2}}{(q^2;q^2)_{n_1}} \cdot \frac{q^{2n_2^2+2n_2}}{(q^4;q^4)_{n_2}} \cdot (-q;q^2)_{n_2}. \tag{3.1}$$

If the expression in (3.1) is summed over all non-negative integers n_1 and n_2, it yields

$$\begin{aligned}
&\sum_{n_1}\sum_{n_2} \frac{q^{n_1^2+2n_1n_2+2n_2^2+2n_2}(-q;q^2)_{n_2}}{(q^2;q^2)_{n_1}(q^4;q^4)_{n_2}} \\
&= \sum_{n_2} \frac{q^{2n_2^2+2n_2}(-q;q^2)_{n_2}}{(q^4;q^4)_{n_2}} \sum_{n_1} \frac{q^{n_1^2+2n_1n_2}}{(q^2;q^2)_{n_1}} \\
&= \sum_{n_2} \frac{q^{2n_2^2+2n_2}(-q;q^2)_{n_2}}{(q^4;q^4)_{n_2}} (-q^{2n_2+1};q^2)_\infty \\
&= (-q;q^2)_\infty \sum_{n_2} \frac{q^{2n_2^2+2n_2}}{(q^4;q^4)_{n_2}} \\
&= (-q;q^2)_\infty (-q^4;q^4)_\infty \\
&= (-q;q^4)_\infty(-q^3;q^4)_\infty(-q^4;q^4)_\infty = \sum_n Q_2(n)q^n.
\end{aligned} \tag{3.2}$$

By just following the above steps we can actually get a two parameter refinement of (3.2), namely,

$$\begin{aligned}
&\sum_{n_1}\sum_{n_2} \frac{z^{n_1}\omega^{n_2} q^{n_1^2+2n_1n_2+2n_2^2+2n_2}(-zq;q^2)_{n_2}}{(q^2;q^2)_{n_1}(q^4;q^4)_{n_2}} \\
&= (-zq;q^4)_\infty(-zq^3;q^4)_\infty(-\omega q^4;q^4)_\infty.
\end{aligned} \tag{3.3}$$

One may view (3.2) as the analytic version of Theorem 3. In reality, the correct way to view (3.2) is that, if the summand on the left is decomposed into three factors as (3.1), then (3.2) is the analytic version of the statement that the number of partitions of an integer n into the triple of partitions (π_1, π_3, π_4) is equal to $Q_2(n)$. This is of course only the final step of the proof given above. and (3.2), which is quite simple, is equivalent to it.

The advantage in the two parameter refinement (3.3) is that by suitable choice of the parameters we get similar representations involving $Q_i(n)$ for $i = 0, 1, 3$. For example, if we replace ω by ωq^{-2} in (3.3) we get

$$\begin{aligned}\sum_{n_1}\sum_{n_2} &\frac{z^{n_1}\omega^{n_2} q^{n_1^2+2n_1n_2+2n_2^2}(-zq;q^2)_{n_2}}{(q^2;q^2)_{n_1}(q^4;q^4)_{n_2}} \\ &= (-zq;q^4)_\infty(-zq^3;q^4)_\infty(-\omega q^2;q^4)_\infty,\end{aligned} \tag{3.4}$$

which is the analytic representation of Theorem 4 above.

Next, replacing z by zq and ω by ωq^{-1} in (3.3) we get

$$\begin{aligned}\sum_{n_1}\sum_{n_2} &\frac{z^{n_1}\omega^{n_2} q^{n_1^2+2n_1n_2+2n_2^2+n_1+n_2}(-zq^2;q^2)_{n_2}}{(q^2;q^2)_{n_1}(q^4;q^4)_{n_2}} \\ &= (-zq^2;q^4)_\infty(-\omega q^3;q^4)_\infty(-zq^4;q^4)_\infty.\end{aligned} \tag{3.5}$$

Now choose $z = 1$ in (3.5). Then the double series on the left becomes

$$\begin{aligned}\sum_{n_1}\sum_{n_2} &\frac{\omega^{n_2} q^{n_1^2+2n_1n_2+2n_2^2+n_1+n_2}}{(q^2;q^2)_{n_1}(q^2;q^2)_{n_2}} \\ &= \sum_{n_1}\sum_{n_2} \frac{\omega^{n_2} q^{(n_1+n_2)^2+n_2^2+n_1+n_2}}{(q^2;q^2)_{n_1}(q^2;q^2)_{n_2}}.\end{aligned} \tag{3.6}$$

If we now put $n = n_1 + n_2$ and $j = n_2$, then (3.6) could be rewritten in the form

$$\begin{aligned}\sum_{n} &\frac{q^{n^2+n}}{(q^2;q^2)_n} \sum_{j=0}^{n} \frac{\omega^j q^{j^2}(q^2;q^2)_n}{(q^2;q^2)_j(q^2;q^2)_{n-j}} \\ &= \sum_{n=0}^{\infty} \frac{q^{n^2+n}(-\omega q;q^2)_n}{(q^2;q^2)_n} = (-q^2;q^4)_\infty(-\omega q^3;q^4)_\infty(-q^4;q^4)_\infty,\end{aligned} \tag{3.7}$$

which is the single series identity (1.1) in a refined form.

Similarly, replacing ω by ωq^{-3} and z by zq in (3.2) we get

$$\sum_{n_1}\sum_{n_2} \frac{z^{n_1}\omega^{n_2}q^{n_1^2+2n_1n_2+2n_2^2+n_1-n_2}(-zq^2;q^2)_{n_2}}{(q^2;q^2)_{n_1}(q^4;q^4)_{n_2}}$$
$$= (-zq^2;q^4)_\infty(-\omega q;q^4)_\infty(-zq^4;q^4)_\infty. \tag{3.8}$$

Now the choice $z=1$ makes the double series in (3.8) as

$$\sum_{n_1}\sum_{n_2} \frac{\omega^{n_2}q^{n_1^2+2n_1n_2+2n_2^2+n_1-n_2}}{(q^2;q^2)_{n_1}(q^2;q^2)_{n_2}} = \sum_{n_1}\sum_{n_2} \frac{\omega^{n_2}q^{(n_1+n_2)^2+n_2^2+n_1-n_2}}{(q^2;q^2)_{n_1}(q^2;q^2)_{n_2}}. \tag{3.9}$$

Once again, putting $n = n_1 + n_2$ and $j = n_2$ makes (3.9) into

$$\sum_n \frac{q^{n^2+n}}{(q^2;q^2)_n}\sum_{j=0}^{n} \frac{\omega^j q^{j^2-2j}(q^2;q^2)_n}{(q^2;q^2)_j(q^2;q^2)_{n-j}}$$

$$= \sum_{n=0}^{\infty} \frac{q^{n^2+n}(-\omega q^{-1};q^2)_n}{(q^2;q^2)_n} = (-q^2;q^4)_\infty(-\omega q;q^4)_\infty(-q^4;q^4)_\infty, \tag{3.10}$$

which is a refinement of the single series identity (1.2). Thus precisely in the cases $i = 1, 3$, can the double series be reduced to single series by setting one of the parameters $z = 1$.

4. A new infinite hierarchy

Identity (3.2) given above is just the case $k = 2$ of a new infinite hierarchy of multiple series identities (4.12) given below.

To derive this hierarchy, we will need the definition of a Bailey pair, and a special case of Bailey's lemma which produces a new Bailey pair from a given Bailey pair [2].

Definition: A pair of sequences $\alpha_n(q), \beta_n(q)$ is called a Bailey pair (relative to 1) if for all $n \geq 0$

$$\beta_n(q) = \sum_{i=0}^{n} \frac{\alpha_i(q)}{(q)_{n-i}(q)_{n+i}}. \tag{4.1}$$

By setting $a = 1, \rho_1 = -q^{\frac{1}{2}}$, and letting $\rho_2 \to \infty$ in the formulas (3.29) and (3.30) of [2], we obtain the following limiting case of Bailey's lemma:

Lemma 3. *Suppose $(\alpha_n(q), \beta_n(q))$ is a Bailey pair. Then $(\alpha_n^{(1)}(q), \beta_n^{(1)}(q))$ is another Bailey pair, where*

$$\alpha_n^{(1)}(q) = q^{\frac{n^2}{2}} \alpha_n(q), \tag{4.2}$$

$$\beta_n^{(1)}(q) = \sum_{i=0}^{n} \frac{(-\sqrt{q})_i}{(q)_{n-i}(-\sqrt{q})_n} q^{\frac{i^2}{2}} \beta_i(q). \tag{4.3}$$

From $(\alpha_n^{(1)}(q), \beta_n^{(1)}(q))$ one can produce next Bailey pair $(\alpha_n^{(2)}(q), \beta_n^{(2)}(q))$ simply using $(\alpha_n^{(1)}(q), \beta_n^{(1)}(q))$ as the initial Bailey pair. It is easy to check that the k-fold iteration of (the limiting case of) Bailey's Lemma yields

$$\alpha_n^{(k)}(q) = q^{k\frac{n^2}{2}} \alpha_n(q), \tag{4.4}$$

$$\beta_n^{(k)}(q) = \sum_{\vec{n}} \frac{q^{\frac{N_1^2+N_2^2+\cdots+N_k^2}{2}} (-\sqrt{q})_{n_k}}{(q)_{n-N_1}(-\sqrt{q})_n (q)_{n_1} \cdots (q)_{n_{k-1}}} \beta_{n_k}(q), \tag{4.5}$$

where $\vec{n} = (n_1, n_2, \cdots, n_k)$ and $N_i = n_i + n_{i+1} + \cdots + n_k$, with $i = 1, 2, \ldots, k$. In [8], [9] Slater derived A-M families of Bailey pairs to produce the celebrated list of 130 identities of the Rogers-Ramanujan type. We shall need her $E(4)$ pair:

$$\alpha_n = \begin{cases} (-1)^n q^{n^2}(q^n + q^{-n}), & \text{if } n > 0, \\ 1, & \text{if } n = 0, \end{cases}$$

$$\beta_n = \frac{q^n}{(q^2; q^2)_n}. \tag{4.6}$$

It follows from (4.1) and (4.4)–(4.6) that

$$\sum_{\vec{n}} \frac{q^{\frac{1}{2}(N_1^2+N_2^2+\cdots+N_k^2)+N_k} (-\sqrt{q})_{n_k}}{(q)_{n-N_1}(q)_{n_1}(q)_{n_2} \cdots (q)_{n_{k-1}}(q^2; q^2)_{n_k}}$$

$$= \frac{(-\sqrt{q})_n}{(q)_n} \sum_{j=-n}^{n} (-1)^j q^{\frac{k+2}{2}j^2+j} \begin{bmatrix} 2n \\ n+j \end{bmatrix}_q, \tag{4.7}$$

where q-binomial coefficients are defined as

$$\begin{bmatrix} n+m \\ n \end{bmatrix}_q = \frac{(q^{m+1})_n}{(q)_n}. \tag{4.8}$$

It is easy to check that

$$\lim_{n\to\infty} \begin{bmatrix} n \\ m \end{bmatrix}_q = \frac{1}{(q)_m}, \tag{4.9}$$

and

$$\lim_{n\to\infty} \begin{bmatrix} 2n \\ n+j \end{bmatrix}_q = \frac{1}{(q)_\infty}. \tag{4.10}$$

Next, we recall Jacobi's triple product identity

$$\sum_{n=-\infty}^{\infty} q^{n^2} z^n = (q^2, -qz, -\frac{q}{z}; q^2)_\infty, \tag{4.11}$$

where $(a_1, a_2, \dots, a_m; q)_\infty = (a_1)_\infty (a_2)_\infty \dots (a_m)_\infty$.
If we let n tend to infinity in (4.7) with $q \to q^2$, we obtain with the aid of (4.10) and (4.11) the desired identity

$$\begin{aligned}
&\sum_{\vec{n}} \frac{q^{N_1^2+\cdots+N_k^2+2N_k}(-q;q^2)_{n_k}}{(q^2;q^2)_{n_1}\cdots(q^2;q^2)_{n_{k-1}}(q^4;q^4)_{n_k}} \\
&= \frac{(-q;q^2)_\infty}{(q^2;q^2)_\infty}(q^{2k+4}, q^k, q^{k+4}; q^{2k+4})_\infty \\
&= \frac{(q^2;q^4)_\infty}{(q)_\infty}(q^{2k+4}, q^k, q^{k+4}; q^{2k+4})_\infty.
\end{aligned} \tag{4.12}$$

Here we used the simple relation

$$\frac{(q^2;q^4)_\infty}{(q)_\infty} = \frac{(q,-q;q^2)_\infty}{(q,q^2;q^2)_\infty} = \frac{(-q;q^2)_\infty}{(q^2;q^2)_\infty}.$$

Making use of

$$\frac{(-q;q^2)_\infty}{(q^2;q^2)_\infty}(q^8, q^2, q^6; q^8) = \frac{(-q;q^2)_\infty}{(q^4;q^8)_\infty} = (-q;q^2)_\infty(-q^4;q^4)_\infty, \tag{4.13}$$

it is straightforward to verify that (4.12) with $k = 2$ yields (3.2), as claimed.

When $k = 1$, (4.12) becomes

$$\sum_{n\geq 0} \frac{q^{n^2+2n}(-q;q^2)_n}{(q^4;q^4)_n} = \frac{(q^2;q^4)_\infty(q^6, q^1, q^5; q^6)_\infty}{(q)_\infty} = \frac{(-q^3;q^6)_\infty}{(q^4, q^8; q^{12})_\infty}. \tag{4.14}$$

Surprisingly, (4.14) is missing from the Slater list. It was given by Andrews in [3].

By using the statistic $s(b;\pi)$ = number of even parts of the partition π which are less than the part b, it can be shown that the the following partition theorem is a combinatorial interpretation of (4.14):

Theorem 5. *Let $G(N)$ denote the number of partitions π of N into distinct parts such that no gap between consecutive parts is $\equiv 1 \pmod 4$, and where the k-th smallest part b is $\equiv 1+2k+2s(b;\pi) \pmod 4$ if b is odd, and $\equiv 2+2k+2s(b;\pi) \pmod 4$, if b is even.*
Let $P(N)$ denote the number of partitions of N into parts $\equiv \pm 3, \pm 4 \pmod{12}$, such that parts $\equiv 3 \pmod 6$ are distinct. Then,

$$G(N) = P(N).$$

Remark: Theorem 5 can be stated without appeal to the statistic $s(b;\pi)$, but we preferred to state it this way to emphasise a different parity condition and to show similarity with Theorems 3 and 4.

It would be interesting to find partition theoretical interpretation of (4.12) with $k > 2$. To this end we observe that the product on the right of (4.12) with $k \equiv 0 \pmod 4$ can be interpreted as a generating function for partitions into parts $\not\equiv 2 \pmod 4$, $\not\equiv 0, \pm k \pmod{2k+4}$.

It is instructive to compare this product

$$\prod_{\substack{n\geq 1 \\ n\not\equiv 2 \pmod 4 \\ n\not\equiv 0,\pm(2K-2) \pmod{4K}}} (1-q^n)^{-1}$$

and the generalized Göllnitz-Gordon product ((7.4.4); [4])

$$\prod_{\substack{n\geq 1 \\ n\not\equiv 2 \pmod 4 \\ n\not\equiv 0,\pm(2\widetilde{k}-1) \pmod{4\widetilde{k}}}} (1-q^n)^{-1}.$$

Here $K = 1+\frac{k}{2}$ with $k \equiv 0 \pmod 4$ and $\widetilde{k}$ is a positive integer.

The right hand side of (4.12) can be rewritten as

$$\frac{(q^2;q^4)_\infty (q^k, q^{k+4}, q^{k+2}, -q^{k+2}; q^{2k+4})_\infty (q^{4k+8};q^{4k+8})_\infty}{(q)_\infty},$$

if k is odd, and

$$\frac{(q^2;q^4)_\infty (q^{2k+4};q^{2k+4})_\infty (q^{\frac{k}{2}}, -q^{\frac{k}{2}}, q^{2+\frac{k}{2}}, -q^{2+\frac{k}{2}}; q^{k+2})_\infty}{(q)_\infty},$$

if $k \equiv 2 \pmod 4$.

This enables us to interpret the right hand side of (4.12) as:

A. $k \equiv 1 \pmod 2$. RHS (4.12) is the generating function for partitions into parts $\not\equiv 2 \pmod 4$, $\not\equiv \pm k \pmod{2k+4}$, $\not\equiv 0 \pmod{4k+8}$, such that parts $\equiv k+2 \pmod{2k+4}$ are distinct.

B. $k \equiv 2 \pmod 4$. RHS (4.12) is the generating function for partitions into parts $\not\equiv 2 \pmod 4$, $\not\equiv 0 \pmod{2k+4}$, such that parts $\not\equiv \pm\frac{k}{2} \pmod{k+2}$ are distinct.

We would like to conclude with the following observation. The hierarchy (4.12) follows in the limit $l, m \to \infty$ from the doubly bounded polynomial identity

$$\begin{aligned}
&\sum_{\vec{n},s} q^{N_1^2+\cdots+N_k^2+s^2+2N_k} \begin{bmatrix} l+m-N_1 \\ m-N_1 \end{bmatrix}_{q^2} \\
&\quad\times \prod_{j=1}^{k-1} \begin{bmatrix} l-\sum_{i=1}^{j} N_i + n_j \\ n_j \end{bmatrix}_{q^2} \begin{bmatrix} n_k + \lfloor \frac{l-1-\sum_{i=1}^{k} N_i - s}{2} \rfloor \\ n_k \end{bmatrix}_{q^4} \begin{bmatrix} n_k \\ s \end{bmatrix}_{q^2} \\
&= \sum_{j=-\infty}^{\infty} \Big\{ q^{(4k+8)j^2+4j} \widetilde{U}(l, m, 2(k+2)j+1, 2j, q^2) \\
&\quad - q^{(4k+8)j^2+4(k+1)j+k} \widetilde{U}(l, m, 2(k+2)j+k+1, 2j+1, q^2) \Big\}, \qquad (4.15)
\end{aligned}$$

where $\lfloor x \rfloor$ is the largest integer $\le x$, $\widetilde{U}(l, m, a, b, q) = T_w(l, m, a, b, q) + T_w(l, m, a+1, b, q)$, and the refined q-trinomial coefficients [10] are defined as

$$\begin{aligned}
&T_w(l, m, a, b, q) \\
&:= \sum_{\substack{n=0 \\ n+l \equiv a \pmod 2}}^{l} q^{\frac{n^2}{2}} \begin{bmatrix} m \\ n \end{bmatrix}_q \begin{bmatrix} m+b+\frac{l-a-n}{2} \\ m+b \end{bmatrix}_q \begin{bmatrix} m-b+\frac{l+a-n}{2} \\ m-b \end{bmatrix}_q . \qquad (4.16)
\end{aligned}$$

Using (4.9) together with Warnaar's limiting formula ((2.26); [10])

$$\lim_{l\to\infty} \widetilde{U}(l, m, a, b, q) = \frac{(-\sqrt{q})_m}{(q)_{2m}} \begin{bmatrix} 2m \\ m+b \end{bmatrix}_q, \qquad (4.17)$$

we obtain (4.7) with $q \to q^2$ and $n \to m$ as $l \to \infty$ in (4.12). On the other hand, if we let $m \to \infty$ in (4.16) we find that

$$\lim_{m\to\infty} T_w(l, m, a, b, q) = \frac{1}{(q)_l} T_{AB}(l, a, q), \qquad (4.18)$$

where the Andrews-Baxter q-trinomial coefficients [5] are defined as

$$T_{AB}(l,a,q) := \sum_{\substack{n=0 \\ n+l\equiv a \pmod 2}}^{l} q^{\frac{n^2}{2}} \begin{bmatrix} l \\ n \end{bmatrix}_q \begin{bmatrix} l-n \\ \frac{l-a-n}{2} \end{bmatrix}_q . \tag{4.19}$$

And so, (4.15) becomes in the limit $m \to \infty$

$$\begin{aligned} &\sum_{\vec{n},s} q^{N_1^2+\cdots+N_k^2+s^2+2N_k} \\ &\qquad \times \prod_{j=1}^{k-1} \begin{bmatrix} l-\sum_{i=1}^{j} N_i + n_j \\ n_j \end{bmatrix}_{q^2} \begin{bmatrix} n_k + \lfloor \frac{l-1-\sum_{i=1}^{k} N_i - s}{2} \rfloor \\ n_k \end{bmatrix}_{q^4} \begin{bmatrix} n_k \\ s \end{bmatrix}_{q^2} \\ &= \sum_{j=-\infty}^{\infty} \left\{ q^{(4k+8)j^2+4j} U(l, 2(k+2)j+1, q^2) \right. \\ &\quad \left. - q^{(4k+8)j^2+4(k+1)j+k} U(l, 2(k+2)j+k+1, q^2) \right\}, \end{aligned} \tag{4.20}$$

where

$$U(l,a,q) = T_{AB}(l,a,q) + T_{AB}(l,a+1,q). \tag{4.21}$$

The proof of (4.15) will be given elsewhere.

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PARTITION IDENTITIES FOR THE MULTIPLE ZETA FUNCTION

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Abstract We define a class of expressions for the multiple zeta function, and show how to determine whether an expression in the class vanishes identically. The class of such identities, which we call partition identities, is shown to coincide with the class of identities that can be derived as a consequence of the stuffle multiplication rule for multiple zeta values.

Keywords: Multiple zeta values, harmonic algebra, quasi-shuffles, stuffles

1. Introduction

For positive integer n and real $s_j \geq 1$ $(j = 1, 2, \ldots, n)$ the multiple zeta function may be defined by

$$\zeta(s_1, s_2, \ldots, s_n) = \sum_{k_1 > k_2 > \cdots > k_n > 0} \prod_{j=1}^{n} k_j^{-s_j}. \tag{1.1}$$

The nested sum (1.1) is over all positive integers $k_1, \ldots, k_n$ satisfying the indicated inequalities, and is finite if and only if $s_1 > 1$ also holds. An elementary property of the multiple zeta function is that it satisfies the so-called stuffle multiplication rule [1]: If $\vec{u} = (u_1, \ldots, u_m)$ and $\vec{v} = (v_1, \ldots, v_n)$, then

$$\zeta(\vec{u})\zeta(\vec{v}) = \sum_{\vec{w} \in \vec{u} * \vec{v}} \zeta(\vec{w}), \tag{1.2}$$

where $\vec{u} * \vec{v}$ is the multi-set of size [2]

$$|\vec{u} * \vec{v}| = \sum_{k=0}^{\min(m,n)} \binom{m}{k} \binom{n}{k} 2^k$$

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defined by the recursion

$$(s,\vec{u}) * (t,\vec{v}) = \{(s,\vec{w}) : \vec{w} \in \vec{u} * (t,\vec{v})\} \cup \{(t,\vec{w}) : \vec{w} \in (s,\vec{u}) * \vec{v}\} \\ \cup \{(s+t,\vec{w}) : \vec{w} \in \vec{u} * \vec{v}\},$$

with initial conditions $\vec{u} * () = () * \vec{u} = \vec{u}$. Thus, for example,

$$\begin{aligned}(s,u) * (t,v) =&\{(s,u,t,v), (s,u+t,v), (s,t,u,v), (s,t,u+v), (s,t,v,u)\} \\ &\cup\{(t,s,u,v), (t,s,u+v), (t,s,v,u), (t,s+v,u), (t,v,s,u)\} \\ &\cup\{(s+t,u,v), (s+t,u+v), (s+t,v,u)\},\end{aligned}$$

and correspondingly, we have the stuffle identity

$$\begin{aligned}&\zeta(s,u)\zeta(t,v) \\ &= \zeta(s,u,t,v) + \zeta(s,u+t,v) + \zeta(s,t,u,v) + \zeta(s,t,u+v) + \zeta(s,t,v,u) \\ &+ \zeta(t,s,u,v) + \zeta(t,s,u+v) + \zeta(t,s,v,u) + \zeta(t,s+v,u) + \zeta(t,v,s,u) \\ &+ \zeta(s+t,u,v) + \zeta(s+t,u+v) + \zeta(s+t,v,u).\end{aligned}$$

The sum on the right hand side of equation (1.2) accounts for all possible interlacings of the summation indices when the two nested series on the left are multiplied.

In this paper, we consider a certain class of expressions ("legal expressions") for the multiple zeta function, consisting of a finite linear combination of terms. Roughly speaking, a term is a product of multiple zeta functions, each of which is evaluated at a sequence of sums selected from a common argument list $(s_1, \ldots, s_n)$ in such a way that each variable s_j appears exactly once in each term. A more precise definition is given in Section 2. Once the legal expressions have been defined, we consider the problem of determining when a legal expression vanishes identically. For reasons which will become clear, we call such identities *partition identities.* It will be seen that the problem of verifying or refuting an alleged partition identity reduces to finite arithmetic over a polynomial ring. Alternatively, one can first rewrite any legal expression as a sum of single multiple zeta functions by applying the stuffle multiplication rule to each term. As we shall see, it is then easy to determine whether or not the original expression vanishes identically.

2. Definitions

Our definition of a partition identity makes use of the concept of a set partition. It is helpful to distinguish between set partitions that are ordered and those that are unordered.

Definition 1 (Unordered Set Partition). Let S be a finite non-empty set. An *unordered* set partition of S is a finite non-empty set

$\mathscr{P}$ whose elements are disjoint non-empty subsets of S with union S. That is, there exists a positive integer $m = |\mathscr{P}|$ and non-empty subsets $P_1, \ldots, P_m$ of S such that $\mathscr{P} = \{P_1, \ldots, P_m\}$, $S = \cup_{k=1}^m P_k$, and $P_j \cap P_k$ is empty if $j \neq k$.

Definition 2 (Ordered Set Partition). Let S be a finite non-empty set. An *ordered* set partition of S is a finite ordered tuple $\vec{P}$ of disjoint non-empty subsets of S such that the union of the components of $\vec{P}$ is equal to S. That is, there exists a positive integer m and non-empty subsets $P_1, \ldots, P_m$ of S such that $\vec{P}$ can be identified with the ordered m-tuple $(P_1, \ldots, P_m)$, $\cup_{k=1}^m P_k = S$, and $P_j \cap P_k$ is empty if $j \neq k$.

Definition 3 (Legal Term). Let n be a positive integer and let $\vec{s} = (s_1, \ldots, s_n)$ be an ordered tuple of n real variables with $s_j > 1$ for $1 \leq j \leq n$. Let $\mathscr{P} = \{P_1, \ldots, P_m\}$ be an unordered set partition of the first n positive integers $\{1, 2, \ldots, n\}$. For each positive integer k such that $1 \leq k \leq m$, let $\vec{P_k} = (P_k^{(1)}, P_k^{(2)}, \ldots, P_k^{(\alpha_k)})$ be an ordered set partition of P_k, and let

$$t_k^{(r)} = \sum_{j \in P_k^{(r)}} s_j, \qquad 1 \leq r \leq \alpha_k = |\vec{P_k}|.$$

A *legal term* for $\vec{s}$ is a product of the form

$$\prod_{k=1}^{m} \zeta\big(t_k^{(1)}, t_k^{(2)}, \ldots, t_k^{(\alpha_k)}\big), \tag{2.1}$$

and every legal term for $\vec{s}$ has the form (2.1) for some unordered set partition $\mathscr{P}$ of $\{1, 2, \ldots, n\}$ and ordered subpartitions $\vec{P_k}$, $1 \leq k \leq |\mathscr{P}|$.

Example 1. The product $\zeta(s_6, s_2+s_5, s_1+s_8+s_9)\zeta(s_3+s_4, s_{10})\zeta(s_7)$ is a legal term for the 10-tuple $(s_1, s_2, s_3, s_4, s_5, s_6, s_7, s_8, s_9, s_{10})$ arising from the partition $\{P_1, P_2, P_3\}$ of the set $\{1, 2, 3, 4, 5, 6, 7, 8, 9, 10\}$, where $P_1 = \{1, 2, 5, 6, 8, 9\}$ has ordered subpartition $\vec{P_1} = (\{6\}, \{2, 5\}, \{1, 8, 9\})$, $P_2 = \{3, 4, 10\}$ has ordered subpartition $\vec{P_2} = (\{3, 4\}, \{10\})$, and $P_3 = \{7\}$ has ordered subpartition $\vec{P_3} = (\{7\})$.

Definition 4 (Legal Expression). Let n be a positive integer, and let $\vec{s} = (s_1, \ldots, s_n)$ be an ordered tuple of n real variables with $s_j > 1$ for $1 \leq j \leq n$. A *legal expression* for $\vec{s}$ is a finite $\mathbf{Z}$-linear combination of legal terms for $\vec{s}$. That is, for any positive integer q, integers a_h, and legal terms T_h for $\vec{s}$ ($1 \leq h \leq q$), the sum $\sum_{h=1}^{q} a_h T_h$ is a legal expression for $\vec{s}$, and every legal expression for $\vec{s}$ has this form.

Definition 5 (Partition Identity). A *partition identity* is an equation of the form LHS $= 0$ for which there exists a positive integer n and real variables $s_j > 1$ ($j = 1, 2, \ldots, n$) such that LHS is a legal expression for $(s_1, \ldots, s_n)$, and the equation holds true for all real values of the variables $s_j > 1$.

Example 2. The equation

$$\begin{aligned} 2\zeta(s_1+s_2+s_3) - \zeta(s_2)\zeta(s_1+s_3) - \zeta(s_3)\zeta(s_1+s_2) + \zeta(s_1+s_2, s_3) \\ + \zeta(s_2, s_1+s_3) + \zeta(s_1+s_3, s_2) + \zeta(s_3, s_1+s_2) = 0 \end{aligned}$$

is a partition identity, and is easily verified by expanding the two products $\zeta(s_2)\zeta(s_1+s_3)$ and $\zeta(s_3)\zeta(s_1+s_2)$ using the stuffle multiplication rule (1.2) and then collecting multiple zeta functions with identical arguments. A natural question is whether *every* partition identity can be verified in this way. We provide an affirmative answer to this question in Section 4. An alternative method for verifying partition identities is given in Section 3.

3. Rational Functions

Here, we describe a method by which one can determine whether or not a legal expression vanishes identically, or equivalently, whether or not an alleged partition identity is in fact a true identity. It will be seen that the problem reduces to that of checking whether or not an associated rational function identity is true. This latter check can be accomplished in a completely deterministic and mechanical fashion by clearing denominators and expanding the resulting multivariate polynomials. More specifically, we associate rational functions with legal terms in such a way that the alleged partition identity holds if and only if the corresponding rational function identity, in which each legal term is replaced by its associated rational function, holds. The rational function corresponding to (2.1) is the function of n real variables $x_1 > 1, \ldots, x_n > 1$ defined by

$$R(x_1, x_2, \ldots, x_n) := \prod_{k=1}^{m} \prod_{\beta=1}^{\alpha_k} \left(\prod_{\lambda=1}^{\beta} \prod_{j \in P_k^{(\lambda)}} x_j - 1 \right)^{-1}. \tag{3.1}$$

Theorem 1. *Let q be a positive integer, and let $E = \sum_{h=1}^{q} a_h T_h$ be a legal expression for $\vec{s} = (s_1, \ldots, s_n)$ (i.e. each $a_h \in \mathbf{Z}$ and T_h is a legal term for $\vec{s}$, $1 \le h \le q$). Let $L = \sum_{h=1}^{q} a_h r_h$ be the expression obtained by replacing each legal term T_h by its corresponding rational function* *according to the rule that associates* (3.1) *with* (2.1). *Then E vanishes identically if and only if L does.*

Example 3. The rational function identity which Theorem 1 asserts is equivalent to the partition identity of Example 2 is

$$\begin{aligned}&\frac{2}{x_1x_2x_3-1}-\frac{1}{x_2-1}\cdot\frac{1}{x_1x_3-1}-\frac{1}{x_3-1}\cdot\frac{1}{x_1x_2-1}\\&+\frac{1}{(x_1x_2-1)(x_1x_2x_3-1)}+\frac{1}{(x_2-1)(x_1x_2x_3-1)}\\&+\frac{1}{(x_1x_3-1)(x_1x_2x_3-1)}+\frac{1}{(x_3-1)(x_1x_2x_3-1)}=0,\end{aligned}$$

which can be readily verified by hand, or with the aid of a suitable computer algebra system.

Proof of Theorem 1. It is immediate from the partition integral [1] representation for the multiple zeta function that every legal term on $(s_1,\ldots,s_n)$ is an n-dimensional integral transform of its associated rational function multiplied by the common kernel $\prod_{j=1}^n(\log x_j)^{s_j-1}/\Gamma(s_j)x_j$. Explicitly,

$$\begin{aligned}&\prod_{k=1}^m\zeta\Bigg(\sum_{j\in P_k^{(1)}}s_j,\sum_{j\in P_k^{(2)}}s_j,\ldots,\sum_{j\in P_k^{(\alpha_k)}}s_j\Bigg)\\&=\int_1^\infty\cdots\int_1^\infty\left\{\prod_{k=1}^m\prod_{\beta=1}^{\alpha_k}\Bigg(\prod_{\lambda=1}^{\beta}\prod_{j\in P_k^{(\lambda)}}x_j-1\Bigg)^{-1}\right\}\prod_{j=1}^n\frac{(\log x_j)^{s_j-1}}{\Gamma(s_j)x_j}\,dx_j.\end{aligned}$$

Linearity of the integral implies that if $L\equiv 0$ then $E\equiv 0$. The real content of Theorem 1 is that the converse also holds. To prove this, we first note that the rational function (3.1) is continuous on the n-fold Cartesian product of open intervals $(1..\infty)^n=\{(x_1,\ldots,x_n)\in\mathbf{R}^n : x_j>1, 1\le j\le n\}$ and $|R(x_1,\ldots,x_n)\prod_{j=1}^n x_j|$ is bounded on any n-fold Cartesian product of half-open intervals of the form $[c..\infty)^n=\{(x_1,\ldots,x_n)\in\mathbf{R}^n : x_j\ge c, 1\le j\le n\}$ with $c>1$. These properties obviously extend to linear combinations of rational functions of the form (3.1), and thus to complete the proof of Theorem 1, it suffices to establish the following result. $\square$

Lemma 1. *Let n be a positive integer and let R be a continuous real-valued function of n real variables defined on the n-fold Cartesian product of open intervals $(1..\infty)^n$. Suppose there exists a constant $c>1$ such that $|R(x_1,x_2,\ldots,x_n)\prod_{j=1}^n x_j|$ is bounded on the n-fold Cartesian product of* *half-open intervals* $[c..\infty)^n$*. Suppose further that there exist non-negative real numbers* $s_1^*, s_2^*, \ldots, s_n^*$ *such that the* n*-dimensional multiple integral*

$$\int_1^\infty \cdots \int_1^\infty R(x_1, x_2, \ldots, x_n) \prod_{j=1}^n (\log x_j)^{s_j} \frac{dx_j}{x_j}$$

vanishes whenever $s_j > s_j^*$ *for* $1 \le j \le n$*. Then* R *vanishes identically.*

Proof. Fix $s_j > s_j^*$ for $1 \le j \le n$. Let $T : [1..\infty) \to \mathbf{R}$ be given by the convergent $(n-1)$-dimensional multiple integral

$$T(x) := \int_1^\infty \cdots \int_1^\infty R(x_1, \ldots, x_{n-1}, x) \prod_{j=1}^{n-1} (\log x_j)^{s_j} \frac{dx_j}{x_j}.$$

Then $T(x) = O(1/x)$ as $x \to \infty$. It follows that the Laplace Transform

$$F(z) := \int_0^\infty e^{-zu}\, T(e^u)\, du$$

is analytic in the right half-plane $\{z \in \mathbf{C} : \Re(z) > -1\}$, and for all positive integers $m > s_n^*$,

$$\left(-\frac{d}{dz}\right)^m F(z)\bigg|_{z=0} = \int_0^\infty u^m\, T(e^u)\, du = \int_1^\infty (\log x)^m\, T(x)\, \frac{dx}{x} = 0.$$

By Taylor's theorem, F is a polynomial. Letting $z \to +\infty$ in the definition of F, we see that in fact, F must be the zero polynomial. By the uniqueness theorem for Laplace transforms (see eg. [4]), the set of $x > 1$ for which $T(x) \neq 0$ is of Lebesgue measure zero. Since T is continuous, it follows that $T(x) = 0$ for all $x > 1$. If $n = 1$, then $T = R$ and we're done. Otherwise, fix $x > 1$, and suppose the result holds for $n - 1$. Since in the above argument, $s_1 > s_1^*, \ldots, s_{n-1} > s_{n-1}^*$ were arbitrary, $T(x) = 0$ implies $R(x_1, x_2, \ldots, x_{n-1}, x) = 0$ for all $x_1, x_2, \ldots, x_{n-1}$ by the inductive hypothesis. Since this is true for each fixed $x > 1$, the result follows. □

4. Stuffles and Partition Identities

As in [1], we define the class of stuffle identities to be the set of all identities of the form (1.2). In [1], it is shown that every stuffle identity is a consequence of a corresponding rational function identity. In the previous section of the present paper, using a different method of proof, we established the more general result that every partition identity is a consequence of a corresponding rational function identity. Clearly every stuffle identity is a partition identity, but not conversely. Nevertheless, we shall see that every partition identity is a consequence of the stuffle multiplication rule. More specifically, we provide an affirmative answer to the question raised at the end of Example 2 in Section 2.

Notation. We introduce the concatenation operator **Cat**, which will be useful for expressing argument sequences without recourse to ellipses. For example, $\mathbf{Cat}_{k=1}^{m} t_j$ denotes the sequence $t_1, \dots, t_m$.

As we noted previously, by applying the stuffle multiplication rule (1.2) to legal terms, any legal expression on $(s_1, \dots, s_n)$ can be rewritten as a finite $\mathbf{Z}$-linear combination of single multiple zeta functions of the form

$$\sum_{h=1}^{q} a_h\, \zeta\big(\operatorname*{\mathbf{Cat}}_{k=1}^{\alpha_h} \sum_{j\in P_k} s_j\big) = \sum_{h=1}^{q} a_h\, \zeta\big(\sum_{j\in P_1} s_j, \sum_{j\in P_2} s_j, \dots, \sum_{j\in P_{\alpha_h}} s_j\big),$$

where the coefficients a_h are integers, q is a positive integer, and $(P_1, \dots, P_{\alpha_h})$ is an ordered set partition of the first n positive integers $\{1, 2, \dots, n\}$ for each $h = 1, 2, \dots, q$. Thus, it suffices to prove the following result.

Theorem 2. *Let F be a finite non-empty set of positive integers, and let $\{s_j : j \in F\}$ be a set of real variables, each exceeding 1. Suppose that for all $s_j > 1$,*

$$\sum_{\vec{P}\models F} c_{\vec{P}}\, \zeta\big(\operatorname*{\mathbf{Cat}}_{k=1}^{|\vec{P}|} \sum_{j\in P_k} s_j\big) = 0, \tag{4.1}$$

where the sum is over all ordered set partitions $\vec{P}$ of F, P_k denotes the k^{th} component of $\vec{P}$, and the coefficients $c_{\vec{P}}$ are real numbers depending only on $\vec{P}$. Then each $c_{\vec{P}} = 0$.

Proof. We argue by induction on the cardinality of F, the case $|F| = 1$ being trivial. To clarify the argument, we present the cases $|F| = 2$ and $|F| = 3$ before proceeding to the inductive step.

When $|F| = 2$, the identity (4.1) takes the form

$$c_1\zeta(s,t) + c_2\zeta(t,s) + c_3\zeta(s+t) = 0, \qquad s > 1,\ t > 1.$$

By Theorem 1, this is equivalent to the rational function identity

$$\frac{c_1}{(x-1)(xy-1)} + \frac{c_2}{(y-1)(xy-1)} + \frac{c_3}{xy-1} = 0, \qquad x > 1,\ y > 1.$$

Letting $x \to 1+$ shows that we must have

$$\frac{c_1}{y-1} = 0 \quad\Longrightarrow\quad c_1\zeta(t) = 0 \quad\Longrightarrow\quad c_1 = 0.$$

Similarly, letting $y \to 1+$ shows that $c_2 = 0$. Since the remaining term must vanish, we must have $c_3 = 0$ as well.

When $|F| = 3$, the identity (4.1) takes the form

$$\begin{aligned}
0 &= c_1\zeta(s,t,u) + c_2\zeta(s,u,t) + c_3\zeta(t,s,u) + c_4\zeta(t,u,s) \\
&\quad + c_5\zeta(u,s,t) + c_6\zeta(u,t,s) + c_7\zeta(s,t+u) + c_8\zeta(t+u,s) \\
&\quad + c_9\zeta(t,s+u) + c_{10}\zeta(s+u,t) + c_{11}\zeta(u,s+t) + c_{12}\zeta(s+t,u) \\
&\quad + c_{13}\zeta(s+t+u), \qquad s>1,\ t>1,\ u>1,
\end{aligned}$$

which, by Theorem 1, is equivalent to the rational function identity

$$\begin{aligned}
0 &= \frac{c_1}{(x-1)(xy-1)(xyz-1)} + \frac{c_2}{(x-1)(xz-1)(xyz-1)} \\
&\quad + \frac{c_3}{(y-1)(xy-1)(xyz-1)} + \frac{c_4}{(y-1)(yz-1)(xyz-1)} \\
&\quad + \frac{c_5}{(z-1)(xz-1)(xyz-1)} + \frac{c_6}{(z-1)(yz-1)(xyz-1)} \\
&\quad + \frac{c_7}{(x-1)(xyz-1)} + \frac{c_8}{(yz-1)(xyz-1)} + \frac{c_9}{(y-1)(xyz-1)} \\
&\quad + \frac{c_{10}}{(xz-1)(xyz-1)} + \frac{c_{11}}{(z-1)(xyz-1)} \\
&\quad + \frac{c_{12}}{(xy-1)(xyz-1)} + \frac{c_{13}}{xyz-1}, \qquad x>1,\ y>1,\ z>1. \qquad (4.2)
\end{aligned}$$

If we let $x \to 1+$ in (4.2), then for the singularities to cancel, we must have

$$0 = \frac{c_1}{(y-1)(yz-1)} + \frac{c_2}{(z-1)(yz-1)} + \frac{c_7}{yz-1}, \qquad y>1,\ z>1,$$

which, in light of Theorem 1, implies the identity

$$0 = c_1\zeta(t,u) + c_2\zeta(u,t) + c_7\zeta(t+u), \qquad t>1,\ u>1.$$

Having proved the $|F| = 2$ case of our result, we see that this implies $c_1 = c_2 = c_7 = 0$. Similarly, letting $y \to 1+$ in (4.2) gives $c_3 = c_4 = c_9 = 0$, and letting $z \to 1+$ in (4.2) gives $c_5 = c_6 = c_{11} = 0$. At this point, only 4 terms in (4.2) remain. Letting $yz \to 1+$ now shows that $c_8 = 0$, and the remaining coefficients can be shown to vanish similarly.

For the inductive step, let $|F| > 1$ and suppose Theorem 2 is true for all non-empty sets of positive integers of cardinality less than $|F|$. Suppose also that (4.1) holds. By Theorem 1, it follows that the rational function identity

$$\sum_{\vec{P}\models F} c_{\vec{P}} \prod_{m=1}^{|\vec{P}|} \Big(\prod_{k=1}^{m} \prod_{j\in P_k} x_j - 1\Big)^{-1} = 0 \qquad (4.3)$$

holds for all $x_j > 1$, $j \in F$. Fix $f \in F$ and let $x_f \to 1+$ in (4.3). For the singularities to cancel, we must have

$$\sum_{\substack{\vec{P} \models F \\ P_1 = \{f\}}} c_{\vec{P}} \prod_{m=2}^{|\vec{P}|} \Big(\prod_{k=2}^{m} \prod_{j \in P_k} x_j - 1 \Big)^{-1} = 0,$$

which, by Theorem 1, implies that

$$\sum_{\substack{\vec{P} \models F \\ P_1 = \{f\}}} c_{\vec{P}} \, \zeta\Big(\operatorname*{\mathbf{Cat}}_{m=2}^{|\vec{P}|} \sum_{j \in P_m} s_j \Big) = \sum_{\vec{P} \models F \setminus \{f\}} c_{\vec{P}} \, \zeta\Big(\operatorname*{\mathbf{Cat}}_{m=1}^{|\vec{P}|} \sum_{j \in P_m} s_j \Big) = 0.$$

By the inductive hypothesis, $c_{\vec{P}} = 0$ for every ordered set partition $\vec{P}$ of F whose first component P_1 is the singleton $\{f\}$. Since $f \in F$ was arbitrary, it follows that $c_{\vec{P}} = 0$ for every ordered set partition $\vec{P}$ of F whose first component P_1 consists of a single element.

Proceeding inductively, suppose we've shown that $c_{\vec{P}} = 0$ for every ordered set partition $\vec{P}$ of F with $|P_1| = r - 1 < |F|$. Let G be a subset of F of cardinality r. If in (4.3) we now let $x_g \to 1+$ for each $g \in G$, then as the singularities in the remaining terms (4.3) must cancel, we must have

$$\sum_{\substack{\vec{P} \models F \\ P_1 = G}} c_{\vec{P}} \prod_{m=2}^{|\vec{P}|} \Big(\prod_{k=2}^{m} \prod_{j \in P_k} x_j - 1 \Big)^{-1} = 0.$$

Theorem 1 then implies that

$$\sum_{\substack{\vec{P} \models F \\ P_1 = G}} c_{\vec{P}} \, \zeta\Big(\operatorname*{\mathbf{Cat}}_{m=2}^{|\vec{P}|} \sum_{j \in P_m} s_j \Big) = \sum_{\vec{P} \models F \setminus G} c_{\vec{P}} \, \zeta\Big(\operatorname*{\mathbf{Cat}}_{m=1}^{|\vec{P}|} \sum_{j \in P_m} s_j \Big) = 0.$$

By the inductive hypothesis, $c_{\vec{P}} = 0$ for every ordered set partition $\vec{P}$ of F with first component equal to G. Since G was an arbitrary subset of F of cardinality r, it follows that $c_{\vec{P}} = 0$ for every ordered set partition $\vec{P}$ of F whose first component has cardinality r. By induction on r, it follows that $c_{\vec{P}} = 0$ for every ordered set partition $\vec{P}$ of F, as claimed. □

Since every partition identity is thus a consequence of the stuffle multiplication rule, it follows that any multi-variate function that obeys a stuffle multiplication rule will satisfy every partition identity satisfied by the multiple zeta function. For example, suppose we fix a positive integer N and a set F of functions $f : \mathbf{Z}^+ \to \mathbf{C}$ closed under point-wise addition. For positive integer n and $f_1, \dots, f_n \in F$, define

$$z_N(f_1, f_2, \dots, f_n) := \sum_{N>k_1>k_2>\cdots>k_n>0} \prod_{j=1}^{n} \exp(f_j(k_j)),$$

where the sum is over all positive integers $k_1, \dots, k_n$ satisfying the indicated inequalities. Then for all $g, h \in F$, we have $z_N(g)z_N(h) = z_N(g,h) + z_N(h,g) + z_N(g+h)$, and more generally, if $\vec{g} = (g_1, \dots, g_m)$ and $\vec{h} = (h_1, \dots, h_n)$ are vectors of functions in F, then z_N obeys the stuffle multiplication rule

$$z_N(\vec{g})z_N(\vec{h}) = \sum_{\vec{f} \in \vec{g} * \vec{h}} z_N(\vec{f}).$$

We assert that z_N satisfies every partition identity satisfied by ζ. For example, let n be a positive integer, and let $\mathfrak{S}_n$ denote the group of $n!$ permutations of the first n positive integers $\{1, 2, \dots, n\}$. Let $s_1, \dots, s_n$ be real variables, each exceeding 1. Using a counting argument, Hoffman [3] proved the partition identity

$$\sum_{\sigma \in \mathfrak{S}_n} \zeta\Big(\operatorname*{\mathbf{Cat}}_{k=1}^{n} s_{\sigma(k)}\Big) = \sum_{\mathscr{P} \vdash \{1,\dots,n\}} (-1)^{n-|\mathscr{P}|} \prod_{P \in \mathscr{P}} (|P|-1)!\, \zeta\Big(\sum_{j \in P} s_j\Big), \quad (4.4)$$

in which the sum on the right extends over all unordered set partitions $\mathscr{P}$ of the first n positive integers $\{1, 2, \dots, n\}$, and of course $|\mathscr{P}|$ denotes the number of parts in the partition $\mathscr{P}$. In light of Theorem 2, it follows that Hoffman's identity (4.4) depends on only the stuffle multiplication property (1.2) of the multiple zeta function; whence any function satisfying a stuffle multiplication rule will also satisfy (4.4). In particular, with z_N defined as above,

$$\sum_{\sigma \in \mathfrak{S}_n} z_N\Big(\operatorname*{\mathbf{Cat}}_{k=1}^{n} f_{\sigma(k)}\Big) = \sum_{\mathscr{P} \vdash \{1,\dots,n\}} (-1)^{n-|\mathscr{P}|} \prod_{P \in \mathscr{P}} (|P|-1)!\, z_N\Big(\sum_{j \in P} f_j\Big).$$

Finally, we note that by Theorem 1, the rational function identity

$$\sum_{\sigma \in \mathfrak{S}_n} \prod_{k=1}^{n} \Big(\prod_{j=1}^{k} x_{\sigma(j)} - 1\Big)^{-1} = \sum_{\mathscr{P} \vdash \{1,\dots,n\}} (-1)^{n-|\mathscr{P}|} \prod_{P \in \mathscr{P}} (|P|-1)!\, \Big(\prod_{j \in P} x_j - 1\Big)^{-1}$$

is equivalent to (4.4).

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A PERTURBATIVE THEORY OF THE EVOLUTION OF THE CENTER OF TYPHOONS

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Abstract We develop the theory of quasi linear systems of PDE introduced by V. P. Maslov. According to this theory many 2-D quasi linear systems of PDE possess only three algebras of singular solutions with properties of "structural" self-similarity and stability. They are the algebras of shock waves, "narrow" solitons and "square root" point singularities (solitary vortices). Their propagation is described by an infinite chain of ODE (the Hugoniót-Maslov chains)obtained by a Taylor expansion of the solution of the shallow water equation around the point of the singularity . We consider the case of the "square root" singularity and connect it with the description of typhoons. We show the connection of this theory with the evolution of the center of typhoons.

1. Introduction

About twenty years ago V. P. Maslov [21, 20] stated the conjecture that a wide class of quasi linear hyperbolic systems, including the hydrodynamic equations, admits only a few types of particular singular solutions. These solutions are characterized by the property of "self similarity" (i.e. they conserve their singular structures for some time in-

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terval) and stability (i.e. small perturbations do not destroy the singular structure). These are strong conditions for the quasi non linear case. While in the case of linear hyperbolic systems the solutions, at least for a small time interval, conserve any type of singularity of the initial condition for the quasi non linear case these conditions restrict the class of solutions of such type. Shock waves, "infinitely narrow" solitons and solitary vortices belong to this class. All the mentioned singular solutions can be described by a formula similar to either "nonlinear WKB" (Whitham) solutions or distorted Riemann waves (see [35]):

$$w = \mathbf{f}(\mathbf{x}, \mathbf{t}) + \mathbf{g}(\mathbf{x}, \mathbf{t}) F(S(x, t)) \tag{1.1}$$

where w is a vector or scalar function describing either the velocity field of the atmosphere or its geopotential, $x \in \mathbb{R}^2$, $F(\tau)$ is a scalar function smooth outside the set $\tau = 0$ and having a singularity at the point $\tau = 0$, and the phase $S(x, t)$, as well as the vector or scalar background $\mathbf{f}(\mathbf{x}, \mathbf{t})$ and the amplitude $\mathbf{g}(\mathbf{x}, \mathbf{t})$, are a smooth function. The solutions of this equation can have all kind of singularities but the properties of self similarity and stability select only the square root singularity which we consider in this work. *Thus we take* $F = \sqrt{\tau}$ (see [21, 33, 5]). All the other special solutions are apparently destroyed by small perturbations. The proof of this conjecture is not trivial, it has been given in [14] for the system of the shallow water Equations. All the singular solutions of the type (1.1) satisfy an infinite system of ODE (chains) which describe their dynamics. These are the equations obtained for the set of their Taylor coefficients of the singular solutions evaluated in the singular points $\mathbf{x} = X(t)$, as well as on the trajectory $\mathbf{x} = X(t)$. We call these equations *the Hugoniót–Maslov chain.*

The chains for the shock waves and solitons for gas dynamic equations were studied many years ago (see [20, 22, 9] and also [30, 18]). For the chains corresponding to vortex singularities there are only a small number of results up to now.

The Hugoniót-Maslov chain is nonclosed since the first N equations contain more than N unknowns, and hence the position of the singularity cannot be uniquely determined from these systems in general. As we already mentioned our chain is obtained from the shallow water (SW) equations. The system of shallow water equations is well known as the simplest 2-dimensional dispersion-free zero-viscosity approximation in modelling various evolution physical processes, including (which is important for this paper) the propagation of the mesoscale vortices in the atmosphere [24, 6]. This system with variable Coriolis force, in the so called β-plane approximation, has the form

$$\frac{\partial \eta}{\partial t} + \langle \nabla, \eta \mathbf{u} \rangle = 0, \quad \frac{\partial \mathbf{u}}{\partial t} + \langle \mathbf{u}, \nabla \rangle \mathbf{u} - \omega \mathbf{T} \mathbf{u} + \nabla \eta = 0. \qquad (1.2)$$

Here $x = {}^t(x_1, x_2) \in \mathbf{R}^2$, and the unknowns $\mathbf{u}(x,t) = {}^t(u_1(x,t), u_2(x,t))$ are two dimensional vectors, and the function $\eta(x,t)$ is the geopotential of the atmosphere or the free surface elevation in the water waves theory, $\mathbf{T} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, $\nabla = {}^t(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2})$, $\omega = \widetilde{\omega} + \beta x_2$ is the doubled Coriolis frequency on the β-plane, and $\widetilde{\omega}$, β are parameters (physical constants), β is assumed to be sufficiently small. We also denote by $<,>$ the inner product and by left upper index t the transposition of matrices and vectors.

The system (1.2) has some important properties, like the existence of the conservation law, Hamiltonian representation etc. For us it is important the existence of a Lagrangian invariant which is the so called *potential vorticity* or *Rossby invariant*

$$\mathbf{\Pi} = \frac{u_{2x_1} - u_{1x_2} + \omega}{\eta}. \qquad (1.3)$$

The invariant property means that $\mathbf{\Pi}$ is conserved along the trajectories of the velocity vector field $\mathbf{u}$: $\mathbf{\Pi}_t + < \mathbf{u}, \nabla > \mathbf{\Pi} = 0$.

We shall study in the present paper the square root type singular vortical solution of this system taking into account its possible application to the physics of atmosphere.

Although we deal finally with very special solutions of the system (1.2), there are many solutions of this kind, and in fact we deal with a family of solutions depending on some parameters. These parameters should be determined from the experimental data in order to predict the trajectory of the center of the typhoons. Let $\Gamma = (\gamma_1, \gamma_2 \ldots)$ denote these parameters, in general, the number of parameters may be infinite. Since the parameters $(\gamma_1, \gamma_2 \ldots)$ have different physical meanings, we shall sometimes denote them by other letters, while the entire collection will always be denoted by Γ. Suppose that we have constructed a family of such solutions and that the trajectory of the motion is described by some functions $X(t, \Gamma) = (X_1(t, \Gamma), X_2(t, \Gamma))$. Then, starting from the conjecture that the functions (1.1) describe the mesoscale vortices (typhoons) and knowing the trajectory of the vortex center (typhoon eye) for $t \in [0, T]$, we can try to recover the subsequent motion of the center as follows. Let $\Gamma^N = (x_1 = X_1^N(t),\ x_3 = X_2^N(t)),\ t \in [t_1, t_2])$, be the trajectory of the center (eye) of an actual vortex. Wechoose the parameters $\Gamma = (\gamma_1, \gamma_2 \ldots)$ from the condition that the trajectories Γ and Γ^N must be close on the interval $[0, T_0]$, say, by minimizing the mean root square deviation between theoretical and observed trajectory of the typhoon. Then, once we know the parameters $\gamma_1, \gamma_2, \ldots$, we can uniquely determine the trajectory Γ for $t > t_2$. Thus, we have arrived at a classical optimization problem. Although we have no place to solve this problem here we give some insight on the solution of this optimization task.

2. Dynamics of vortex square-root type singularities and Hugoniót–Maslov chains

2.1 Statement of the problem.

Thus our aim is to construct solutions of system (1.2) in the form

$$\begin{aligned} \eta &= \rho(x,t) + \widetilde{\rho}(x,t), & \widetilde{\rho}(x,t) &= R(x,t)F(S(x,t)), \\ \mathbf{u} &= u(x,t) + \widetilde{u}(x,t), & \widetilde{u}(x,t) &= U(x,t)F(S(x,t)), \end{aligned} \tag{2.1}$$

Here $x = {}^t(x_1, x_2) \in R^2$ and $t \in [0, T]$; furthermore, ρ, R, and S are smooth scalar functions and $u = {}^t(v, w)$ and $U = {}^t(U_1, U_2)$ are smooth 2-dimensional vector functions. The function $S(x, t)$ is assumed to satisfy the following conditions:

i) $S(x, t) \geq 0$, and for each t the equality $S(x, t) = 0$ holds at a single point $x = X(t) = {}^t(X_1(t), X_2(t))$. The set $\Gamma = (x = X(t), t \in [0, T])$ will be called the *trajectory* of the singular solution (2.1) of (1.2) on the interval $[0, T]$.

The functions S, U and R are "generic" in the sense that

ii) The matrix $\mathbf{H}(t) = \|\frac{\partial^2 S}{\partial x_i \partial x_j}\|\Big|_\Gamma = \operatorname{Hess} S\Big|_\Gamma$ of second derivatives is nondegenerate (and hence positive) on Γ.

iii) The eigenvalues of the matrix $\operatorname{Hess} S|_\Gamma$ are distinct[1]. (In what follows we show that if there exist solutions (2.1) such that $S(x, t)$ satisfies the above assumptions at $t = t_0$, then these assumptions hold for $t > t_0$ as well.)

iv)The expansions of U and R in powers of $(x - X(t))$ start from the minimum possible powers[2].

v) (v-a.) $F(\tau)$ is a continuous functions for $\tau \geq 0$, $F(0) = 0$; (v-b.) $F(\tau)$ is smooth for $\tau > 0$, $\lim_{\tau \to +0} F'(\tau) = \infty$.

Obviously, the function F in (2.1) is not determined uniquely by the condition v): we can multiply it with any non-vanishing smooth function and add any smooth function (depending on S) vanishing on the trajectory $X(t)$. Moreover, sometimes the function S can be also multiplied by some non-vanishing smooth function of (x, t).

As we mentioned before the nonlinearity in system (1.2) together with the assumptions about "self similarity and stability" of the singular structure "eliminate" the possibility to choose the function F in an arbitrary way. So the problem is to describe all suitable functions F in (2.1) and then to construct at least some characteristics of solutions (2.1), and, the most important aim, to determine the trajectories Γ and the values on Γ of the functions ρ, R, u, U, some of their derivatives, $\operatorname{Hess} S|_\Gamma$, etc., that is, the characteristics of the solution in the vicinity of Γ.

First we choose the approximation from asymptotic considerations. Namely, we wish our approximate solution to be, in a sense, the leading term of the formal asymptotic expansion with respect to smoothness (or powers of $x - X(t)$). The dependence of the trajectory X on the parameters will not be indicated explicitly.

2.2 The Hugoniót–Maslov chains are necessary conditions for the existence of vortical solutions.

Let us now state some results. We start from an assertion that describes the discontinuous part of the solution (2.1) and which was stated and proved earlier in a somewhat different form in [21, 33] for the case in which $\omega = 0$.

We adopt the following notation. (1) A dot over a letter indicates differentiation with respect to time. (2) An asterisk in the position of a superscript indicates the adjoint matrix, while the left superscript "t" stands for transposition. (3) Let $G(x,t)$ be a smooth function or vector, and let $X(t)$ be a trajectory. Then we consider the Taylor expansion

$$G \sim \sum_{k=0}^{\infty} G^{(k)}(x,t), \qquad \text{where} \tag{2.2}$$

$$G^{(k)}(x,t) = \sum_{m_1+m_2=k} G^{(k)}_{m_1 m_2}(t)(x_1 - X_1(t))^{m_1}(x_2 - X_2(t))^{m_2},$$

$G^{(m_1+m_2)}_{m_1,m_2}(t) = \frac{1}{m_1!m_2!}\frac{\partial^{(m_1+m_2)}G}{\partial x_1^{m_1}\partial x_2^{m_2}}(X(t),t)$, so that the $G^{(k)}$ are kth-order homogeneous polynomials and the $G^{(m_1+m_2)}_{m_1 m_2}$ are the Taylor coefficients[3]. The superscript on these coefficients is superfluous, and we omit it in this section. However, in the awkward computations in the subsequent sections, it is convenient not to omit the superscript. Furthermore, to simplify the notation, we write $\rho_0(t)$ instead of $\rho^{(0)}_{00}$. The function η must be strictly positive (according to its physical meaning), and in what follows we consider only solutions of system (1.2) which satisfy this condition. Hence $\rho_0(t)$ should be positive for the trajectory Γ, we shall see that our solutions preserve this property in time.

We also denote

$$q(t) = \frac{1}{2}\operatorname{div} u(X(t), t), \tag{2.3}$$

$$p(t) = \frac{1}{2}\left(\frac{\partial v}{\partial x_2}(X(t), t) - \frac{\partial w}{\partial x_1}(X(t), t)\right) \equiv -\frac{1}{2}\operatorname{curl}_3 u(X(t), t), \tag{2.4}$$

$$\omega_0 = \widetilde{\omega} + \beta X_2(t). \tag{2.5}$$

Theorem 1. If the system (1.2) has a solution of the form (2.1) satisfying conditions $i) - -v)$, then the following assertions hold.

1. Without loss of generality one can assume that in (2.1) $F = \sqrt{\tau}$.

2a. The trajectory $X(t)$ is frozen in the velocity field $\mathbf{u}$ (and u):

$$\dot{X}(t) = u(X(t), t) \equiv \mathbf{u}(X(t), t) \equiv V(t) \Longleftrightarrow \dot{X}_1 = V_1, \quad \dot{X}_2 = V_2. \tag{2.6}$$

2b. The complex velocities $u(x, t) = v(x, t) + iw(x, t)$ (and $\mathbf{u}_1(x, t) + i\mathbf{u}_2(x, t)$) on the trajectory $X(t)$ satisfy the Cauchy–Riemann conditions

$$\frac{\partial v}{\partial x_1} = \frac{\partial w}{\partial x_2}|_\Gamma = q(t), \quad \frac{\partial v}{\partial x_2}|_\Gamma = -\frac{\partial w}{\partial x_1}|_\Gamma = p(t) \tag{2.7}$$

and

$$\rho_{20}|_\Gamma = \rho_{02}|_\Gamma + \beta V_1/2, \quad \rho_{11}|_\Gamma = \beta V_2/2. \tag{2.8}$$

2c. The "potential vorticity" $\mathbf{\Pi}$ (1.3) is conserved along the trajectory Γ:

$$\mathbf{\Pi}|_\Gamma = \frac{\omega_0 - 2p}{\rho_0} = -c = const. \tag{2.9}$$

2d. The functions $\widetilde{\rho} = R\sqrt{S}$ and $\widetilde{u} = U\sqrt{S}$ are given by

$$\begin{pmatrix} \widetilde{u} \\ \widetilde{\rho} \end{pmatrix} = \varphi\sqrt{S}\begin{pmatrix} \mathbf{T}P \\ 0 \end{pmatrix} + \frac{2}{3}S\sqrt{S}\begin{pmatrix} \mathbf{T}(\nabla(\varphi\rho))^{(1)} \\ \varphi c\rho_0(t)) \end{pmatrix} + O(|x - X(t)|^4) \tag{2.10}$$

Here the smooth function S, φ and the vector functions P are

$$S = \frac{\rho_0(t)}{2}(x - X(t), \Pi(t)B\Pi^*(t)(x - X(t)) + O(|x - X(t)|^3),$$

$$P = \nabla S \equiv \rho_0(t)\Pi(t)B\Pi^*(t)(x - X(t)) + O(|x - X(t)|^2,$$

$\Pi(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$ is the matrix of rotation by the angle

$$\theta(t) = \theta_0 + \int_0^t p(t)dt \equiv \theta_0 - \frac{1}{2}\int_0^t \operatorname{curl}_3 u(X(t), t)dt, \tag{2.11}$$

$$\varphi = A + O(|x - X(t)|), \quad A = const, \tag{2.12}$$

$B = \begin{pmatrix} 1+b & 0 \\ 0 & 1-b \end{pmatrix}$, b, θ_0 and A are real constants characterizing the initial structure of the vortical solution, $|b| < 1$.

2e. The derivatives ρ_{lj}, v_{lj}, w_{lj}, the functions $V_1 = v(X(t))$, $V_2 = w(X(t))$, $\omega_0(t)$, ρ_0, $p(t)$, $q(t)$ and

$$r = \rho_{20} - \beta V_1/4 \equiv \rho_{02} + \beta V_1/4 \tag{2.13}$$

satisfy the following equations in addition to (2.6) and (2.7) (the initial relations of the Hugoniót–Maslov chain):

$$\dot V_1 - \omega_0 V_2 + \rho_{10} = 0, \quad \dot V_2 + \omega_0 V_1 + \rho_{01} = 0, \tag{2.14}$$

$$\dot\rho_0 + 2q\rho_0 = 0, \tag{2.15}$$

$$\dot\rho_{10} + 3q\rho_{10} - p\rho_{01} + \rho_0(w_{11} + 2v_{20}) = 0, \tag{2.16}$$

$$\dot\rho_{01} + 3q\rho_{01} + p\rho_{10} + \rho_0(v_{11} + 2w_{02}) = 0, \tag{2.17}$$

$$\dot q - p^2 + q^2 + \omega_0 p + 2r + \beta V_1/2 = 0, \tag{2.18}$$

$$\dot p + 2pq - \omega_0 q - \beta V_2/2 = 0, \tag{2.19}$$

$$\dot r + 4qr + \frac{1}{2}\rho_{10}(3v_{20} + w_{11} + v_{02}) + \frac{1}{2}\rho_{01}(v_{11} + 3w_{02} + w_{20}) = f_0, \tag{2.20}$$

$$\dot v_{20} + 3qv_{20} - \omega_0 w_{20} - p(v_{11} - w_{20}) = f_1, \tag{2.21}$$

$$\dot v_{11} + 3qv_{11} - \omega_0 w_{11} - p(2v_{02} - 2v_{20} - w_{11}) + \beta p = f_2, \tag{2.22}$$

$$\dot v_{02} + 3qv_{02} - \omega_0 w_{02} + p(v_{11} + w_{02}) - \beta q = f_3, \tag{2.23}$$

$$\dot w_{20} + 3qw_{20} + \omega_0 v_{20} - p(w_{11} + v_{20}) = f_4, \tag{2.24}$$

$$\dot w_{11} + 3qw_{11} + \omega_0 v_{11} - p(-2w_{20} + 2w_{02} + v_{11}) + \beta q = f_5, \tag{2.25}$$

$$\dot w_{02} + 3qw_{02} + \omega_0 v_{02} + p(w_{11} - v_{02}) + \beta p = f_6, \tag{2.26}$$

$$\dot\omega_0 - \beta V_2 = 0, \tag{2.27}$$

$$\begin{aligned} &\rho_{10}(v_{11} + w_{02}) + \rho_{01}(v_{20} + w_{11}) \\ &\quad + \rho_0(v_{21} + w_{12}) + \beta(\dot V_2/4 + qV_2 + pV_1/2) = 0, \end{aligned} \tag{2.28}$$

$$\begin{aligned} &\rho_{10}(3v_{20} + w_{11} - v_{02}) - \rho_{01}(v_{11} + 3w_{02} - w_{20}) \\ &\quad + \rho_0(3v_{30} + w_{21} - v_{12} - 3w_{03}) + \beta(\dot V_1/2 + 2qV_1 - pV_2) = 0. \end{aligned} \tag{2.29}$$

Here $f_0 = -\rho_0(3v_{30} + 3w_{03} + w_{21} + v_{12})$, $f_1 = -3\rho_{30}$, $f_2 = -2\rho_{21}$, $f_3 = -\rho_{12}$, $f_4 = -\rho_{21}$, $f_5 = -2\rho_{12}$, $f_6 = -3\rho_{03}$.

3. Conditions (2.6)–(2.8) and (2.14)–(2.29) and the representations (2.10)–(2.12) are necessary and sufficient for the function (2.1) to satisfy the original system with accuracy $O(|x - X(t)|^3)$.

The proof of this theorem is given in the paper [14]. The relations given in the theorem are analogous to the Hugoniót conditions and higher-order corrections for solitary vortices of Eqs. (1.2). The "freeze-in" conditions (2.6) for the vortex and the Cauchy–Riemann conditions (2.7) follow from the presence of a nonsmooth part in the solution (2.1), and the derivation of these conditions is based on arguments closely similar to that of the eikonal or WKB method applied to expansions with respect to smoothness. We point out that the derivation of these conditions substantially uses the vortex asymmetry condition iii). The equations (2.14)–(2.29) are essentially derived by successive differentiation of the original system with regard to (2.6)–(2.8) and evaluating the results at the points of the trajectory $x = X(t)$. This part of the proof requires only some awkward computations. The content of the point $2d$ explains the connection with the typhoon's phenomenology see [14].

Remarks.

- Equation (2.27) is obtained from (2.5) by differentiation; as will be clear in the following, it is advisable to use (2.5) instead of (2.27).

- As it was mentioned already,the system (1.2) generates a variable that is constant along the trajectories of the vector field $\mathbf{u}$, namely, the "potential vorticity" $\mathbf{\Pi}$. It is well known that when one applies asymptotic procedures, some special properties like conservation laws or Hamiltonian structure manifest themselves also in the equations for the functions specifying the asymptotic. For example, the conservation laws play an important role in the Whitham's averaging method for the Korteweg–de Vries equation: the averaged conservation laws are the equations for the slowly varying parameters of cnoidal waves (e.g., see [35, 15]). In that connection, it is of interest to understand what the existence of conserved potential vorticity for the Hugoniót–Maslov chain means. It turns out that for the smooth part we have the identity (2.9) and for the non smooth part this fact implies the Cauchy–Riemann conditions (2.7). Moreover the existence of $\mathbf{\Pi}$ implies some other interesting facts, like the integrability of the truncated chain etc.

- Equations (2.8) follow from the Cauchy–Riemann conditions, that is, from the conservation of the potential vorticity.

- The function φ in (2.10) describes the corrections of the asymptotic expansion of $\widetilde{\rho}$ and $\widetilde{u}$. The representation (2.10) includes also the correction $U^{(2)}$, which can be expressed via the phase correction $S^{(3)}$ and contains a new unknown function $\varphi^{(1)}$, which depends linearly on $x - X(t)$ and smoothly on t :

$$U^{(2)} = AP_{\perp}^{(2)} + \varphi^{(1)}P_{\perp}^{(1)} + \frac{2}{3\rho_0}S^{(2)}\mathbf{T}\nabla(\varphi^{(1)}\rho_0 + \varphi_0\rho^{(1)}). \quad (2.30)$$

Here $P_{\perp}^{(2)} = \mathbf{T}\nabla S^{(3)}$. Then in (2.10) $\varphi = A + \varphi^{(1)}$. To find the functions $S^{(3)}$ and $\varphi^{(1)}$, one must construct the corrections $U^{(3)}$ and $R^{(3)}$, that is, an asymptotic solution satisfying the original system modulo $|x - X(t)|^4$. Theorem 1 remains valid for an arbitrary choice of the functions $\varphi^{(1)}$ and $S^{(3)}$; for example, we can take these functions to be zero identically. Representing $\widetilde{\rho}$ and $\widetilde{u}$ in the form (2.10) one can see that actually the expansion "with respect to smoothness" (or with respect to the powers of $(x_j - X_j(t))$ for solutions (2.1) is an expansion with respect to the powers $S^{k+1/2}$. Also we hope that (2.10) may allow one to guess the structure of higher approximations.

- As we mentioned before the choice of the phase S is not unique: it is possible to multiply it by any smooth positive function; this changes the amplitude (U, R). It is shown in ([14]) that, modulo this transformation, the phase S satisfies as a *necessary* condition the *eikonal or Hamilton-Jacobi* equation $S_t + \langle u, \nabla S\rangle = 0$, which is one of the characteristic equations corresponding to the linearization of the original system (1.2) on the smooth back ground u, ρ. In hydrodynamics this characteristics are called "hydrodynamic" or "slow" mode. The linearized equation have also two other characteristics which are called "acoustic" or "fast" modes. Hence the pure mathematical constructions show that a necessary condition is that the considered vortex propagates along the trajectory of the slow mode. One can consider the Cauchy problem $S|_{t=o} = S_0(x)$ with a smooth initial function S_0 for the eikonal equation. The smooth solution to this problem exists for any t from $(-\infty, \infty)$. The question is: does any arbitrary initial phase S_0 satisfying conditions i)-iii) imply the phase S which is suitable for the solution (2.1)? The quadratic form $S^{(2)}$ is the approximate solution of this equation, and in the initial moment of time this quadratic form can be chosen more or less arbitrary. The question about the complete solution S and about higher approximations $S^{(3)}, S^{(4)}$, etc. is open.

- The compressibility in system (1.2) plays an important role both in the derivation of the chain and in the relative analysis. If instead of system (1.2) we consider the two-dimensional Euler equation for an incompressible fluid (formally, this means that the continuity equation in system (1.2) is replaced by the equation $div\,\mathbf{u} = \mathbf{0}$), then, as G. Koval showed, the vector functions $(X(t), V(t))$ will not be coupled with the other derivatives of u and ρ, that is, the trajectory Γ can be specified arbitrarily. This is due to the fact that the Euler equations in the entire space are invariant with respect to the change to a noninertial frame of reference. From the physical viewpoint, this fact can apparently be explained as follows: the boundary effects in an incompressible medium affect the trajectory of the singularity even in the zero approximation, whereas in a compressible medium the problem of the propagation of singularities can be localized in some approximation. The presence of compressibility in the derivation of the Hugoniót–Maslov chain for point singularities agrees fairly well with the fact that the Hugoniót conditions for shock waves are obtained from the gas dynamic equations, where compressibility is also present. Let us also add that the linearized Euler equations have only one type of (real) characteristics corresponding to hydrodynamical or slow mode, the fast modes are absent in this case. As we just mentioned the requirement of "structural self-similarity" of the solution (2.1) implies that asymptotically the singularity moves only along the "slow" (or "hydrodynamic") mode and lends no energy to the "rapid" ("acoustic") modes," whose presence is due to compressibility. We see that although the trajectory can be included in the chain only by virtue of the presence of acoustic modes, the "main part" of the vortex is carried by the hydrodynamic mode rather than the acoustic modes.

The chain can be closed by putting the third order terms equal to zero

$$f_j = 0, \quad j = 0, \ldots, 6. \tag{2.31}$$

We analyze the system obtained in this way in the following sections. We first show a simple method for getting the chain of equations of Hogoniót-Maslov type and then we analyze a system of first integrals.

3. Equation for the smooth and singular part of the solutions Cauchy-Riemann conditions

In this section we show a method for deriving the equations of the chain of Theorem **1**. First we derive two subsystems of equations which come from the singular and smooth part of the solution of the system (1.2). Putting the solution of the form (1.1) in the system (1.2) and separating the smooth parts from the singular parts we get two subsystems of equations:

$$\begin{aligned} &\tfrac{\partial}{\partial t}\rho + (\nabla, \rho u + RUS) = 0, \\ &\tfrac{\partial}{\partial t}u + (u,\nabla)u + \nabla\rho - \omega \mathbf{T} u + (U\sqrt{S},\nabla)(U\sqrt{S}) = 0; \end{aligned} \tag{3.1}$$

$$\begin{aligned} &\tfrac{\partial}{\partial t}(R\sqrt{S}) + (\nabla, uR\sqrt{S} + \rho U\sqrt{S}) = 0, \\ &\tfrac{\partial}{\partial t}(U\sqrt{S}) + (u,\nabla)(U\sqrt{S}) + (U\sqrt{S},\nabla)u + \nabla R\sqrt{S} - \omega \mathbf{T} U\sqrt{S} = 0. \end{aligned}$$

Making the derivatives and eliminating $\sqrt{S}$ the second subsystem gets the form

$$\begin{aligned} &\Lambda R + \rho(P,U) + 2Sf = 0, \\ &\Lambda U + PR + 2SF = 0, \end{aligned} \tag{3.2}$$

where $\Lambda = S_t + (u,P)$, $P = \nabla S$, $f = R_t + (\nabla, uR + \rho U)$, $F = U_t + (u,\nabla)U + (U,\nabla)u - \omega TU + \nabla R$. Thus we get six equations for seven unknown variables ρ, u_1, u_2, R, U_1, U_2, S. It is possible to see that, without loss of generality, the function S satisfies the equation of the "eikonal" (Hamilton-Jacobi) which corresponds to the "hydrodynamical mode" or "slow mode" [28]:

$$S_t + (u,\nabla)S = 0. \tag{3.3}$$

The equation (3.3) and the condition that the phase S in the first order approximation is a quadratic form in the variables $x - X(t)$, are the conditions for the existence of the frozen velocity field on the trajectory Γ of the center of typhoons:

$$\dot{X}(t) = u(X(t),t) \stackrel{\text{def}}{=} V(t).$$

using the equation (3.3) the system (3.2) may be written in the form:

$$\begin{aligned} &S(R_t + (\nabla, uR + \rho U)) + \frac{1}{2}\rho(U,\nabla)S = 0, \\ &S(U_t + (u,\nabla)U + (U,\nabla)u - \omega TU + \nabla R) + \frac{1}{2}R\nabla S = 0, \end{aligned} \tag{3.4}$$

The equations (3.1), (3.3), (3.4) are a closed system for the evaluation of the seven functions ρ, u_1, u_2, R, U_1, U_2, S.

In this way we have a system with a singular term which has degenerate solutions. The smooth solutions can be found only introducing further hypotheses for its coefficients, i.e. for the functions u and ρ. Surprisingly, the first of such additional hypotheses are just the Cauchy-Riemann conditions for the complex velocities on the trajectory Γ [14]:

$$\frac{\partial u_1}{\partial x_1}|_\Gamma = \frac{\partial u_2}{\partial x_2}|_\Gamma \stackrel{\text{def}}{=} q(t), \quad \frac{\partial u_1}{\partial x_2}|_\Gamma = -\frac{\partial u_2}{\partial x_1}|_\Gamma \stackrel{\text{def}}{=} p(t). \tag{3.5}$$

The conditions (3.5) are obtained by equating to zero all the Taylor coefficients only up to the third order in (3.4). We observe that we didn't suppose a priori the analyticity of the complex velocity $u(x,t)$, beside this property doesn't hold: it takes place only on the trajectory Γ. It turns out that (3.5) in some sense it is a consequence of the conservation of the potential vorticity. A complete explanation of the appearance of the property of Cauchy-Riemann conditions is still not available.

4. Derivation of the Hugoniót-Maslov chain using complex variables and its integrals

We give now the derivation of the Hugoniót-Maslov chain using complex variables. This approach to the problem is new and differs from the previous ones where the real variables were used [12], [14]. The use of complex variables simplifies the necessary computations and allows to write the new variables with which the system is written in a more comprehensible and compact form as it is shown in this section. The simplifications arise also from the Cauchy-Riemann conditions. Let us define these new variables. The vectors X, V, u are substituted by the complex variables $X = X_1 + iX_2$, $V = V_1 + iV_2$ and $u = u_1 + iu_2$. Instead of $\rho_0 = \rho(X(t), t)$, q, p (these last variables are defined by the Taylor second order coefficients of the expansion of u) and the other coefficients of the Taylor expansion up to the second order of ρ and u we introduce the real variables c, μ, ω, λ and the complex ones Y, Z, W, U:

$$\begin{aligned}
&c = (2p - \omega_0)/\rho_0 \\
&\mu = 1/\sqrt{|c|\rho_0} \\
&Y = \mu^3|c|^{-1}(2\frac{\partial^2}{\partial z\partial \bar{z}}u - \beta/3)|_\Gamma \\
&Z = \mu^3|c|^{-1}(\frac{\partial^2}{\partial z\partial z}u + \beta/3)|_\Gamma \\
&U = \mu^3|c|^{-1}\frac{\partial^2}{\partial \bar{z}\partial \bar{z}}u|_\Gamma \\
&W = 2\mu^3|c|^{-1}(-ic\rho_{\bar{z}} - \frac{\partial^2}{\partial z\partial \bar{z}}u + \frac{\partial^2}{\partial \bar{z}\partial \bar{z}}\mathbf{u} + \beta/2)|_\Gamma \equiv -\frac{2i}{|c|^{5/2}\rho_0^{1/2}}\frac{\partial \mathbf{\Pi}}{\partial \bar{z}}|_\Gamma \\
&\lambda = 1/4 - 2r\mu^4 + |c|\,\mathrm{Re}(2(Z - \bar{Y})W + 3YZ)) \\
&X = X_1 + iX_2 \\
&V = V_1 + iV_2.
\end{aligned} \tag{4.1}$$

The symbol $\bar{\alpha}$ indicates the complex conjugate of α, $\partial/\partial z = (\partial/\partial x_1 - i\partial/\partial x_2)/2$, $r = \frac{\partial^2}{\partial z\partial \bar{z}}\rho|_\Gamma$. It is easy to check that

$$\begin{aligned}
&c = \text{const} \\
&p = (\omega + \sigma\mu^{-2})/2 \\
&\sigma = \text{sign} c.
\end{aligned} \tag{4.2}$$

The closed Hugoniót-Maslov chain in the way (2.31) takes this form in the new variables:

$$\begin{aligned}
&\dot V + i\omega V + i\sigma\mu^{-3}(Y + W - 2\bar Z) = 0,\\
&\dot Y = i(p-\omega)Y - \tfrac{i\beta}{3|c|}(2p+\omega)\mu^3,\\
&\dot Z = i(3p-\omega)Z + \tfrac{i\beta}{3|c|}\omega\mu^3,\\
&\dot W = -ipW,\\
&\dot\lambda = \beta\mu^3(\omega\,\mathrm{Im}\,Y - (2p+\omega)\,\mathrm{Im}\,Z - 4p\,\mathrm{Im}\,W/3),\\
&\dot\omega = \beta\,\mathrm{Im}\,V \equiv \beta V_2,\\
&\ddot\mu + b^2\mu = \mu^{-3}(\lambda + 2|c|\,\mathrm{Re}((Z-\bar Y)W + 3ZY/2)),\\
&b^2 = (\omega_2 + 2\beta\,\mathrm{Re}\,V)/4.
\end{aligned} \tag{4.3}$$

It is possible to show that the equations (4.3) can be easily derived from the system (3.1) and from the conservation law of the potential vorticity if one changes variables. For convenience, one has to pass to coordinates relative to the center of the point singularity. Instead of the variables x_1, x_2 one has to use the variables $x_1' = x_1 - X_1(t)$, $x_2' = x_2 - X_2(t)$, and use the velocity $u' = u - V$ instead u. Then instead of using the variables (x_1', x_2'), one can use the complex variables $(z, \bar z)$, where $z = x_1' + ix_2'$ and $\bar z = x_1' - ix_2'$. To simplify the notation we omit primes on variables. After the introduction of the new variables the equations for the background part of the flow will be written in the form:

$$\begin{aligned}
&\tfrac{\partial}{\partial t}\rho + (u,\nabla)\rho + \rho\,\mathrm{div}\,u = \mathcal{F}(R,U,S),\\
&\tfrac{\partial}{\partial t}u + (u,\nabla)u + \dot V + i\omega(u+V) + 2\tfrac{\partial}{\partial\bar z}\rho = \mathcal{G}(U,S),
\end{aligned} \tag{4.4}$$

In order to simplify the notations we use the symbols: $(u,\nabla) = u\frac{\partial}{\partial z} + \bar u\frac{\partial}{\partial\bar z}$, $\mathrm{div}\,u = \frac{\partial}{\partial z}u + \frac{\partial}{\partial\bar z}\bar u = 2\,\mathrm{Re}\,(\frac{\partial}{\partial z}u)$.

$$\omega(z,\bar z,t) = \omega_0 - i\frac{\beta}{2}(z - \bar z),$$

where $\omega_0(t) = \widetilde\omega + \beta X_2(t)$. $\mathcal{F} = -\,\mathrm{div}(RUS)$, $\mathcal{G} = -S(U,\nabla)U - \frac{1}{2}U(U,\nabla)S$ is the right hand side which depends on the singular part of the solution (1.1).

Let us denote with $g^{(k)}$ the k order homogeneous polynomial of the Taylor expansion of the function g in powers of z, $\bar z$:

$$g^{(k)} = \sum_{i=0}^{k}\frac{1}{i!(k-i)!}\,g_{i,k-i}z^i\bar z^{k-i}.$$

For example

$$u = u^{(0)} + u^{(1)} + u^{(2)} + O(|z|^3),$$

where $u^{(0)} = 0$ as a consequence of the "freezing" hypothesis, and, as a consequence of condition (3.5), $u^{(1)} = (q - ip)z$. Let us remark that $\rho_{m,n} = \bar{\rho}_{n,m}$ since ρ is a real function.

Now the chain can be derived by equating the coefficients of the powers of the same order appearing in (4.4). The differentiation with respect to t doesn't change the order of the polynomial in z, $\bar{z}$ in the Taylor expansion. The derivative with respect to z and $\bar{z}$ decreases the order of the corresponding polynomial by one. The multiplication of the polynomial with z^m, $\bar{z}^n$ increases it by $m+n$. Thus the system (4.4) can be rewritten in the following way.

$$\begin{aligned}
&\frac{\partial \rho^{(k)}}{\partial t} + (u^{(1)}, \nabla)\rho^{(k)} + \rho^{(k)} \operatorname{div} u^{(1)} + (u^{(k)}, \nabla)\rho^{(1)} + \rho^{(1)} \operatorname{div} u^{(k)} = \\
&\qquad \mathcal{M}_k + \mathcal{F}^{(k)}, \\
&\frac{\partial u^{(k)}}{\partial t} + (u^{(1)}, \nabla)u^{(k)} + (u^{(k)}, \nabla)u^{(1)} + i\omega_0 u^{(k)} = \mathcal{N}_k + \mathcal{G}^{(k)}.
\end{aligned} \tag{4.5}$$

Here the functions $\mathcal{M}_k$, $\mathcal{N}_k$ are the k-st order homogeneous polynomials depending on $\rho^{(0)}, \dots, \rho^{(k-1)}$, $u^{(2)}, \dots, u^{(k-1)}$, $u^{(k+1)}$, $\rho^{(k+1)}$ and their derivatives by z, $\bar{z}$.

The system (4.5) is a non homogenous linear equation for $v = {}^t(\rho^{(k)}, u^{(k)})$: $\widehat{L}v = f$, where $\widehat{L}$ is a linear operator, f is the right hand side independent from v and its derivatives.

Lemma 2. The monomials $z^m \bar{z}^n$ are eigenfunctions of the operator $(u^{(1)}, \nabla)$ with eigenvalues $(q(m+n) - ip(m-n))$:

$$(u^{(1)}, \nabla) z^m \bar{z}^n = (q(m+n) - ip(m-n)) z^m \bar{z}^n.$$

Proof. It follows simply from (3.5) and the expression $(u, \nabla) = u\frac{\partial}{\partial z} + \bar{u}\frac{\partial}{\partial \bar{z}}$. □

Differentiating the last equation in (4.5) with respect to z and $\bar{z}$ and taking into account the statement of Lemma 2, we get a system of equations for the Taylor coefficients of the form:

$$\begin{aligned}
&\frac{\partial}{\partial t} u_{m,n} + ((1+m+n)q - i(1+m-n)p + i\omega_0) u_{m,n} \\
&= \frac{\partial^{m+n}}{\partial z^m \partial \bar{z}^n} (\mathcal{N}_{m+n} + \mathcal{G}^{(m+n)}),
\end{aligned} \tag{4.6}$$

Making the change of variables:

$$u_{m,n} = \rho_0^{(1+m+n)/2} \widetilde{u}_{m,n}$$

we obtain the system

$$\frac{\partial}{\partial t}\widetilde{u}_{m,n} + i(\omega_0 - (1+m-n)p)\widetilde{u}_{m,n}$$
$$= \frac{1}{\rho_0^{(1+m+n)/2}} \frac{\partial}{\partial z^m} \frac{\partial}{\partial \bar{z}^n} (\mathcal{N}_{m+n} + \mathcal{G}^{(m+n)}),$$

Making a Taylor expansion of the background field in the equation (4.4) and collecting the term containing the same powers of z,$\bar{z}$, we get the following set of equations:

$$\frac{\partial \rho_0}{\partial t} + \rho_0 \operatorname{div} u^{(1)} = 0, \tag{4.7}$$

$$\frac{\partial \rho^{(1)}}{\partial t} + (u^{(1)}, \nabla)\rho^{(1)} + \rho^{(1)} \operatorname{div} u^{(1)} + \rho_0 \operatorname{div} u^{(2)} = 0, \tag{4.8}$$

$$\frac{\partial \rho^{(2)}}{\partial t} + (u^{(1)}, \nabla)\rho^{(2)} + \rho^{(2)} \operatorname{div} u^{(1)} + (u^{(2)}, \nabla)\rho^{(1)} + \rho^{(1)} \operatorname{div} u^{(2)} + $$
$$+ \rho_0 \operatorname{div} u^{(3)} = 0, \tag{4.9}$$

$$\frac{dV}{dt} + i\omega_0 V + 2\frac{\partial}{\partial \bar{z}}\rho^{(1)} = 0, \tag{4.10}$$

$$\frac{\partial u^{(1)}}{\partial t} + (u^{(1)}, \nabla)u^{(1)} + i\omega_0 u^{(1)} + 2\frac{\partial}{\partial \bar{z}}\rho^{(2)} + \beta(z-\bar{z})V/2 = 0, \tag{4.11}$$

$$\frac{\partial u^{(2)}}{\partial t} + (u^{(1)}, \nabla)u^{(2)} + u^{(2)}\frac{\partial}{\partial z}u^{(1)} + i\omega_0 u^{(2)} + 2\frac{\partial}{\partial \bar{z}}\rho^{(3)} +$$
$$+ \beta(z-\bar{z})u^{(1)}/2 = 0. \tag{4.12}$$

The first equation gives:

$$\dot{\rho}_0 + 2q\rho_0 = 0. \tag{4.13}$$

Substituting $u^{(1)} = (q - ip)z$ in (4.11) we get

$$(\dot{q} - i\dot{p})z + (q-ip)^2 z + 2\rho_{11} z + 2\rho_{02}\bar{z} + i\omega_0(q-ip)z + \beta(z-\bar{z})V/2 = 0.$$

Applying $\partial/\partial\bar{z}$ to the last equation we get

$$\bar{\rho}_{20} = \rho_{02} = \beta V/4,$$

Applying the operator $\partial/\partial z$ and separating the real and imaginary parts we obtain two equations:

$$\dot{q} - p^2 + q^2 + \omega_0 p + 2r + \beta V_1/2 = 0, \tag{4.14}$$

$$\dot{p} + 2pq - \omega_0 q - \beta V_2/2 = 0. \tag{4.15}$$

Where $r = r(t) = \rho_{11}$ is a real function. The seventh equation in (4.3) for $\ddot{\mu}$ follows from the equations (4.13)–(4.15)

If we collect the coefficients of the monomial $z\bar{z}$ in (4.12), then from the representation (4.6) we get the equation

$$\frac{d}{dt}u_{11} + 2qu_{11} + (q - ip)u_{11} + i\omega u_{11} + 2\rho_{12} - \beta(q - ip)/2 = 0.$$

Introducing the function

$$Y(t) = \frac{1}{|c|^{5/2}} \frac{1}{\rho_0^{3/2}}(2u_{11} - \frac{\beta}{3})|_\Gamma,$$

and using (4.13) we get

$$\dot{Y} = i(p - \omega_0)Y - \frac{i\beta(2p + \omega_0)}{3|c|^{5/2}\rho_0^{3/2}} - 4\frac{\rho_{12}}{|c|^{5/2}\rho_0^{3/2}}. \tag{4.16}$$

Taking the coefficients of zz and $\bar{z}\bar{z}$ in (4.12) we obtain two equations:

$$\frac{d}{dt}u_{20} + 2(q - ip)u_{20} + (q - ip)u_{zz} + i\omega u_{20} + 2\rho_{21}^{(3)} + \beta(q - ip) = 0,$$

$$\frac{d}{dt}u_{02} + 2(q + ip)u_{02} + (q - ip)u_{02} + i\omega_0 u_{02} + 2\rho_{03}^{(3)} = 0,$$

Introducing the functions

$$Z = \frac{1}{|c|^{5/2}\rho_0^{3/2}}(u_{20} + \frac{\beta}{3})|_\Gamma,$$

and

$$U = \frac{1}{|c|^{5/2}\rho_0^{3/2}}u_{02},$$

we have:

$$\dot{Z} = i(3p - \omega_0)Z + \frac{i\omega_0\beta}{3|c|^{5/2}\rho_0^{3/2}} - 2\frac{\rho_{21}}{|c|^{5/2}\rho_0^{3/2}}.$$

$$\dot{U} = -i(p + \omega_0)U - 2\frac{\rho_{03}}{|c|^{5/2}\rho_0^{3/2}}.$$

The equation (4.16) and the last two equations follow the equations for $\dot{Y}$, $\dot{Z}$, $\dot{U}$ in (2.31).

Let us show how it is possible to obtain some integrals of the chain starting from the equation of the potential vorticity. From the expression of the non regular part of the solution it follows that the conservation of potential vorticity takes the form

$$\Pi_t + (u, \nabla)\Pi + O(|z|^3) = 0, \tag{4.17}$$

where $\Pi = (\operatorname{rot} u + \omega)/\rho = \Omega/\rho$, $\operatorname{rot} u = \frac{1}{i}(\frac{\partial}{\partial z} u - \frac{\partial}{\partial \bar{z}} \bar{u})$.

Projecting (4.17) on Γ

$$c \stackrel{\text{def}}{=} \frac{2p - \omega_0}{\rho_0} = -\Pi^{(0)} = const.$$

This equation can be derived using (4.13), (4.15) and the equation for ω_0:

$$\dot{\omega}_0 = \beta \operatorname{Im} V. \tag{4.18}$$

So if one introduces the constant c it is possible to drop the function $p(t)$ and the equation (4.15) from the chain. Let us consider the following approximation of (4.17). Applying the operator $\partial/\partial\bar{z}$ (4.17) we get

$$\frac{d}{dt}\Pi_{01} + (q + ip)\Pi_{01} = 0.$$

Introducing the function $W(t) = -\frac{2i}{|c|^{5/2}\rho_0^{1/2}}\Pi_{01}$ we get

$$\dot{W} = -ipW.$$

The Taylor expansion of the function Π gives

$$\Pi^{(1)} = \frac{\Omega^{(1)}}{\rho_0} + c\frac{\rho^{(1)}}{\rho_0},$$

from which

$$\rho^{(1)} = \frac{1}{c}(\Pi^{(1)}\rho_0 - \Omega^{(1)}) = \frac{1}{c}(\Pi^{(1)}\rho_0 + i(\frac{\partial u^{(2)}}{\partial z} - \frac{\partial \bar{u}^{(2)}}{\partial \bar{z}}))$$

if $c \neq 0$. Differentiating the last equation with respect to $\bar{z}$ we get

$$\begin{aligned} 2\rho_{\bar{z}} &= 2\frac{1}{c}(\Pi_{\bar{z}}\rho_0 + i(u_{z\bar{z}} - \bar{u}_{\bar{z}\bar{z}})) \\ &= \frac{\rho_0^{3/2}}{c}(\frac{2\Pi_{\bar{z}}}{\rho_0^{1/2}} + i\frac{2u_{z\bar{z}}}{\rho_0^{3/2}} - i\frac{2\bar{u}_{\bar{z}\bar{z}}}{\rho_0^{3/2}}) = i\frac{\rho_0^{3/2}}{c}(W + Y - 2\bar{Z}). \end{aligned}$$

From this equation we have

$$\dot{V} + i\omega_0 V + \frac{i\rho_0^{3/2}}{c}(Y + W - 2\bar{Z}) = 0.$$

Applying the operator $\partial^2/\partial z\partial\bar{z}$ to (4.9) and substituting Y, Z, U, and W in the corresponding Taylor coefficients we get

$$\dot{r} + 4qr - 2\frac{\rho_0^3}{c}\operatorname{Im}((Z + \bar{Y})W + 3YZ) = 0 \tag{4.19}$$

From this equation follows the equation for $\dot{\lambda}$.

This system of equations obtained from the second order terms of the chain is more easy to analyze because it is easy to see that the variables Y, Z, U, W are all first integrals of motion for $\beta = 0$. Moreover it is easier to study the stability of the fixed points of the system and their stable and unstable manifolds.

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Notes

1. This assumption is not invariant with respect to choice of the coordinate system on the plane (x_1, x_2). The invariant assumption is that the ratio of eigenvalues of the matrix $\mathrm{Hess}S|_\Gamma$ and the matrix $\mathrm{Hess}(\nabla S)^2|_\Gamma$ are different.
2. It is possible to omit this assumption, but it looks natural from the point of view of possible application, as well it allows to simplify future considerations.
3. Let us emphasize that we *include the factorials* into the coefficients.

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ALGEBRAIC ASPECTS OF MULTIPLE ZETA VALUES

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Abstract Multiple zeta values have been studied by a wide variety of methods. In this article we summarize some of the results about them that can be obtained by an algebraic approach. This involves "coding" the multiple zeta values by monomials in two noncommuting variables x and y. Multiple zeta values can then be thought of as defining a map $\zeta : \mathfrak{H}^0 \to \mathbf{R}$ from a graded rational vector space $\mathfrak{H}^0$ generated by the "admissible words" of the noncommutative polynomial algebra $\mathbf{Q}\langle x, y\rangle$. Now $\mathfrak{H}^0$ admits two (commutative) products making ζ a homomorphism–the shuffle product and the "harmonic" product. The latter makes $\mathfrak{H}^0$ a subalgebra of the algebra QSym of quasi-symmetric functions. We also discuss some results about multiple zeta values that can be stated in terms of derivations and cyclic derivations of $\mathbf{Q}\langle x, y\rangle$, and we define an action of QSym on $\mathbf{Q}\langle x, y\rangle$ that appears useful. Finally, we apply the algebraic approach to relations of finite partial sums of multiple zeta value series.

Keywords: Multiple zeta values, shuffle product, quasi-symmetric functions, Hopf algebra

1. Introduction

The last fifteen years have seen a great deal of work on the multiple zeta values (MZVs)

$$\zeta(i_1, i_2, \dots, i_k) = \sum_{n_1 > n_2 > \cdots > n_k \geq 1} \frac{1}{n_1^{i_1} n_2^{i_2} \cdots n_k^{i_k}}, \tag{1.1}$$

where $i_1, i_2, \dots, i_k$ are positive integers. The case $k = 2$ goes back to Euler [8], and was revisited by Nielsen [28] and Tornheim [35]. The general case was introduced in [17] and [39]. These quantities have appeared in a surprising variety of contexts, including knot theory [25], quantum field theory [4, 24], and even mirror symmetry [20].

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Much work on MZVs has focused on discovering and proving identities about them, particularly those that express MZVs of "length" (k in equation (1.1)) greater than one in terms of ordinary (length one) zeta values. Even in the length-two case, it appears that there are MZVs that are "irreducible" in the sense that they can't be expressed (polynomially with rational coefficients) in terms of length one zeta values, e.g., $\zeta(6,2)$. (Of course it isn't known how to prove even that $\zeta(3)^2/\zeta(2)^3$ is irrational, so we have to say "appears": but everyone since Euler who has looked for some reduction of $\zeta(6,2)$ hasn't found one.)

Many approaches have been used to obtain MZV identities. Analytic techniques are emphasized in the surveys [5] and [3]. In this article we will focus on algebraic techniques. It is evident that sums of form (1.1) constitute an algebra by simple multiplication of series: this was the starting point of [18], which formalized the "harmonic algebra" of MZVs. But, as has become fairly well known by now, there are two distinct algebra structures on the set of MZVs, the harmonic (or "stuffle") algebra and the shuffle algebra.

Before proceeding further it is useful to introduce an algebraic notation for MZVs. Series of form (1.1) can be specified by the composition (finite sequence of positive integers) $(i_1, i_2, \dots, i_k)$; to this composition we assign the word $x^{i_1-1}yx^{i_2-1}y\cdots x^{i_k-1}y$ in noncommuting letters x and y. A series of form (1.1) converges exactly when $i_1 > 1$, i.e., when the corresponding word starts with x and ends with y. We call such words "admissible", and we can think of ζ as assigning a real number to each admissible word. (It is convenient to treat the empty word 1 as admissible and set $\zeta(1) = 1$.) Note that if w is the word corresponding to a composition $(i_1, \dots, i_k)$, the weight $i_1 + \cdots + i_k$ is the total degree $|w|$ of w. In this case the length k of the composition is the y-degree of w; we denote this by $\ell(w)$. We will find it convenient to call $|w| - \ell(w)$ (i.e., the x-degree of w) the colength of w, denoted $c(w)$.

Let $\mathfrak{H}$ be the underlying rational vector space of $\mathbf{Q}\langle x, y\rangle$, and let $\mathfrak{H}^0$ be the subspace generated by the admissible words. Then we think of ζ as a $\mathbf{Q}$-linear map $\zeta : \mathfrak{H}^0 \to \mathbf{R}$. Now x and y are not admissible, but $\mathfrak{H}^0$ is a noncommutative polynomial algebra on the words $v_{p,q} = x^p y^q$ for $p, q \geq 1$ (Of course ζ is not a homomorphism for this algebra structure). We call the length of a word $w \in \mathfrak{H}^0$ in terms of the $v_{p,q}$ its height, denoted $\mathrm{ht}(w)$. For example, $\mathrm{ht}(xyx^2y^2) = 2$.

With this notation, it is easy to state two identities whose proof motivated much of the early work on MZVs, the sum theorem and the duality theorem. (Both appeared in [17] as conjectures: the sum theorem was proved by Granville [13] and independently by Zagier; the duality theorem was proved via the iterated integral discussed below–

see [39]–unfortunately without any notice of the conjecture!) The sum theorem can be stated as

$$\sum_{w\in\mathfrak{H}^0,\ |w|=n,\ \ell(w)=k} \zeta(w) = \zeta(n)$$

for $n \geq 2$. For the duality theorem, define an antiautomorphism τ of the noncommutative polynomial ring $\mathbf{Q}\langle x, y\rangle$ by $\tau(x) = y$ and $\tau(y) = x$; note that τ is an involution that exchanges length and colength, and preserves height. The duality theorem states that

$$\zeta(w) = \zeta(\tau(w))$$

for admissible words w.

Another of "early" results on MZVs was the Le-Murakami theorem of [25]. This is the identity

$$\sum_{w\in\mathfrak{H}^0,\ |w|=2n,\ \mathrm{ht}(w)=k} (-1)^{\ell(w)}\zeta(w) = (-1)^n\zeta((xy)^n)\sum_{j=0}^{n-k}\binom{2n+1}{2j}(2-2j)B_{2j},$$

which they proved by examining the Kontsevich integral of the unknot.

One reason for the efficacy of the "algebraic" notation is apparent–it corresponds to the expression of MZVs by iterated integrals, as follows. Let $w = a_1a_2\cdots a_n$ be the factorization of an admissible word into x's and y's. Then it is easy to show that

$$\zeta(w) = \int_0^1\int_0^{t_n}\cdots\int_0^{t_2}\frac{dt_1}{A_n(t_1)}\cdots\frac{dt_{n-1}}{A_2(t_{n-1})}\frac{dt_n}{A_1(t_n)}, \tag{1.2}$$

where

$$A_i(t) = \begin{cases} t, & \text{if } a_i = x,\\ 1-t, & \text{if } a_i = y.\end{cases}$$

The duality theorem follows immediately from the change of variable $(t_1,\dots,t_n) \to (1-t_n,\dots,1-t_1)$ in the iterated integral. In addition, the fact that iterated integrals multiply via shuffle product (see the Section 2 below) implies the existence of the shuffle product structure on the set of MZVs.

But the series multiplication (or "stuffle product") can also be formated in terms of the algebraic notation; this is the "harmonic algebra" of [18]. The formulation in [18] led to the discovery that the harmonic algebra of MZVs is a subalgebra of the quasi-symmetric functions. We discuss this in detail in Section 3.

Another remarkable success for the algebraic method is the result of [17] that I have since (see [21]) called the derivation theorem. Let D be the derivation of $\mathbf{Q}\langle x, y\rangle$ with $D(x) = 0$ and $D(y) = xy$. Then D takes $\mathfrak{H}^0$ to itself, as does the derivation $\tau D\tau$. We can state the derivation theorem as

$$\zeta(D(w)) = \zeta(D(\tau(w)))$$

for admissible words w. The proof of this in [17] is an elementary but messy partial-fractions argument. It seems to have nothing to do with iterated integrals, but the algebraic notation is working some magic here– just compare the formulation above with the one given as Theorem 5.1 of [17]: for any admissible composition $(i_1, \dots, i_k)$,

$$\sum_{j=1}^{k} \zeta(i_1, \dots, i_j + 1, \dots, i_k)$$
$$= \sum_{\substack{1\le j\le k \\ i_j \ge 2}} \sum_{p=0}^{i_j-2} \zeta(i_1, \dots, i_{j-1}, i_j - p, p+1, i_{j+1}, \dots, i_k).$$

The sum, duality, and derivation theorems are all subsumed in a remarkable identity proved in 1999 by Ohno [29]. It can be stated nicely in the algebraic notation, but to do so will require some more machinery: see Section 4 below. More recently, I conjectured, and Ohno proved, a somewhat mysterious "cyclic" analogue of the derivation theorem [21]. As with the derivation theorem, the statement in the algebraic notation is very simple, but the proof is a tricky partial-fractions argument. We discuss this in Section 5.

The "magic" of the algebraic notation seems to extend to the finite partial sums of the MZVs. Here the harmonic algebra still applies, although the shuffle algebra does not. In Section 6 we state some results on finite multiple sums, including some mod p results (p a prime). The main result of this section appears to be new.

2. The Shuffle Algebra

As above, let $\mathfrak{H}$ be the underlying graded rational vector space of $\mathbf{Q}\langle x, y\rangle$, with x and y both given degree 1. We define a multiplication $\sqcup\!\sqcup$ on $\mathfrak{H}$ by requiring that it distribute over the addition, and that it satisfy the following axioms:

S1. For any word w, $1 \sqcup\!\sqcup\, w = w \sqcup\!\sqcup\, 1 = w$;

S2. For any words w_1, w_2 and $a, b \in \{x, y\}$,

$$aw_1 \sqcup\!\sqcup\, bw_2 = a(w_1 \sqcup\!\sqcup\, bw_2) + b(aw_1 \sqcup\!\sqcup\, w_2).$$

Induction on total degree then establishes the following.

Theorem 2.1. The $\sqcup\!\sqcup$ -product is commutative and associative.

Recall from the previous section that τ is the anti-automorphism of $\mathbf{Q}\langle x, y\rangle$ the exchanges x and y. Then we have the following fact.

Theorem 2.2. τ is an automorphism of $(\mathfrak{H}, \sqcup\!\sqcup)$.

Proof. Since evidently $\tau^2 = \mathrm{id}$, it suffices to show that τ is a $\sqcup\!\sqcup$ -homomorphism. Using the axioms S1, S2 above and induction on $|w_1 w_2|$, it is straightforward to prove that

$$w_1 a \sqcup\!\sqcup w_2 b = (w_1 \sqcup\!\sqcup w_2 b)a + (w_1 a \sqcup\!\sqcup w_2)b$$

for any words w_1, w_2 and letters a, b. Now suppose inductively that $\tau(w_1 \sqcup\!\sqcup w_2) = \tau(w_1) \sqcup\!\sqcup \tau(w_2)$ for $|w_1 w_2| < n$, and let w_1, w_2 be words with $|w_1 w_2| = n$. We can assume both w_1 and w_2 are nonempty; write $w_1 = w_1' a$ and $w_2 = w_2' b$. Then

$$\begin{aligned}
\tau(w_1 \sqcup\!\sqcup w_2) &= \tau((w_1' \sqcup\!\sqcup w_2)a + (w_1 \sqcup\!\sqcup w_2')b) \\
&= \tau(a)\tau(w_1' \sqcup\!\sqcup w_2) + \tau(b)\tau(w_1 \sqcup\!\sqcup w_2') \\
&= \tau(a)(\tau(w_1') \sqcup\!\sqcup \tau(w_2)) + \tau(b)(\tau(w_1) \sqcup\!\sqcup \tau(w_2')) \\
&= \tau(a)\tau(w_1') \sqcup\!\sqcup \tau(b)\tau(w_2') \\
&= \tau(w_1) \sqcup\!\sqcup \tau(w_2).
\end{aligned}$$

□

Now order the words of $\mathfrak{H}$ as follows. For any words w_1, w_2, w_3, set $w_1 x w_2 < w_1 y w_3$; and if u, v are words with v nonempty, set $u < uv$. A nonempty word w is called Lyndon if it is smaller than any of its nontrivial right factors; i.e., $w < v$ whenever $w = uv$ and $u \neq 1 \neq v$. From [31] we have the following result.

Theorem 2.3. As a commutative algebra, $(\mathfrak{H}, \sqcup\!\sqcup)$ is freely generated by the Lyndon words.

The link between the shuffle algebra and MZVs is given by the iterated integral representation (1.2), together with the well-known fact [32] that iterated integrals multiply by shuffle product. We can state this as follows.

Theorem 2.4. The map $\zeta : (\mathfrak{H}^0, \sqcup\!\sqcup) \to \mathbf{R}$ is a τ-equivariant homomorphism.

The shuffle-product structure has been used to prove some MZV identities. For example, in [2] it is first established that

$$\sum_{r=-n}^{n} (-1)^r [(xy)^{n-r} \sqcup\!\sqcup (xy)^{n+r}] = 4^n (x^2 y^2)^n$$

in $\mathfrak{H}$, and then ζ is applied to get

$$\sum_{r=-n}^{n} (-1)^r \zeta((xy)^{n-r})\zeta((xy)^{n+r}) = 4^n \zeta((x^2y^2)^n).$$

Using the known result

$$\zeta((xy)^k) = \frac{\pi^{2k}}{(2k+1)!} \tag{2.1}$$

(for which see the remarks following Theorem 3.5 below), together with some arithmetic, one then obtains the result conjectured by Zagier [39] several years earlier:

$$\zeta((x^2y^2)^n) = \frac{1}{2n+1}\zeta((xy)^{2n}).$$

Other shuffle convolutions are used to prove some instances of the "cyclic insertion conjecture" for MZVs in the same paper, and the topic has been revisited in [6].

3. The Harmonic Algebra and Quasi-Symmetric Functions

We can define another commutative multiplication $*$ on $\mathfrak{H}$ by requiring that it distribute over the addition and that it satisfy the following axioms:

H1. For any word w, $1 * w = w * 1 = w$;

H2. For any word w and integer $n \geq 1$,

$$x^n * w = w * x^n = wx^n;$$

H3. For any words w_1, w_2 and integers $p, q \geq 0$,

$$x^p y w_1 * x^q y w_2 = x^p y(w_1 * x^q y w_2) + x^q y(x^p y w_1 * w_2) + x^{p+q+1} y(w_1 * w_2).$$

Note that axiom (H3) allows the $*$-product of any pair of words to be computed recursively, since each $*$-product on the right has fewer factors of y than the $*$-product on the left-hand side. Induction on y-degree establishes the counterpart of Theorem 2.1.

Theorem 3.1. The $*$-product is commutative and associative.

We refer to $\mathfrak{H}$ together with its commutative multiplication $*$ as the harmonic algebra $(\mathfrak{H}, *)$. Evidently τ is *not* an automorphism of $(\mathfrak{H}, *)$.

But we do have counterparts of Theorems 2.3 and 2.4, which are proved in [18].

Theorem 3.2. As a commutative algebra, $(\mathfrak{H}, *)$ is freely generated by the Lyndon words.

Theorem 3.3. $(\mathfrak{H}^0, *)$ is a subalgebra of $(\mathfrak{H}, *)$, and $\zeta : (\mathfrak{H}^0, *) \to \mathbf{R}$ is a homomorphism.

Because the multiplications $*$ and $ш$ are quite different, Theorems 2.4 and 3.3 imply that ζ has a large kernel. For example, since

$$xy * xy = 2(xy)^2 + x^3y$$
$$xy \sqcup\!\sqcup\, xy = 2(xy)^2 + 4x^2y^2$$

we must have

$$\zeta(x^3y - 4x^2y^2) = 0.$$

In fact, it has been conjectured that all identities of MZVs come from comparing the two multiplications. The derivation theorem can be recovered, since

$$y \sqcup\!\sqcup\, w - y * w = \tau D \tau(w) - D(w)$$

for $w \in \mathfrak{H}^0$ (Theorem 4.3 of [21]). Zudilin [41] states the conjecture as

$$\ker \zeta = \{u \sqcup\!\sqcup\, v - u * v \mid u \in \mathfrak{H}^1, v \in \mathfrak{H}^0\};$$

for other formulations see [16] and [38].

Let $\mathfrak{H}^1$ be the vector subspace $\mathbf{Q}1 + \mathfrak{H}y$ of $\mathfrak{H}$; it is evidently a subalgebra of $(\mathfrak{H}, *)$. In fact, since x is the only Lyndon word ending in x, it is easy to see that $\mathfrak{H}^1$ is the subalgebra of $(\mathfrak{H}, *)$ generated by the Lyndon words other than x. Note that any word $w \in \mathfrak{H}^1$ can be written in terms of the elements $z_i = x^{i-1}y$, and that the y-degree $\ell(w)$ is the length of w when expressed this way. We can rewrite the inductive rule (H3) for the $*$-product as

$$z_p w_1 * z_q w_2 = z_p(w_1 * z_q w_2) + z_q(z_p w_1 * w_2) + z_{p+q}(w_1 * w_2). \tag{3.1}$$

Now for each positive integer n, define a map $\phi_n : \mathfrak{H}^1 \to \mathbf{Q}[t_1, \dots, t_n]$ (where $|t_i| = 1$ for all i) as follows. Let $\phi_n(1) = 1$ and

$$\phi_n(z_{i_1} z_{i_2} \cdots z_{i_k}) = \sum_{n \geq n_1 > n_2 > \cdots > n_k \geq 1} t_{n_1}^{i_1} t_{n_2}^{i_2} \cdots t_{n_k}^{i_k}$$

for words of length $k \leq n$, and let $\phi(w) = 0$ for words of length greater than n; extend ϕ_n linearly to $\mathfrak{H}^1$. Because the rule (3.1) corresponds to multiplication of series, ϕ_n is a homomorphism, and ϕ_n is evidently injective through degree n. For each $m \geq n$, there is a restriction map

$$\rho_{m,n} : \mathbf{Q}[t_1, \ldots, t_m] \to \mathbf{Q}[t_1, \ldots, t_n]$$

such that

$$\rho(t_i) = \begin{cases} t_i, & i \leq n \\ 0, & i > n. \end{cases}$$

The inverse limit

$$\mathfrak{P} = \operatorname*{proj\,lim}_n \mathbf{Q}[t_1, \ldots, t_n]$$

is the subalgebra of $\mathbf{Q}[[t_1, t_2, \ldots]]$ consisting of those formal power series of bounded degree. Since the maps ϕ_n commute with the restriction maps, they define a homomorphism $\phi : \mathfrak{H}^1 \to \mathfrak{P}$.

Inside $\mathfrak{P}$ is the algebra of symmetric functions

$$\mathrm{Sym} = \operatorname*{proj\,lim}_n \mathbf{Q}[t_1, \ldots, t_n]^{\Sigma_n}$$

and also the algebra of quasi-symmetric functions (first described in [12]). We can define the algebra QSym of quasi-symmetric functions as follows. A formal series $p \in \mathfrak{P}$ is in QSym if the coefficient of $t_{i_1}^{p_1} \cdots t_{i_k}^{p_k}$ in p is the same as the coefficient of $t_{j_1}^{p_1} \cdots t_{j_k}^{p_k}$ in p whenever $i_1 < i_2 < \cdots < i_k$ and $j_1 < j_2 < \cdots < j_k$. Evidently Sym $\subset$ QSym. A vector space basis for QSym is given by the monomial quasi-symmetric functions

$$M_{(p_1, p_2, \ldots, p_k)} = \sum_{i_1 < i_2 < \cdots < i_k} t_{i_1}^{p_1} t_{i_2}^{p_2} \cdots t_{i_k}^{p_k},$$

which are indexed by compositions $(p_1, \ldots, p_k)$. Since evidently $\phi(z_{i_1} \cdots z_{i_k}) = M_{(i_k, \ldots, i_1)}$, we have the following result.

Theorem 3.4. ϕ is an isomorphism of $\mathfrak{H}^1$ onto QSym.

As is well known, the algebra Sym of symmetric functions is generated by the elementary symmetric functions e_i, as well as by the power-sum symmetric functions p_i (Note that we are working over $\mathbf{Q}$). It is easy to see that $\phi^{-1}(e_i) = z_1^i$ and $\phi^{-1}(p_i) = z_i$. Let Sym^0 be the subalgebra of the symmetric functions generated by the power-sum symmetric functions p_i with $i \geq 2$. Then $\phi^{-1}(\mathrm{Sym}) \cap \mathfrak{H}^0 = \phi^{-1}(\mathrm{Sym}^0)$. Since ϕ is a homomorphism, we have the following result.

Theorem 3.5. If $a \in \phi^{-1}(\mathrm{Sym}^0)$, then $\zeta(a)$ is a sum of products of values of $\zeta(i)$ of the zeta function with $i \geq 2$.

In fact, the problem of expressing MZVs $\zeta(a)$ with $a \in \phi^{-1}(\mathrm{Sym}^0)$ in terms of values of the zeta function is entirely equivalent to writing particular monomial symmetric functions in terms of power-sum symmetric functions p_i, for which there are well-known algorithms [26]. This includes cases like

$$\zeta(z_i^k) = \zeta(i, i, \dots, i)$$

(Note $i = 2$ occurs in equation (2.1) above), treated by analytical methods in [1]. For example, since $M_{22} = \frac{1}{2}(p_2^2 - p_4)$ in Sym^0, we have

$$\zeta(2,2) = \frac{1}{2}(\zeta(2)^2 - \zeta(4)) = \frac{1}{2}\left(\frac{\pi^4}{36} - \frac{\pi^4}{90}\right) = \frac{\pi^4}{120}.$$

(For a general proof of equation (2.1) by this method, see Corollary 2.3 of [17].)

Since y is the only Lyndon word that begins with y, we can write $\mathfrak{H}^1 = \mathfrak{H}^0[y]$ (for either the $ш$ or the $*$ product). So we can extend ζ to a map $\hat{\zeta} : \mathfrak{H}^1 \to \mathbf{R}$ by defining $\hat{\zeta}(y)$. Since

$$y * y = 2y^2 + xy \quad \text{and} \quad y \,ш\, y = 2y^2,$$

there is no way to do this consistently for both multiplications, but if we restrict our attention to the $*$-multiplication it turns out that $\hat{\zeta}(y) = \gamma$ (Euler's constant) is a happy choice. If

$$H(t) = 1 + yt + (y^2 + xy)t^2 + (y^3 + yxy + xy^2 + x^2y)t^3 + \cdots$$

is the generating function for the complete symmetric functions, then the following result is easy to show (see [18]).

Theorem 3.6. $\hat{\zeta}(H(t)) = \Gamma(1 - t)$.

Now one can show (e.g., using differential equations) that

$$\sum_{w \in \mathfrak{H}^0,\ \mathrm{ht}(w)=1} \zeta(w) u^{c(w)} v^{\ell(w)} = 1 - \frac{\Gamma(1-u)\Gamma(1-v)}{\Gamma(1-u-v)}.$$

Putting this together with Theorem 3.6, we have

$$\sum_{w \in \mathfrak{H}^0,\ \mathrm{ht}(w)=1} \zeta(w) u^{c(w)} v^{\ell(w)} = \zeta\left(1 - \frac{H(u)H(v)}{H(u+v)}\right). \tag{3.2}$$

Hence $\zeta(w) \in \zeta(\phi^{-1}(\mathrm{Sym}^0))$ for any word w of height 1 (i.e., of the form $x^p y^q$), and thus can be written in terms of ordinary zeta values $\zeta(n) = \zeta(z_n)$.

Remarkably, Ohno and Zagier [30] have recently proved that equation (3.2) is just the constant term of the following result.

Theorem 3.7.

$$\sum_{w\in\mathfrak{H}^0}\zeta(w)u^{c(w)}v^{\ell(w)}z^{\mathrm{ht}(w)-1}=\frac{1}{1-z}\zeta\left(1-\frac{H(u)H(v)}{H(\alpha)H(\beta)}\right),$$

where

$$\alpha=\frac{1}{2}\left((u+v)+\sqrt{(u+v)^2-4uvz}\right)$$
$$\beta=\frac{1}{2}\left((u+v)-\sqrt{(u+v)^2-4uvz}\right).$$

The theorem implies that any sum of MZVs of fixed weight, length, and height, e.g.,

$$\sum_{|w|=6,\ \mathrm{ht}(w)=2,\ \ell(w)=3}\zeta(w)=\zeta(3,2,1)+\zeta(2,3,1)+\zeta(2,1,3)+\zeta(3,1,2)$$

is in $\zeta(\phi^{-1}(\mathrm{Sym}^0))$ and hence expressible in terms of $\zeta(n)$'s. But the theorem implies much more. For example, taking the limit as $z\to 1$ gives the sum theorem, and setting $v=-u$ gives the Le-Murakami theorem.

For another application of Theorem 3.6 see [20].

4. Derivations and an Action by Quasi-Symmetric Functions

As mentioned in the introduction, the derivation theorem has a far-reaching generalization proved by Ohno [29]. In this section we give a succinct statement of Ohno's theorem and some of its equivalents using the Hopf algebra structure of QSym.

We begin by motivating the use of a Hopf algebra structure in this context. (The standard references on Hopf algebras are [34] and [27], but the reader may find a source like [23] more convenient.) Let $\mathcal{O}$ be an algebra of operators (with composition as multiplication) acting on an algebra $\mathcal{A}$. Then elements of the tensor product $\mathcal{O}\otimes\mathcal{O}$ act naturally on products pq for $p,q\in\mathcal{A}$: $\alpha\otimes\beta(pq)=\alpha(p)\beta(q)$. To say that $\alpha\in\mathcal{O}$ is a derivation is to say that the action of α on a products agrees with the action of $\alpha\otimes 1+1\otimes\alpha$:

$$\alpha(pq)=\alpha(p)q+p\alpha(q)=(\alpha\otimes 1+1\otimes\alpha)(pq).$$

A Hopf algebra structure on $\mathcal{O}$ is essentially a "coproduct" $\Delta:\mathcal{O}\to\mathcal{O}\otimes\mathcal{O}$ compatible with the multiplication in $\mathcal{O}$. We require that $\alpha(pq)=$

$\Delta(\alpha)(pq)$ for all $\alpha \in \mathcal{O}$. Elements α with $\Delta(\alpha) = \alpha \otimes 1 + 1 \otimes \alpha$ are called primitive, so the primitives in $\mathcal{O}$ are exactly those that act as derivations. The "fine print" of the definition of a (graded connected) Hopf algebra requires that $\Delta(\alpha)$ always contain the terms $\alpha \otimes 1$ and $1 \otimes \alpha$ for α of positive degree, so primitive elements are those whose coproducts are as simple as possible. We can generalize the notion of derivation by allowing extra terms in the coproduct. For example, a set $\{\alpha_0 = 1, \alpha_1, \alpha_2, \dots\}$ of elements is called a set of divided powers if

$$\Delta(\alpha_n) = \sum_{i+j=n} \alpha_i \otimes \alpha_j;$$

if we think of the α_n as operators, they are sometimes called a "higher derivation". Thus, a Hopf algebra of operators is a natural extension of the notion of a Lie algebra acting by derivations.

Now $(\mathfrak{H}^1, *) \cong \mathrm{QSym}$ has a Hopf algebra structure with coproduct Δ defined by

$$\Delta(z_{i_1} z_{i_2} \cdots z_{i_n}) = \sum_{j=0}^{n} z_{i_1} \cdots z_{i_j} \otimes z_{i_{j+1}} \cdots z_{i_n},$$

(and counit ε with $\varepsilon(u) = 0$ for all elements u of positive degree). This extends the well-known Hopf algebra structure on the algebra Sym (as described in [10]), in which the elementary symmetric functions e_i ($\leftrightarrow y^i$) and complete symmetric functions h_i are divided powers, while the power sums p_i ($\leftrightarrow z_i$) are primitive. The Hopf algebra $(\mathfrak{H}^1, *, \Delta)$ is commutative but not cocommutative. Its (graded) dual is the Hopf algebra of noncommutative symmetric functions as defined in [11].

Now define $\cdot : \mathfrak{H}^1 \otimes \mathbf{Q}\langle x, y\rangle \to \mathbf{Q}\langle x, y\rangle$ by setting $1 \cdot w = w$ for all words w,

$$z_k \cdot 1 = 0, \quad z_k \cdot x = 0, \quad z_k \cdot y = x^k y$$

for all $k \geq 1$, and

$$u \cdot w_1 w_2 = \sum_u (u' \cdot w_1)(u'' \cdot w_2) \tag{4.1}$$

where $\Delta(u) = \sum_u u' \otimes u''$; the coassociativity of Δ insures this is well-defined. It turns out (Lemma 5.2 of [21]) that $u \cdot w$ just consists of those terms of $u * w$ having the same y-degree as w, so it follows (from the associativity of $*$) that $\cdot$ is really an action, i.e., $u \cdot (v \cdot w) = (u * v) \cdot w$. Also, equation (4.1) says the action makes $\mathbf{Q}\langle x, y\rangle$ a QSym-module algebra, in the terminology of [23].

We note that the action of z_1 on $\mathbf{Q}\langle x, y\rangle$ is just the derivation D defined in the introduction, since $z_1 \cdot x = 0$ and $z_1 \cdot y = xy$. In fact, for each $n \geq 1$ we have a derivation D_n given by $D_n(w) = z_n \cdot w$, since the z_n are primitive in QSym.

In terms of this action, we can now state Ohno's theorem [29] as follows.

Theorem 4.1. For any word $w \in \mathfrak{H}^0$ and nonnegative integer i,

$$\zeta(h_i \cdot w) = \zeta(h_i \cdot \tau(w)).$$

Recall that the h_n are divided powers, i.e., $\Delta(h_n) = \sum_{i+j=n} h_i \otimes h_j$. Only $h_1 = z_1$ is primitive, in which case we recover the derivation theorem. Taking $h_0 = 1$ gives the duality theorem, and with a little manipulation the sum theorem can also be obtained.

M. Kaneko sought to generalize the derivation theorem in another way. One can formulate the derivation theorem as saying that $(\tau D \tau - D)(w) \in \ker \zeta$ for all $w \in \mathfrak{H}^0$. Are there derivations of higher degree for which this is still true? Kaneko defined a degree-n derivation ∂_n of $\mathbf{Q}\langle x, y\rangle$ by

$$\partial_n(x) = -\partial_n(y) = x(x+y)^{n-1}y,$$

and conjectured that $\partial_n(w) \in \ker \zeta$ for all $w \in \mathfrak{H}^0$. Note $\partial_1 = \tau D \tau - D$, so the conjecture holds for $n = 1$; and the case $n = 2$ follows easily from Theorem 4.1.

Eventually Kaneko and K. Ihara proved the conjecture [22] by showing it equivalent to Theorem 4.1. One way to see this involves the action we have just defined. Extend the action of QSym on $\mathfrak{H}$ to an action of QSym$[[t]]$ on $\mathfrak{H}[[t]]$ in the obvious way, and (as in the previous section) let

$$H(t) = 1 + h_1 t + h_2 t^2 + \cdots \in \mathrm{QSym}[[t]]$$

be the generating function of the complete symmetric functions. If we set $\sigma_t(u) = H(t) \cdot u$ for $u \in \mathfrak{H}$, then Theorem 4.1 is equivalent to $\zeta(\bar{\sigma}_t(u) - \sigma_t(u)) = 0$ for $u \in \mathfrak{H}$, where $\bar{\sigma}_t = \tau \sigma_t \tau$. Now σ_t is an automorphism of $\mathfrak{H}^0[[t]]$: in fact $\sigma_t^{-1}(u) = E(-t) \cdot u$, where

$$E(t) = 1 + yt + y^2 t + \cdots \in \mathrm{QSym}[[t]]$$

is the generating function of the elementary symmetric functions. Thus, Theorem 4.1 is equivalent to

$$\bar{\sigma}_t \sigma_t^{-1}(u) - u \in \ker \zeta$$

for all $u \in \mathfrak{H}^0[[t]]$. Then following result implies Kaneko's conjecture.

Theorem 4.2.

$$\bar{\sigma}_t \sigma_t^{-1} = \exp\left(\sum_{n=1}^{\infty} \frac{t^n}{n} \partial_n\right).$$

This result can be proved by showing both sides are automorphisms of $\mathfrak{H}[[t]]$ that fix t and $x+y$, and take x to $x(1-ty)^{-1}$ (see [21]). The derivations ∂_n are related to the derivations D_n mentioned above as follows. Since

$$\frac{d}{dt}\log H(t) = \frac{H'(t)}{H(t)} = \sum_{n=1}^{\infty} p_n t^{n-1},$$

the map σ_t can also be written

$$\sigma_t = \exp\left(\sum_{n=1}^{\infty} \frac{t^n}{n} D_n\right).$$

Hence Theorem 4.2 says that

$$\exp\left(\sum_{n=1}^{\infty} \frac{t^n}{n}\partial_n\right) = \exp\left(\sum_{n=1}^{\infty} \frac{t^n}{n}\bar{D}_n\right)\exp\left(-\sum_{n=1}^{\infty} \frac{t^n}{n} D_n\right),$$

where $\bar{D}_n = \tau D_n \tau$. Thus, the ∂_n can be written in terms of the D_n and $\bar{D}_n$ via the Campbell-Hausdorff formula. For example,

$$\partial_2 = \bar{D}_2 - D_2 - [\bar{D}_1, D_1],$$

and

$$\partial_3 = \bar{D}_3 - D_3 - \frac{3}{4}[\bar{D}_1, D_2] - \frac{3}{4}[\bar{D}_2, D_1] + \frac{1}{4}[[\bar{D}_1, D_1], D_1] - \frac{1}{4}[\bar{D}_1, [\bar{D}_1, D_1]].$$

5. Cyclic Derivations

There is an analogue of the derivation theorem involving a "cyclic derivation" $C : \mathfrak{H} \to \mathfrak{H}$. We can define C as the composition $\widetilde{\mu}\hat{C}$, where $\hat{C} : \mathfrak{H} \to \mathfrak{H} \otimes \mathfrak{H}$ is the derivation sending x to 0 and y to $y \otimes x$, and $\widetilde{\mu}(a \otimes b) = ba$. Here we regard $\mathfrak{H} \otimes \mathfrak{H}$ as a two-sided module over $\mathfrak{H}$ via $a(b \otimes c) = ab \otimes c$ and $(a \otimes b)c = a \otimes bc$. Thus, e.g.,

$$\begin{aligned} C(x^3yxy) &= \widetilde{\mu}(x^3(y \otimes x)xy + x^3yx(y \otimes x)) \\ &= \widetilde{\mu}(x^3y \otimes x^2y + x^3yxy \otimes x) \\ &= x^2yx^3y + x^4yxy. \end{aligned}$$

This particular definition follows D. Voiculescu's version of the cyclic derivative [37]: cyclic derivatives were first studied by Rota, Sagan and Stein [33].

In terms of the composition notation, C differs from D in that the entries are permuted cyclically, e.g.,

$$D(4,2) = (5,2) + (4,3) \quad \text{versus} \quad C(4,2) = (5,2) + (3,4).$$

The following result was conjectured by myself and proved by Ohno [21].

Theorem 5.1. For any word $w \in \mathfrak{H}^1$ that is not a power of y,

$$\zeta(C(w)) = \zeta(\tau C \tau(w)).$$

As mentioned in the introduction, the proof uses partial fractions.

The difference between C and D is most striking when applied to periodic words. For example, Theorem 5.1 applied to $w = (x^2y)^n$ gives (in the composition notation)

$$\zeta(4, 3, \dots, 3) = \zeta(3, 3, \dots, 3, 1) + \zeta(2, 3, \dots, 3, 2).$$

Theorem 5.1 also gives a very nice proof of the sum theorem. Here is the idea: Let $u = x + ty$. Then the coefficient of t^k in $xu^{n-2}y$ is the sum of all words $w \in \mathfrak{H}^0$ with $|w| = n$ and $\ell(w) = k$. Now

$$C(u^{n-1}) = (n-1)txu^{n-2}y \quad \text{while} \quad \tau C \tau(u^{n-1}) = (n-1)xu^{n-2}y,$$

so the cyclic derivation theorem implies that ζ applied to the coefficient of t^{k-1} equals ζ applied to the coefficient of t^k. That is, the sum of MZVs of fixed weight n and length k must be independent of k (and so must be $\zeta(n)$).

Here is another corollary of Theorem 5.1, stated in terms of the action of QSym on $\mathbf{Q}\langle x, y\rangle$.

Theorem 5.2. For $m, n \geq 1$, $\zeta(z_n \cdot xy^m) = \zeta(z_m \cdot xy^n)$.

Just as the derivation theorem extends to Theorem 4.1, it is natural to ask if the cyclic derivation theorem can be extended. It is easy to define cyclic derivations C_n analogous to the D_n of the last section: just set $C_n = \widetilde{\mu}\hat{C}_n$, where $\hat{C}_n(x) = 0$ and $\hat{C}_n(y) = y \otimes x^n$. One could then try to define cyclic derivations analogous to Kaneko's derivations ∂_n (which are expressible in terms of commutators of the D_n and $\bar{D}_n$). The difficulty appears to be in defining the commutator of cyclic derivations.

6. Finite Multiple Sums and Mod p Results

In this section we consider the finite sums

$$A_{(i_1,\dots,i_k)}(n) = \sum_{n \geq n_1 > n_2 > \cdots > n_k \geq 1} \frac{1}{n_1^{i_1} \cdots n_k^{i_k}}$$

and

$$S_{(i_1,\dots,i_k)}(n) = \sum_{n \geq n_1 \geq n_2 \geq \cdots \geq n_k \geq 1} \frac{1}{n_1^{i_1} \cdots n_k^{i_k}}$$

where the notation is patterned after that of [17]; the multiple zeta values of the previous sections are

$$\zeta(i_1,\dots,i_k)=\lim_{n\to\infty}A_{(i_1,\dots,i_k)}(n),$$

when the limit exists (i.e., when $i_1>1$).

The sums $A_I(n)$ and $S_I(n)$ are related in an obvious way, e.g.,

$$S_{(4,2,1)}(n)=A_{(4,2,1)}(n)+A_{(6,1)}(n)+A_{(4,3)}(n)+A_{(7)}(n).$$

We can formalize the relation as follows. For compositions I,J, we say I refines J (denoted $I\succ J$) if J can be obtained from I by combining some of its parts. Then

$$S_I(n)=\sum_{I\succeq J}A_J(n). \tag{6.1}$$

Of course $S_{(m)}(n)=A_{(m)}(n)$ for all m,n.

It will be useful to have some additional notations for compositions. We adapt the notation used in previous sections for words, so for $I=(i_1,\dots,i_k)$ the weight of I is $|I|=i_1+\dots+i_k$, and $k=\ell(I)$ is the length of I. For $I=(i_1,\dots,i_k)$, the reversed composition $(i_k,\dots,i_1)$ will be denoted $\bar{I}$: of course reversal preserves weight, length and refinement (i.e., $I\succeq J$ implies $\bar{I}\succeq\bar{J}$).

Compositions of weight n are in 1-to-1 correspondence with subsets of $\{1,2,\dots,n-1\}$ via partial sums

$$(i_1,i_2,\dots,i_k)\to\{i_1,i_1+i_2,\dots,i_1+\dots+i_{k-1}\},$$

and $I\preceq J$ if and only if the subset corresponding to I contains that corresponding to J. Complementation in the power set then gives rise to an involution $I\to I^*$; e.g., $(1,1,2)^*=(3,1)$. Evidently $|I^*|=|I|$ and $\ell(I)+\ell(I^*)=|I|+1$. Also, $I\preceq J$ if and only if $I^*\succeq J^*$. Finally, for two compositions I and J we write $I\sqcup J$ for their juxtaposition.

From [17] we have formulas for symmetric sums of $A_I(n)$ and $S_I(n)$ in terms of length one sums $S_{(m)}(n)$. (Though the proofs in [17] are given for infinite series, they carry over to the finite case.) They require some notation to state. For a partition $\Pi=\{P_1,\dots,P_l\}$ of the set $\{1,2,\dots,k\}$, let

$$c(\Pi)=\prod_{s=1}^{l}(\operatorname{card}P_s-1)!\quad\text{and}\quad\tilde{c}(\Pi)=(-1)^{k-l}\prod_{s=1}^{l}(\operatorname{card}P_s-1)!,$$

and if also $I=(i_1,\dots,i_k)$ is a composition of length k, let

$$S(n,\Pi,I)=\prod_{s=1}^{l}S_{(p_s)}(n),\quad\text{where}\quad p_s=\sum_{j\in P_s}i_j.$$

If $I = (i_1, \ldots, i_k)$ is a composition of length k, then elements $\sigma \in \Sigma_k$ of the symmetric group act on I via $\sigma \cdot I = (i_{\sigma(1)}, \ldots, i_{\sigma(k)})$. Then Theorems 2.1 and 2.2 of [17] give us the following result.

Theorem 6.1. For all positive integers k and n and compositions I of length k,

$$\sum_{\sigma \in \Sigma_k} S_{\sigma \cdot I}(n) = \sum_{\text{partitions of } \{1,\ldots,k\}} c(\Pi) S(n, \Pi, I)$$

$$\sum_{\sigma \in \Sigma_k} A_{\sigma \cdot I}(n) = \sum_{\text{partitions of } \{1,\ldots,k\}} \tilde{c}(\Pi) S(n, \Pi, I)$$

Because of the correspondence between compositions and noncommutative words in $\mathfrak{H}^1$, we have (for any fixed n) a map $\rho_n : \mathfrak{H}^1 \to \mathbf{Q}$ sending $w \in \mathfrak{H}^1$ to $A_{I(w)}(n)$, where $I(w)$ is the composition associated with w. Note that ρ_n is the composition $\mathrm{ev} \circ T \circ \phi_n$, where ϕ_n is the map defined in Section 3, T is the automorphism of QSym sending M_I to $M_{\bar{I}}$, and ev is the function that sends t_i to $\frac{1}{i}$. Thus, $\rho_n : (\mathfrak{H}^1, *) \to \mathbf{R}$ is a homomorphism. We can combine the homomorphisms ρ_n into a homomorphism ρ that sends $w \in \mathfrak{H}^1$ to the real-valued sequence $n \to \rho_n(w)$. We shall write A_I for the real-valued sequence $n \to A_I(n)$ (and similarly for S_I), so ρ sends w to $A_{I(w)}$.

Now QSym has various integral bases besides the M_I. In the literature one often sees the fundamental quasi-symmetric functions

$$F_I = \sum_{J \succeq I} M_J,$$

but we will be concerned with what we call the "essential" quasi-symmetric functions

$$E_I = \sum_{J \preceq I} M_J.$$

In view of equation (6.1), the homomorphism ρ_n sends E_I to $S_I(n)$.

Since QSym is a commutative Hopf algebra, its antipode S is an automorphism of QSym and $S^2 = \mathrm{id}$. Now S can be given by the following explicit formulas: for proof see [7] or [19].

Theorem 6.2. The antipode S of QSym is given by

1. $S(M_I) = \sum_{I_1 \sqcup I_2 \sqcup \cdots \sqcup I_l = I} (-1)^l M_{I_1} M_{I_2} \cdots M_{I_l}$;
2. $S(M_I) = (-1)^{\ell(I)} E_{\bar{I}}$.

Part (2) of this result says that the E_I have essentially the same multiplication rules as the M_I: if T is the automorphism of QSym defined above, then $S \circ T$ takes any identity among the M_I to an identity among the E_I that differs only in signs. For example, since

$$M_{(2)}M_{(3)} = M_{(2,3)} + M_{(3,2)} + M_{(5)}$$

we have

$$E_{(2)}E_{(3)} = E_{(2,3)} + E_{(3,2)} - E_{(5)}.$$

Now define an automorphism ψ of $\mathbf{Q}\langle x, y\rangle$ by

$$\psi(x) = x + y, \quad \psi(y) = -y$$

Evidently $\psi^2 = \mathrm{id}$, and $\psi(\mathfrak{H}^1) = \mathfrak{H}^1$. Thus ψ defines a linear involution of $\mathfrak{H}^1 \cong \mathrm{QSym}$ (which is *not*, however, a homomorphism for the $*$-product). We can describe the action of ψ on the integral bases for QSym as follows.

Theorem 6.3. For any composition I,

1. $\psi(M_I) = (-1)^{\ell(I)} F_I$
2. $\psi(E_I) = -E_{I^*}$

Proof. Suppose $w = w(I)$ is the word in x and y corresponding to a composition I. Then evidently substituting y in place of any particular factor x in w corresponds to splitting a part of I. With this observation, part (1) is clear (there is also one factor of -1 for each occurrence of y in w).

Now we prove part (2). We have

$$\psi(E_I) = \sum_{J \preceq I} \psi(M_J) = \sum_{J \preceq I} (-1)^{\ell(J)} F_J$$

from part (1). From Example 1 of [19], $S(F_I) = (-1)^{|I|} F_{\bar{I}^*}$, where S is the antipode of QSym. Thus

$$\begin{aligned} S\psi(E_I) = \sum_{J \preceq I} (1)^{\ell(J)+|J|} F_{\bar{J}^*} &= -\sum_{J \preceq I} (-1)^{\ell(J^*)} F_{\bar{J}^*} \\ &= -\sum_{\bar{J}^* \succeq \bar{I}^*} (-1)^{\ell(\bar{J}^*)} F_{\bar{J}^*} = -\sum_{K \succeq \bar{I}^*} (-1)^{\ell(K)} F_K. \end{aligned}$$

Now by Möbius inversion,

$$F_I = \sum_{I \preceq J} M_J \quad \text{implies} \quad M_I = \sum_{I \preceq J} (-1)^{\ell(I)-\ell(J)} F_J,$$

and so

$$S\psi(E_I) = -(-1)^{\ell(\bar{I}^*)} M_{\bar{I}^*}$$

Apply S be both sides to get

$$\psi(E_I) = -(-1)^{\ell(I^*)}(-1)^{\ell(\bar{I}^*)} E_{I^*} = -E_{I^*}. \qquad \square$$

We consider two operators on the space $\mathbf{R}^{\mathbf{N}}$ of real-valued sequences. First, there is the partial-sum operator Σ, given by

$$\Sigma a(n) = \sum_{i=0}^{n} a(i)$$

for $a \in \mathbf{R}^{\mathbf{N}}$. Second, there is the operator ∇ given by

$$\nabla a(n) = \sum_{i=0}^{n} \binom{n}{i} (-1)^i a(i).$$

It is easy to show that Σ and ∇ generate a dihedral group within the automorphisms of $\mathbf{R}^{\mathbf{N}}$, i.e., $\nabla^2 = \mathrm{id}$ and $\Sigma\nabla = \nabla\Sigma^{-1}$. It follows that $(\Sigma\nabla)^2 = \mathrm{id}$. We have the following result on multiple sums.

Theorem 6.4. For any composition I, $\Sigma\nabla S_I = -S_{I^*}$.

Proof. We proceed by induction on $|I|$. The weight one case is $\Sigma\nabla S_{(1)} = \nabla\Sigma^{-1} S_1 = -S_{(1)}$, i.e.

$$\sum_{k=1}^{n} \frac{(-1)^k}{k} \binom{n}{k} = -\sum_{k=1}^{n} \frac{1}{k},$$

which is a classical (but often rediscovered) formula; it actually goes back to Euler [9]. For $I = (i_1, i_2, \ldots, i_k)$, it is straightforward to show that $\nabla S_I(n) = \frac{1}{n}\nabla f(n)$, where $f \in \mathbf{R}^{\mathbf{N}}$ is given by

$$f(n) = \begin{cases} S_{(i_2,\ldots,i_k)}(n), & \text{if } i_1 = 1; \\ \Sigma^{-1} S_{(i_1-1,i_2,\ldots,i_k)}(n), & \text{otherwise.} \end{cases}$$

Now suppose the theorem has been proved for all I of weight less than n, and let $I = (i_1, \ldots, i_k)$ have weight n. There are two cases: $i_1 = 1$, and $i_1 > 1$. In the first case, let $(i_2, \ldots, i_k)^* = J = (j_1, \ldots, j_r)$. By the assertion of the preceding paragraph and the induction hypothesis,

$$\Sigma\nabla S_I(n) = \Sigma(\frac{1}{n}\nabla S_{J^*}(n)) = -\Sigma(\frac{1}{n}\Sigma^{-1} S_J(n)) = -S_{(j_1+1,j_2,\ldots,j_r)}(n).$$

But evidently $I^* = (j_1 + 1, j_2, \ldots, j_r)$, so the theorem holds in this case

If $i_1 > 1$, we instead write $(i_1 - 1, i_2, \ldots, i_k)^* = J = (j_1, \ldots, j_r)$. Then

$$\begin{aligned}\Sigma\nabla S_I(n) &= \Sigma(\frac{1}{n}\nabla\Sigma^{-1}S_{J^*}(n)) = \Sigma(\frac{1}{n}\Sigma\nabla S_{J^*}(n)) \\ &= -\Sigma(\frac{1}{n}S_J(n)) = -S_{(1,j_1,\ldots,j_r)}(n).\end{aligned}$$

But in this case $I^* = (1, j_1, \ldots, j_r)$, so the theorem holds in this case as well. □

The proof of the preceding result is essentially a formalization of the procedure in App. B of [36]. (For a recent occurrence of the special case $I = (1,1,1)$ as a problem, see [15].) Theorem 6.4, together with part (2) of Theorem 6.3, says that the diagram

$$\begin{tikzcd} \mathrm{QSym} \arrow[r, "\psi"] \arrow[d, "\rho"'] & \mathrm{QSym} \arrow[d, "\rho"'] \\ \mathbf{R}^{\mathbf{N}} \arrow[r, "\Sigma\nabla"] & \mathbf{R}^{\mathbf{N}} \end{tikzcd} \tag{6.2}$$

commutes.

For the rest of this section, we discuss mod p results about $S_I(p-1)$ and $A_I(p-1)$, where p is a prime. (Some results of this type appear in [40].) For prime p, the sums $A_I(p-1)$ and $S_I(p-1)$ contain no factors of p in the denominators, and can be regarded as elements of the field $\mathbf{Z}/p\mathbf{Z}$. The following result about length one harmonic sums is well known (cf. [14], pp. 86-88).

Theorem 6.5. $S_{(k)}(p-1) \equiv 0 \mod p$ for all prime $p > k+1$.

Because Theorem 6.1 expresses symmetric sums of $S_I(p-1)$ and $A_I(p-1)$ in terms of length one sums, any such symmetric sum is zero mod p for $p > |I| + 1$. In particular, for $I = (k, k, \ldots, k)$ (r repetitions), we have

$$A_I(p-1) \equiv S_I(p-1) \equiv 0 \mod p$$

for prime $p > rk + 1$ (cf. Theorem 1.5 of [40]). There is the following result relating sums associated to I and $\bar{I}$ (cf. Lemma 3.2 of [40]).

Theorem 6.6. For any composition I, $A_I(p-1) \equiv (-1)^{|I|}A_{\bar{I}}(p-1)$ mod p, and similarly $S_I(p-1) \equiv (-1)^{|I|}S_{\bar{I}}(p-1) \mod p$.

Proof. Let $I = (i_1, \dots, i_k)$. Working mod p, we have

$$\begin{aligned} &A_I(p-1) \\ &\equiv \sum_{p>a_1>\cdots>a_k>0} \frac{1}{a_1^{i_1}\cdots a_k^{i_k}} \equiv \sum_{p>a_1>\cdots>a_k>0} \frac{(-1)^{i_1+\cdots+i_k}}{(p-a_1^{i_1})\cdots(p-a_k^{i_k})} \\ &\equiv \sum_{0<b_1<\cdots<b_k<p} \frac{(-1)^{i_1+\cdots+i_k}}{b_1^{i_1}\cdots b_k^{i_k}} = (-1)^{|I|}A_{\bar{I}}(p-1), \end{aligned}$$

and similarly for S_I. □

An immediate consequence is that $S_I(p-1) \equiv A_I(p-1) \equiv 0 \mod p$ if $I = \bar{I}$ and $|I|$ is odd. Another consequence is that $S_{(i,j)}(p-1) \equiv A_{(i,j)}(p-1) \equiv 0 \mod p$ when $p > i+j+1$ and $i+j$ is even. This is because

$$S_{(i,j)}(p-1) + S_{(j,i)}(p-1) \equiv 0 \mod p$$

for $p > i+j+1$ by Theorem 6.1, while $S_{(i,j)}(p-1) \equiv S_{(j,i)}(p-1) \mod p$ when $i+j$ is even by Theorem 6.6.

We have the following result relating S_I and S_{I^*}.

Theorem 6.7. $S_I(p-1) \equiv -S_{I^*}(p-1) \mod p$ for all primes p.

Proof. Let f be a sequence. From the definition of ∇

$$\Sigma\nabla f(n) = \sum_{i=0}^{n} \binom{n+1}{i+1}(-1)^i f(i),$$

so taking $n = p-1$ gives

$$\Sigma\nabla f(p-1) \equiv (-1)^{p-1} f(p-1) \equiv f(p-1) \mod p.$$

Now take $f = S_I$ and apply Theorem 6.4. □

This result has the following corollary for the A_I, which may be compared with Theorem 4.4 of [17]. (We use superscripts for repetition, so $(n, 1^k)$ means the composition of weight $n+k$ with k repetitions of 1.)

Theorem 6.8. If p is a prime with $p > \max\{k+1, n\}$, then

$$A_{(n,1^k)}(p-1) \equiv A_{(k+1,1^{n-1})}(p-1) \mod p.$$

Proof. First note that $(n, 1^k)^* = (1^{n-1}, k+1)$. So, combining Theorems 6.7 and 6.6,

$$S_{(n,1^k)}(p-1) \equiv -S_{(1^{n-1},k+1)} \equiv (-1)^{n+k+1} S_{(k+1,1^{n-1})}(p-1) \mod p. \tag{6.3}$$

Now equate the right-hand sides of parts (1) and (2) of Theorem 6.2 and then apply ρ_{p-1} to get

$$(-1)^{\ell(I)} S_{\bar{I}}(p-1) = \sum_{I_1 \sqcup \cdots \sqcup I_l = I} (-1)^l A_{I_1}(p-1) \cdots A_{I_l}(p-1)$$

for any composition I; if we set $I = (1^k, n)$, the hypothesis insures that all the terms on the right-hand side are zero mod p except the one with $l = 1$, giving $(-1)^k S_{(n,1^k)}(p-1) \equiv A_{(1^k,n)}(p-1) \mod p$. Apply Theorem 6.6 to get $S_{(n,1^k)}(p-1) \equiv (-1)^n A_{(n,1^k)}(p-1) \mod p$. By the same argument, $S_{(k+1,1^{n-1})}(p-1) \equiv (-1)^{k+1} A_{(k+1,1^{n-1})}(p-1) \mod p$, and equation (6.3) gives the conclusion. □

We can state Theorem 6.7 in algebraic language as follows. Define, for each prime p, a map $\chi_p : \mathfrak{H}^1_{\mathbf{Z}} \to \mathbf{Z}/p\mathbf{Z}$ by $\chi_p(w) = \rho_{p-1}(w)$. (Here $\mathfrak{H}^1_{\mathbf{Z}}$ is the integral version of $\mathfrak{H}^1$, i.e., the graded $\mathbf{Z}$-module in $\mathbf{Z}\langle x, y\rangle$ generated by words ending in y.) The commutative diagram (6.2) gives the following algebraic version of Theorem 6.7, which can be considered a mod p counterpart of the duality theorem for MZVs.

Theorem 6.9. As elements of $\mathbf{Z}/p\mathbf{Z}$, $\chi_p(w) = \chi_p(\psi(w))$ for words w of $\mathfrak{H}^1$.

For example, since $\psi(x^2y^3) = -x^2y^3 - xy^4 - yxy^3 - y^5$, we have

$$\begin{aligned} A_{(3,1,1)}(p-1) \equiv & -A_{(3,1,1)}(p-1) - A_{(2,1,1,1)}(p-1) \\ & - A_{(1,2,1,1)}(p-1) - A_{(1,1,1,1,1)}(p-1) \mod p. \end{aligned}$$

For $p > 6$ this reduces to

$$2A_{(3,1,1)}(p-1) \equiv -A_{(2,1,1,1)}(p-1) - A_{(1,2,1,1)}(p-1) \mod p.$$

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ON THE LOCAL FACTOR OF THE ZETA FUNCTION OF QUADRATIC ORDERS

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Abstract We prove by an elementary method the Riemann hypothesis for the local Euler factor of the zeta function of quadratic orders.

Keywords: zeta function, Riemann hypothesis.

Let K be a quadratic number field, $\mathcal{O}_K$ its ring of integers, and for each integer $f \geq 1$ let $\mathcal{O}_f$ be the order of conductor f in $\mathcal{O}_K = \mathcal{O}_1$. As shown in [1] and [3], the zeta function $\zeta_{\mathcal{O}_f}(s)$ of $\mathcal{O}_f$, which is defined by

$$\zeta_{\mathcal{O}_f}(s) = \sum_{\mathfrak{a}} \frac{1}{N(\mathfrak{a})^s},$$

where the sum extends over all *proper* ideals $\mathfrak{a}$ of $\mathcal{O}_f$ with norm $N(\mathfrak{a})$, has the following form:

$$\zeta_{\mathcal{O}_f}(s) = \zeta_K(s) \prod_{p|f} \frac{(1-p^{-s})(1-\chi(p)p^{-s}) - p^{n_p-1-2n_ps}(1-p^{1-s})(\chi(p)-p^{1-s})}{(1-p^{1-2s})}.$$

Here, $\zeta_K(s)$ is the Dedekind zeta function of K, the product is over the prime factors p of the conductor f, with n_p being the exact power of p in f, and χ is the Dirichlet character corresponding to the extension $K/\mathbf{Q}$.

The main purpose of this short note is to provide proofs of the following properties, including the "Riemann hypothesis," for the local factor

$$\varepsilon_{f,p}(s) := \frac{(1-p^{-s})(1-\chi(p)p^{-s}) - p^{n_p-1-2n_ps}(1-p^{1-s})(\chi(p)-p^{1-s})}{(1-p^{1-2s})}$$

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of $\zeta_{\mathcal{O}_f}(s)/\zeta_K(s)$:

Theorem 1. *1)* The function $\varepsilon_{f,p}(s)$ is a polynomial of degree $2n_p$ in p^{-s} and satisfies the functional equation

$$\varepsilon_{f,p}(1-s) = p^{-n_p(1-2s)}\varepsilon_{f,p}(s).$$

2) All the zeros of $\varepsilon_{f,p}(s)$ lie on the line $\mathrm{Re}(s) = 1/2$.

Proof. Setting $u = p^{-s}$ and $n = n_p$, we rewrite $\varepsilon_{f,p}(s)$ as the function $P_n(u)$, given as follows:

$$\begin{aligned} &P_n(u) \\ &= \frac{(1-u)(1-\chi(p)u) - p^{n-1}u^{2n}(1-pu)(\chi(p)-pu)}{1-pu^2} \\ &= \frac{1-p^{n+1}u^{2(n+1)} - (1+\chi(p))u(1-p^n u^{2n}) + \chi(p)u^2(1-p^{n-1}u^{2(n-1)})}{1-pu^2}. \end{aligned}$$

The numerator of this expression vanishes if we set $u = \pm 1/\sqrt{p}$ and hence is divisible by the denominator $1-pu^2$. Thus $P_n(u)$ is indeed a polynomial of degree $2n$. By direct division, we find

$$P_n(u) = 1 - (1+\chi(p))u + \cdots - p^{n-1}(1+\chi(p))u^{2n-1} + p^n u^{2n}.$$

The functional equation can be verified straightforwardly. This ends the proof of assertion 1).

To prove the Riemann hypothesis 2), put $s = 1/2 + it/\log p$. Then we have $u = p^{-1/2}e^{-it}$ and

$$\begin{aligned} P_n(u) = \frac{1}{1-e^{-2it}}\Big(&1 - e^{-2(n+1)it} - (1+\chi(p))p^{-1/2}e^{-it}(1-e^{-2nit}) \\ &+\chi(p)p^{-1}e^{-2it}(1-e^{-2(n-1)it})\Big). \end{aligned}$$

Then, using the relation

$$\frac{1-e^{-2mit}}{1-e^{-2it}} = \frac{e^{-mit}}{e^{-it}}\frac{\sin mt}{\sin t},$$

we obtain

$$P_n(u) = \frac{e^{-nit}}{p}\left(p\,\frac{\sin(n+1)t}{\sin t} - \sqrt{p}\,(1+\chi(p))\,\frac{\sin nt}{\sin t} - \chi(p)\,\frac{\sin(n-1)t}{\sin t}\right).$$

We have to show that if the right-hand side of this is zero, then t is real. Recall that, for any integer $m \geq 0$, the quotient $\sin(m+1)t/\sin t$

is a polynomial of degree m in $x = \cos t$, which is referred to as the Chebyshev polynomial of the second kind, denoted by $U_m(x)$. The first several of these are as follows:

$$U_0(x) = 1, \quad U_1(x) = 2x, \quad U_2(x) = 4x^2 - 1, \quad U_3(x) = 8x^3 - 4x.$$

Note that the function $U_m(x)$ can also be defined for $m < 0$; in particular, we have $U_{-1}(x) = 0$ and $U_{-2}(x) = -1$. Using the $U_m(x)$, the proof is reduced to showing that all the roots of the polynomial (of degree n)

$$Q_n(x) := p\,U_n(x) - \sqrt{p}\,(1 + \chi(p))\,U_{n-1}(x) + \chi(p)\,U_{n-2}(x) \quad (n \geq 1)$$

are in the real interval $[-1, 1]$.

Because of the recurrence of the Chebyshev polynomials

$$U_n(x) = 2xU_{n-1}(x) - U_{n-2}(x),$$

the polynomials $Q_n(x)$ satisfy the same recurrence:

$$Q_n(x) = 2xQ_{n-1}(x) - Q_{n-2}(x) \quad (n \geq 2),$$

with $Q_0(x) = p - \chi(p)$. We show that the n roots of $Q_n(x)$ are all in the interval $(-1, 1)$ by making use of the theorem of Sturm (cf. [2, §92]), thereby utilizing the fact that $Q_n(x), Q_{n-1}(x), \ldots, Q_0(x)$ forms a "Strum sequence." Since $U_n(1) = n + 1$ and $U_n(-1) = (-1)^n(n + 1)$, we have

$$\begin{aligned} Q_n(1) &= p(n+1) - \sqrt{p}(1 + \chi(p))n + \chi(p)(n-1) \\ &= (\sqrt{p} - 1)(\sqrt{p} - \chi(p))n + p - \chi(p) > 0 \end{aligned}$$

and

$$\begin{aligned} &Q_n(-1) \\ &= p(-1)^n(n+1) - \sqrt{p}(1 + \chi(p))(-1)^{n-1}n + \chi(p)(-1)^{n-2}(n-1) \\ &= (-1)^n \{p(n+1) + \sqrt{p}(1 + \chi(p))n + \chi(p)(n-1)\} \\ &= (-1)^n \{(\sqrt{p} + 1)(\sqrt{p} + \chi(p))n + p - \chi(p)\}. \end{aligned}$$

The sign of the last expression is $(-1)^n$, and hence the number of "variations," as defined in [2, §92], is n. Then, noting the theorem of Sturm, we conclude that $Q_n(x)$ has n roots in the interval $(-1, 1)$. (Note that, since the degree of $Q_n(x)$ is n, condition 4 of [2, §92] need not be verified.) $\square$

Remarks and questions. 1) It is amusing that the properties stated in the above theorem are precisely those enjoyed by the congruence zeta function (or, rather, its essential part) of a curve of genus $n = n_p$ over the prime field $\mathbf{F}_p$. This naturally leads us to wonder if $\varepsilon_{f,p}(s)$ admits a cohomological (or any other "nice") interpretation and if the above theorem can be proved "conceptually" using such an interpretation.

2) The theorem proved here shows in particular that the quotient $\zeta_{\mathcal{O}_f}(s)/\zeta_K(s)$ is entire and that the Riemann hypothesis holds for $\zeta_{\mathcal{O}_f}(s)$ only if it holds for $\zeta_K(s)$. It is known that for a Galois extension k'/k of number fields, the quotient of the Dedekind zeta functions $\zeta_{k'}(s)/\zeta_k(s)$ is entire. Thus the zeta function of the *over* field is divisible by that of the base field. On the contrary, in the case considered above, the zeta function of the *subring* $\mathcal{O}_f$ is divisible by that of the over ring. What is the reason for this?

3) The generating function of the polynomials $P_n(x)$ takes the simple form

$$F(u,X) := 1 + \sum_{n=1}^{\infty} P_n(u)X^n = \frac{(1-uX)(1-\chi(p)uX)}{(1-X)(1-pu^2X)},$$

and the functional equation for $P_n(u)$, which is written as

$$p^n u^{2n} P_n(\frac{1}{pu}) = P_n(u),$$

is encoded as

$$F(\frac{1}{pu}, pu^2X) = F(u,X).$$

4) For another zeta function

$$\zeta^*_{\mathcal{O}_f}(s) = \sum_{\mathfrak{a}} \frac{1}{N(\mathfrak{a})^s},$$

where $\mathfrak{a}$ runs over *all* (not necessarily proper) ideals of $\mathcal{O}_f$, the Euler product is (*cf.* [3])

$$\zeta_K(s) \cdot \prod_{p|f} \frac{1 - p^{(n_p+1)(1-2s)} - \chi(p)p^{-s}(1 - p^{n_p(1-2s)})}{1 - p^{1-2s}}.$$

It can be shown similarly that the local factor

$$\frac{1 - p^{(n_p+1)(1-2s)} - \chi(p)p^{-s}(1 - p^{n_p(1-2s)})}{1 - p^{1-2s}}$$

possesses the same properties as those for $\varepsilon_{f,p}(s)$.

5) It would be nice to have a generalization of our theorem to the zeta functions of orders of number fields of higher degree.

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SUMS INVOLVING THE HURWITZ ZETA-FUNCTION VALUES

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Dedicated to Professor Masaki Sudo for his sixtieth birthday

Abstract By interpreting the Hurwitz zeta-function ζ^* as its Fourier series, we find a closed form for the sum $S(s,a) = \sum_{a=0}^{n-1} \zeta^*(1-s, 1-\{\frac{a^2 m}{n} + x\})$ for coprime integers $m, n, \Re s > 1$ or $s = 1$ and $x \in \mathbb{R}$ in terms of the invariants of the associated quadratic field.

Keywords: Hurwitz zeta-function, fractional part sums, Dirichlet L-functions

1. Introduction and statement of results

For the complex variable s with $\sigma = \Re s > 1$, the polylogarithm function $\ell_s(x)$ of order s is defined by its "Fourier series"

$$\ell_s(x) = \sum_{\nu=1}^{\infty} \frac{e^{2\pi i \nu x}}{\nu^s} \tag{1.1}$$

for all $x \in \mathbb{R}$. By Abel's continuity theorem, $\ell_1(x)$ is defined by (1.1) for $x \notin \mathbb{Z}$, and further it holds that

$$\ell_1(x) = -\log 2|\sin \pi x| - \pi i \overline{B}_1(x),$$

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whence, in particular,

$$\Im\ell_1(x) = -\pi\overline{B}_1(x) = \sum_{\nu=1}^{\infty} \frac{\sin 2\pi\nu x}{\nu}, \quad 0 < x < 1, \tag{1.2}$$

where $\overline{B}_1(x) = x - [x] - \frac{1}{2}$ is the first periodic Bernoulli polynomial. The Fourier series for $\overline{B}_1(x)$ in (1.2) converges to 0 for $x \in \mathbb{Z}$, and this suggests the definition

$$\overline{B}_1^*(x) = \begin{cases} \overline{B}_1(x), & x \notin \mathbb{Z} \\ 0, & x \in \mathbb{Z}. \end{cases} \tag{1.3}$$

Then (1.2) allows us to extend the definition of $\Im\ell_1(x)$ for $x \in \mathbb{Z}$ also as 0.

Let $\zeta(s,x)$ denote the Hurwitz zeta-function defined in the first instance by

$$\zeta(s,x) = \sum_{\nu=0}^{\infty} \frac{1}{(\nu+x)^s}, \quad \sigma > 1,\ 0 < x < 1$$

and then continued meromorphically over the whole complex plane, the analytic continuation furnished by the Hurwitz functional equation ([16, 13·15])

$$\zeta(1-s,1-x) = \frac{\Gamma(s)}{(2\pi)^s}\left\{e^{-\frac{\pi i s}{2}}\ell_s(1-x) + e^{\frac{\pi i s}{2}}\ell_s(x)\right\} \tag{1.4}$$

valid for $\sigma < 0$ and $0 < x < 1$, which for $s \in \mathbb{N} \cup \{0\}$ degenerates into

$$-s\zeta(1-s,1-x) = B_s(1-x) = (-1)^s B_s(x), \tag{1.5}$$

where $B_s(x)$ is the s-th Bernoulli polynomial ([16, 13·14]).

Since (1.5) for $s = 1$ reads $-\zeta(0,x) = B_1(x)$, we are led to extend the definition of $\zeta(0, 1-x)$ by putting $\zeta^*(0,1-x) = \overline{B}_1^*(x)$. This means that the functional equation (1.4) holds in the form

$$\zeta^*(1-s,1-x) = \frac{\Gamma(s)}{(2\pi)^s}\left\{e^{-\frac{\pi i s}{2}}\ell_s(1-x) + e^{\frac{\pi i s}{2}}\ell_s(x)\right\} \tag{1.6}$$

for $0 \le x < 1$, where we understand the right-hand side as given by Fourier series (1.1), and in particular, for $s = 1$, we are to understand

$$\zeta^*(0,1-x)\left(= \frac{-1}{\pi}\Im\ell_1(x)\right) = \overline{B}_1^*(x).$$

We note that (1.6) entails one unconventional implication $\zeta^*(0) = \zeta^*(0,1) = 0$, but otherwise, it has the merit that we may constantly use the Fourier series (1.1) in all cases.

In this note we are going to find a closed form for the sum

$$S(s,x)=\sum_{a=0}^{n-1}\zeta^*\left(1-s,1-\left\{\frac{a^2m}{n}+x\right\}\right) \tag{1.7}$$

for coprime positive integers $m,n,\sigma>1$ or $s=1$ and $x\in\mathbb{R}$ to be specified as one of the values $0,\frac{1}{2},\frac{1}{4}$ and where $\{y\}=y-[y]$ means the fractional part of y.

Our main result is the following

Theorem. *For all $x\in\mathbb{R}$ and $\sigma>1$ or $s=1$, we have*

$$S(s,x)=\frac{2\Gamma(s)}{(2\pi)^s}\sum_{dd'=n}d'^{1-s}\left(\left(\frac{d}{m}\right)\phi_1(d'x,d,s)-\left(\frac{-d}{m}\right)\phi_{-1}(d'x,d,s)\right), \tag{1.8}$$

where

$$\phi_1(z,d,s)=\begin{cases}\sqrt{d}\displaystyle\sum_{\nu=1}^{\infty}\frac{\left(\frac{d}{\nu}\right)}{\nu^s}\cos\left(\frac{\pi s}{2}+2\pi\nu z\right) & \text{if } d\equiv 0,1\,(4)\\ 0 & \text{otherwise}\end{cases} \tag{1.9}$$

and

$$\phi_{-1}(z,d,s)=\begin{cases}\sqrt{d}\displaystyle\sum_{\nu=1}^{\infty}\frac{\left(\frac{-d}{\nu}\right)}{\nu^s}\sin\left(\frac{\pi s}{2}+2\pi\nu z\right) & \text{if } d\equiv 0,3\,(4)\\ 0 & \text{otherwise}\end{cases} \tag{1.10}$$

and where $(\frac{d}{\nu})$ signifies the Kronecker-Jacobi symbol.

The functions in (1.9) and (1.10) are slight extensions of those introduced by the second author [13].

We now state some special cases of our Theorem as corollaries. Naturally, we are not going to be exhaustive, the unspecified cases being read off easily, in the same manner.

Corollary 1. For coprime positive integers m,n, we have

$$\begin{aligned}S(1,x)&=\sum_{\substack{a=0\\ \{\frac{a^2m}{n}+x\}\neq 0}}^{n-1}\left(\left\{\frac{a^2m}{n}+x\right\}-\frac{1}{2}\right)\\ &=-\sum_{dd'=n}\left\{\left(\frac{d}{m}\right)\phi_1(d'x,d)+\left(\frac{-d}{m}\right)\phi_{-1}(d'x,d)\right\},\end{aligned} \tag{1.11}$$

where $\phi_\pm(z,d) = \mp\phi_{\pm 1}(z,d,1)/\pi$ are those adopted in [13]; further particular cases are

$$S(1,0) = -\frac{1}{\pi} \sum_{\substack{d|n \\ d\equiv 0,3\,(4)}} \left(\frac{-d}{m}\right) \sqrt{d}\, L\left(1, \left(\frac{-d}{\cdot}\right)\right)$$

$$= - \sum_{\substack{d|n \\ d\equiv 0,3\,(4)}} \left(\frac{-d}{m}\right) c_d h(-d), \tag{1.12}$$

where $L(s, (\frac{-d}{\cdot}))$ stands for the Dirichlet L-function with character $(\frac{-d}{\cdot})$, $h(-d)$ the class number of primitive quadratic forms with discriminant $-d$, w_d the number of automorphs of them, and finally $c_d = 2/w_d$;

$$S\left(1, \frac{1}{2}\right) = \sum_{\substack{dd'=n \\ d\equiv 0,3\,(4) \\ d'\equiv 1\,(2)}} \left(\frac{-d}{m}\right) c_d \left(1 - \left(\frac{-d}{2}\right)\right) h(-d)$$

$$- \sum_{\substack{dd'=n \\ d\equiv 0,3\,(4) \\ d'\equiv 0\,(2)}} \left(\frac{-d}{m}\right) c_d h(-d); \tag{1.13}$$

in the case $n \equiv 2\,(4)$, we have

$$S\left(1, \frac{1}{4}\right) = \sum_{\substack{dd'=n \\ d\equiv 3\,(4)}} \left(\frac{-d}{m}\right) \left(1 - \left(\frac{-d}{2}\right)\right) c_d h(-d) \tag{1.14}$$

We remark that

$$S(1,x) = \sum_{a=0}^{n-1} \left(\left\{\frac{a^2 m}{n} + x\right\} - \frac{1}{2}\right) + \frac{1}{2} \sum_{\substack{a=0 \\ \{\frac{a^2m}{n}+x\}=0}}^{n-1} 1,$$

and that

$$\sum_{\substack{a=0 \\ \{\frac{a^2m}{n}\}=0}}^{n-1} 1 = q, \qquad \sum_{\substack{a=0 \\ \{\frac{a^2m}{n}+\frac{1}{2}\}=0}}^{n-1} 1 = \frac{1+(-1)^{n/q^2}}{2} q$$

and

$$\sum_{\substack{a=0 \\ \{\frac{a^2m}{n}+\frac{1}{4}\}=0}}^{n-1} 1 = 0 \quad (\text{ in the case } n \equiv 2\,(4)),$$

where q^2 signifies the largest square divisor of n.

Hence we contend that (1.12) is equivalent to [13, Corollary], while (1.13) and (1.14) give those formulas stated on p. 115 of [13] (in the case of (1.14), notice that $(\frac{-d}{2}) = 1$ if $d \equiv -3\,(8)$, which are generalizations of Lerch's results [9–11].

Now we shall give general results for positive integer value l.

Corollary 2. Let $\delta(h)$ denote 0 or 1 according as h is even or odd. Then for integers $l \geq 1$ and coprime positive integers m, n, we have

$$S(l,0) = \frac{2\Gamma(l)n^{1-l}}{(2\pi)^l}(-1)^{[\frac{l+1}{2}]} \times \sum_{\substack{d|n \\ d\equiv 0,(-1)^{\delta(l)}\,(4)}} d^{l-\frac{1}{2}} \left(\frac{(-1)^{\delta(l)}d}{m}\right) L\left(l, \left(\frac{(-1)^{\delta(l)}d}{\cdot}\right)\right), \tag{1.15}$$

$$S\left(l,\frac{1}{2}\right) = \frac{2\Gamma(l)n^{1-l}}{(2\pi)^l}(-1)^{[\frac{l+1}{2}]} \sum_{\substack{d|n \\ d\equiv 0,(-1)^{\delta(l)}\,(4)}} d^{l-\frac{1}{2}} \left(\frac{(-1)^{\delta(l)}d}{m}\right) \times \left(2^{1-l}\left(\frac{(-1)^{\delta(l)}d}{m}\right) - 1\right)^{\delta(n/d)} L\left(l, \left(\frac{(-1)^{\delta(l)}d}{\cdot}\right)\right) \tag{1.16}$$

In the case n being odd, we have for $k \geq 1$

$$S\left(2k,\frac{1}{4}\right) = \frac{2\Gamma(2k)n^{1-2k}(-1)^k}{(2\pi)^{2k}} \times \left\{ \sum_{\substack{d|n \\ d\equiv 0,1\,(4)}} d^{2k-\frac{1}{2}} \left(\frac{d}{2m}\right) 2^{-2k}\left(2^{1-2k}\left(\frac{d}{2}\right) - 1\right) L\left(2k, \left(\frac{d}{\cdot}\right)\right) - \sum_{\substack{d|n \\ d\equiv 0,3\,(4)}} d^{2k-\frac{1}{2}} \left(\frac{-d}{m}\right) (-1)^{\frac{1}{2}(\frac{n}{d}-1)} L\left(2k, \chi_4\left(\frac{-d}{\cdot}\right)\right) \right\} \tag{1.17}$$

and

$$S\left(2k+1,\frac{1}{4}\right)=\frac{2\Gamma(2k+1)n^{1-(2k+1)}(-1)^{k+1}}{(2\pi)^{2k+1}}\times$$

$$\times\left\{\sum_{\substack{d|n\\ d\equiv 0,1\,(4)}} d^{(2k+1)-\frac{1}{2}}\left(\frac{d}{m}\right)(-1)^{\frac{1}{2}(\frac{n}{d}-1)}L\left(2k+1,\chi_4\left(\frac{d}{\cdot}\right)\right)\right.$$

$$+\sum_{\substack{d|n\\ d\equiv 0,3\,(4)}} d^{(2k+1)-\frac{1}{2}}\left(\frac{-d}{2m}\right)2^{-(2k+1)}\left(2^{-2k}\left(\frac{-d}{2}\right)-1\right)\times$$

$$\left.\times L\left(2k+1,\left(\frac{-d}{\cdot}\right)\right)\right\}, \qquad (1.18)$$

where χ_4 signifies the primitive character mod 4.

2. Proof of results

The proof is typical, once-put-into-proper-form-it's-easy-to-prove-type. By (1.3), the sum $S(s,x)$ can be written as

$$S(s,x)=\frac{\Gamma(s)}{(2\pi)^s}\left\{e^{-\frac{\pi is}{2}}T_1(s,x)+e^{\frac{\pi is}{2}}T_2(s,x)\right\}, \qquad (2.1)$$

where

$$T_1(s,x)=\sum_{a=0}^{n-1}\ell_s^*\Big(1-\Big\{\frac{a^2m}{n}+x\Big\}\Big), \qquad (2.2)$$

and

$$T_2(s,x)=\sum_{a=0}^{n-1}\ell_s^*\Big(-1+\Big\{\frac{a^2m}{n}+x\Big\}\Big), \qquad (2.3)$$

under the convention that $\ell_1^*(x)=0$ for $x\in\mathbb{Z}$; for other values of x, $\ell_s^*(x)=\ell_s(x)$.

For coprime positive integers m,n, the quadratic Gauss sum

$$\varphi(m,n)=\sum_{a=0}^{n-1}e^{2\pi i\frac{a^2m}{n}} \qquad (2.4)$$

has been considered by several authors (e.g. cf. [7], [8, p.87]) and this general case was treated by the second author [13] in his Lemma;

$$\varphi(m,n)=\begin{cases}\left(\dfrac{n}{m}\right)\sqrt{n} & \text{if } n\equiv 1\,(4),\\ \left(\dfrac{-n}{m}\right)\sqrt{n} & \text{if } n\equiv -1\,(4),\\ 0 & \text{if } n\equiv 2\,(4),\\ \left(\left(\dfrac{n}{m}\right)+\left(\dfrac{-n}{m}\right)i\right)\sqrt{n} & \text{if } n\equiv 0\,(4),\end{cases} \tag{2.5}$$

and

$$\varphi(dm,dn)=d\varphi(m,n). \tag{2.6}$$

Interchanging the order of summation in (2.2), we see that

$$T_1(s,x)=\sum_{\nu'=1}^{\infty}\frac{e^{-2\pi i\nu' x}}{\nu'^s}\overline{\varphi}(m\nu',n), \tag{2.7}$$

where the bar means the complex conjugate. Let $(n,\nu')=d'$, $n=dd'$ and $\nu'=\nu d'$ in (2.7). Then

$$T_1(s,x)=\sum_{d|n}\sum_{\substack{\nu=1\\(\nu,d)=1}}^{\infty}\frac{e^{-2\pi i d'\nu x}}{(d'\nu)^s}d'\,\overline{\varphi}(m\nu,d) \tag{2.8}$$

and ν runs through all integers satisfying $(m\nu,d)=1$.

Substituting from (2.5), thereby distinguishing three cases $d\equiv 0,1,3\,(4)$, we contend that

$$\begin{aligned}T_1(s,x)=&\sum_{\substack{d|n\\ d\equiv 0,1\,(4)}} d'^{1-s}\left(\frac{d}{m}\right)\sqrt{d}\sum_{\substack{\nu=1\\(\nu,d)=1}}^{\infty}\frac{(\frac{d}{\nu})e^{-2\pi i\frac{n\nu}{d}x}}{\nu^s}\\ &-i\sum_{\substack{d|n\\ d\equiv 0,3\,(4)}} d'^{1-s}\left(\frac{-d}{m}\right)\sqrt{d}\sum_{\substack{\nu=1\\(\nu,d)=1}}^{\infty}\frac{(\frac{-d}{\nu})e^{-2\pi i\frac{n\nu}{d}x}}{\nu^s}\end{aligned} \tag{2.9}$$

where the condition $(\nu,d)=1$ may be suppressed in view of the presence of the character $(\frac{\pm d}{\nu})$.

Similarly,

$$\begin{aligned} T_2(s,x) = &\sum_{\substack{d|n \\ d\equiv 0,1\,(4)}} {d'}^{1-s}\left(\frac{d}{m}\right)\sqrt{d}\sum_{\nu=1}^{\infty}\frac{(\frac{d}{\nu})e^{2\pi i\frac{n\nu}{d}x}}{\nu^s} \\ &+ i\sum_{\substack{d|n \\ d\equiv 0,3\,(4)}} {d'}^{1-s}\left(\frac{-d}{m}\right)\sqrt{d}\sum_{\nu=1}^{\infty}\frac{(\frac{-d}{\nu})e^{2\pi i\frac{n\nu}{d}x}}{\nu^s} \end{aligned} \tag{2.10}$$

Substituting (2.9) and (2.10) in (2.1) and transforming the exponentials into sines and cosines, we complete the proof of (1.8).

To illustrate the way of deducing corollaries from our Theorem, we give a proof of (1.14), which contains most of the ingredients and is most instructive.

We have

$$\begin{aligned} S\left(1,\frac{1}{4}\right) = -\frac{1}{\pi}&\left\{\sum_{\substack{d|n \\ d\equiv 0,1\,(4)}}\left(\frac{d}{m}\right)\sqrt{d}\sum_{\nu=1}^{\infty}\frac{(\frac{d}{\nu})\sin(\frac{\pi}{2}\frac{n\nu}{d})}{\nu}\right. \\ &\left.+\sum_{\substack{d|n \\ d\equiv 0,3\,(4)}}\left(\frac{-d}{\nu}\right)\sqrt{d}\sum_{\nu=1}^{\infty}\frac{(\frac{-d}{\nu})\cos(\frac{\pi}{2}\frac{n\nu}{d})}{\nu}\right\}. \end{aligned} \tag{2.11}$$

Since we assume $n \equiv 2\,(4)$, we observe that if $d|n$, then $d \not\equiv 0\,(4)$, and hence that $\sin\frac{\pi n\nu}{2d} = 0$ and $\cos\frac{\pi n\nu}{2d} = (-1)^{\frac{n\nu}{2d}} = (-1)^{\nu}$. Hence

$$S\left(1,\frac{1}{4}\right) = -\frac{1}{\pi}\sum_{\substack{d|n \\ d\equiv 3(4)}}\left(\frac{-d}{m}\right)\sqrt{d}\sum_{\nu=1}^{\infty}\frac{(\frac{-d}{\nu})(-1)^{\nu}}{\nu}, \tag{2.12}$$

whose inner sum is

$$\begin{aligned} \sum_{2|\nu}-\sum_{2\nmid\nu} &= -\sum_{\nu=1}^{\infty}\frac{(\frac{-d}{\nu})}{\nu}+2\sum_{\substack{\nu=1 \\ 2|\nu}}\frac{(\frac{-d}{\nu})}{\nu} \\ &= -L\left(1,\left(\frac{-d}{\cdot}\right)\right)+2\sum_{\nu_1=1}^{\infty}\frac{(\frac{-d}{2\nu_1})}{2\nu_1} \\ &= \left(\left(\frac{-d}{2}\right)-1\right)L\left(1,\left(\frac{-d}{\cdot}\right)\right). \end{aligned}$$

Hence

$$S\left(1, \frac{1}{4}\right) = -\frac{1}{\pi} \sum_{\substack{d|n \\ d\equiv 3\,(4)}} \left(\frac{-d}{m}\right) \left(\left(\frac{-d}{2}\right) - 1\right) \sqrt{d} L\left(1, \left(\frac{-d}{\cdot}\right)\right)$$

$$= \frac{1}{\pi} \sum_{\substack{d|n \\ d\equiv 3\,(4)}} \left(\frac{-d}{m}\right) \left(1 - \left(\frac{-d}{2}\right)\right) c_d h(-d). \tag{2.13}$$

In order to deduce Lerch's formula, it suffices to note that those integers $d \equiv -1\,(4)$ split into two congruence classes $d \equiv 3\,(8)$ and $d \equiv 7\,(8)$, the latter giving $\frac{d^2-1}{8} \equiv 0(2)$, whence $1 - (\frac{-d}{2}) = 0$ on appealing to the complementary reciprocity law $(\frac{-d}{2}) = (\frac{-2}{d}) = (-1)^{\frac{d^2-1}{8}}$.

Remark. The evaluation of (1.7) seems to be closely related to that of short-interval character sums as expanded in [1, 14, 15] and through it, to the evaluation of Maillet determinants [2, 5, 6]. It might also be interesting to consider similar sums as (1.7) with the derivatives of ζ (cf. e.g. [3]). We hope to return to these problems at another occasion.

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CRYSTAL SYMMETRY VIEWED AS ZETA SYMMETRY

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Dedicated to Professor Yukio Ueda on his seventieth birthday

Abstract In this paper we study two kinds of energy invariants – the Madelung constant and the screened Coulomb potential associated to a crystal lattice though the lattice zeta-function, which is manifested as the Epstein zeta-function. We take into account the lattice structure (crystal symmetry) in our study through the functional equation of the Epstein zeta-function (zeta symmetry).

Keywords: Bessel series, incomplete gamma series, functional equation, crystal lattice, Epstein zeta-function, screened Coulomb potential, Abel mean

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1. Introduction

In this paper we are going to study two kinds of energy invariants associated to a crystal lattice.

One is the Madelung constant associated to a lattice about which numerous papers have appeared so far. Main references in book form are [6], [14] and [27]. The main feature of our paper in this regard is that we incorporate the lattice structure in its full extent, especially, the relationships between mutually dual lattice structures are revealed as those between the associated lattice zeta-functions, which are in turn manifested as the Epstein zeta-functions. I.e. unlike previous work (save for Terras), we are going to express the distance and ion charges of the crystal structure in the form of a quadratic form and construct the Epstein zeta-functions associated to it, and then apply decomposition of the coefficient matrices to the Epstein zeta-function as is seen in Terras [25].

As the second main feature, we shall present a rather complete version of the theory of Epstein zeta-functions, which include generalizations of the theory of Berndt [4], Chowla-Selberg and Terras as well as a unification of the theory of lattice zeta-values developed so far. They are manifested as the special values like $\zeta(1/2)$, $\beta(1/2)$, and we may efficiently incorporate our recent results on special values (see [18]).

The second object of study is the screened Coulomb potential, which we view as Abel mean of the modular relation, or what is the same thing, the functional equation, i.e. the zeta symmetry. Here the main references are [8]-[11], [16] and further developed by [7] and [15]. These papers, however, lack the view point of Abel mean and the relevant zeta-functions, and give impressions that there is no ad hoc structure implemented.

As the third main feature, we shall appeal to the symmetry of the associated general Epstein zeta-function and show that the Abel mean considered by Chaba-Pathria is indeed equivalent to (or a consequence of) the functional equation, or the zeta symmetry. This type of Abel mean was considered by F.V. Atkinson [1] using the integral representation of the zeta-function and then more thoroughly by B.C. Berndt [3] using a perturbed Dirichlet series, or the Mellin-Barnes integrals (cf. Paris-Kaminski [23]).

First we recall the theory of functional equation of Hecke type and then state the special case of Epstein zeta-functions.

As is well-known (cf. e.g. [18]), the Hecke type functional equation is stated as

I. Let $\varphi(s)$ and $\psi(s)$ denote Dirichlet series with abscissas of absolute convergence σ_a and σ_a^* respectively:

$$\varphi(s) = \sum_{n=1}^{\infty} \frac{a_n}{\lambda_n^s}, \quad \psi(s) = \sum_{n=1}^{\infty} \frac{b_n}{\mu_n^s}, \tag{1.1}$$

where $\{a_n\}$, $\{b_n\}$ are complex sequences and $\{\lambda_n\}$, $\{\mu_n\}$ are real increasing sequences tending to ∞ with $\lambda_1 > 0$, $\mu_1 > 0$.

$\varphi(s)$ and $\psi(s)$ are said to satisfy the functional equation of Hecke type

$$\Gamma(s)\varphi(s) = \Gamma(\delta - s)\psi(\delta - s) \tag{1.2}$$

if there exist a constant $\delta \in \mathbb{R}$ and a function $\chi(s)$ analytic outside of a compact set $\mathcal{S}$ such that

$$\chi(s) = \Gamma(s)\varphi(s), \quad \sigma > \sigma_a \tag{1.3}$$

$$\chi(s) = \Gamma(\delta - s)\psi(\delta - s), \quad \sigma < \delta - \sigma_a^* \tag{1.4}$$

and all poles of $\chi(s)$ lie in $\mathcal{S}$.

The functional equation I is equivalent to

II. Modular relation (due to S. Bochner [5])

$$\Phi(x) = x^{-\delta}\Psi(x^{-1}) + P(x),$$

where $P(x)$ signifies the residual function given by

$$P(x) = \frac{1}{2\pi i}\int_{\mathcal{C}} \chi(s)x^{-s}ds,$$

with $\mathcal{C}$ signifying a curve or curves in $\mathcal{S}$ encircling all the singularities of χ.

Here $\Phi(x)$ and $\Psi(x)$ stand for the Lambert series associated to $\varphi(s)$ and $\psi(s)$, respectively:

$$\Phi(x) = \sum_{n=1}^{\infty} a_n e^{-\lambda_n x}, \quad \Psi(x) = \sum_{n=1}^{\infty} b_n e^{-\mu_n x}, \tag{1.5}$$

for $\Re x > 0$.

In [18] we stated other equivalent conditions; one is an incomplete gamma series (due to Kuz'min-Linnik-Lavrik [22] and Terras [27], the origin going back to Riemann), another is a Bessel series expression due to Chowla-Selberg, Berndt [3] and Terras [25], [27, Part I]. We shall state these conditions independently for Epstein zeta-functions; in section 2, we shall state the Bessel series expression which reflects the coefficient matrix decomposition, in section 3, we shall state the incomplete gamma series.

We now introduce the notation (from Terras [27]) concerning the Epstein zeta-functions, which will be used throughout in what follows.

Notation. Let $\boldsymbol{g}$, $\boldsymbol{h} \in \mathbb{R}^n$ be n-dimensional real vectors which (in the first place) give rise to the perturbation and the (additive) characters, respectively.

Let $Y = (y_{ij})$ be a positive definite $n \times n$ real symmetric matrix. Define the Epstein zeta-function associated to the quadratic form

$$Y[\mathbf{a}] = \mathbf{a} \cdot Y\mathbf{a} = {}^t\mathbf{a}Y\mathbf{a} = \sum_{i,j=1}^{n} y_{ij}a_i a_j, \tag{1.6}$$

where $\mathbf{a} = (a_1, \ldots, a_n) \in \mathbb{R}^n$ and "$\cdot$" means the scalar product, by

$$Z(Y, \mathbf{0}, \mathbf{0}, s) = \sum_{\substack{\mathbf{a}\in\mathbb{Z}^n \\ \mathbf{a}\neq\mathbf{0}}} \frac{1}{Y[\mathbf{a}]^s}, \quad \sigma > \frac{n}{2}, \tag{1.7}$$

where $\sigma = \Re s$.

For $\boldsymbol{g}$, $\boldsymbol{h} \in \mathbb{R}^n$ define the general Epstein zeta-function (of Hurwitz-Lerch type) by

$$Z(Y, \boldsymbol{g}, \boldsymbol{h}, s) = \sum_{\substack{\mathbf{a}\in\mathbb{Z}^n \\ \mathbf{a}+\boldsymbol{g}\neq\mathbf{0}}} \frac{e^{2\pi i \boldsymbol{h}\cdot\mathbf{a}}}{Y[\mathbf{a}+\boldsymbol{g}]^s}, \quad \sigma > \frac{n}{2}, \tag{1.8}$$

and incorporate the completion

$$\Lambda(Y, \boldsymbol{g}, \boldsymbol{h}, s) = \pi^{-s}\Gamma(s)Z(Y, \boldsymbol{g}, \boldsymbol{h}, s), \tag{1.9}$$

which satisfies the functional equation of the form (1.2) with an additional factor and replacement of parameters (proof given in section 3):

$$\Lambda(Y, \boldsymbol{g}, \boldsymbol{h}, s) = \frac{1}{\sqrt{|Y|}} e^{-2\pi i \boldsymbol{g}\cdot\boldsymbol{h}} \Lambda\left(Y^{-1}, \boldsymbol{h}, -\boldsymbol{g}, \frac{n}{2} - s\right). \tag{1.10}$$

In what follows we always denote the special vector ${}^t\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$ by $\boldsymbol{c}_0$:

$$\boldsymbol{c}_0 = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}.$$

We shall now give some illustrative examples.

Example 1.1. The relationship between the Madelung constants of the *NaCl* and *CsCl* structure.

In [16, p.1724], it is stated that the cations of *CsCl* are at $\mathbf{a} \in \left(\frac{2}{\sqrt{3}}\left(\mathbb{Z}+\frac{1}{2}\right)\right)^3$ and anions are at $\mathbf{a} \in \left(\frac{2}{\sqrt{3}}\mathbb{Z}\right)^3$. The Madelung constant M_{CsCl} is defined, in the first place, by

$$M_{CsCl} = \frac{\sqrt{3}}{2} \sum_{\mathbf{a}\in\mathbb{Z}^3} |\mathbf{a}+\boldsymbol{c}_0|^{-1} - \frac{\sqrt{3}}{2} \sum_{\substack{\mathbf{a}\in\mathbb{Z}^3 \\ \mathbf{a}\neq\mathbf{0}}} |\mathbf{a}|^{-1}, \tag{1.11}$$

which, in our notation above, is

$$\frac{\sqrt{3}}{2} Z\left(I, \boldsymbol{c}_0, \mathbf{0}, \frac{1}{2}\right) - \frac{\sqrt{3}}{2} Z\left(I, \mathbf{0}, \mathbf{0}, \frac{1}{2}\right) \tag{1.12}$$

and is in turn equal to

$$-\sqrt{3} Z\left(B, \mathbf{0}, \boldsymbol{c}_0, \frac{1}{2}\right), \tag{1.13}$$

where

$$I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{(identity matrix)},$$

and

$$B = \begin{pmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{pmatrix}. \tag{1.14}$$

Hautot [16], without giving any reasons, transforms (1.11) into the form

$$\begin{aligned} \frac{2}{\sqrt{3}} M_{CsCl} =& 2M_{NaCl} \\ &+ 6 \sum\sum\sum \left[\left\{ (2l)^2 + (2m+1)^2 + (2n+1)^2 \right\}^{-1/2} \right. \\ &\left. - \left\{ (2l)^2 + (2m+1)^2 + (2n)^2 \right\}^{-1/2} \right], \end{aligned} \tag{1.15}$$

and then proceeds to transfer the triple sum using the Schlömilch series technique (cf. [19] also). Thus (1.15) suggests that there may be a relationship between M_{NaCl} and M_{CsCl} structure. This suggestion is strengthened by the comparison of numerical values

$$\begin{aligned} M_{NaCl} &= 1.74756459463\ldots, \\ M_{CsCl} &= 1.76267477307\ldots. \end{aligned} \tag{1.16}$$

The real situation is the following duality relations (1.17) and (1.18), which can be found only through the study of lattice structure.

Between the Madelung constants $M_{NaCl} = -Z(I, \mathbf{0}, \boldsymbol{c}_0, \frac{1}{2})$ and $M_{CsCl} = -\sqrt{3}Z(B, \mathbf{0}, \boldsymbol{c}_0, \frac{1}{2})$, the duality relations hold (under the notation (1.14)):

$$M_{NaCl} = -Z\left(I, \mathbf{0}, \boldsymbol{c}_0, \frac{1}{2}\right) = -\frac{2}{\pi}\left\{Z(B, \mathbf{0}, \mathbf{0}, 1) - Z(B, \mathbf{0}, \boldsymbol{c}_0, 1)\right\} \tag{1.17}$$

and

$$M_{CsCl} = -\sqrt{3}Z\left(B, \mathbf{0}, \boldsymbol{c}_0, \frac{1}{2}\right) = -\frac{\sqrt{3}}{2\pi}\left\{Z(I, \mathbf{0}, \mathbf{0}, 1) - Z(I, \mathbf{0}, \boldsymbol{c}_0, 1)\right\} \tag{1.18}$$

(cf. Formula on p.4 of [20]; proof given in Example 1.2 below).

In the case of M_{ZnS}, Hautot states another relation corresponding to (1.15), again without giving any reason why the Madelung constants M_{ZnS} and M_{CsCl} should be related:

$$\frac{4}{\sqrt{3}}M_{ZnS} = \frac{2}{\sqrt{3}}M_{CsCl} - 6\sum\sum\sum \frac{1}{\sqrt{(2l)^2 + (2m+1)^2 + (2n+1)^2}}, \tag{1.19}$$

where we note that the Madelung constant M_{ZnS} is to be defined by

$$M_{ZnS} = \frac{\sqrt{3}}{2}Z\left(A, \frac{1}{2}\boldsymbol{c}_0, \mathbf{0}, \frac{1}{2}\right) - \frac{\sqrt{3}}{2}Z\left(A, \mathbf{0}, \mathbf{0}, \frac{1}{2}\right), \tag{1.20}$$

where

$$A = \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}. \tag{1.21}$$

Comparing (1.18) and (1.20) and the numerical values (1.16) and (1.22) below does not give much to expect a relation between them;

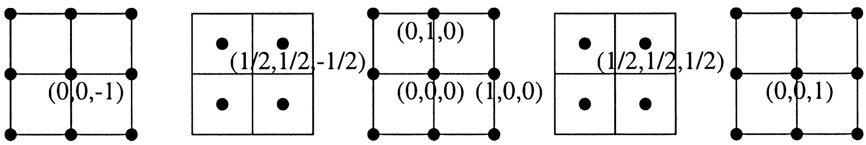
$$M_{ZnS} = 1.63805505338\ldots. \tag{1.22}$$

Surprisingly enough, there holds a remarkable relation

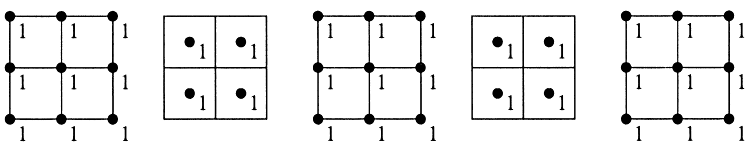
$$M_{ZnS} = \frac{\sqrt{3}}{4}M_{NaCl} + \frac{1}{2}M_{CsCl}. \tag{1.23}$$

The proof given below is based on the figures and it contains the proof of (2.31) simultaneously.

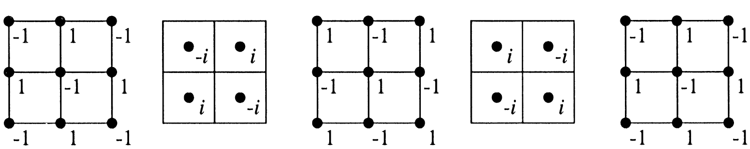
Let $z_k(s) = Z\left(\frac{1}{4}B, \mathbf{0}, \frac{k}{2}\boldsymbol{c}_0, s\right) = 2^{2s} Z\left(B, \mathbf{0}, \frac{k}{2}\boldsymbol{c}_0, s\right)$ $(k = 0, 1, 2, 3)$. We express the coordinates schematically in 2-dimensions.



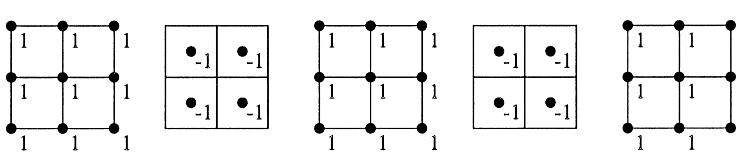
$$z_0(s) = Z\left(\frac{1}{4}B, \mathbf{0}, \mathbf{0}, s\right)$$



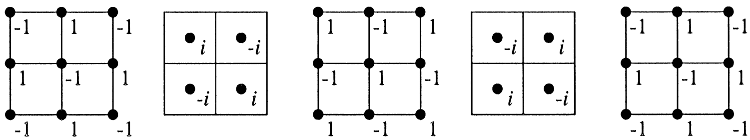
$$z_1(s) = Z\left(\frac{1}{4}B, \mathbf{0}, \frac{1}{2}\boldsymbol{c}_0, s\right)$$



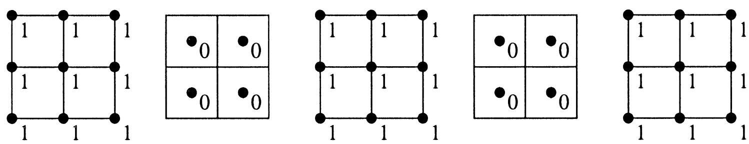
$$z_2(s) = Z\left(\frac{1}{4}B, \mathbf{0}, \mathbf{0}, s\right)$$



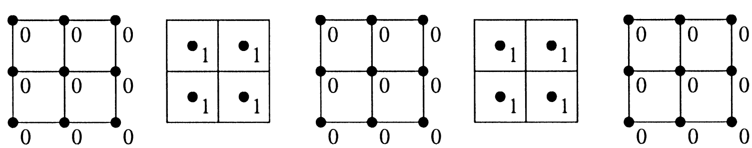
$$z_3(s) = Z\left(\frac{1}{4}B, \mathbf{0}, \boldsymbol{c}_0, s\right)$$



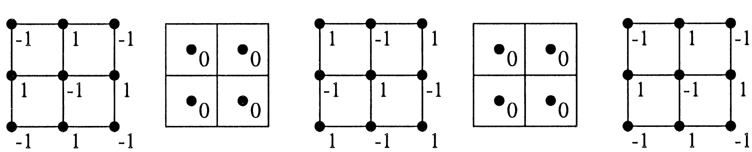
$$\frac{1}{2}(z_0(s) + z_2(s)) = Z(I, \mathbf{0}, \mathbf{0}, s)$$



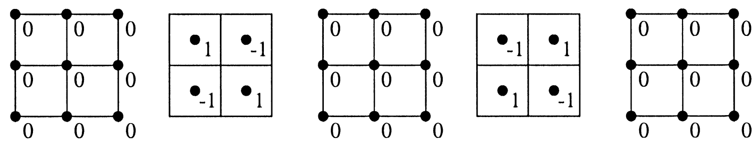
$$\frac{1}{2}(z_0(s) - z_2(s)) = Z(I, \boldsymbol{c}_0, \mathbf{0}, s)$$



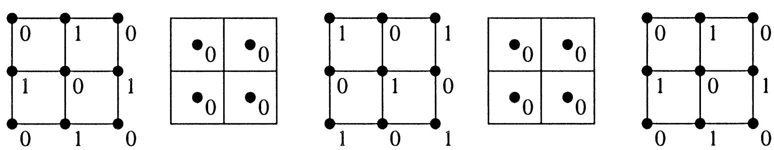
$$\frac{1}{2}(z_1(s) + z_3(s)) = Z(I, \mathbf{0}, \boldsymbol{c}_0, s)$$



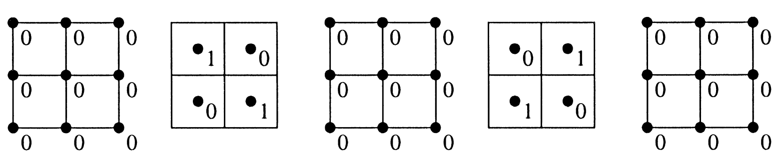
$$\frac{1}{2}(iz_1(s) - iz_3(s)) = Z(I, \boldsymbol{c}_0, \boldsymbol{c}_0, s) = 0$$



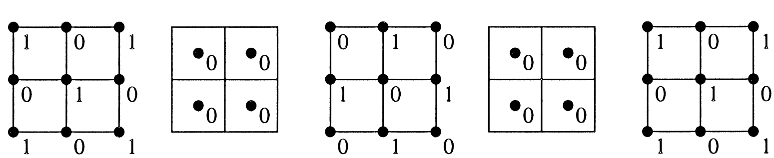
$$\frac{1}{4}(z_0(s) + z_1(s) + z_2(s) + z_3(s)) = Z(A, \mathbf{0}, \mathbf{0}, s)$$



$$\frac{1}{4}(z_0(s) + iz_1(s) - z_2(s) - iz_3(s)) = Z\left(A, \frac{1}{2}\boldsymbol{c}_0, \mathbf{0}, s\right)$$



$$\frac{1}{4}(z_0(s) - z_1(s) + z_2(s) - z_3(s)) = Z\left(A, \boldsymbol{c}_0, \mathbf{0}, s\right)$$



From the figures, it follows that

$$\begin{aligned}
M_{CaF_2} &= \frac{1}{2}\left\{\frac{\sqrt{3}}{2}Z\left(I, \boldsymbol{c}_0, \mathbf{0}, \frac{1}{2}\right) - \sqrt{3}Z\left(A, \mathbf{0}, \mathbf{0}, \frac{1}{2}\right)\right\} \\
&\quad + \frac{1}{2}\left\{\sqrt{3}Z(A, \frac{1}{2}\boldsymbol{c}_0, \mathbf{0}, \frac{1}{2}) - \frac{\sqrt{3}}{2}Z\left(I, \mathbf{0}, \mathbf{0}, \frac{1}{2}\right)\right\} \\
&= \frac{\sqrt{3}}{2}Z\left(A, \frac{1}{2}\boldsymbol{c}_0, \mathbf{0}, \frac{1}{2}\right) - \frac{\sqrt{3}}{2}Z\left(A, \mathbf{0}, \mathbf{0}, \frac{1}{2}\right) \\
&\quad + \frac{\sqrt{3}}{4}Z\left(I, \boldsymbol{c}_0, \mathbf{0}, \frac{1}{2}\right) - \frac{\sqrt{3}}{4}Z\left(I, \mathbf{0}, \mathbf{0}, \frac{1}{2}\right) \\
&= M_{ZnS} + \frac{1}{2}M_{CsCl} \\
&= \frac{\sqrt{3}}{4}M_{NaCl} + M_{CsCl},
\end{aligned}$$

namely (2.32).

In Example 1.2 we are going to reveal those identities given in Example 1.1 as special cases of zeta-function relations.

We introduce the general principle.

Principle. Suppose L is a lattice with basis $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$:

$$L = \mathbb{Z}\boldsymbol{e}_1 \oplus \mathbb{Z}\boldsymbol{e}_2 \oplus \mathbb{Z}\boldsymbol{e}_3. \tag{1.24}$$

With $M = (\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$, the associated Gram matrix Y is defined by ${}^tMM$:

$$Y = {}^tMM = \begin{pmatrix} \boldsymbol{e}_1\cdot\boldsymbol{e}_1 & \boldsymbol{e}_1\cdot\boldsymbol{e}_2 & \boldsymbol{e}_1\cdot\boldsymbol{e}_3 \\ \boldsymbol{e}_2\cdot\boldsymbol{e}_1 & \boldsymbol{e}_2\cdot\boldsymbol{e}_2 & \boldsymbol{e}_2\cdot\boldsymbol{e}_3 \\ \boldsymbol{e}_3\cdot\boldsymbol{e}_1 & \boldsymbol{e}_3\cdot\boldsymbol{e}_2 & \boldsymbol{e}_3\cdot\boldsymbol{e}_3 \end{pmatrix} \tag{1.25}$$

Let $\boldsymbol{f}_1 = \boldsymbol{e}_2 + \boldsymbol{e}_3$, $\boldsymbol{f}_2 = \boldsymbol{e}_3 + \boldsymbol{e}_1$, $\boldsymbol{f}_3 = \boldsymbol{e}_1 + \boldsymbol{e}_2$, and

$$J = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}. \tag{1.26}$$

Then the matrix ${}^tJ\rangle YJ = J\rangle YJ$ is the Gram matrix associated to the sublattice $L_1 = \mathbb{Z}\boldsymbol{f}_1 \oplus \mathbb{Z}\boldsymbol{f}_2 \oplus \mathbb{Z}\boldsymbol{f}_3$ of L, and we have

$$L = L_1 \cup \left(L_1 + \frac{1}{2}\boldsymbol{f}_1 + \frac{1}{2}\boldsymbol{f}_2 + \frac{1}{2}\boldsymbol{f}_3\right). \tag{1.27}$$

We appeal to the fact to be proved in section 2 that the zeta-function of a lattice coincides with the Epstein zeta-function of the corresponding Gram matrix under suitable identification. It follows that

$$\Lambda(Y,\mathbf{0},\boldsymbol{c}_0,s)=\Lambda({}^tJ\rangle YJ,\mathbf{0},\mathbf{0},s)-\Lambda({}^tJ\rangle YJ,\boldsymbol{c}_0,\mathbf{0},s), \tag{1.28}$$

and

$$\Lambda(Y,\mathbf{0},\mathbf{0},s)=\Lambda({}^tJ\rangle YJ,\mathbf{0},\mathbf{0},s)+\Lambda({}^tJ\rangle YJ,\boldsymbol{c}_0,\mathbf{0},s). \tag{1.29}$$

Now note that the inverse matrix $({}^tJ\rangle YJ)^{-1}$ is the Gram matrix associated to the dual lattice $L_1'(\cong \mathrm{Hom}(L_1,\mathbb{Z}))$ or recall the functional equation (1.10) to transform the right-hand side of (1.28) further into

$$\frac{1}{\sqrt{|{}^tJ\rangle YJ|}}\left\{\Lambda\left(({}^tJ\rangle YJ)^{-1},\mathbf{0},\mathbf{0},\frac{3}{2}-s\right)-\Lambda\left(({}^tJ\rangle YJ)^{-1},\mathbf{0},-\boldsymbol{c}_0,\frac{3}{2}-s\right)\right\},$$

so that

$$\begin{aligned}\Lambda(Y,\mathbf{0},\boldsymbol{c}_0,s)=\frac{1}{\sqrt{|{}^tJ\rangle YJ|}}&\left\{\Lambda\left(({}^tJ\rangle YJ)^{-1},\mathbf{0},\mathbf{0},\frac{3}{2}-s\right)\right.\\&\left.-\Lambda\left(({}^tJ\rangle YJ)^{-1},\mathbf{0},-\boldsymbol{c}_0,\frac{3}{2}-s\right)\right\}.\end{aligned} \tag{1.30}$$

Now we apply the above principal to some lattice sums.

Example 1.2. First choose ${}^tJ\rangle YJ=A=\begin{pmatrix}2&1&1\\1&2&1\\1&1&2\end{pmatrix}$ ((1.21)). Then $Y=I$ and (1.28) reads

$$Z(I,\mathbf{0},\boldsymbol{c}_0,s)=Z(A,\mathbf{0},\mathbf{0},s)-Z(A,\boldsymbol{c}_0,\mathbf{0},s). \tag{1.31}$$

This explains the reason why the proper definition (given in section 2) of the Madelung constant M_{NaCl} as the value at $s=\frac{1}{2}$ of

$$Z(A,\boldsymbol{c}_0,\mathbf{0},s)-Z(A,\mathbf{0},\mathbf{0},s)$$

coincides with the value at $s=\frac{1}{2}$ of $-Z(I,\mathbf{0},\boldsymbol{c}_0,s)$ i.e.

$$\begin{aligned}M_{NaCl}&=Z\left(A,\boldsymbol{c}_0,\mathbf{0},\frac{1}{2}\right)-Z\left(A,\mathbf{0},\mathbf{0},\frac{1}{2}\right)\\&=-Z\left(I,\mathbf{0},\boldsymbol{c}_0,\frac{1}{2}\right).\end{aligned} \tag{1.32}$$

Next, we choose $Y=\frac{1}{4}B$ ((1.14)). Then ${}^tJ\rangle YJ=I$, and

$$Z\left(\frac{1}{4}B,\mathbf{0},\boldsymbol{c}_0,s\right)=Z(I,\mathbf{0},\mathbf{0},s)-Z(I,\boldsymbol{c}_0,\mathbf{0},s). \tag{1.33}$$

We make an important remark, which will be in effect as the Abel mean in section 3, that for $c > 0$

$$Z(cY, \boldsymbol{g}, \boldsymbol{h}, s) = c^{-s} Z(Y, \boldsymbol{g}, \boldsymbol{h}, s), \tag{1.34}$$

i.e. we may incorporate the parameter c in Y by just multiplying by the factor c^{-s}.

Using (1.34) and (1.33), we have for $s = \frac{1}{2}$

$$\frac{\sqrt{3}}{2}\left\{Z\left(I, \boldsymbol{c}_0, \boldsymbol{0}, \frac{1}{2}\right) - Z\left(I, \boldsymbol{0}, \boldsymbol{0}, \frac{1}{2}\right)\right\} = -\sqrt{3} Z\left(B, \boldsymbol{0}, \boldsymbol{c}_0, \frac{1}{2}\right), \tag{1.35}$$

which asserts that (1.12) and (1.13) are equal.

We turn to the proof of duality relations (1.17) and (1.18).

As we deduced (1.31), we choose ${}^tJ\rangle YJ = A$, and so $Y = I$. Then (1.30) gives

$$-\Lambda(I, \boldsymbol{0}, \boldsymbol{c}_0, s) = \frac{1}{\sqrt{|A|}}\left\{\Lambda\left(A^{-1}, \boldsymbol{0}, -\boldsymbol{c}_0, \frac{3}{2} - s\right) - \Lambda\left(A^{-1}, \boldsymbol{0}, \boldsymbol{0}, \frac{3}{2} - s\right)\right\}.$$

Since $A^{-1} = \frac{1}{4}B$, we apply (1.34) to obtain

$$-\Lambda(I, \boldsymbol{0}, \boldsymbol{c}_0, s) = \frac{1}{2} 4^{\frac{3}{2}-s}\left\{\Lambda\left(B, \boldsymbol{0}, -\boldsymbol{c}_0, \frac{3}{2} - s\right) - \Lambda\left(B, \boldsymbol{0}, \boldsymbol{0}, \frac{3}{2} - s\right)\right\},$$

or

$$\begin{aligned} -\pi^{-s}\Gamma(s) Z(I, \boldsymbol{0}, \boldsymbol{c}_0, s) &= 2^{2-2s}\pi^{-(\frac{3}{2}-s)}\Gamma\left(\frac{3}{2} - s\right) \\ &\times \left\{Z\left(B, \boldsymbol{0}, -\boldsymbol{c}_0, \frac{3}{2} - s\right) - Z\left(B, \boldsymbol{0}, \boldsymbol{0}, \frac{3}{2} - s\right)\right\}, \end{aligned} \tag{1.36}$$

which in turn gives (1.17) for $s = \frac{1}{2}$.

Also, for the choice $Y = \frac{1}{4}B$, ${}^tJ\rangle YJ = I$, (1.30) reads, as in (1.35),

$$\Lambda(B, \boldsymbol{0}, \boldsymbol{c}_0, s) = 4^{-s}\left\{\Lambda\left(I, \boldsymbol{0}, \boldsymbol{0}, \frac{3}{2} - s\right) - \Lambda\left(I, \boldsymbol{0}, -\boldsymbol{c}_0, \frac{3}{2} - s\right)\right\},$$

or

$$\begin{aligned} \pi^{-s}\Gamma(s) Z(B, \boldsymbol{0}, \boldsymbol{c}_0, s) &= 4^{-s}\pi^{-(\frac{3}{2}-s)}\Gamma\left(\frac{3}{2} - s\right) \\ &\times \left\{Z\left(I, \boldsymbol{0}, \boldsymbol{0}, \frac{3}{2} - s\right) - Z\left(I, \boldsymbol{0}, -\boldsymbol{c}_0, \frac{3}{2} - s\right)\right\}, \end{aligned} \tag{1.37}$$

which gives (1.18) for $s = \frac{1}{2}$.

2. Lattice zeta-functions and Epstein zeta-functions

In this section we shall clarify the relationship between the zeta-functions mentioned in the title and apply them to Madelung constants.

First of all we shall give a precise meaning of Madelung constants.

2.1 A precise meaning of Madelung constants

Recall Coulomb's law which asserts that the electric force on a charge q at $\boldsymbol{r}$ by another charge q_i at $\boldsymbol{r}_i$ which are at rest is

$$\boldsymbol{F}(\boldsymbol{r}_i) = \frac{1}{4\pi\varepsilon_0}\frac{qq_i(\boldsymbol{r}-\boldsymbol{r}_i)}{|\boldsymbol{r}-\boldsymbol{r}_i|^3}, \tag{2.1}$$

where $\frac{1}{4\pi\varepsilon_0} = c^2 \times 10^{-7}$, with c signifying the speed of light.

Then consider the situation where there are (infinitely, we shall so regard) many charges q_i at position $\boldsymbol{r}_i$. Then the total electrostatic force, $\boldsymbol{F}(\boldsymbol{r})$ exerted on one of them, say q at $\boldsymbol{r}$, is, by the principle of superposition, the sum of the electric force $\boldsymbol{F}(\boldsymbol{r}_i)$ of the form of (2.1) other than $\boldsymbol{r}$. Denoting by $U(\boldsymbol{r})$ the electrostatic energy of q at $\boldsymbol{r}$, we deduce from $\boldsymbol{F}(\boldsymbol{r}) = -\nabla U(\boldsymbol{r})$ that

$$U(\boldsymbol{r}) = \frac{1}{4\pi\varepsilon_0}\sum_i \frac{qq_i}{|\boldsymbol{r}-\boldsymbol{r}_i|} \tag{2.2}$$

(Note that $\lim_{\boldsymbol{r}\to 0} U(\boldsymbol{r}) = 0$).

We adopt the empirical formula for the crystal structure X:

$$X = C_{n_+}A_{n_-},$$

where C is a cation of electric charge $+N_+\mathrm{e}$ and A is an anion of electric charge $-N_-\mathrm{e}$ and where e means the elementary electric charge. We understand conventionally $n_+N_+ = n_-N_-$.

We adopt the coordinate system such that the shortest distance between the ions is equal to 1, i.e. we factor out r in (2.2). We denote by S_{++} the coordinates of cations and by S_{+-} those of anions, both with respect to a coordinate system with a cation at the origin. Similarly, we denote by S_{-+} and S_{--} the coordinates of cations and anions, respectively, with respect to a coordinate system with an anion at the origin.

For $S = S_{++}, S_{+-}, S_{-+}, S_{--}$, we introduce the zeta-function (more general case given in 2.2)

$$Z_S(s) = \sum_{\substack{\boldsymbol{x}\in S\\ \boldsymbol{x}\neq \boldsymbol{0}}} \frac{1}{(x_1^2+x_2^2+x_3^2)^s} \tag{2.3}$$

for σ large enough. Then the electrostatic energy U_+ of a cation is formally

$$U_+ = \frac{1}{4\pi\varepsilon_0 r}\left(N_+^2 \mathrm{e}^2 Z_{S_{++}}\left(\frac{1}{2}\right) - N_+N_-\mathrm{e}^2 Z_{S_{+-}}\left(\frac{1}{2}\right)\right), \tag{2.4}$$

but the series for $Z_{S_{++}}\left(\frac{1}{2}\right)$, $Z_{S_{+-}}\left(\frac{1}{2}\right)$ are divergent. Similarly, for the electrostatic energy of U_- of an anion is

$$U_- = \frac{1}{4\pi\varepsilon_0 r}\left(N_-^2 \mathrm{e}^2 Z_{S_{--}}\left(\frac{1}{2}\right) - N_+N_-\mathrm{e}^2 Z_{S_{-+}}\left(\frac{1}{2}\right)\right), \tag{2.5}$$

again the series are divergent.

Thus we are led to assign the definite value $Z_S\left(\frac{1}{2}\right)$ of (the analytic continuation of) the zeta-function of $Z_S(s)$.

The electrostatic energy of the crystal X being formally given by

$$\begin{aligned} U_X &= \frac{1}{2}\left(n_+U_+ + n_-U_-\right) \\ &= \frac{1}{4\pi\varepsilon_0}\frac{N_+N_-\mathrm{e}^2}{r}\left(\frac{n_-}{2}Z_{S_{++}}\left(\frac{1}{2}\right) - \frac{n_+}{2}Z_{S_{+-}}\left(\frac{1}{2}\right)\right. \\ &\qquad \left. - \frac{n_-}{2}Z_{S_{-+}}\left(\frac{1}{2}\right) + \frac{n_+}{2}Z_{S_{--}}\left(\frac{1}{2}\right)\right), \end{aligned} \tag{2.6}$$

after slight modification.

As stated above, we adopt the zeta-regularization here to assign definite values to divergent series. We define the zeta-function $Z_X(s)$ of the crystal structure X by

$$Z_X(s) = \frac{n_+}{2}Z_{S_{+-}}(s) - \frac{n_-}{2}Z_{S_{++}}(s) - \frac{n_-}{2}Z_{S_{-+}}(s) + \frac{n_+}{2}Z_{S_{--}}(s) \tag{2.7}$$

and the Madelung constant M_X of X by

$$M_X = Z_X\left(\frac{1}{2}\right), \tag{2.8}$$

whereby

$$U_X = -\frac{1}{4\pi\varepsilon_0}\frac{N_+N_-\mathrm{e}^2}{r}M_X \tag{2.9}$$

by (2.6).

2.2 Lattice zeta-function

Let L be a lattice, i.e. a free Abelian group of finite rank (n, say) with a positive definite biadditive form $(\ ,\ )_L$. We form the zeta-function $Z_L(s) = Z(L,0,0,s)$ corresponding to (1.7) by

$$Z_L(s) = Z(L,0,0,s) = \sum_{\substack{x\in L\\ x\neq 0}} \frac{1}{(x,x)_L^s}, \tag{2.10}$$

absolutely convergent for $\sigma > \frac{n}{2}$.

If, in particular, $L \subset \mathbb{R}^m$ and $(\mathbf{a},\boldsymbol{b})_L$ means the scalar product $\mathbf{a}\cdot\boldsymbol{b} = {}^t\mathbf{a}\boldsymbol{b} = \sum_{i=1}^m a_i b_i$, then

$$Z(L,0,0,s) = \sum_{\substack{x\in L\\ x\neq 0}} \frac{1}{(x_1^2+\cdots+x_m^2)^s} \tag{2.11}$$

of which (2.3) is a special case.

As usual, let L' denote the dual lattice of L: $L' = \mathrm{Hom}(L,\mathbb{Z})$. Then for lattice elements p, q with real coefficients, $p \in L\otimes\mathbb{R}$, $q \in L'\otimes\mathbb{R}$, we introduce the general lattice zeta-function $Z(L,p,q,s)$ corresponding to (1.8) by

$$Z(L,p,q,s) = \sum_{\substack{x\in L\\ x+p\neq 0}} \frac{e^{2\pi i q(x)}}{(x+p,x+p)_{L\otimes\mathbb{R}}^s}, \tag{2.12}$$

absolutely convergent for $\sigma > \frac{n}{2}$. Here we understand the meaning of $q(x)$ through

$$L'\otimes\mathbb{R} \cong \mathrm{Hom}(L,\mathbb{R}) \cong \mathrm{Hom}_{\mathbb{R}}(L\otimes\mathbb{R},\mathbb{R})$$

and the completion corresponding to (1.9):

$$\Lambda(L,p,q,s) = \pi^{-s}\Gamma(s)Z(L,p,q,s). \tag{2.13}$$

We recall the Principle in section 1 in the following form.

Associated to a lattice L with basis $\boldsymbol{e}_1,\ldots,\boldsymbol{e}_n$, $L = \mathbb{Z}\boldsymbol{e}_1\oplus\cdots\oplus\mathbb{Z}\boldsymbol{e}_n$, is its Gram matrix

$$Y = {}^tMM = \begin{pmatrix} (\boldsymbol{e}_1\cdot\boldsymbol{e}_1)_L & \cdots & (\boldsymbol{e}_1\cdot\boldsymbol{e}_n)_L \\ \vdots & \ddots & \vdots \\ (\boldsymbol{e}_n\cdot\boldsymbol{e}_1)_L & \cdots & (\boldsymbol{e}_n\cdot\boldsymbol{e}_n)_L \end{pmatrix}, \tag{2.14}$$

where $M = (\boldsymbol{e}_1,\ldots,\boldsymbol{e}_n)$.

Let ϕ be the canonical isomorphism

$$\phi : \mathbb{Z}^n \longrightarrow L, \quad x = \phi(\mathbf{a}) = a_1\boldsymbol{e}_1 + \cdots + a_n\boldsymbol{e}_n, \tag{2.15}$$

for $\mathbf{a} = (a_1, \ldots, a_n)$, or $\phi(\mathbf{a}) = M\mathbf{a}$. Through ϕ, we may interpret the bilinear form $(x, x)_L$ as $(\phi(\mathbf{a}), \phi(\mathbf{a}))_L$, which we may think of as $Y[\mathbf{a}]$. Thus,

$$Z_L(s) = Z(L, 0, 0, s) = Z(Y, \mathbf{0}, \mathbf{0}, s). \tag{2.16}$$

We may extend ϕ to the isomorphism

$$\phi : \mathbb{R}^n \longrightarrow L \otimes \mathbb{R}, \quad x = \phi(\mathbf{a}) = a_1\boldsymbol{e}_1 + \cdots + a_n\boldsymbol{e}_n,$$

for $\mathbf{a} = (a_1, \ldots, a_n) \in \mathbb{R}^n$. Then we have

$$(\phi(\mathbf{a}), \phi(\mathbf{a}))_{L\otimes\mathbb{R}} = Y[\mathbf{a}].$$

If further we put $p = \phi(\boldsymbol{g})$ and $q(x) = q \circ \phi(\mathbf{a}) = \boldsymbol{h} \cdot \mathbf{a}$ $(\mathbf{a} \in \mathbb{R}^n)$, then

$$\begin{aligned} Z(L, p, q, s) &= \sum_{\substack{\mathbf{a}\in\mathbb{Z}^n \\ \mathbf{a}+\boldsymbol{g}\neq\mathbf{0}}} \frac{e^{2\pi i q\circ\phi(\mathbf{a})}}{(\phi(\mathbf{a}+\boldsymbol{g}), \phi(\mathbf{a}+\boldsymbol{g}))_{L\otimes\mathbb{R}}^s} \\ &= \sum_{\substack{\mathbf{a}\in\mathbb{Z}^n \\ \mathbf{a}+\boldsymbol{g}\neq\mathbf{0}}} \frac{e^{2\pi i \boldsymbol{h}\cdot\mathbf{a}}}{Y[\mathbf{a}+\boldsymbol{g}]^s} = Z(Y, \boldsymbol{g}, \boldsymbol{h}, s). \end{aligned} \tag{2.17}$$

Thus,

Proposition. *Under above notation, we have*

$$\Lambda(L, p, q, s) = \Lambda(Y, \boldsymbol{g}, \boldsymbol{h}, s).$$

Hence, whenever we speak about a lattice zeta-function, we may do well with the corresponding Epstein zeta-function with the Gram matrix.

Example 2.1. (i) The simple cubic structure (s.c.), $\mathbb{Z}^3 = \mathbb{Z}\begin{pmatrix}1\\0\\0\end{pmatrix} \oplus \mathbb{Z}\begin{pmatrix}0\\1\\0\end{pmatrix} \oplus \mathbb{Z}\begin{pmatrix}0\\0\\1\end{pmatrix}$ with Gram matrix $I = \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$. The zeta-function is

$$Z(\mathbb{Z}^3, 0, 0, s) = Z(I, \mathbf{0}, \mathbf{0}, s) = \sum_{\substack{\mathbf{a}\in\mathbb{Z}^3 \\ \mathbf{a}\neq\mathbf{0}}} \frac{1}{|\mathbf{a}|^{2s}}. \tag{2.18}$$

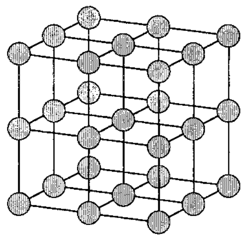


Figure 1. the simple cubic structure (s.c.)

(ii) The face-centered cubic structure (f.c.c.),

$$\begin{aligned} L_f &= \left\{ \mathbf{a} \in \mathbb{Z}^3 \,\middle|\, (-1)^{a_1+a_2+a_3} = 1 \right\} \\ &= \mathbb{Z}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \oplus \mathbb{Z}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \oplus \mathbb{Z}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \end{aligned}$$

with Gram matrix $A = \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$ ((1.21)).

The zeta-function is

$$\begin{aligned} Z_{L_f}(s) &= Z(A, \mathbf{0}, \mathbf{0}, s) \\ &= \sum_{\substack{\mathbf{a} \in \mathbb{Z}^3 \\ \mathbf{a} \neq \mathbf{0}}} \frac{1}{(2a_1^2 + 2a_2^2 + 2a_3^2 + 2a_1a_2 + 2a_2a_3 + 2a_3a_1)^s}. \end{aligned}$$

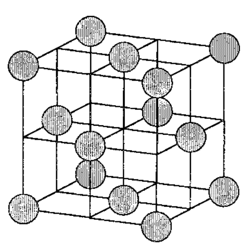


Figure 2. the face-centered cubic structure (f.c.c.)

With $\boldsymbol{c}_0 = {}^t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, $Z(I, \mathbf{0}, \boldsymbol{c}_0, s) = \sum_{\substack{\mathbf{a} \in \mathbb{Z}^3 \\ \mathbf{a} \neq \mathbf{0}}} \frac{(-1)^{a_1+a_2+a_3}}{I[\mathbf{a}]^s}$ can be written as

$$Z(I, \mathbf{0}, \boldsymbol{c}_0, s) = 2Z(A, \mathbf{0}, \mathbf{0}, s) - Z(I, \mathbf{0}, \mathbf{0}, s).$$

Solving in $Z(A,\mathbf{0},\mathbf{0},s)$, we have

$$Z(A,\mathbf{0},\mathbf{0},s) = \frac{1}{2}\left(Z(I,\mathbf{0},\mathbf{0},s) + Z(I,\mathbf{0},\mathbf{c}_0,s)\right). \tag{2.19}$$

(iii) The body-centered cubic structure (b.c.c.),

$$\begin{aligned} L_b &= \left\{\mathbf{a}\in\mathbb{Z}^3 | a_2+a_3, a_3+a_1, a_1+a_2 \in 2\mathbb{Z}\right\} \\ &= \left\{\mathbf{a}\in\mathbb{Z}^3 | (-1)^{a_2+a_3} + (-1)^{a_3+a_1} + (-1)^{a_1+a_2} = 3\right\} \end{aligned}$$

with Gram matrix $B = \begin{pmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{pmatrix}$ ((1.14)). The zeta-function is

$$\begin{aligned} Z_{L_b}(s) &= Z(B,\mathbf{0},\mathbf{0},s) \\ &= \sum_{\substack{\mathbf{a}\in\mathbb{Z}^3 \\ \mathbf{a}\neq\mathbf{0}}} \frac{1}{(3a_1^2+3a_2^2+3a_3^2-2a_1a_2-2a_2a_3-2a_3a_1)^s}. \end{aligned}$$

Since

$$\begin{aligned} 3Z(I,\mathbf{0},\begin{pmatrix}\frac12\\\frac12\\0\end{pmatrix},s) &= Z(I,\mathbf{0},\begin{pmatrix}0\\\frac12\\\frac12\end{pmatrix},s) + Z(I,\mathbf{0},\begin{pmatrix}\frac12\\0\\\frac12\end{pmatrix},s) + Z(I,\mathbf{0},\begin{pmatrix}\frac12\\\frac12\\0\end{pmatrix},s) \\ &= \sum_{\substack{\mathbf{a}\in\mathbb{Z}^3 \\ \mathbf{a}\neq\mathbf{0}}} \frac{(-1)^{a_2+a_3} + (-1)^{a_3+a_1} + (-1)^{a_1+a_2}}{I[\mathbf{a}]^s}, \end{aligned}$$

we get, on resorting to the definition of L_b,

$$\begin{aligned} 3Z(I,\mathbf{0},\begin{pmatrix}\frac12\\\frac12\\0\end{pmatrix},s) &= \sum_{\substack{\mathbf{a}\in L_b \\ \mathbf{a}\neq\mathbf{0}}} \frac{3}{I[\mathbf{a}]^s} + \sum_{\mathbf{a}\in\mathbb{Z}^3-L_b} \frac{-1}{I[\mathbf{a}]^s} \\ &= 4Z(B,\mathbf{0},\mathbf{0},s) - Z(I,\mathbf{0},\mathbf{0},s), \end{aligned}$$

whence

$$Z(B,\mathbf{0},\mathbf{0},s) = \frac{1}{4}\left\{Z(I,\mathbf{0},\mathbf{0},s) + 3Z(I,\mathbf{0},\begin{pmatrix}\frac12\\\frac12\\0\end{pmatrix},s)\right\}. \tag{2.20}$$

Using 'square root' of A and B, i.e. J from (1.26) and

$$K = \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix} \tag{2.21}$$

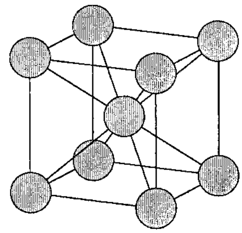


Figure 3. the body-centered cubic structure (b.c.c.)

($J^2 = A, K^2 = B, J^{-1} = \frac{1}{2}K$), we obtain generalizations of formulas (2.19) and (2.20):

$$Z(JYJ, \boldsymbol{g}, \boldsymbol{h}, s) = \frac{1}{2}\left\{ Z(Y, J\boldsymbol{g}, J^{-1}\boldsymbol{h}, s) + Z(Y, J\boldsymbol{g}, J^{-1}\boldsymbol{h} + \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}, s) \right\} \tag{2.22}$$

$$\begin{aligned} Z(KYK, \boldsymbol{g}, \boldsymbol{h}, s) &= \frac{1}{4}\left\{ Z(Y, K\boldsymbol{g}, K^{-1}\boldsymbol{h}, s) + Z(Y, K\boldsymbol{g}, K^{-1}\boldsymbol{h} + \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}, s) \right. \\ &\left. + Z(Y, K\boldsymbol{g}, K^{-1}\boldsymbol{h} + \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix}, s) + Z(Y, K\boldsymbol{g}, K^{-1}\boldsymbol{h} + \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}, s) \right\}. \end{aligned} \tag{2.23}$$

Example 2.2. (i) The $NaCl$ (Sodium Chloride) structure. Here the data is

$$\begin{aligned} &n_+ = n_- = 1, \\ &S_{++} = S_{--} = \{\mathbf{a} \in \mathbb{Z}^3 | a_1 + a_2 + a_3 \in 2\mathbb{Z}\} \qquad \text{(f.c.c.)}, \\ &S_{+-} = S_{+-} = \{\mathbf{a} \in \mathbb{Z}^3 | a_1 + a_2 + a_3 \in 2\mathbb{Z} + 1\} \qquad \text{(f.c.c.)}, \end{aligned}$$

so that by (2.7) and then by (1.32)

$$\begin{aligned} Z_{NaCl}(s) &= Z(A, \boldsymbol{c}_0, \mathbf{0}, s) - Z(A, \mathbf{0}, \mathbf{0}, s) \\ &= -Z(I, \mathbf{0}, \boldsymbol{c}_0, s). \end{aligned} \tag{2.24}$$

Formula (2.24) justifies the first equality in (1.17).

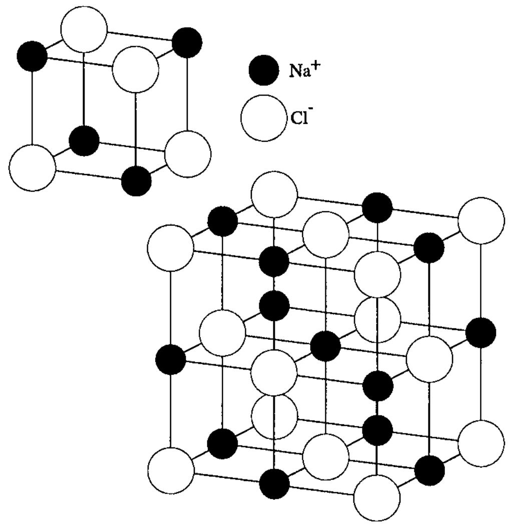


Figure 4. the $NaCl$ (Sodium Chloride) structure (s.c.)

Thus, by (2.8), the Madelung constant M_{NaCl} is given by

$$\begin{aligned} M_{NaCl} &= -Z\left(I, \mathbf{0}, \boldsymbol{c}_0, \frac{1}{2}\right) \\ &= -\sum_{\mathbf{a}\in\mathbb{Z}^3} \frac{(-1)^{a_1+a_2+a_3}}{|\mathbf{a}|} = 1.7475645849\ldots \end{aligned} \tag{2.25}$$

as stated in (1.16) and (1.17).

(ii) The $CsCl$ (Caesium Chloride) structure. Here the data is

$$\begin{aligned} n_+ &= n_- = 1, \\ S_{++} &= S_{--} = \left(\frac{2}{\sqrt{3}}\mathbb{Z}\right)^3 \text{ (s.c.)}, \\ S_{+-} &= S_{+-} = \left(\frac{2}{\sqrt{3}}\left(\mathbb{Z}+\frac{1}{2}\right)\right)^3 \text{ (s.c.)}, \end{aligned}$$

and the zeta-function is, as discussed in Example 1.2, (1.33)–(1.35),

$$\begin{aligned} Z_{CsCl}(s) &= Z\left(\frac{4}{3}I, \boldsymbol{c}_0, \mathbf{0}, s\right) - Z\left(\frac{4}{3}I, \mathbf{0}, \mathbf{0}, s\right) \\ &= \left(\frac{3}{4}\right)^s Z(I, \boldsymbol{c}_0, \mathbf{0}, s) - \left(\frac{3}{4}\right)^s Z(I, \mathbf{0}, \mathbf{0}, s) \\ &= -3^s Z(B, \mathbf{0}, \boldsymbol{c}_0, s). \end{aligned} \tag{2.26}$$

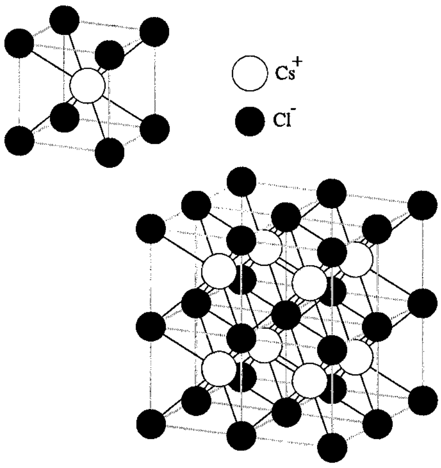


Figure 5. the $CsCl$ (Caesium Chloride) structure (b.c.c.)

Hence

$$M_{CsCl} = \frac{\sqrt{3}}{2} Z\left(I, \boldsymbol{c}_0, \mathbf{0}, \frac{1}{2}\right) - \frac{\sqrt{3}}{2} Z\left(I, \mathbf{0}, \mathbf{0}, \frac{1}{2}\right)$$
$$= -\sqrt{3} Z\left(B, \mathbf{0}, \boldsymbol{c}_0, \frac{1}{2}\right) \tag{2.27}$$

as in (1.35), whence (1.18) ensues.

(iii) The ZnS (Zincblende) structure. The data is

$$n_+ = n_- = 1,$$
$$S_{++} = S_{--} = \left\{ \frac{2}{\sqrt{3}}\mathbf{a} \;\middle|\; \mathbf{a} \in \mathbb{Z}^3, a_1 + a_2 + a_3 \in 2\mathbb{Z} \right\} \qquad \text{(f.c.c.)},$$
$$S_{+-} = S_{+-} = \left\{ \frac{2}{\sqrt{3}}\mathbf{a} \;\middle|\; \mathbf{a} \in \left(\mathbb{Z} + \frac{1}{2}\right)^3, a_1 + a_2 + a_3 \in 2\mathbb{Z} + \frac{1}{2} \right\} \quad \text{(f.c.c.)},$$

and the zeta-function is

$$Z_{ZnS}(s) = Z\left(\frac{4}{3}A, \frac{1}{2}\boldsymbol{c}_0, \mathbf{0}, s\right) - Z\left(\frac{4}{3}A, \mathbf{0}, \mathbf{0}, s\right)$$
$$= \left(\frac{3}{4}\right)^s Z\left(A, \frac{1}{2}\boldsymbol{c}_0, \mathbf{0}, s\right) - \left(\frac{3}{4}\right)^s Z\left(A, \mathbf{0}, \mathbf{0}, s\right), \tag{2.28}$$

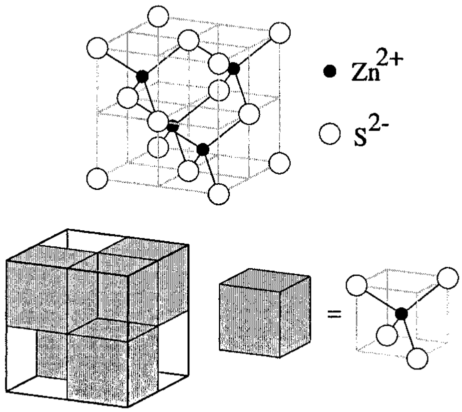


Figure 6. the ZnS (Zincblende) structure (diamond)

i.e. (1.20). Further in a similarly way as we prove (2.31), we may prove

$$Z_{ZnS}(s) = \frac{1}{2}\left(\frac{3}{4}\right)^s Z_{NaCl}(s) + \frac{1}{2}Z_{CsCl}(s), \tag{2.29}$$

whence as in (1.22) and (1.23)

$$\begin{aligned} M_{ZnS} &= \frac{\sqrt{3}}{4}M_{NaCl} + \frac{1}{2}M_{CsCl} \\ &= 1.63805805338\ldots. \end{aligned} \tag{2.30}$$

(iv) The CaF_2 (Fluorite) structure. The data:

$n_+ = 1, n_- = 2,$

$$S_{++} = \left\{ \frac{2}{\sqrt{3}}\mathbf{a} \,\middle|\, \mathbf{a} \in \mathbb{Z}^3,\ a_1 + a_2 + a_3 \in 2\mathbb{Z} \right\} \qquad \text{(f.c.c.)},$$

$$S_{+-} = \left(\frac{2}{\sqrt{3}}\left(\mathbb{Z} + \frac{1}{2}\right)\right)^3 \qquad \text{(s.c.)},$$

$$S_{--} = \left(\frac{2}{\sqrt{3}}\mathbb{Z}\right)^3 \qquad \text{(s.c.)},$$

$$S_{-+} = \left\{ \frac{2}{\sqrt{3}}\mathbf{a} \,\middle|\, \mathbf{a} \in \left(\mathbb{Z} + \frac{1}{2}\right)^3,\ a_1 + a_2 + a_3 \in 2\mathbb{Z} + \frac{1}{2} \right\} \qquad \text{(f.c.c.)}.$$

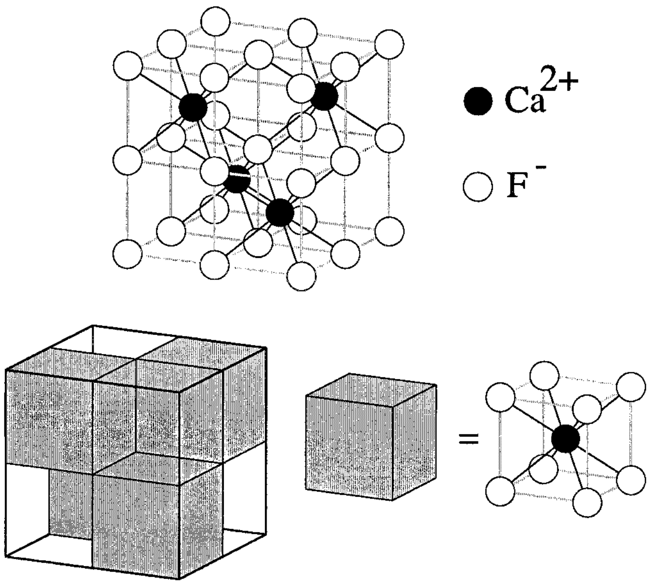


Figure 7. the CaF_2 (Fluorite) structure

The zeta-function is

$$\begin{aligned} Z_{CaF_2}(s) &= \frac{1}{2}\left\{Z\left(\frac{4}{3}I, \boldsymbol{c}_0, \mathbf{0}, s\right) - 2Z\left(\frac{4}{3}A, \mathbf{0}, \mathbf{0}, s\right)\right\} \\ &\quad + \frac{1}{2}\left\{2Z\left(\frac{4}{3}A, \frac{1}{2}\boldsymbol{c}_0, \mathbf{0}, s\right) - Z\left(\frac{4}{3}I, \mathbf{0}, \mathbf{0}, s\right)\right\} \\ &= \frac{1}{2}\left(\frac{3}{4}\right)^s Z(I, \boldsymbol{c}_0, \mathbf{0}, s) - \frac{1}{2}\left(\frac{3}{4}\right)^s Z(I, \mathbf{0}, \mathbf{0}, s) \\ &\quad + \left(\frac{3}{4}\right)^s Z\left(A, \frac{1}{2}\boldsymbol{c}_0, \mathbf{0}, s\right) - \left(\frac{3}{4}\right)^s Z(A, \mathbf{0}, \mathbf{0}, s). \end{aligned}$$

In a similar way as we prove (2.30), we may prove

$$Z_{CaF_2}(s) = \frac{1}{2}\left(\frac{3}{4}\right)^s Z_{NaCl}(s) + Z_{CsCl}(s), \tag{2.31}$$

whence

$$\begin{aligned} M_{CaF_2} &= \frac{\sqrt{3}}{4} M_{NaCl} + M_{CsCl} \\ &= 2.51939243992\ldots. \end{aligned} \tag{2.32}$$

2.3 Bessel series expansions for Epstein zeta-functions

In this subsection we shall prove a Bessel series expansion of Chowla-Selberg type (Theorem 2) for the Epstein zeta-function $\Lambda(Y, \boldsymbol{g}, \boldsymbol{h}, s)$ corresponding to a block decomposition of the matrix Y. The proof depends on another Bessel series expansion (Theorem 1) for the generalized Epstein zeta-function $\sum_{\mathbf{a}\in\mathbb{Z}^n} \frac{e^{2\pi i \boldsymbol{h}\cdot\mathbf{a}}}{(Y[\mathbf{a}+\boldsymbol{g}]+b)^s}$ for $b > 0$, which is interesting in its own right and which we call the Mellin-Barnes type, being dependent on the Mellin-Barnes integrals.

As a corollary to Theorem 1, we shall prove the Benson-Mackenzie formula (Corollary 1) and as one to Theorem 2, the Hautot formula (Corollary 2).

Theorem 1 (Mellin-Barnes type formula). Notation being as above, we have for $b > 0$,

$$\begin{aligned} &\pi^{-s}\Gamma(s) \sum_{\mathbf{a}\in\mathbb{Z}^n} \frac{e^{2\pi i \boldsymbol{h}\cdot\mathbf{a}}}{(Y[\mathbf{a}+\boldsymbol{g}]+b)^s} \\ &= \frac{2}{\sqrt{|Y|}} \sum_{\substack{\mathbf{a}\in\mathbb{Z}^n \\ \mathbf{a}+\boldsymbol{h}\neq\mathbf{0}}} e^{-2\pi i \boldsymbol{g}\cdot(\mathbf{a}+\boldsymbol{h})} \sqrt{\frac{Y^{-1}[\mathbf{a}+\boldsymbol{h}]}{b}}^{\,s-\frac{n}{2}} K_{s-\frac{n}{2}}\left(2\sqrt{Y^{-1}[\mathbf{a}+\boldsymbol{h}]b}\,\pi\right) \\ &\quad + \delta(\boldsymbol{h}) \frac{1}{\sqrt{|Y|}} \frac{\Gamma(s-\frac{n}{2})}{\pi^{s-\frac{n}{2}}} \frac{1}{b^{s-\frac{n}{2}}}, \end{aligned} \tag{2.33}$$

where $K_s(z)$ signifies the modified Bessel function of the second kind defined e.g. by

$$K_s(z) = \frac{1}{2}\int_0^\infty e^{-\frac{1}{2}z(t+\frac{1}{t})} t^{s-1} dt, \quad \sigma > -\frac{1}{2}, \quad |\arg z| < \frac{\pi}{4}, \tag{2.34}$$

and

$$\delta(\boldsymbol{h}) = \begin{cases} 0 & \text{if } \boldsymbol{h} \notin \mathbb{Z}^n \\ 1 & \text{if } \boldsymbol{h} \in \mathbb{Z}^n. \end{cases}$$

Proof. This is Formula (1.25) [18] with the term $\varepsilon(\boldsymbol{g})(\pi b)^{-s}\Gamma(s)$ incorporated in the left-side member. There the proof depended on the modular relation, i.e. the Poisson summation modified so as to suit the case. We refer to Terras for a similar but more subtler proof using the Poisson summation formula.

We may deduce (2.33) from the functional equation (1.10) via the Mellin-Barnes integral

$$(1+x)^{-s} = \frac{1}{2\pi i}\int_{(c)} \frac{\Gamma(s-z)\Gamma(z)}{\Gamma(s)} x^{-z} dz \tag{2.35}$$

for $x > 0$, $0 < c < \sigma$, which has been used extensively in various context (cf. e.g. [19], [20] and [23]). The proof starts from expression the sum in the form of the integral (2.35), applying the functional equation, and then finally appealing to the Mellin inversion

$$\frac{1}{2\pi i}\int_{(c)} \Gamma\left(s+\frac{\mu+\nu}{2}\right)\Gamma\left(s+\frac{\mu-\nu}{2}\right)x^{-s}dx = 2x^{\frac{\mu}{2}}K_\nu(2\sqrt{x}). \quad (2.36)$$

Corollary 1 (Benson-Mackenzie (Borweins' [6])). Let as before $I = \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$, $\boldsymbol{c}_0 = \begin{pmatrix}\frac12\\\frac12\\\frac12\end{pmatrix}$ and $I_2 = \begin{pmatrix}1&0\\0&1\end{pmatrix}$, $\boldsymbol{c}_1 = \begin{pmatrix}\frac12\\\frac12\end{pmatrix}$. Then we have

$$Z(I,\mathbf{0},\boldsymbol{c}_0,s) = \frac{6\pi^{s+1}}{\Gamma(s+1)}\sum_{\mathbf{a}\in\left(\mathbb{Z}+\frac12\right)^2}\sum_{\substack{b\in\mathbb{Z}\\ b\neq 0}} b^2(-1)^b\sqrt{\frac{I_2[\mathbf{a}]}{b^2}}^{\,s} K_s\left(2\sqrt{I_2[\mathbf{a}]b^2}\,\pi\right) \quad (2.37)$$

and

$$Z\left(I,\mathbf{0},\boldsymbol{c}_0,\frac12\right) = -12\pi\sum_{a_1=\frac12}^{\infty}\sum_{a_2=\frac12}^{\infty}\left(\operatorname{sech}\left(\sqrt{a_1^2+a_2^2}\,\pi\right)\right)^2, \quad (2.38)$$

Proof. Since for $\sigma > \frac32$

$$Z(I,\mathbf{0},\boldsymbol{c}_0,s) = \sum_{\substack{\mathbf{a}\in\mathbb{Z}^3\\ \mathbf{a}\neq\mathbf{0}}} \frac{(-1)^{a_1+a_2+a_3}(a_1^2+a_2^2+a_3^2)}{(a_1^2+a_2^2+a_3^2)^{s+1}},$$

we may write

$$Z(I,\mathbf{0},\boldsymbol{c}_0,s) = 3\sum_{\substack{b\in\mathbb{Z}\\ b\neq 0}}\sum_{\mathbf{a}\in\mathbb{Z}^2}\frac{(-1)^{a_1+a_2+b}\,b^2}{(a_1^2+a_2^2+b^2)^{s+1}},$$

whence

$$Z(I,\mathbf{0},\boldsymbol{c}_0,s) = 3\sum_{\substack{b\in\mathbb{Z}\\ b\neq 0}}\left(b^2(-1)^b\sum_{\mathbf{a}\in\mathbb{Z}^2}\frac{e^{2\pi i\boldsymbol{c}_1\cdot\mathbf{a}}}{(I_2[\mathbf{a}]+b^2)^{s+1}}\right). \quad (2.39)$$

We apply Theorem 1 to the inner sum on the right of (2.39) to obtain

$$Z(I,\mathbf{0},\boldsymbol{c}_0,s)$$
$$=3\sum_{\substack{b\in\mathbb{Z}\\ b\neq 0}}\left(b^2(-1)^b\frac{2\pi^{s+1}}{\Gamma(s+1)}\sum_{\mathbf{a}\in\mathbb{Z}^2}\sqrt{\frac{I_2[\mathbf{a}+\boldsymbol{c}_1]}{b^2}}^{\,s}K_s\left(2\sqrt{I_2[\mathbf{a}+\boldsymbol{c}_1]b^2}\,\pi\right)\right), \tag{2.40}$$

which is (2.37).

Now put $s=\frac{1}{2}$ and recall the formula

$$K_{\frac{1}{2}}(z)=K_{-\frac{1}{2}}(z)=\sqrt{\frac{\pi}{2z}}e^{-z} \tag{2.41}$$

to deduce that

$$\begin{aligned} Z\left(I,\mathbf{0},\boldsymbol{c}_0,\frac{1}{2}\right) &= 6\pi\sum_{\mathbf{a}\in(\mathbb{Z}+\frac{1}{2})^2}\sum_{\substack{b\in\mathbb{Z}\\ b\neq 0}}|b|(-1)^b\exp\left(-2\sqrt{I_2[\mathbf{a}]}\,|b|\pi\right)\\ &= 12\pi\sum_{\mathbf{a}\in(\mathbb{Z}+\frac{1}{2})^2}\sum_{b=1}^{\infty}b(-\exp(-2\sqrt{I_2[\mathbf{a}]}\,\pi))^b \end{aligned} \tag{2.42}$$

The inner sum can be evaluated to be

$$\frac{-\exp(-2\sqrt{I_2[\mathbf{a}]}\,\pi)}{(1+\exp(-2\sqrt{I_2[\mathbf{a}]}\,\pi))^2}=-\frac{1}{4}\left(\operatorname{sech}\left(\sqrt{a_1^2+a_2^2}\,\pi\right)\right)^2,$$

$\mathbf{a}=\begin{pmatrix}a_1\\ a_2\end{pmatrix}\in\left(\mathbb{Z}+\frac{1}{2}\right)^2$. Hence, splitting the sum over a_1,a_2 into 4 parts, we conclude (2.38), completing the proof.

To state Theorem 2, we introduce new notation.

Let $Y=\left(\begin{array}{c|c}A & B\\ \hline {}^tB & C\end{array}\right)$ be a block decomposition with A an $n\times n$ matrix and B an $m\times m$ matrix. Set

$$D=C-{}^tBA^{-1}B.$$

In accordance with this decomposition, we decompose the vectors $\boldsymbol{g}=\begin{pmatrix}\boldsymbol{g}_1\\ \boldsymbol{g}_2\end{pmatrix}$, $\boldsymbol{h}=\begin{pmatrix}\boldsymbol{h}_1\\ \boldsymbol{h}_2\end{pmatrix}$, $\boldsymbol{g}_1,\boldsymbol{h}_1\in\mathbb{Z}^n$, $\boldsymbol{g}_2,\boldsymbol{h}_2\in\mathbb{Z}^m$.

Theorem 2. (generalized Chowla-Selberg type formula cf. [27, Example 4, p.208]) Under the above notation, we have

$$\begin{aligned}
&\Lambda(Y, \boldsymbol{g}, \boldsymbol{h}, s)\\
&= \delta(\boldsymbol{g}_2) e^{-2\pi i \boldsymbol{g}_2 \cdot \boldsymbol{h}_2} \Lambda(A, \boldsymbol{g}_1, \boldsymbol{h}_1, s) + \delta(\boldsymbol{h}_1) \frac{1}{\sqrt{|A|}} \Lambda\left(D, \boldsymbol{g}_2, \boldsymbol{h}_2, s - \frac{n}{2}\right)\\
&\quad + \frac{2e^{-2\pi i \boldsymbol{g}_1 \cdot \boldsymbol{h}_1}}{\sqrt{|A|}} \sum_{\substack{\mathbf{a} \in \mathbb{Z}^n \\ \mathbf{a}+\boldsymbol{h}_1 \neq \mathbf{0}}} \sum_{\substack{\boldsymbol{b} \in \mathbb{Z}^m \\ \boldsymbol{b}+\boldsymbol{g}_2 \neq \mathbf{0}}} e^{2\pi i(-\boldsymbol{g}_1 \cdot \mathbf{a} + \boldsymbol{h}_2 \cdot \boldsymbol{b})} e^{-2\pi i A^{-1} B(\boldsymbol{b}+\boldsymbol{g}_2) \cdot (\mathbf{a}+\boldsymbol{h}_1)}\\
&\quad \times \sqrt{\frac{A^{-1}[\mathbf{a}+\boldsymbol{h}_1]}{D[\boldsymbol{b}+\boldsymbol{g}_2]}}^{\,s-\frac{n}{2}} K_{s-\frac{n}{2}}\left(2\sqrt{A^{-1}[\mathbf{a}+\boldsymbol{h}_1] D[\boldsymbol{b}+\boldsymbol{g}_2]}\,\pi\right). \qquad (2.43)
\end{aligned}$$

Proof. The case $\boldsymbol{g} = \boldsymbol{h} = \mathbf{0}, n = m = 1$ is due to Chowla and Selberg [12, 24] (cf. also Bateman and Grosswald [2]), the case $m = 1$ is due to Berndt [4] and the general case with $\boldsymbol{g} = \boldsymbol{h} = \mathbf{0}$ is due to Terras [25, 27].

The proof in our most general case runs as follows.

Noting that

$$\Lambda(Y, \boldsymbol{g}, \boldsymbol{h}, s) = \pi^{-s} \Gamma(s) \sum_{\substack{\mathbf{a} \in \mathbb{Z}^n, \boldsymbol{b} \in \mathbb{Z}^m \\ (\mathbf{a}+\boldsymbol{g}_1, \boldsymbol{b}+\boldsymbol{g}_2) \neq \mathbf{0}}} \frac{e^{2\pi i(\boldsymbol{h}_1 \cdot \mathbf{a} + \boldsymbol{h}_2 \cdot \boldsymbol{b})}}{Y[(\mathbf{a}+\boldsymbol{g}_1, \boldsymbol{b}+\boldsymbol{g}_2)]^s},$$

we distinguish three cases: $\boldsymbol{b} + \boldsymbol{g}_2 = \mathbf{0}$ ($\boldsymbol{g}_2 = \mathbf{0}$ or not) and $\boldsymbol{b} + \boldsymbol{g}_2 \neq \mathbf{0}$:

$$\begin{aligned}
\Lambda(Y, \boldsymbol{g}, \boldsymbol{h}, s) &= \delta(\boldsymbol{g}_2) \pi^{-s} \Gamma(s) \sum_{\substack{\mathbf{a} \in \mathbb{Z}^n \\ \mathbf{a}+\boldsymbol{g}_1 \neq \mathbf{0}}} \frac{e^{2\pi i(\boldsymbol{h}_1 \cdot \mathbf{a} - \boldsymbol{h}_2 \cdot \boldsymbol{g}_2)}}{Y[(\mathbf{a}+\boldsymbol{g}_1, \mathbf{0})]^s}\\
&\quad + \pi^{-s} \Gamma(s) \sum_{\substack{\boldsymbol{b} \in \mathbb{Z}^m \\ \boldsymbol{b}+\boldsymbol{g}_2 \neq \mathbf{0}}} \sum_{\mathbf{a} \in \mathbb{Z}^n} \frac{e^{2\pi i(\boldsymbol{h}_1 \cdot \mathbf{a} + \boldsymbol{h}_2 \cdot \boldsymbol{b})}}{Y[(\mathbf{a}+\boldsymbol{g}_1, \boldsymbol{b}+\boldsymbol{g}_2)]^s}. \qquad (2.44)
\end{aligned}$$

We now apply the formula

$$Y[(\mathbf{a}, \boldsymbol{b})] = A[\mathbf{a} + A^{-1} B \boldsymbol{b}] + D[\boldsymbol{b}], \quad \mathbf{a} \in \mathbb{Z}^n, \boldsymbol{b} \in \mathbb{Z}^m \qquad (2.45)$$

to transform (2.44) into

$$\begin{aligned}
&\Lambda(Y,\boldsymbol{g},\boldsymbol{h},s)\\
&=\delta(\boldsymbol{g}_2)\pi^{-s}\Gamma(s)e^{-2\pi i\boldsymbol{h}_2\cdot\boldsymbol{g}_2}\sum_{\substack{\mathbf{a}\in\mathbb{Z}^n\\ \mathbf{a}+\boldsymbol{g}_1\neq\mathbf{0}}}\frac{e^{2\pi i\boldsymbol{h}_1\cdot\mathbf{a}}}{A[(\mathbf{a}+\boldsymbol{g}_1]^s}\\
&\quad+\pi^{-s}\Gamma(s)\sum_{\substack{\boldsymbol{b}\in\mathbb{Z}^m\\ \boldsymbol{b}+\boldsymbol{g}_2\neq\mathbf{0}}}e^{2\pi i\boldsymbol{h}_2\cdot\boldsymbol{b}}\sum_{\mathbf{a}\in\mathbb{Z}^n}\frac{e^{2\pi i\boldsymbol{h}_1\cdot\mathbf{a}}}{(A[\mathbf{a}+\boldsymbol{g}_1+A^{-1}B(\boldsymbol{b}+\boldsymbol{g}_2)]+D[\boldsymbol{b}+\boldsymbol{g}_2])^s}.
\end{aligned}\tag{2.46}$$

The first sum on the right of (2.46) is $\Lambda(A,\boldsymbol{g}_1,\boldsymbol{h}_1,s)$ and to the inner sum in the second term, we apply Theorem 1. Then the second term on the right of (2.46) becomes

$$\begin{aligned}
&\sum_{\substack{\boldsymbol{b}\in\mathbb{Z}^m,\boldsymbol{b}\neq\mathbf{0}\\ \boldsymbol{b}+\boldsymbol{g}_2\neq\mathbf{0}}}e^{2\pi i\boldsymbol{h}_2\cdot\boldsymbol{b}}\Bigg\{\frac{2}{\sqrt{|A|}}\sum_{\substack{\mathbf{a}\in\mathbb{Z}^n\\ \mathbf{a}+\boldsymbol{h}_1\neq\mathbf{0}}}e^{-2\pi i(\boldsymbol{g}_1+A^{-1}B(\boldsymbol{b}+\boldsymbol{g}_2))\cdot(\mathbf{a}+\boldsymbol{h}_1)}\\
&\times\sqrt{\frac{A^{-1}[\mathbf{a}+\boldsymbol{h}_1]}{D[\boldsymbol{b}+\boldsymbol{g}_2]}}^{\,s-\frac{n}{2}}K_{s-\frac{n}{2}}\left(2\pi\sqrt{A^{-1}[\mathbf{a}+\boldsymbol{h}_1]D[\boldsymbol{b}+\boldsymbol{g}_2]}\right)\Bigg\}\\
&+\sum_{\substack{\boldsymbol{b}\in\mathbb{Z}^m\\ \boldsymbol{b}+\boldsymbol{g}_2\neq\mathbf{0}}}e^{2\pi i\boldsymbol{h}_2\cdot\boldsymbol{b}}\delta(\boldsymbol{h}_1)\frac{\Gamma(s-\frac{n}{2})}{\sqrt{|A|}D[\boldsymbol{b}+\boldsymbol{g}_2]^{s-\frac{n}{2}}\pi^{s-\frac{n}{2}}},
\end{aligned}$$

which are the third and second terms on the right of (2.43), whence the result follows.

Corollary 2 (Hautot formula [17]). For the Madelung constant $M_{NaCl}=-Z(I,\mathbf{0},\boldsymbol{c}_0,\frac{1}{2})$ (1.17), we have the representations

$$M_{NaCl}=\frac{\pi}{2}-3\sum_{\substack{\boldsymbol{b}\in\mathbb{Z}^2\\ \boldsymbol{b}\neq\mathbf{0}}}\frac{(-1)^{b_1}}{\sqrt{b_1^2+b_2^2}}\operatorname{cosech}\left(\sqrt{b_1^2+b_2^2}\,\pi\right),\tag{2.47}$$

$$\begin{aligned}
M_{NaCl}&=-\pi+12(1-\sqrt{2})\zeta\left(\frac{1}{2}\right)\beta\left(\frac{1}{2}\right)\\
&\quad-24\sum_{b_1=1}^{\infty}\sum_{b_2=1}^{\infty}\frac{(-1)^{b_1+b_2}}{\sqrt{b_1^2+b_2^2}}\frac{1}{\exp\left(2\sqrt{b_1^2+b_2^2}\,\pi\right)-1},
\end{aligned}\tag{2.48}$$

where $\beta(s)=L(s,\chi_4)$ is the Dirichlet L-function with non-trivial character χ_4 mod 4.

Proof. Recall from Example 2.1 (ii), the formula (cf. (2.19))

$$\Lambda(I, \mathbf{0}, \boldsymbol{c}_0, s) = 2\Lambda(A, \mathbf{0}, \mathbf{0}, s) - \Lambda(I, \mathbf{0}, \mathbf{0}, s).$$

Applying the functional equation (1.10) and arguing as we deduced (1.36), we obtain

$$\Lambda(I, \mathbf{0}, \boldsymbol{c}_0, s) = \Lambda\left(\frac{1}{4}B, \mathbf{0}, \mathbf{0}, \frac{3}{2} - s\right) - \Lambda\left(I, \mathbf{0}, \mathbf{0}, \frac{3}{2} - s\right), \tag{2.49}$$

whence for $s = \frac{1}{2}$,

$$\Lambda\left(I, \mathbf{0}, \boldsymbol{c}_0, \frac{1}{2}\right) = \Lambda\left(\frac{1}{4}B, \mathbf{0}, \mathbf{0}, 1\right) - \Lambda(I, \mathbf{0}, \mathbf{0}, 1). \tag{2.50}$$

On the other hand, from Example 2.1 (iii), we have the formula (cf. (2.20))

$$3\Lambda(I, \mathbf{0}, \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}, s) = 4\Lambda(B, \mathbf{0}, \mathbf{0}, s) - \Lambda(I, \mathbf{0}, \mathbf{0}, s),$$

which gives for $s = 1$

$$3\Lambda(I, \mathbf{0}, \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}, 1) = 4\Lambda(B, \mathbf{0}, \mathbf{0}, 1) - \Lambda(I, \mathbf{0}, \mathbf{0}, 1). \tag{2.51}$$

Combing (2.50) and (2.51) yields

$$\Lambda(I, \mathbf{0}, \boldsymbol{c}_0, \frac{1}{2}) = 3\Lambda(I, \mathbf{0}, \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}, 1). \tag{2.52}$$

We apply Theorem 2 to the left-hand side of (2.52) with the decomposition $I = \left(\begin{array}{c|cc} 1 & 0 & 0 \\ \hline 0 & 1 & 0 \\ 0 & 0 & 1 \end{array}\right)$ to deduce that

$$\begin{aligned} \Lambda(I, \mathbf{0}, \boldsymbol{c}_0, \frac{1}{2}) &= 3\Lambda(I, \mathbf{0}, \frac{1}{2}, 1) \\ &\quad + 3 \sum_{\substack{\boldsymbol{b} \in \mathbb{Z}^2 \\ \boldsymbol{b} \neq 0}} \sum_{a \in \mathbb{Z}} \frac{(-1)^{b_1}}{\sqrt{b_1^2 + b_2^2}} \exp\left(-2\left|a + \frac{1}{2}\right| \sqrt{b_1^2 + b_2^2}\,\pi\right) \\ &= -\frac{\pi}{2} + 3 \sum_{\substack{\boldsymbol{b} \in \mathbb{Z}^2 \\ \boldsymbol{b} \neq \mathbf{0}}} \frac{(-1)^{b_1}}{\sqrt{b_1^2 + b_2^2}} \operatorname{cosech}\left(\sqrt{b_1^2 + b_2^2}\,\pi\right), \end{aligned} \tag{2.53}$$

which lead to (2.47).

Now, corresponding to (2.52), we have

$$\Lambda\left(I, \mathbf{0}, \boldsymbol{c}_0, \frac{1}{2}\right) = 3\Lambda(I, \mathbf{0}, \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}, 1), \tag{2.54}$$

whence corresponding to (2.53),

$$\begin{aligned}\Lambda(I, \mathbf{0}, \boldsymbol{c}_0, \frac{1}{2}) &= 3\Lambda(I, \mathbf{0}, \mathbf{0}, 1) + 3\Lambda\left(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, 0, \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}, \frac{1}{2}\right) \\ &\quad + 3\sum_{\substack{\boldsymbol{b}\in\mathbb{Z}^2 \\ \boldsymbol{b}\neq\mathbf{0}}} \frac{(-1)^{b_1+b_2}}{\sqrt{b_1^2+b_2^2}} \exp\left(-2|a|\sqrt{b_1^2+b_2^2}\,\pi\right) \\ &= \pi + 12(\sqrt{2}-1)\zeta\left(\frac{1}{2}\right)\zeta\left(\frac{1}{2}\right) \\ &\quad + 24\sum_{b_1=1}^{\infty}\sum_{b_2=1}^{\infty} \frac{(-1)^{b_1+b_2}}{\sqrt{b_1^2+b_2^2}} \frac{1}{\exp(2\sqrt{b_1^2+b_2^2}\,\pi)-1},\end{aligned} \tag{2.55}$$

whence (2.48) follows. The proof is now complete.

3. Abel means and screened Coulomb potential

Suppose the pair $\varphi(s)$ and $\psi(s)$ satisfy the Hecke type functional equation prescribed in section 1 and that $\chi(s) = \Gamma(s)\varphi(s)$ has simple poles at $s_1, \ldots, s_m$ with residues $\rho_1, \ldots, \rho_m$, respectively.

Let

$$\widetilde{\varphi}(s, w) = \sum_{n=1}^{\infty} \frac{a_n}{\lambda_n^s} e^{-\lambda_n w} \tag{3.1}$$

and

$$\widetilde{\psi}(s, w) = \sum_{n=1}^{\infty} \frac{b_n}{\mu_n^s} e^{-\mu_n w} \tag{3.2}$$

for $w > 0$ (ultimately we allow $\Re w > 0$) be the weighted Lambert series. We note that they reduce to the Lambert series introduced in section 1:

$$\Phi(w) = \sum_{n=1}^{\infty} a_n e^{-\lambda_n w} = \widetilde{\varphi}(0, w),$$

$$\Psi(w) = \sum_{n=1}^{\infty} b_n e^{-\mu_n w} = \widetilde{\psi}(0, w).$$

F.V. Atkinson [1] was the first to consider the limit as $w \to 0$ of (3.1) or (3.2) and call it Abel mean. Then B.C. Berndt [3] gave a general result which holds true for all Dirichlet series φ and ψ.

Theorem (Berndt [3], Theorem 4.1). *We have*

$$\lim_{w\to 0+}\left\{\widetilde{\varphi}(s,w)-\sum_{k=1}^{m}\frac{\Gamma(s_k-s)}{\Gamma(s_k)}w^{s-s_k}\rho_k\right\}=\varphi(s).$$

Our first result is the following theorem whose proof is to appear elsewhere [21].

Theorem 3. We have

$$\lim_{w\to 0+}\left\{\widetilde{\varphi}(s,w)-\sum_{k=1}^{m}\frac{\Gamma(s_k-s)}{\Gamma(s_k)}w^{s-s_k}\rho_k\right\}=\frac{\Gamma(\delta-s)}{\Gamma(s)}\psi(\delta-s).$$

Remark 1. (i) By the functional equation (1.2), the right-hand side is $\varphi(s)$, so that our Theorem 3 implies Berndt's Theorem 4.1.

(ii) If $\sigma > \sigma_a$ (and $\delta/2$), then we may take the limits as $w \to 0_+$ separately on the left to obtain

$$\varphi(s)=\sum_{n=1}^{\infty}\frac{a_n}{\lambda_n^s}=\frac{\Gamma(\delta-s)}{\Gamma(s)}\psi(\delta-s).$$

Thus,

Corollary 3. Atkinson-Berndt Abel mean amounts to another proof of the functional equation (1.2).

Now we confine ourselves to the Epstein zeta-function through which we clarify the meaning of screened Coulomb potential considered by Chaba-Pathria [8]-[11], Borweins [7], Hall [15], Hautot [16] in 2- and 3-dimensional lattice structure.

By screened Coulomb potentials are meant the Dirichlet series

$$S(\beta;a):=\sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^3\\ \boldsymbol{r}\neq\boldsymbol{0}}}\frac{\exp(2\pi i\beta\cdot\boldsymbol{r}-ar^2)}{r^2}\tag{3.3}$$

and

$$T(\beta;a):=\sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^3\\ \boldsymbol{r}+\beta\neq\boldsymbol{0}}}\frac{\exp(-a|\boldsymbol{r}+\beta|^2)}{|\boldsymbol{r}+\beta|^2},\tag{3.4}$$

where $\boldsymbol{r}$ signifies the position vector (x, y, z), r its length $\sqrt{x^2+y^2+z^2}$, $\beta \in \mathbb{R}^3$ giving rise to the additive character and $a > 0$ (eventually $\Re a > 0$ is allowed). "Screened" means that they decay exponentially as $a \to \infty$ (cf. Chaba-Pathria [9], (48) and (54), respectively).

Screened Coulomb potential was first studied by Hautot [16] and then extensively by Chaba-Pathria [8]-[11]. The 2-dimensional case was taken up by Borweins. We shall interpret all of these results as special cases (Abel mean) of our general result, which in turn is a slight generalization (i.e. the poles being taken into account) of Terras (Exercise 17 pp.81–82) and Ewald [13].

We use the notation given in section 1.

Theorem 4. For $c > 0$ (or $\Re c > 0$) we have

$$
\begin{aligned}
&\Lambda(Y, \boldsymbol{g}, \boldsymbol{h}, s) = c^s \Lambda(cY, \boldsymbol{g}, \boldsymbol{h}, s) \\
&= \frac{1}{\sqrt{|Y|}} e^{-2\pi i \boldsymbol{g}\cdot\boldsymbol{h}} \sum_{\substack{\mathbf{a}\in\mathbb{Z}^n \\ \mathbf{a}+\boldsymbol{h}\neq\mathbf{0}}} e^{-2\pi i \boldsymbol{g}\cdot\mathbf{a}} \frac{\Gamma\left(\frac{n}{2}-s, \frac{\pi}{c} Y^{-1}[\mathbf{a}+\boldsymbol{h}]\right)}{\pi^{\frac{n}{2}-s} Y^{-1}[\mathbf{a}+\boldsymbol{h}]^{\frac{n}{2}-s}} + \delta(\boldsymbol{h}) \frac{1}{\sqrt{|Y|}} \frac{c^{s-\frac{n}{2}}}{s-\frac{n}{2}} \\
&\quad + \sum_{\substack{\mathbf{a}\in\mathbb{Z}^n \\ \mathbf{a}+\boldsymbol{g}\neq\mathbf{0}}} e^{2\pi i \boldsymbol{h}\cdot\mathbf{a}} \frac{\Gamma(s, \pi c Y[\mathbf{a}+\boldsymbol{g}])}{\pi^s Y[\mathbf{a}+\boldsymbol{g}]^s} - \delta(\boldsymbol{g}) e^{-2\pi i \boldsymbol{g}\cdot\boldsymbol{h}} \frac{c^s}{s},
\end{aligned}
$$

where $\delta(\cdot)$ is the delta symbol and as in section 1, $\Gamma(s, z)$ signifies the incomplete gamma function.

Remark 2. Theorem 4 entails those results corresponding to Theorem 3 and Corollary 3.

Indeed, for $0 < \sigma < \frac{n}{2}$, we let $c \to 0+$ to obtain

$$
\begin{aligned}
&\lim_{c\to 0+} \left\{ \sum_{\substack{\mathbf{a}\in\mathbb{Z}^n \\ \mathbf{a}+\boldsymbol{g}\neq\mathbf{0}}} e^{2\pi i \boldsymbol{h}\cdot\mathbf{a}} \frac{\Gamma(s, \pi c Y[\mathbf{a}+\boldsymbol{g}])}{\pi^s Y[\mathbf{a}+\boldsymbol{g}]^s} + \delta(\boldsymbol{h}) \frac{1}{\sqrt{|Y|}} \frac{c^{s-\frac{n}{2}}}{s-\frac{n}{2}} \right\} \\
&= \Lambda(Y, \boldsymbol{g}, \boldsymbol{h}, s).
\end{aligned}
$$

For $\sigma < 0$, let $c \to \infty$ to obtain

$$
\Lambda(Y, \boldsymbol{g}, \boldsymbol{h}, s) = \frac{1}{\sqrt{|Y|}} e^{-2\pi i \boldsymbol{g}\cdot\boldsymbol{h}} \Lambda\left(Y^{-1}, \boldsymbol{h}, -\boldsymbol{g}, \frac{n}{2} - s\right),
$$

i.e. the functional equation (1.10) follows, as stated by Terras, p.82.

Corollary 4. For $a > 0$, $n = 3$ and $\beta \notin \mathbb{Z}^3$,

(i)
$$S(\beta; a) = a + A(\beta) - \pi \sum_{\boldsymbol{r} \in \mathbb{Z}^3} \frac{\operatorname{erfc}\left(\frac{\pi}{\sqrt{a}}|\boldsymbol{r} + \beta|\right)}{|\boldsymbol{r} + \beta|},$$

(ii)
$$\begin{aligned} V(\beta; a) &:= \sum_{\boldsymbol{r} \in \mathbb{Z}^3} \frac{\exp(-a|\boldsymbol{r} + \beta|)}{|\boldsymbol{r} + \beta|} \\ &= \frac{4\pi}{a^2} + \frac{A(\beta)}{\pi} - \frac{a^2}{4\pi^3} \sum_{\substack{\boldsymbol{r} \in \mathbb{Z}^3 \\ \boldsymbol{r} \neq \boldsymbol{0}}} \frac{\exp(2\pi i \beta \cdot \boldsymbol{r})}{r^2 \left(r^2 + \frac{a^2}{4\pi^2}\right)}, \end{aligned}$$

where $A(\beta) = S(\beta; 0) = \sum_{\substack{\boldsymbol{r} \in \mathbb{Z}^3 \\ \boldsymbol{r} \neq \boldsymbol{0}}} \frac{\exp(2\pi i \beta \cdot \boldsymbol{r})}{r^2}$.

(iii)
$$T(\beta; a) = \frac{2\pi^{3/2}}{\sqrt{a}} + B(\beta) - \pi \sum_{\substack{\boldsymbol{r} \in \mathbb{Z}^3 \\ \boldsymbol{r} \neq \boldsymbol{0}}} \frac{\exp(2\pi i \beta \cdot \boldsymbol{r}) \operatorname{erfc}\left(\frac{\pi}{\sqrt{a}} r\right)}{r},$$

(iv)
$$\begin{aligned} U(\beta; a) &:= \sum_{\substack{\boldsymbol{r} \in \mathbb{Z}^3 \\ \boldsymbol{r} \neq \boldsymbol{0}}} \frac{\exp(2\pi i \beta \cdot \boldsymbol{r} - ar)}{r} \\ &= a + \frac{B(\beta)}{\pi} - \frac{a^2}{4\pi^3} \sum_{\boldsymbol{r} \in \mathbb{Z}^3} \frac{1}{|\boldsymbol{r} + \beta|^2 \left(|\boldsymbol{r} + \beta|^2 + \frac{a^2}{4\pi^2}\right)}, \end{aligned}$$

where $B(\beta) = \lim_{a \to 0+} \left(T(\beta; a) - 2\pi^{3/2} a^{-1/2}\right)$, and where $\operatorname{erfc}(z) = \frac{1}{\sqrt{\pi}} \Gamma(1/2, z^2)$ is the error function usually so denoted.

Proof. Formulas (i) and (iii) are direct specializations of the formula in Theorem 4 with the following known formulas taken into account:

$$\Gamma(1, z) = e^{-z}, \quad \Gamma\left(\frac{1}{2}, z\right) = \sqrt{\pi} \operatorname{erfc}(\sqrt{z}), \tag{3.5}$$

while formulas in (ii) and (iv) are Laplace transforms of (i) and (iii), respectively, when the following known formulas incorporated:

$$\mathcal{L}\left[\operatorname{erfc}\left(at^{-1/2}\right)\right](p) = \frac{1}{p} e^{-2a\sqrt{p}} \tag{3.6}$$

or more generally,

$$\mathcal{L}\left[\Gamma\left(\nu, \frac{a}{t}\right)\right](p) = 2a^{\frac{\nu}{2}} p^{\frac{\nu}{2} - 1} K_\nu(2\sqrt{ap}), \tag{3.7}$$

which for $\nu = \frac{1}{2}$ reduces to (3.6) in view of (2.41) and

$$\mathcal{L}[\Gamma(\nu, at)](p) = \frac{\Gamma(\nu)}{p}\left(1 - \frac{1}{(1+\frac{p}{a})^{\nu}}\right). \tag{3.8}$$

We choose $Y = I$ (identity matrix), once and for all, so that $Y[\mathbf{a}] = I[\mathbf{a}] = |\mathbf{a}|^2$, and $c = \frac{a}{\pi}$ (we write $\boldsymbol{r}$ for $\mathbf{a}$).

To prove (i) we choose $s = 1$, $\boldsymbol{g} = \mathbf{0}$, $\boldsymbol{h} = \beta$. Then

$$\pi^{-1} \sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^3 \\ \boldsymbol{r}\neq\mathbf{0}}} \frac{e^{2\pi i\beta\cdot\boldsymbol{r}}}{r^2} = \sum_{\boldsymbol{r}\in\mathbb{Z}^3} \frac{\operatorname{erfc}(\frac{\pi}{\sqrt{a}}|\boldsymbol{r}+\beta|)}{|\boldsymbol{r}+\beta|} - \frac{a}{\pi} + \pi^{-1} \sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^3 \\ \boldsymbol{r}\neq\mathbf{0}}} \frac{e^{2\pi i\beta\cdot\boldsymbol{r}}e^{-ar^2}}{r^2},$$

which is Chaba-Pathria [9], (48), p.1419.

Taking Laplace transform $\mathcal{L}[\cdot](p)$ of (i) with (3.7) and (3.8) in mind, we conclude that

$$\begin{aligned}\frac{4\pi^2}{a^2}\Lambda(I,\mathbf{0},\beta,1) &= \frac{4\pi^2}{a^2} \sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^3 \\ \boldsymbol{r}+\beta\neq\mathbf{0}}} \frac{\exp(-a|\boldsymbol{r}+\beta|)}{|\boldsymbol{r}+\beta|} \\ &\quad + \frac{1}{\pi} \sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^3 \\ \boldsymbol{r}\neq\mathbf{0}}} \frac{\exp(-2\pi i\beta\cdot\boldsymbol{r})}{r^2(r^2+\frac{a^2}{4\pi^2})} - \frac{1}{\pi}\left(\frac{4\pi^2}{a^2}\right)^2,\end{aligned}$$

where we put $p = \frac{a^2}{4\pi^2}$. This proves (ii), i.e. [9, (62)].

It may be worth while recording the general Laplace transform of the formula in Theorem 4.

$$\begin{aligned}&\frac{4\pi^2}{a^2}\Lambda(Y,\boldsymbol{g},\boldsymbol{h},s) \\ &= \frac{1}{\sqrt{|Y|}} e^{-2\pi i\boldsymbol{g}\cdot\boldsymbol{h}} \sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^n \\ \boldsymbol{r}+\boldsymbol{h}\neq\mathbf{0}}} \frac{2(\pi^2 Y^{-1}[\boldsymbol{r}+\boldsymbol{h}])^{\frac{n/2-s}{2}}}{\pi^{n/2-s}(Y^{-1}[\boldsymbol{r}+\boldsymbol{h}])^{n/2-s}} \left(\frac{a}{2\pi}\right)^{\frac{n}{2}-s-2} \times \\ &\times K_{\frac{n}{2}-s}\left(2\sqrt{\pi^2 Y^{-1}[\boldsymbol{r}+\boldsymbol{h}](\frac{a^2}{4\pi^2})}\right) \\ &+ \delta(\boldsymbol{h})\frac{1}{\sqrt{|Y|}}\frac{\pi^{\frac{n}{2}-s}}{s-\frac{n}{2}}\left(\frac{a^2}{4\pi^2}\right)^{\frac{n}{2}-s-1}\Gamma\left(s-\frac{n}{2}+1\right) \\ &+ \Gamma(s)\frac{4\pi^2}{a^2}\sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^n \\ \boldsymbol{r}+\boldsymbol{g}\neq\mathbf{0}}} e^{-2\pi i\boldsymbol{h}\cdot\boldsymbol{r}} \frac{1}{\pi^s(Y[\boldsymbol{r}+\boldsymbol{g}])^s}\left(1 - \frac{1}{(1+\frac{a^2}{4\pi^2}(Y[\boldsymbol{r}+\boldsymbol{g}])^{-1})^s}\right) \\ &- \delta(\boldsymbol{g})e^{-2\pi i\boldsymbol{g}\cdot\boldsymbol{h}}\frac{\pi^{-s}}{s}\Gamma(s+1)p^{-s-1}\end{aligned} \tag{3.9}$$

for $\Re(s) > \frac{n}{2} - 1$. Formula (iv) is a special case of (3.9) with $\boldsymbol{g} = \beta$, $\boldsymbol{h} = \mathbf{0}$, $s \to 1$ ($c = a/\pi$, $n = 3, \ldots$). We note that $B(\beta) = \pi U(\beta; 0)$.

The same specialization yields that

$$Z(I, \beta, \mathbf{0}, 1) = \pi \sum_{\substack{\boldsymbol{r} \in \mathbb{Z}^3 \\ \boldsymbol{r} \neq \mathbf{0}}} \frac{e^{-2\pi i \beta \cdot \boldsymbol{r}} e^{-\pi a^{-1/2} r}}{r} - \frac{2\pi^{3/2}}{a^{1/2}} + \sum_{\substack{\boldsymbol{r} \in \mathbb{Z}^3 \\ \boldsymbol{r}+\beta \neq \mathbf{0}}} \frac{e^{-a|\boldsymbol{r}+\beta|^2}}{|\boldsymbol{r}+\beta|^2}, \tag{3.10}$$

which amounts to (iii). Of course, the Laplace transform of (3.10) leads to (iv). This completes the proof.

Some comments on the limiting cases as $a \to 0$ (or $\beta \to \mathbf{0}$) of above formulas are in order.

Remark 3. (i) Chaba-Pathria [9] state that the limiting case as $\beta \to \mathbf{0}$ of (i)

$$S(0; a) = \sum_{\substack{\boldsymbol{r} \in \mathbb{Z}^3 \\ \boldsymbol{r} \neq \mathbf{0}}} \frac{e^{-ar^2}}{r^2} = \frac{2\pi^{3/2}}{a^{1/2}} + C_3 + a - \pi \sum_{\substack{\boldsymbol{r} \in \mathbb{Z}^3 \\ \boldsymbol{r} \neq 0}} \frac{\operatorname{erfc}(\pi a^{-1/2} r)}{r^2} \tag{3.11}$$

appeared already in [8], but (3.11) does not follow from (i), and to deduce it, we need to appeal to our Theorem 4 with $\boldsymbol{g} = \boldsymbol{h} = \mathbf{0}$, $s \to 1$:

$$\begin{aligned} Z(I, \mathbf{0}, \mathbf{0}, 1) &= \lim_{s \to 1} Z(I, \mathbf{0}, \mathbf{0}, s) \\ &= \sum_{\substack{\boldsymbol{r} \in \mathbb{Z}^3 \\ \boldsymbol{r} \neq \mathbf{0}}} \frac{e^{-ar^2}}{r^2} - \frac{2\pi^{3/2}}{a^{1/2}} - a + \pi \sum_{\substack{\boldsymbol{r} \in \mathbb{Z}^3 \\ \boldsymbol{r} \neq \mathbf{0}}} \frac{\operatorname{erfc}(\pi a^{-1/2} r)}{r^2}. \end{aligned} \tag{3.12}$$

Chaba-Pathria [9, (50)] introduce the constant (introduced in [8])

$$C_3 = \lim_{a \to 0+} \left(S(0, a) - 2\pi^{3/2} a^{-1/2} \right),$$

but cannot state its source. We have an advantage over them to the effect that C_3 is exactly the special value at $s = 1$ of the (analytic continuation of the) Epstein zeta-function $Z(I, \mathbf{0}, \mathbf{0}, s) = \sum_{\substack{\boldsymbol{r} \in \mathbb{Z}^3 \\ \boldsymbol{r} \neq \mathbf{0}}} \frac{1}{r^{2s}}$:

$$C_3 = Z(I, \mathbf{0}, \mathbf{0}, 1). \tag{3.13}$$

(ii) In the case of $B(\beta)$ we have the same advantage of assigning the definite value $Z(I, \beta, \mathbf{0}, 1)$ to it:

$$B(\beta) = Z(I, \beta, \mathbf{0}, 1). \tag{3.14}$$

Chaba-Pathria [9] give Formula (55) connecting $B(\beta)$ to $\pi \sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^3 \\ \boldsymbol{r}\neq\mathbf{0}}} \frac{e^{-2\pi i\beta\cdot\boldsymbol{r}}}{r}$, but it is not clear how they deduce this. Only through (3.14), we get the following, on resorting to the functional equation (1.10)

$$B(\beta) = Z(I, \beta, \mathbf{0}, 1) = \sqrt{\pi} Z\left(I, \mathbf{0}, -\beta, \frac{1}{2}\right). \tag{3.15}$$

We now turn to the case $n = 2$ and recover Borweins' result [7].

Corollary 5. For $\Re a > 0$, we have

(i)
$$Z\left(I, \beta, \mathbf{0}, \frac{1}{2}\right) = \sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^2 \\ \boldsymbol{r}\neq\mathbf{0}}} e^{-2\pi i\beta\cdot\boldsymbol{r}} \frac{\operatorname{erfc}\left(\frac{\pi}{\sqrt{a}} r\right)}{r} + \sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^2 \\ \boldsymbol{r}+\beta\neq\mathbf{0}}} \frac{\operatorname{erfc}(\sqrt{a}|\boldsymbol{r}+\beta|)}{|\boldsymbol{r}+\beta|} - 2\sqrt{\frac{\pi}{a}},$$

(i)$'$
$$Z\left(I, \beta, \mathbf{0}, \frac{1}{2}\right) = \sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^2 \\ \boldsymbol{r}\neq\mathbf{0}}} e^{-2\pi i\beta\cdot\boldsymbol{r}} \frac{\operatorname{erfc}(\sqrt{a} r)}{r} + \sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^2 \\ \boldsymbol{r}+\beta\neq\mathbf{0}}} \frac{\operatorname{erfc}\left(\frac{\pi}{\sqrt{a}}|\boldsymbol{r}+\beta|\right)}{|\boldsymbol{r}+\beta|} - 2\sqrt{\frac{a}{\pi}},$$

(ii)
$$\sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^2 \\ \boldsymbol{r}\neq\mathbf{0}}} e^{-2\pi i\beta\cdot\boldsymbol{r}} \frac{e^{ar}}{r} = Z\left(I, \beta, \mathbf{0}, \frac{1}{2}\right) + a - \sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^2 \\ \boldsymbol{r}+\beta\neq\mathbf{0}}} \left(\frac{1}{|\boldsymbol{r}+\beta|} - \frac{1}{\sqrt{|\boldsymbol{r}+\beta|^2 + \frac{a^2}{4\pi^2}}}\right).$$

We have further

(iii)
$$\sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^2 \\ \boldsymbol{r}\neq\mathbf{0}}} \frac{e^{-ar}}{r} = \frac{2\pi}{a} + Z\left(I, \mathbf{0}, \mathbf{0}, \frac{1}{2}\right) + a - \sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^2 \\ \boldsymbol{r}\neq\mathbf{0}}} \left(r^{-1} - \left(r^2 + \frac{a^2}{4\pi^2}\right)^{-1/2}\right),$$

(iii)′
$$\lim_{a\to 0+}\left(\sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^2\\ \boldsymbol{r}\neq\boldsymbol{0}}}\frac{e^{-ar}}{r}-\frac{2\pi}{a}\right)=4\zeta\left(\frac{1}{2}\right)\beta\left(\frac{1}{2}\right).$$

Proof. Formula (i) is a specialization of our formula in Theorem 4 with $n=2$, $Y=I$, $\boldsymbol{g}=\beta$, $\boldsymbol{h}=\boldsymbol{0}$, $s\to\frac{1}{2}$, while (i)′ is a restatement of (i) with $\frac{\pi^2}{a}$ in place of a. Formula (i) is Chaba-Pathria [9, (33)] and Formula (i)′ is (39).

Formula (ii) is Chaba-Pathria [9, (41)] and Borweins' (8). Both Chaba-Pathria and Borweins deduce (ii) using Fetter et al's technique. However, as is pointed out by Chaba-Pathria, we may prove (ii) by taking the Laplace transform $\mathcal{L}[\cdot](p)$ and put $p=\frac{a^2}{4\pi^2}$ in the same way as we proved Corollary 4.

To prove Formula (iii), we use a specialization of our formula in Theorem 4 with $n=2$, $Y=I$, $\boldsymbol{g}=\boldsymbol{h}=\boldsymbol{0}$, $s\to\frac{1}{2}$:

$$Z\left(I,\boldsymbol{0},\boldsymbol{0},\frac{1}{2}\right)=\sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^2\\ \boldsymbol{r}\neq\boldsymbol{0}}}\frac{\operatorname{erfc}\left(\frac{\pi}{\sqrt{a}}r\right)}{r}+\sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^2\\ \boldsymbol{r}\neq\boldsymbol{0}}}\frac{\operatorname{erfc}(\sqrt{a}r)}{r}-2\sqrt{\frac{\pi}{a}}-2\sqrt{\frac{a}{\pi}}.\tag{3.16}$$

Taking the Laplace transforms of (3.16), we obtain (iii). Formula (iii) is Chaba-Pathria [9, (42)] and Borweins (9).

Formula (iii)′ follows from (iii) and is denoted by D ([9, (36)]), which should be defined as (iii)′. It is given as Formula (7) in Borweins.

Corollary 6. For the special choice $\beta=\underline{\frac{1}{2}}=\left(\frac{1}{2},\frac{1}{2}\right)$, we write $E_\beta(a)=E_-(a)$ and let $\rho=\frac{1}{2}\sqrt{(2m+1)^2+(2n+1)^2}$ instead of r. Then we have

$$\lim_{x\to 0+}E_-(x+i\theta)=i\theta+\gamma\left(\frac{1}{2}\right)-\sum_{m,n}\left(\frac{1}{\rho}-\frac{1}{\sqrt{\rho^2-\frac{\theta^2}{4\pi^2}}}\right).\tag{3.17}$$

This is Borweins' formula (11), from which their Abel mean formulas for

$$S_\pm(\theta)=\sum_{n=1}^{\infty}\frac{(\pm 1)^n r(n)}{\sqrt{n}}\sin(\sqrt{n}\theta),$$
$$C_\pm(\theta)=\sum_{n=1}^{\infty}\frac{(\pm 1)^n r(n)}{\sqrt{n}}\cos(\sqrt{n}\theta)$$

can be read off immediately, where $r(n)$ stands for the number of representations of n as the sum of two squares.

More general questions concerning $S_\beta(\theta) = \sum_{\substack{\boldsymbol{r}\in\mathbb{Z}^2\\ \boldsymbol{r}\neq\boldsymbol{0}}} \frac{e^{-2\pi i\beta\cdot r}}{r} e^{2\pi i r\theta}$ and generalizations will be considered elsewhere.

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SUM RELATIONS FOR MULTIPLE ZETA VALUES

To the memory of Professor Tsuneo Arakawa

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Abstract In this note we shall present some identities between sums of multiple zeta values and Riemann zeta values after an overview of our results in [13],[18] and [20]. An application of the identities to the Arakawa-Kaneko zeta functions shall also be given. Throughout this note, we shall point out the importance of classifying multiple zeta values by the indices called weight, depth and height, and we shall also indicate the significance of multiple zeta-star values.

1. Introduction

Recently, the multiple zeta values have been appeared in various fields of mathematics and physics and are studied with many interests. These values are defined as follows: For any multi-index $\mathbf{k} = (k_1, k_2, \ldots, k_n)$ ($k_i \in \mathbf{Z}$, $k_i > 0$, the *weight* $\mathrm{wt}(\mathbf{k})$, *depth* $\mathrm{dep}(\mathbf{k})$, and *height* $\mathrm{ht}(\mathbf{k})$ of $\mathbf{k}$ are by definition the integers $k = k_1 + k_2 + \cdots + k_n$, n, and $s = \#\{i | k_i > 1\}$, 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 $k_1 \geq 2$. 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

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

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Various relations among these values have been studied. Here we review two well known basic identities, one is called the *duality* and the other is called the *sum formula* of multiple zeta values.

First, we define the *dual index.* For any admissible index $\mathbf{k}$, positive integers s and $a_1, b_1, a_2, b_2, \ldots, a_s, b_s$ are uniquely determined, so that $\mathbf{k}$ is written in the form

$$\mathbf{k} = (a_1 + 1, \underbrace{1, \ldots, 1}_{b_1 - 1}, a_2 + 1, \underbrace{1, \ldots, 1}_{b_2 - 1}, \ldots, a_s + 1, \underbrace{1, \ldots, 1}_{b_s - 1}).$$

Then the dual index $\mathbf{k}'$ of $\mathbf{k}$ is defined by

$$\mathbf{k}' = (b_s + 1, \underbrace{1, \ldots, 1}_{a_s - 1}, b_{s-1} + 1, \underbrace{1, \ldots, 1}_{a_{s-1} - 1}, \ldots, b_1 + 1, \underbrace{1, \ldots, 1}_{a_1 - 1}).$$

By the definition, $\mathbf{k}'$ is obviously an admissible index and

$$\mathrm{wt}(\mathbf{k}') = \mathrm{wt}(\mathbf{k}), \quad \mathrm{dep}(\mathbf{k}') = \mathrm{wt}(\mathbf{k}) - \mathrm{dep}(\mathbf{k}), \quad \mathrm{ht}(\mathbf{k}') = \mathrm{ht}(\mathbf{k})$$

are satisfied.

Theorem 1 (Duality). For any admissible index $\mathbf{k}$ and its dual index $\mathbf{k}'$, we have

$$\zeta(\mathbf{k}') = \zeta(\mathbf{k}).$$

Theorem 2 (Sum formula). For any integers $k > n > 0$, we have

$$\sum_{\substack{\mathbf{k}:\text{admissible}, \\ \mathrm{wt}(\mathbf{k})=k, \quad \mathrm{dep}(\mathbf{k})=n}} \zeta(\mathbf{k}) = \zeta(k).$$

Here the right-hand side denotes the Riemann zeta value.

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

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

then the left-hand side of the sum formula can be written as

$$\sum_{s=1}^{\min(n, \ k-n)} G_0(k, n, s) .$$

The sum formula was firstly proved by A. Granville ([9]) and D. Zagier ([27]). We state three kinds of generalization of this formula in the next section.

2. Generalizations of the sum formula

In this section we shall see three types of generalization of the sum formula. We end each subsection by mentioning several special cases of each theorem which were previously known or are of special interest.

2.1 A simultaneous generalization of duality and sum formula

Here we review a simultaneous generalization of duality and the sum formula presented in [18]. This formula was reproved in the context of derivation relations by K. Ihara, M. Kaneko and D. Zagier in [14] and in terms of the Mellin transform of Landen's connection formula for polylogarithms by J. Okuda and K. Ueno in [21]. As we stated in the original paper, the formula also contaions M. E. Hoffman's result (see below).

For any admissible index $\mathbf{k} = (k_1, k_2, \ldots, k_n)$ and for any integer $l \geq 0$, we define $Z(\mathbf{k}; l)$ by

$$Z(\mathbf{k}; l) = \sum_{\substack{\varepsilon_1+\varepsilon_2+\cdots+\varepsilon_n=l, \\ \forall \varepsilon_j \geq 0}} \zeta(k_1+\varepsilon_1, k_2+\varepsilon_2, \ldots, k_n+\varepsilon_n).$$

Theorem 3 ([18]). For any admissible index $\mathbf{k}$ and its dual $\mathbf{k}'$ and for any integer $l \geq 0$, we have

$$Z(\mathbf{k}'; l) = Z(\mathbf{k}; l). \tag{2.1}$$

(a) If we put $l = 0$ then we get duality formula from (2.1).

(b) When $\mathrm{dep}(\mathbf{k}) = 1$, (2.1) implies the sum formula. In fact, for any integers $k > n > 1$, if we take $\mathbf{k} = (n+1)$ then the dual index of $\mathbf{k}$ is

$$\mathbf{k}' = (2, \underbrace{1, 1, \ldots, 1}_{n-1})$$

and we have

$$\begin{aligned} Z(\mathbf{k}'; k-n-1) &= \sum_{\substack{\varepsilon_1+\varepsilon_2+\cdots+\varepsilon_n=k-n-1, \\ \forall \varepsilon_j \geq 0}} \zeta(2+\varepsilon_1, 1+\varepsilon_2, 1+\varepsilon_3, \ldots, 1+\varepsilon_n) \\ &= \sum_{\substack{\mathbf{k}'': \text{admissible}, \\ \mathrm{wt}(\mathbf{k}'')=k, \quad \mathrm{dep}(\mathbf{k}'')=n}} \zeta(\mathbf{k}''). \end{aligned}$$

On the other hand, we have $Z(\mathbf{k}; k-n-1) = \zeta(k)$ on the right.

(c) If we put $l = 1$ on (2.1) and apply the duality formula for each term of the right-hand side of the equality, then we get Hoffman's relation (Theorem 5.1 of [10]).

2.2 Sum of Multiple zeta values and Riemann zeta values

Another generalization of the sum formula has been given by our joint research ([20]) with D. Zagier. This general formula contains the sum formula, Le-Murakami's formula and a few other known relations (see below).

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

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

If the indices k, n and s satisfy the conditions $n \ge s \ge 1$ and $k \ge n+s$, then the set $I_0(k,n,s)$ is non-empty and $G_0(k,n,s)$ has a positive value and so we can collect all the numbers $G_0(k,n,s)$ into a single generating function

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

Theorem 4 ([20]). The power series Φ_0 is given by

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

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

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

or alternatively by the identity

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

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.

We can also restate the formula in the alternative form

$$1 \,-\, (xy-z)\,\Phi_0(x,y,z) \;=\; \prod_{m=1}^{\infty}\left(1 \,-\, \frac{xy-z}{(m-x)(m-y)}\right), \tag{2.2}$$

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

(a) Specializing Theorem 4 to $z = xy$ we get

$$\Phi_0(x, y, xy) = \sum_{k>n>0} G_0(k, n) x^{k-n-1} y^{n-1}$$

where $G_0(k, n) = \displaystyle\sum_{s=1}^{\min(n,\ k-n)} G_0(k, n, s)$ 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 the alternative form (2.2), 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 $G_0(k, n) = \zeta(k)$ stated above.

(b) If we put $s = 1$, then $G_0(k, n, 1) = \zeta(k - n + 1, \underbrace{1, \ldots, 1}_{n-1})$. On the other hand, we have $S_n(x, y, 0) = x^n + y^n - (x + y)^n$, so $\Phi_0(x, y, 0)$ reduces to

$$\begin{aligned} &\sum_{a,\, b \geq 1} \zeta(a + 1, \underbrace{1, \ldots, 1}_{b-1})\, x^a y^b \\ &\qquad = \frac{1}{xy} \left(1 - \exp\left(\sum_{n=2}^{\infty} \zeta(n)\, \frac{x^n + y^n - (x + y)^n}{n}\right)\right), \end{aligned}$$

a formula given in [27].

(c) Specializing Theorem 4 to $x = y = 0$ corresponds to the unique zeta value $\zeta(2, \ldots, 2)$ (with $k = 2n = 2s$), so we get

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

and hence $\zeta(\underbrace{2, \ldots, 2}_{s}) = \dfrac{\pi^{2s}}{(2s + 1)!}$ a formula reproved many times by many mathematicians.

(d) If we put $y = -x$, we obtain the formula proved by T. Q. T. Le and J. Murakami([16]);

$$\sum_{n=s}^{2k-s} \sum_{\mathbf{k} \in I_0(2k,n,s)} (-1)^n \zeta(\mathbf{k}) = \frac{(-1)^k}{(2k+1)!} \sum_{r=0}^{k-s} \binom{2k+1}{2r} (2 - 2^{2r}) B_{2r} \pi^{2k}$$

where the integers k, s satisfy $k \geq s \geq 1$ and B_m denotes the m-th Bernoulli number.

2.3 Cyclic sum formula

The remainder of this section will be devoted to state the cyclic sum formula. The formula was conjectured by M. E. Hoffman and proved by the author([13]). Sum formula is an easy consequence of this formula. One of the open questions for mathematicians interested in multiple zeta values is "Can we generalize the cyclic sum formula?". For the reader's convenience, we review the proof of the formula.

First, we define *cyclic equivalence classes* of multiple indices in the set

$$I(k,n) = \bigcup_{s=1}^{\min(n,\ k-n)} I(k,n,s) .$$

We say two elements of $I(k,n)$ are cyclically equivalent if they are cyclic permutations of each other, i.e., for $\sigma = (k_1, k_2, \ldots, k_n)$ and for $j = 1, 2, \ldots, n$, we define $(k_1, k_2, \ldots, k_n) \equiv (\sigma^j(k_1), \sigma^j(k_2), \ldots, \sigma^j(k_n))$. Let $\Pi(k,n)$ be the set of cyclic equivalence classes of $I(k,n)$. For any $\alpha \in \Pi(k,n)$, it is easy to see that the dual indices of all admissible indices in α are cyclic permutations of each other. Thus, we postulate that $\beta \in \Pi(k, k-n)$ is the "dual" of $\alpha \in \Pi(k,n)$, if the dual index of an admissible index in α is in β.

Theorem 5 (Cyclic sum formula [13]). For any integers $k > n > 0$, and for $\alpha \in \Pi(k,n)$ and its dual $\beta \in \Pi(k, k-n)$, we have

$$\sum_{(k_1,\ldots,k_n)\in\alpha} \zeta(k_1+1, k_2, \ldots, k_n) = \sum_{(k'_1,\ldots,k'_{k-n})\in\beta} \zeta(k'_1+1, k'_2, \ldots, k'_{k-n}).$$

Theorem 6 (Cyclic sum formula without duality [13]). For any index set $\alpha \in \Pi(k,n)$ with $n < k$, we have

$$\sum_{(k_1,k_2,\ldots,k_n)\in\alpha} \zeta(k_1+1, k_2, k_3, \ldots, k_n)$$

$$= \sum_{(k_1,k_2,\ldots,k_n)\in\alpha} \sum_{i=0}^{k_1-2} \zeta(k_1 - i, k_2, \ldots, k_n, i+1)$$

where the inner sum on the right-hand side is treated as 0 whenever $k_1 = 1$.

We can easily see that Theorem 5 and Theorem 6 are equivalent to each other up to the duality formula.

In the proof of the cyclic sum formula, we treated a key lemma on a infinite series T defined as follows. For any positive integers $n,\ k_1, \dots, k_n$ with $k_1 + \cdots + k_n > n$ (i.e., at least one of the k_i's is > 1), let $T(k_1, k_2, \dots, k_n)$ be defined as the convergent series

$$T(k_1, k_2, \dots, k_n) = \sum_{a_1 > a_2 > \cdots > a_n > a_{n+1} \geq 0} \frac{1}{a_1^{k_1} a_2^{k_2} \cdots a_n^{k_n} (a_1 - a_{n+1})}.$$

Key Lemma 1. For any positive integers $n,\ k_1, \dots, k_n$ with $k_i > 1$ for some i, we have

$$T(k_1, k_2, \dots, k_n) - T(k_2, k_3, \dots, k_n, k_1)$$

$$= \zeta(k_1 + 1, k_2, \dots, k_{n-1}, k_n) - \sum_{i=0}^{k_1-2} \zeta(k_1 - i, \dots, k_{n-1}, k_n, i+1),$$

where the sum on the right is understood to be 0 if $k_1 = 1$.

Proof of Key lemma 1 For any integers $r \geq 2$ and $i \geq 0$, we have

$$\begin{aligned}
&\sum_{a_1 > \cdots > a_n > a_{n+1} > 0} \frac{1}{a_1^{r} a_2^{k_2} \cdots a_n^{k_n} a_{n+1}^{i} (a_1 - a_{n+1})} \\
&= \sum_{a_1 > \cdots > a_n > a_{n+1} > 0} \frac{1}{a_1^{r-1} a_2^{k_2} \cdots a_n^{k_n} a_{n+1}^{i+1}} \Big(\frac{1}{a_1 - a_{n+1}} - \frac{1}{a_1} \Big) \\
&= \sum_{a_1 > \cdots > a_n > a_{n+1} > 0} \frac{1}{a_1^{r-1} a_2^{k_2} \cdots a_n^{k_n} a_{n+1}^{i+1} (a_1 - a_{n+1})} \\
&\qquad - \zeta(r, k_2, \dots, k_n, i+1).
\end{aligned}$$

Putting $r = k_1 - i$ and adding up the above equality for $i = 0, 1, \dots, k_1 - 2$, we obtain

$$\sum_{a_1>\cdots>a_n>a_{n+1}>0} \frac{1}{a_1^{k_1}a_2^{k_2}\cdots a_n^{k_n}(a_1-a_{n+1})}$$
$$= \sum_{a_1>\cdots>a_n>a_{n+1}>0} \frac{1}{a_1 a_2^{k_2}\cdots a_n^{k_n}a_{n+1}^{k_1-1}(a_1-a_{n+1})}$$
$$-\sum_{i=0}^{k_1-2}\zeta(k_1-i,k_2,\ldots,k_n,i+1).$$

The left-hand side of this equality becomes

$$T(k_1,k_2,\ldots,k_n)-\zeta(k_1+1,k_2,\ldots,k_n)$$

and the first sum on the right-hand side can be written as

$$\sum_{a_1>\cdots>a_n>a_{n+1}>0} \frac{1}{a_2^{k_2}\cdots a_n^{k_n}a_{n+1}^{k_1}}\Big(\frac{1}{a_1-a_{n+1}}-\frac{1}{a_1}\Big)$$
$$= \sum_{a_2>\cdots>a_n>a_{n+1}>0} \frac{1}{a_2^{k_2}\cdots a_{n-1}^{k_{n-1}}a_n^{k_n}a_{n+1}^{k_1}} \sum_{a_1=a_2+1}^{\infty}\Big(\frac{1}{a_1-a_{n+1}}-\frac{1}{a_1}\Big)$$
$$= \sum_{a_2>\cdots>a_n>a_{n+1}>0} \frac{1}{a_2^{k_2}\cdots a_n^{k_n}a_{n+1}^{k_1}} \sum_{a_{n+2}=0}^{a_{n+1}-1}\frac{1}{a_2-a_{n+2}}$$
$$= \sum_{a_1>\cdots>a_n>a_{n+1}>a_{n+2}\geq 0} \frac{1}{a_2^{k_2}\cdots a_n^{k_n}a_{n+1}^{k_1}(a_2-a_{n+2})}$$
$$= T(k_2,\ldots,k_n,k_1).$$

Q.E.D.

Proof of Theorem 6 The cyclic sum formula is readily proved when we apply the Key Lemma 1 for all cyclic permutations of $(k_1,k_2,\ldots,k_n)$ and add them up. Q.E.D.

(a) It is worth pointing out that Theorem 6 provides another proof of the sum formula.

Proof We add up the equality in Theorem 6 for all cyclic equivalence classes of $I(k,n)$ to obtain

$$\sum_{(k_1,k_2,\ldots,k_n)\in I(k,n)} \zeta(k_1+1,k_2,\ldots,k_n)$$
$$= \sum_{(k_1,k_2,\ldots,k_n)\in I(k,n)} \sum_{i=0}^{k_1-2}\zeta(k_1-i,\ldots,k_n,i+1). \tag{2.3}$$

Now, we use the following lemma:

Lemma 1. For any integers k and n with $0 < n < k$,

$$\sum_{(k_1,k_2,\dots,k_{n+1})\in I(k,n+1)} \zeta(k_1+1,k_2,\dots,k_{n+1})$$
$$= \sum_{(t,k_2,k_3,\dots,k_n)\in I(k,n)} \sum_{i=0}^{t-2} \zeta(t-i,k_2,\dots,k_n,i+1) \tag{2.4}$$

Proof of lemma 1 The left-hand side of (2.4) is a sum of $\binom{k-1}{n}$ terms and the right-hand side has $\left(\sum_{t=2}^{k-n+1}(t-1)\binom{k-t-1}{n-2}\right)$ terms, and by using the formula $\sum_{i=1}^{n} i\binom{n+s-i-1}{n-i} = \binom{n+s}{s+1}$, we can see that these two numbers are the same.

For any index $(k_1,k_2,\dots,k_{n+1}) \in I(k,n+1)$, we have $(k_1+k_{n+1},\ k_2,\ k_3,\dots,k_n) \in I(k,n)$ and so on the right-hand side of (2.4), the terms

$$\sum_{i=0}^{k_1+k_{n+1}-2} \zeta(k_1+k_{n+1}-i,k_2,\dots,k_n,i+1)$$

occur. If we fix $i = k_{n+1}-1$, then the condition $0 \le i = k_n - 1 \le k_0+k_n-2$ is satisfied, so on the right-hand side, the term $\zeta(k_1+1,k_2,\dots,k_{n+1})$ occurs. Thus, the entries of both sides are the same and each entry appears exactly once, so the equality is valid. Q.E.D.

By using the lemma, (2.3) gives the following equality for any integers $0 < n < k$,

$$\sum_{(k_1,k_2,\dots,k_n)\in I(k,n)} \zeta(k_1+1,k_2,\dots,k_n)$$
$$= \sum_{(k_1,k_2,\dots,k_{n+1})\in I(k,n+1)} \zeta(k_1+1,k_2,\dots,k_{n+1}).$$

Thus, the sum formula follows by induction on n. Q.E.D.

(b) We can also prove the sum formula by using Theorem 5 and the duality theorem, i.e., if we add up the equality of Theorem 5 for all entries of $\Pi(k,n)$, then we get the equality between $G_0(k+1,n)$ and $G_0(k+1,k-n)$. Duality theorem implies the identity $G_0(k+1,k-n) = G_0(k+1,n+1)$. We apply this identity to the right-hand side of the equality thus obtained, we get the same formula as in the last part of the above proof.

3. Identities associated with Arakawa-Kaneko zeta functions

3.1 New formula and its application

Here we state a family of relations between the sums of multiple zeta values and the rational multiple of Riemann zeta values. The result also gives some information on the Arakawa-Kaneko zeta functions.

Theorem 7. For any integer $k > 1$, we have

$$\sum_{n=1}^{k-1}\sum_{l=1}^{n}\sum_{\substack{a_i>0\ (i=1,2,\ldots,n),\\ a_1+\cdots+a_l=n}} \zeta(k-n+a_1, a_2, a_3, \ldots, a_l) \;=\; 2(k-1)(1-2^{1-k})\zeta(k).$$

This theorem shall be restated in the next section in terms of *multiple zeta-star values.*

As an application of Theorem 7, we can express sums of special values of the Arakawa-Kaneko zeta functions in terms of Riemann zeta values.

For any positive integer $k \geq 1$, T. Arakawa and M. Kaneko [3] defined the function $\xi_k(s)$ by

$$\xi_k(s) = \frac{1}{\Gamma(s)}\int_0^{\infty}\frac{t^{s-1}}{e^t-1}\mathrm{Li}_k(1-e^{-t})dt,$$

where $\mathrm{Li}_k(s)$ denotes the k-th polylogarithm $\mathrm{Li}_k(s) = \sum_{m=1}^{\infty}\frac{s^m}{m^k}$. The integral converges for $\mathrm{Re}(s) > 0$ and the function $\xi_k(s)$ continues to an entire function of whole s-plane. They proved that the special values of $\xi_k(s)$ at non-positive integers are given by poly-Bernoulli numbers and the values at positive integers are given in terms of multiple zeta values. Thereafter we gave in [18] the following representation for the values of $\xi_k(s)$ at positive integers.

Proposition 1. For any positive integers k and n, we have

$$\xi_k(n) \;=\; \sum_{m_1\geq m_2\geq\cdots\geq m_n\geq 1}\frac{1}{{m_1}^{k+1}m_2\cdots m_n}.$$

Using this representation, we have the following proposition.

Proposition 2. For any positive integer k, we have

$$\sum_{n=1}^{k-1}\xi_{k-n}(n) = 2(k-1)(1-2^{1-k})\zeta(k).$$

3.2 Proof of Theorem 7

By using the iterated integral expression of multiple zeta values (cf. [26] or (2) of [12]), we can rewrite the left-hand side of the equality of Theorem 7 as follows:

$$
\begin{aligned}
&\sum_{n=1}^{k-1}\sum_{l=1}^{n}\sum_{a_1+\cdots+a_l=n}\zeta(k-n+a_1,a_2,a_3,\ldots,a_l)\\
&=\sum_{n=1}^{k-1}\int\cdots\int_{0<t_1<\cdots<t_k<1}\frac{1}{1-t_1}\left(\frac{1}{t_2}+\frac{1}{1-t_2}\right)\cdots\left(\frac{1}{t_n}+\frac{1}{1-t_n}\right)\\
&\qquad\qquad\times\frac{1}{t_{n+1}}\frac{1}{t_{n+2}}\cdots\frac{1}{t_k}\,dt_1\cdots dt_k\\
&=\sum_{n=1}^{k-1}\frac{1}{(k-n-1)!(n-1)!}\iint_{0<t_1<t_{n+1}<1}\frac{1}{1-t_1}\left(\int_{t_1}^{t_{n+1}}\left(\frac{1}{t}+\frac{1}{1-t}\right)dt\right)^{n-1}\\
&\qquad\qquad\times\frac{1}{t_{n+1}}\left(\int_{t_{n+1}}^{1}\frac{1}{t}dt\right)^{k-n-1}dt_1\;dt_{n+1}\\
&=\sum_{n=1}^{k-1}\frac{1}{(k-n-1)!(n-1)!}\iint_{0<t_1<t_2<1}\left(\log\frac{t_2}{t_1}+\log\frac{1-t_1}{1-t_2}\right)^{n-1}\\
&\qquad\qquad\times\left(\log\frac{1}{t_2}\right)^{k-n-1}\frac{dt_1dt_2}{(1-t_1)t_2}\\
&=\frac{1}{(k-2)!}\iint_{0<t_1<t_2<1}\left(\log\frac{1}{t_1}+\log\frac{1-t_1}{1-t_2}\right)^{k-2}\frac{dt_1dt_2}{(1-t_1)t_2}.
\end{aligned}\tag{3.1}
$$

We change the variables as

$$x=\log\frac{1}{t_1}+\log\frac{1-t_1}{1-t_2}\quad,\quad y=\log\frac{1}{t_1},$$

$$\frac{dt_1dt_2}{(1-t_1)t_2}=\frac{dxdy}{e^x-e^y+1},$$

then (3.1) becomes

$$\begin{aligned}
&\frac{1}{(k-2)!}\int_0^\infty \int_0^x \frac{x^{k-2}}{e^x-e^y+1}dx\ dy \\
&= \frac{1}{(k-2)!}\int_0^\infty \left(\frac{-x^{k-2}}{e^x+1}[\log(e^{x-y}+e^{-y}-1)]_{y=0}^{y=x}\right)\ dx \\
&= \frac{2}{(k-2)!}\int_0^\infty \frac{x^{k-1}}{e^x+1}dx \\
&= 2(k-1)(1-2^{1-k})\zeta(k).
\end{aligned}$$

So we get Theorem 7. Q.E.D.

4. Multiple zeta-star values and restriction on weight, depth, and height

For any admissible index $\mathbf{k}=(k_1,k_2,\ldots,k_n)$, another type of multiple zeta values shall be concerned in this section. *Multiple zeta-star values* $\zeta^*(\mathbf{k})$ are defined as follows:

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

Note that, there are linear relations among ζ^* and ζ, for example,

$$\zeta^*(k_1,k_2)=\zeta(k_1,k_2)+\zeta(k_1+k_2),\quad \zeta(k_1,k_2)=\zeta^*(k_1,k_2)-\zeta^*(k_1+k_2),$$

$$\zeta^*(k_1,k_2,k_3)=\zeta(k_1,k_2,k_3)+\zeta(k_1+k_2,k_3)+\zeta(k_1,k_2+k_3)+\zeta(k_1+k_2+k_3),$$

$$\zeta(k_1,k_2,k_3)=\zeta^*(k_1,k_2,k_3)-\zeta^*(k_1+k_2,k_3)-\zeta^*(k_1,k_2+k_3)+\zeta^*(k_1+k_2+k_3),$$

and so on. Multiple zeta-star values ζ^* had been studied by Euler[7], and his study is the origin of various researches of multiple zeta values ζ.

In terms of multiple zeta-star values, we can restate Theorem 7 as follows. We see that the statement becomes much simpler in the context of ζ^*.

Theorem 8. For any integer $k>1$, we have

$$\sum_{n=1}^{k-1}\zeta^*(k-n+1,\underbrace{1,\ldots,1}_{n-1})\ =\ 2(k-1)(1-2^{1-k})\zeta(k).$$

If we denote by $G_0^*(k,n,s)$ the value of the sum

$$G_0^*(k,n,s)\ =\ \sum_{\mathbf{k}\in I_0(k,n,s)}\zeta^*(\mathbf{k})\ ,$$

then Theorem 8 is

$$\sum_{n=1}^{k-1} G_0^*(k,n,1) \;=\; 2(k-1)(1-2^{1-k})\zeta(k)\ . \qquad (4.1)$$

Farther generalization

$$\sum_{n=s}^{k-s} G_0^*(k,n,s) \;=\; 2\binom{k-1}{2s-1}(1-2^{1-k})\zeta(k)$$

of (4.1) shall be shown in terms of connection formulas for the Gauss hypergeometric function in [1] by our joint work with T. Aoki.

On the other hand, the well known formula

$$\sum_{s=1}^{\min(n,\ k-n)} G_0^*(k,n,s) \;=\; \binom{k-1}{n-1}\zeta(k).$$

(sum formula for ζ^*) is also reproved recently by using a differential equation of first order ([15]).

In the results stated in this note, especially in Theorems 2,3,4 and 8, it seems that the sums of all zeta values ζ (or ζ^*) of fixed weight, depth and height (namely G_0 or G_0^*) are good objects to treat, and their generating function fits to a certain kind of differential equations and their connection formulas.

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THE SUM FORMULA FOR MULTIPLE ZETA VALUES AND CONNECTION PROBLEM OF THE FORMAL KNIZHNIK-ZAMOLODCHIKOV EQUATION

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Abstract The sum formula for multiple zeta values are derived, via the Mellin transform, from the Euler connection formula and the Landen connection formula for polylogarithms. These connection formulas for multiple polylogarithms will be considered in the framework of the theory of the formal Knizhnik-Zamolodchikov equation.

1. Introduction

In this paper, we will derive the sum formula [Gra97] for multiple zeta values (MZVs, for short) in two ways: We will show that the Mellin transform of the Euler connection formula and the Landen connection formula for polylogarithms gives the sum formula, respectively. Furthermore we will clarify the meaning of these connection formulas for multiple polylogarithms (MPLs, briefly) in the framework of the connection problem of the formal Knizhnik-Zamolodchikov equation.

In [OU04], we considered the Ohno relation for MZVs [Ohn99] by means of the generating functional method: That is, we introduced the two generating functions $f((a_i, b_i)_{i=1}^{s}; \lambda)$, $g((a_i, b_i)_{i=1}^{s}; \lambda)$ by which the Ohno relation is represented as $f = g$, and found the subfamily $F_{\mathbf{k}}(\lambda) = G_{\mathbf{k}}(\lambda)$ of the Ohno relation which is converted to the Landen connection

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formula for MPLs by the inverse Mellin transform. This subfamily was called the reduced Ohno relation.

The multiple polylogarithm is, by definition,

$$\mathrm{Li}_{k_1,k_2,\ldots,k_m}(z)=\sum_{n_1>n_2>\cdots>n_m>0}\frac{z^{n_1}}{n_1^{k_1}n_2^{k_2}\cdots n_m^{k_m}},\tag{1.1}$$

and the Landen connection formula [OU04]

$$\mathrm{Li}_{k_1,\ldots,k_m}(z)=(-1)^n\sum_{\substack{\mathbf{c}_1,\ldots,\mathbf{c}_m\\ \text{weight of }\mathbf{c}_j=k_j}}\mathrm{Li}_{\mathbf{c}_1,\ldots,\mathbf{c}_m}\left(\frac{z}{z-1}\right)\tag{1.2}$$

can be thought of the connection formula between $z=1$ and $z=\infty$ for MPLs. On the other hand, the Euler inversion formula [Lew81] for the dilogarithm

$$\mathrm{Li}_2(z)+\mathrm{Li}_1(1-z)\mathrm{Li}_1(z)+\mathrm{Li}_2(1-z)=\zeta(2)\tag{1.3}$$

and its generalization (the Euler connection formula) give the connection formula between $z=0$ and $z=1$ for MPLs. Only the polylogarithm case will be treated in this paper. It seems interesting to calculate relations for general MPLs.

These connection formulas can be easily verified by elementary methods, but can be understood in a unified way by considering the connection problem for the formal Knizhnik-Zamolodchikov equation

$$\frac{dG}{dz}=\left(\frac{X}{z}+\frac{Y}{1-z}\right)G.\tag{KZ}$$

This paper is organized as follows: In Section 2, we will briefly review the theory of the shuffle algebra $\mathfrak{h}=(\mathbb{C}\langle x,y\rangle,\,ш)$ and the regularization map defined on it, according to the arguments in [IK01, HPH99] and [Oku03]. As an element in $\mathfrak{H}=\mathbb{C}\langle\langle X,Y\rangle\rangle$, which is thought of to be the topological dual of $\mathfrak{h}$, the Drinfel′d associator φ_{KZ} constructed in [Dri90] is canonically introduced. In Section 3, we will consider the link between the connection formulas for MPLs and the connection problem for (KZ). The solutions G_0, G_1, G_∞ to (KZ) are defined to be unique ones satisfying the prescribed asymptotic properties around each singular point. In particular, G_0 plays a role of the generating function for MPLs, and G_1 and G_∞ are expressed in terms of G_0 and homomorphisms induced from linear fractional transformations preserving the singular points. Thus the connection problem for (KZ) leads to the connection formulas for MPLs. Furthermore, we can verify the so called hexagon relation [Dri90] satisfied by the Drinfel′d associator by using a sort of the braid relation for the induced homomorphisms. These results are parallel to those in [HPH99], however they did not use the regularization map defined on $\mathfrak{h}$ which was firstly introduced by [IK01] and [Kan02]. In Section 4, we will see that the sum formula for MZVs follows from the Mellin transform of the Euler connection formula and the Landen connection formula for polylogarithms. In Section 5, we will consider the connection problem for the system (KZ_3) [Dri90] over the configuration space of ordered three points in the complex line $X_3(\mathbb{C}) = \{(z_1, z_2, z_3) \in \mathbb{C}^3 \mid z_i \neq z_j \ (i \neq j)\}$

$$dW = \left(\sum_{1 \le i < j \le 3} X_{ij} d \log(z_i - z_j) \right) W, \tag{KZ_3}$$

where the coefficients satisfy $X_{ij} = X_{ji}, \quad [X_{ij}, X_{ik} + X_{kj}] = 0$, with the aid of the connection problem for (KZ). Through these investigations, we see that the relations for MPLs which come from the connection problem of (KZ_3) are only the Euler connection formula and the Landen connection formula in a essential sense.

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2. Shuffle Algebra

We define the shuffle product $ш$ on the non-commutative polynomial algebra $\mathfrak{h} = \mathbb{C}\langle x, y \rangle$ of letters x and y, recursively by

$$\begin{aligned} 1 ш w &= w ш 1 = w, \\ l_1 w_1 ш l_2 w_2 &= l_1 (w_1 ш l_2 w_2) + l_2 (l_1 w_1 ш w_2), \end{aligned}$$

where w, w_1 and w_2 are monomials and l_1 and l_2 are the letters. Now let us introduce the subalgebras $\mathfrak{h} \supset \mathfrak{h}^1 \supset \mathfrak{h}^0$ with respect to $ш$ and concatenation product defined by

$$\mathfrak{h}^1 = \mathbb{C}1 \oplus \mathfrak{h} y, \qquad \mathfrak{h}^0 = \mathbb{C}1 \oplus x \mathfrak{h} y. \tag{2.1}$$

For $w = x^{k_1-1}y\cdots x^{k_m-1}y \in \mathfrak{h}^0$, we set a linear map $\widehat{\zeta} : \mathfrak{h}^0 \to \mathbb{C}$ by

$$\widehat{\zeta}(w) = \zeta(k_1,\ldots,k_m) = \sum_{n_1>\cdots>n_m>0} \frac{1}{n_1^{k_1}\cdots n_m^{k_m}}, \tag{2.2}$$

which is a multiple zeta value. Then $\widehat{\zeta}$ is a homomorphism with respect to $\sqcup\!\sqcup$, that is,

$$\widehat{\zeta}(w_1 \sqcup\!\sqcup w_2) = \widehat{\zeta}(w_1)\widehat{\zeta}(w_2). \tag{2.3}$$

It is well known that $\mathfrak{h}$ is a polynomial algebra with respect to the product $\sqcup\!\sqcup$ generated by the Lyndon words (cf. [Reu93]). In particular the Lyndon words contain the letters x and y, and $\mathfrak{h}$ can be decomposed as follows:

$$\begin{aligned}\mathfrak{h} &= \bigoplus_{n=0}^{\infty} \mathfrak{h}^1 \sqcup\!\sqcup x^{\sqcup\!\sqcup n} = \mathfrak{h}^1[x] \\ &= \bigoplus_{m,n=0}^{\infty} y^{\sqcup\!\sqcup m} \sqcup\!\sqcup \mathfrak{h}^0 \sqcup\!\sqcup x^{\sqcup\!\sqcup n} = \mathfrak{h}^0[x,y].\end{aligned} \tag{2.4}$$

Let $\mathrm{reg} : \mathfrak{h} = \mathfrak{h}^0[x,y] \to \mathfrak{h}^0$ be a map to associate the constant term in the decomposition $\mathfrak{h} = \mathfrak{h}^0[x,y]$ to each element in $\mathfrak{h}$. This is called the reguralization map, and is a $\sqcup\!\sqcup$-homomorphism.

Proposition 1 ([IK01]). For $w \in \mathfrak{h}^0$,

$$\mathrm{reg}(y^m w x^n) = \sum_{i=0}^{m}\sum_{j=0}^{n} (-1)^{i+j} y^i \sqcup\!\sqcup y^{m-i} w x^{n-j} \sqcup\!\sqcup x^j, \tag{2.5}$$

or equivalently

$$y^m w x^n = \sum_{i=0}^{m}\sum_{j=0}^{n} y^i \sqcup\!\sqcup \mathrm{reg}(y^{m-i} w x^{n-j}) \sqcup\!\sqcup x^j. \tag{2.6}$$

Let us introduce the algebra $\mathfrak{H} = \mathbb{C}\langle\langle X, Y\rangle\rangle$ of non-commutative formal power series over $\mathbb{C}$ in the letters X and Y. This is thought of to be the topological dual of $\mathfrak{h}$. Then the latter equation (2.6) is expressed by the "formal" Chen series in $\mathfrak{h}\widehat{\otimes}\mathfrak{H}$ [IK01]

$$\begin{aligned}\sum_W wW &= 1 + xX + yY + xxXX + xyXY + yxYX + yyYY + \cdots \\ &= \exp_{\sqcup\!\sqcup}(yY)\left(\sum_W \mathrm{reg}(w)W\right)\exp_{\sqcup\!\sqcup}(xX),\end{aligned} \tag{2.7}$$

where W runs over all the monomials in $\mathfrak{H}$, and $\exp_{ш}$ is a series defined by

$$\begin{aligned}\exp_{ш}(xX) &= 1 + xX + \frac{x^{ш2}X^2}{2!} + \frac{x^{ш3}X^3}{3!} + \cdot \\ &= 1 + xX + x^2X^2 + x^3X^3 + \cdots\end{aligned}$$

as well as $\exp_{ш}(yY)$.

Let $\varphi_{\mathrm{KZ}}(X,Y) \in \mathfrak{H}$ be the series [IK01]

$$\varphi_{\mathrm{KZ}}(X,Y) := \sum_W \widehat{\zeta}(\mathrm{reg}(w))W. \tag{2.8}$$

According to [Kas95], we refer to φ_{KZ} as the Drinfel'd associator.

We define the antipode S of $\mathfrak{h}$ and $\mathfrak{H}$ to be an anti-involution such that

$$\begin{aligned} S: x &\mapsto -x, \qquad & y &\mapsto -y, \\ X &\mapsto -X, & Y &\mapsto -Y. \end{aligned}$$

We note that S is a ш-homomorphism on $\mathfrak{h}$ and yields the inverse of the generating series:

$$\left(\sum_W wW\right)^{-1} = \sum_W S(w)W = \sum_W wS(W). \tag{2.9}$$

3. Multiple Polylogarithms and the formal KZ equation

For $w = x^{k_1-1}yx^{k_2-1}y\cdots x^{k_m-1}y \in \mathfrak{h}^1$ and x we define the multiple polylogarithms on $\mathbb{C}\backslash(-\infty,0]\cup[1,\infty)$ by

$$\mathrm{Li}(x;z) = \log z, \tag{3.1}$$

$$\begin{aligned}\mathrm{Li}(w;z) &= \mathrm{Li}_{k_1,k_2,\ldots,k_m}(z) \\ &= \sum_{n_1>n_2>\cdots>n_r>0} \frac{z^{n_1}}{n_1^{k_1}n_2^{k_2}\cdots n_m^{k_m}} \qquad (|z|<1) \\ &= \underbrace{\int_0^z \frac{dz}{z}\cdots\int_0^z \frac{dz}{z}}_{k_1-1}\int_0^z \frac{dz}{1-z}\cdots\underbrace{\int_0^z \frac{dz}{z}\cdots\int_0^z \frac{dz}{z}}_{k_r-1}(-\log(1-z)),\end{aligned} \tag{3.2}$$

where the branch of $\log z$ is chosen as the principal value. Because $\mathrm{Li}(\bullet;z)$ on $\mathfrak{h}^1$ is a ш-homomorphism [Ree58] and $\mathfrak{h}$ can be decomposed as (2.4), $\mathrm{Li}(\bullet; z)$ extends from $\mathfrak{h}^1$ to the whole $\mathfrak{h}$ as a ш-homomorphism. For word $w \in \mathfrak{h}^0$ the evaluation of $\mathrm{Li}(w; z)$ tending $z \to 1-0$ is

$$\lim_{z\to 1-0} \mathrm{Li}(w; z) = \widehat{\zeta}(w).$$

From this evaluation, (2.3) obviously follows.

Applying $\mathrm{Li}(\bullet; z)$ to the Chen series $\sum_W wW$, we have a $\mathfrak{H}$-valued function

$$G_0(X, Y; z) = G_0(z) = \mathrm{Li}(\bullet; z)\left(\sum_W wW\right) = \sum_W \mathrm{Li}(w; z)W \tag{3.3}$$

holomorphic on $\mathbb{C}\backslash(-\infty, 0] \cup [1, \infty)$. By virtue of (2.7), we have

$$\begin{aligned} G_0(X, Y; z) &= \exp_{ш}(\mathrm{Li}(y; z)Y)\left(\sum_W \mathrm{Li}(\mathrm{reg}(w); z)W\right)\exp_{ш}(\mathrm{Li}(x; z)X) \\ &= \exp(-Y\log(1-z))\left(\sum_W \mathrm{Li}(\mathrm{reg}(w); z)W\right)\exp(X\log z) \\ &= (1-z)^{-Y}\overline{G}_0(X, Y; z)z^X \end{aligned} \tag{3.4}$$

where

$$\overline{G}_0(X, Y; z) = \sum_W \mathrm{Li}(\mathrm{reg}(w); z)W.$$

$G_0(X, Y; z)$ is a unique solution to the system (KZ)

$$dG = \Omega_{\mathrm{KZ}}G, \tag{KZ}$$

where

$$\Omega_{\mathrm{KZ}} = X\,d\log z - Y\,d\log(1-z),$$

with the asymptotic behavior

$$G_0(X, Y; z) \times z^{-X} \longrightarrow 1 \qquad (z \to 0) \tag{3.5}$$

(cf. [HPH99, Oku03]). There also exist unique solutions G_1 and G_∞ of (KZ) with the following asymptotic behavior

$$G_1(X, Y; z) \times (1-z)^Y \longrightarrow 1 \qquad (z \to 1), \tag{3.6}$$

$$G_\infty(X, Y; z) \times (1/z)^{-X+Y} \longrightarrow 1 \qquad (z \to \infty). \tag{3.7}$$

Let us introduce the connection matrices $C^{(jk)}$ by

$$G_k = G_j \times C^{(jk)}, \qquad (j, k = 0, 1 \text{ or } \infty). \tag{3.8}$$

We investigate the explicit form of the solutions G_1, G_∞, and the connection matrices (the connection problem for (KZ)!). To do this, we use the linear fractional transformations following [HPH99, Oku03]. There are six functions preserving the singular points of (KZ):

$$z, \qquad 1-z, \qquad \frac{1}{z}, \qquad \frac{z}{z-1}, \qquad \frac{1}{1-z}, \qquad \frac{z-1}{z}. \tag{3.9}$$

Each function corresponds to the permutation of singular points:

$$e, \qquad (01), \qquad (0\infty), \qquad (1\infty), \qquad (01\infty), \qquad (10\infty). \tag{3.10}$$

The linear fractional transformations f act on functions by the pull-back

$$(f^*G)(z) = G(f(z)). \tag{3.11}$$

We also define the actions on $\mathfrak{h}$, $\mathfrak{H}$, which is denoted by f^*, f_* respectively, by the following rule: Let us identify the letter x as $d\log z$, and the letter y as $-d\log(1-z)$. Then $\Omega_{\mathrm{KZ}} = xX + yY$. We define $f^*(x)$ and $f^*(y)$ to be the pull-back $f^*d\log z = d\log f(z)$, $-f^*d\log(1-z) = -d\log(1-f(z))$, respectively. Note that these 1-forms are again expressed as linear combinations of x and y. We write it as

$$(f^*(x), f^*(y)) = (x, y)A(f),$$

where $A(f)$ is a numerical 2×2 matrix. Then we define $f_*(X)$ and $f_*(Y)$ as

$$\begin{pmatrix} f_*(X) \\ f_*(Y) \end{pmatrix} = A(f)\begin{pmatrix} X \\ Y \end{pmatrix}.$$

So we have

$$f^*\Omega_{\mathrm{KZ}} = f^*(x)X + f^*(y)Y = xf_*(X) + yf_*(Y). \tag{3.12}$$

Then we have the following table:

	x	y	X	Y
z	x	y	X	Y
$1-z$	$-y$	$-x$	$-Y$	$-X$
$\frac{1}{z}$	$-x$	$x+y$	$-X+Y$	Y
$\frac{z}{z-1}$	$x+y$	$-y$	X	$X-Y$
$\frac{1}{1-z}$	y	$-x-y$	$-Y$	$X-Y$
$\frac{z-1}{z}$	$-x-y$	x	$-X+Y$	$-X,$

(3.13)

e.g.

$$1-z : x \mapsto -y, \qquad y \mapsto -x, \qquad X \mapsto -Y, \qquad Y \mapsto -X.$$

These extend to homomorphisms on $\mathfrak{h}$, and $\mathfrak{H}$ respectively, and satisfy

$$(f \circ g)^* = g^* \circ f^*, \qquad (f \circ g)_* = f_* \circ g_* \tag{3.14}$$

$$\sum_W f^*(w)\ W = \sum_W w\ f_*(W) \tag{3.15}$$

and f^* is a ш-homomorphism of $\mathfrak{h}$. Note that $f_* \circ g^* = g^* \circ f_*$ for any f, g.

For any $\mathfrak{H}$-valued function $F(X, Y, ; z) = \sum_W \ell(w; z)W$, we set

$$\begin{aligned}\pi(f)F(X, Y, ; z) &= f_*(f^*)^{-1}F(X, Y; z)\\ &= F(f_*(X), f_*(Y); f^{-1}(z))\\ &= \sum_W \ell(w; f^{-1}(z))f_*(W)\\ &= \sum_W \ell(f^*(w); f^{-1}(z))W.\end{aligned}$$

Since $H = (f^*)^{-1}G_0$ is a solution of the equation $dH = (f^*)^{-1}\Omega_{\mathrm{KZ}}\ H$, applying f_* to $(f^*)^{-1}G_0$,

$$\pi(f)G_0(X, Y; z) = \sum_W \mathrm{Li}(f^*(w); f^{-1}(z))W \tag{3.16}$$

becomes a solution of (KZ) again. Note that this transformation is $\mathbb{C}$-linear, but not $\mathfrak{H}$-linear, and satisfy

$$\pi(f \circ g) = \pi(f) \circ \pi(g) \tag{3.17}$$

for any f and g. The asymptotic behavior of this solution around $f(0)$ can be obtained by

$$\begin{aligned}&\pi(f)G_0(X, Y; z)\\ &= \left(1 - f^{-1}(z)\right)^{-f_*(Y)}\ \overline{G}_0(f_*(X), f_*(Y); f^{-1}(z))\left(f^{-1}(z)\right)^{f_*(X)}.\end{aligned}$$

Thus, from the uniqueness of the solutions satisfying the prescribed asymptotic behavior,

Proposition 2. We have

$$\pi(1-z)(G_0) = G_1, \tag{3.18}$$

$$\pi\left(\frac{1}{z}\right)(G_0) = G_\infty, \tag{3.19}$$

$$\pi\left(\frac{z}{z-1}\right)(G_0) = G_0 \times \exp(\mp X\pi i), \tag{3.20}$$

$$\pi\left(\frac{1}{1-z}\right)(G_0) = G_1 \times \exp(\mp Y\pi i), \tag{3.21}$$

$$\pi\left(\frac{z-1}{z}\right)(G_0) = G_\infty \times \exp(\pm(-X+Y)\pi i), \tag{3.22}$$

where $z \in \mathbf{H}_\pm$.

We should observe that in the latter three cases all the cut of the logarithms which appear in the singular parts of the solutions separate $\mathbb{C}$ to $\mathbf{H}_+ \cup \mathbf{H}_-$, for example,

$$\log\left(\frac{z}{z-1}\right) + \log(1-z) - \log z = \mp\pi i \quad (z \in \mathbf{H}_\pm).$$

In particular (3.20) is explicitly written as

$$\sum_W \mathrm{Li}\left(\left(\frac{z}{z-1}\right)^*(w); \frac{z}{z-1}\right) W = \left(\sum_W \mathrm{Li}(w;z)W\right) \times \exp(\pm X\pi i), \tag{3.23}$$

where

$$\left(\frac{z}{z-1}\right)^* : \qquad x \mapsto x+y, \qquad y \mapsto -y,$$

so that the equality of the coefficient of W (a word $\in \mathfrak{H}Y$) gives rise to the Landen connection formula (1.2):

Proposition 3. We have

$$\mathrm{Li}\left(\left(\frac{z}{z-1}\right)^*(w); \frac{z}{z-1}\right) = \mathrm{Li}(w;z), \tag{3.24}$$

where w is a word $\in \mathfrak{h}^1$.

Using the antipode S, we can describe the inverse of G_1 as follows:

$$\begin{aligned}
G_1(X,Y;z)^{-1} &= \sum_W \mathrm{Li}\left((1-z)^*(w);1-z\right) S(W) \\
&= \sum_W \mathrm{Li}\left((1-z)^* \circ S(w);1-z\right) W \\
&= \exp\left(Y\log(1-z)\right)\left(\sum_W \mathrm{Li}\left(\mathrm{reg}\circ(1-z)^*\circ S(w);1-z\right) W\right) \\
&\qquad \times \exp\left(-X\log z\right) \\
&= \exp\left(Y\log(1-z)\right)\overline{G}_0(-Y,-X;1-z)^{-1}\exp\left(-X\log z\right).
\end{aligned}$$

so that the ratio of these two solutions is computed, by letting $z \to 0$ and $z \to 1$, as follows:

$$\begin{aligned}
C^{(10)} &= G_1(X,Y;z)^{-1}G_0(X,Y;z) \qquad (3.25)\\
&= \exp\left(Y\log(1-z)\right)\overline{G}_0(-Y,-X;1-z)^{-1}\exp\left(-X\log z\right) \\
&\qquad \times \exp\left(-Y\log(1-z)\right)\overline{G}_0(X,Y;z)\exp\left(X\log z\right) \\
&= \overline{G}_0(X,Y;1) = \overline{G}_0(-Y,-X;1)^{-1}.
\end{aligned}$$

Hence we obtain

$$\begin{aligned}
C^{(10)} &= \overline{G}_0(X,Y;1) = \sum_W \mathrm{Li}(\mathrm{reg}(w);1)W \\
&= \sum_W \widehat{\zeta}(\mathrm{reg}(w))W = \varphi_{\mathrm{KZ}}(X,Y)
\end{aligned}$$

and

$$\begin{aligned}
C^{(10)} &= \overline{G}_0(-Y,-X;1)^{-1} = \varphi_{\mathrm{KZ}}(-Y,-X)^{-1} \\
&= \sum_W \mathrm{Li}(\mathrm{reg}\circ\tau(w);1)W = \sum_W \widehat{\zeta}(\mathrm{reg}\circ\tau(w))W,
\end{aligned}$$

where $\tau = \pi(1-z)\circ S$ is an anti-involution which maps $x \mapsto y$, $y \mapsto x$ and preserves $\mathfrak{h}^0$. As a consequence, we have

Proposition 4. The Drinfel′d associator satisfies [Dri90]

$$\varphi_{\mathrm{KZ}}(X,Y)\cdot\varphi_{\mathrm{KZ}}(-Y,-X) = 1, \qquad (3.26)$$

which is equivalent to a generalization of the duality formula in [Zag94]:

$$\widehat{\zeta}(\mathrm{reg}(w)) = \widehat{\zeta}(\mathrm{reg}\circ\tau(w)), \qquad (3.27)$$

where w is an arbitrary word.

(This equivalency was firstly pointed out to the authors by Masanobu Kaneko in private communications.)

Moreover writing down (3.25), we have

$$\sum_W \left(\sum_{w_1 w_2 = w} \mathrm{Li}(\tau(w_1); 1-z)\mathrm{Li}(w_2; z) \right) W = \sum_W \widehat{\zeta}(\mathrm{reg}(w))W,$$

which is equivalent to the Euler connection formula for multiple polylogarithms:

Proposition 5. We have

$$\sum_{w_1 w_2 = w} \mathrm{Li}(\tau(w_1); 1-z)\mathrm{Li}(w_2; z) = \widehat{\zeta}(\mathrm{reg}(w)). \tag{3.28}$$

where w is an arbitrary word.

Let us discuss more on the connection problem of (KZ). The hexagon relations in [Dri90] can be derived from a braid relation

$$\frac{1}{z} = (1-z) \circ \left(\frac{z}{z-1}\right) \circ (1-z) = \left(\frac{z}{z-1}\right) \circ (1-z) \circ \left(\frac{z}{z-1}\right). \tag{3.29}$$

First applying $\pi(1/z)$ to G_0, we have

$$\begin{aligned} G_\infty &= \pi\left(\frac{1}{z}\right)(G_0) = \pi(1-z) \circ \pi\left(\frac{z}{z-1}\right) \circ \pi(1-z)(G_0) \\ &= \pi(1-z) \circ \pi\left(\frac{z}{z-1}\right)(G_0 \times \varphi_{\mathrm{KZ}}(X,Y)^{-1}) \\ &= \pi(1-z)(G_0 \times \exp(\mp X\pi i)) \times \varphi_{\mathrm{KZ}}(X, X-Y)^{-1} \\ &= G_0 \times \varphi(X,Y)^{-1} \times \exp(\mp Y\pi i) \times \varphi_{\mathrm{KZ}}(-Y, X-Y)^{-1}. \end{aligned}$$

By similar computation, we have

$$\begin{aligned} G_\infty &= \pi\left(\frac{1}{z}\right)(G_0) = \pi\left(\frac{z}{z-1}\right) \circ \pi(1-z) \circ \pi\left(\frac{z}{z-1}\right)(G_0) \\ &= \pi\left(\frac{z}{z-1}\right) \circ \pi(1-z)(G_0 \times \exp(\mp X\pi i)) \\ &= \pi\left(\frac{z}{z-1}\right)(G_0 \times \varphi_{\mathrm{KZ}}(X,Y)^{-1} \times \exp(\mp Y\pi i)) \\ &= G_0 \times \exp(\mp X\pi i) \times \varphi_{\mathrm{KZ}}(X, X-Y)^{-1} \times \exp(\mp(-X+Y)\pi i). \end{aligned}$$

Therefore we have the hexagon relations [HPH99]

$$\exp(\pm X\pi i) = \varphi_{\mathrm{KZ}}(-X+Y,-X) \times \exp(\mp(-X+Y)\pi i) \\ \times \varphi_{\mathrm{KZ}}(-X+Y,Y)^{-1} \times \exp(\pm Y\pi i) \times \varphi_{\mathrm{KZ}}(X,Y). \quad (3.30)$$

4. Mellin transforms of polylogarithms and the sum formula for MZVs

The Mellin transform and the inverse Mellin transform were used in [OU04] to show that the reduced Ohno relation is converted to the Landen connection formula for MPLs. In this section, we will consider the Mellin transforms of the Euler connection formula and the Landen connection formula for polylogarithms.

We define the Mellin transform by

$$M[\varphi(z)](\lambda) = \int_0^1 \varphi(z) z^{\lambda-1}\, dz, \quad (4.1)$$

the inverse Mellin transform by

$$\widetilde{M}[f(\lambda)](z) = \frac{1}{2\pi\sqrt{-1}} \int_C f(\lambda) z^{\lambda}\, d\lambda. \quad (4.2)$$

For the details (the integral contour C in (4.2), and the relation between both transforms, for example), see [OU04].

Now we calculate the Mellin transform of the Euler connection formula for the polylogarithms,

$$\mathrm{Li}_k(z) + \mathrm{Li}_{k-1}(z)\mathrm{Li}_1(1-z) + \cdots + \mathrm{Li}_1(z)\mathrm{Li}_{\underbrace{1\ldots1}_{k-1}}(1-z) + \\ + \mathrm{Li}_{\underbrace{21\ldots1}_{k-1}}(1-z) = \zeta(k). \quad (4.3)$$

Since $\mathrm{Li}_k(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^k}$ $(k \geq 2)$ is uniformly convergent for $0 \leq z \leq 1$, and

$$\mathrm{Li}_{\underbrace{1\ldots1}_{j}}(1-z) z^{-\lambda-1} = \frac{1}{j!}(-\log z)^j z^{-\lambda-1} = \frac{1}{j!}\left(\frac{d}{d\lambda}\right)^j z^{-\lambda-1},$$

we have

$$\begin{aligned}
M[\mathrm{Li}_{k-j}(z)\mathrm{Li}_{\underbrace{1\ldots1}_{j}}(1-z)](\lambda) &= \frac{1}{j!}\left(\frac{d}{d\lambda}\right)^j \int_0^1 \mathrm{Li}_{k-j}(z) z^{-\lambda-1}\,dz \\
&= \frac{1}{j!}\left(\frac{d}{d\lambda}\right)^j \sum_{n=1}^{\infty} \frac{1}{n^{k-j}(n-\lambda)} \\
&= \sum_{n=1}^{\infty} \frac{1}{n^{k-j}(n-\lambda)^{j+1}}.
\end{aligned}$$

Hence the sum $\sum_{j=0}^{k-1} M[\mathrm{Li}_{k-j}(z)\mathrm{Li}_{\underbrace{1\ldots1}_{j}}(1-z)](\lambda)$ is shown to be

$$\begin{aligned}
\sum_{j=0}^{k-1}\sum_{n=1}^{\infty} \frac{1}{n^{k-j}(n-\lambda)^{j+1}} &= \sum_{n=1}^{\infty} \frac{1}{n^k} \frac{\dfrac{1}{n-\lambda} - \dfrac{n^k}{(n-\lambda)^{k+1}}}{1-\dfrac{n}{n-\lambda}} \\
&= \sum_{n=1}^{\infty} \frac{1}{-\lambda}\left\{\frac{1}{n^k} - \frac{1}{(n-\lambda)^k}\right\} \\
&= -\frac{\zeta(k)}{\lambda} + \frac{1}{\lambda}\sum_{m=0}^{\infty}\binom{-k}{m}\sum_{n=1}^{\infty}\frac{(-\lambda)^m}{n^{k+m}} \\
&= \frac{\zeta(k)}{\lambda} + \frac{1}{\lambda}\sum_{m=0}^{\infty}\binom{m+k-1}{m}\zeta(k+m)\lambda^m.
\end{aligned}$$

The Mellin transform of the last term in (4.3) can be calculated as follows:

$$\begin{aligned}
&\int_0^1 \mathrm{Li}_{\underbrace{21\ldots1}_{k-1}}(1-z) z^{-\lambda-1}\,dz \\
&= \sum_{n_1>\cdots>n_{k-1}>0} \frac{1}{n_1^2 n_2 \cdots n_{k-1}} \int_0^1 z^{-\lambda-1}(1-z)^{n_1}\,dz
\end{aligned}$$

(by the integral representation of the beta function)

$$= \sum_{n_1>\cdots>n_{k-1}>0} \frac{1}{n_1^2 n_2 \cdots n_{k-1}} \frac{\Gamma(-\lambda)\Gamma(n_1+1)}{\Gamma(n_1-\lambda+1)}$$

$$= \frac{1}{-\lambda} \sum_{n_1>\cdots>n_{k-1}>0} \frac{1}{n_1^2 n_2 \cdots n_{k-1}} \frac{n_1!}{(n_1-\lambda)(n_1-1-\lambda)\cdots(1-\lambda)}$$

$$= \frac{1}{-\lambda} \sum_{n_1>\cdots>n_{k-1}} \sum_{m=0}^{\infty} \sum_{\substack{l_i\geq 0 \\ l_1+\cdots+l_{n_1}=m}} \frac{1}{n_1^2 n_2 \cdots n_{k-1}} \times \frac{\lambda^m}{{n_1}^{l_{n_1}} (n_1-1)^{l_{n_1-1}} \cdots 2^{l_2} 1^{l_1}}$$

(by some combinatorial consideration)

$$= \frac{1}{-\lambda} \sum_{m=0}^{\infty} \sum_{j=0}^{m} \binom{(k-1)+j-1}{j} S(k+m,(k-1)+j)\lambda^m$$

$$= \frac{1}{-\lambda} \sum_{m=0}^{\infty} \sum_{j=0}^{m} \binom{k+j-2}{j} S(k+m,(k-1)+j)\lambda^m,$$

where $S(n,r)$ denotes the sum of all MZVs of weight n and depth r. Thus we obtain, for $k \geq 2$, $m \geq 0$,

$$\sum_{j=0}^{m} \binom{k+j-2}{k-2} S(k+m,k-1+j) = \binom{m+k-1}{k-1} \zeta(k+m). \tag{4.4}$$

which is rewritten, by putting $n = k+m$, $d = k-1+j$, as

$$\sum_{d=k-1}^{n-1} \binom{d-1}{k-2} S(n,d) = \binom{n-1}{k-1} \zeta(n) \quad (2 \leq k \leq n). \tag{$\heartsuit$}$$

From this we can easily prove the sum formula

$$S(n,r) = \zeta(n) \quad (n \geq 2,\ n \geq r \geq 1) \tag{4.5}$$

by induction on r.

Proof. That $S(n,n-1) = \zeta(n)$ follows from ($\heartsuit$) with $k = n$. For $r < n-1$, we write ($\heartsuit$) as

$$S(n,r) + \sum_{d=r+1}^{n-1} \binom{d-1}{r-1} S(n,d) = \binom{n-1}{r} \zeta(n).$$

From the induction hypothesis, we have

$$S(n,r) + \sum_{d=r+1}^{n-1} \binom{d-1}{r-1}\zeta(n) = \binom{n-1}{r}\zeta(n)$$

Noting that

$$\sum_{d=r+1}^{n-1} \binom{d-1}{r-1} = \binom{n-1}{r} - 1,$$

we obtain (4.5). □

Next we consider the Mellin transform of the Landen connection formula for polylogarithms:

$$\mathrm{Li}_m(z) = -\sum_{j=1}^{m} \sum_{\substack{\mathbf{c} \\ \text{weight } m \\ \text{length } m-j+1}} \mathrm{Li}_{\mathbf{c}}\left(\frac{z}{z-1}\right). \tag{4.6}$$

For $m = 2$, it is nothing but the Landen formula for the dilogarithm

$$\mathrm{Li}_2(z) = -\mathrm{Li}_2\left(\frac{z}{z-1}\right) - \mathrm{Li}_{11}\left(\frac{z}{z-1}\right). \tag{4.7}$$

First we compute the Mellin transform of this formula. The Taylor expansion of (4.7) of both sides reads

$$\sum_{n=1}^{\infty} \frac{z^n}{n^2} = \sum_{n_1>n_2>0} \frac{z^{n_2}}{n_1(n_1-n_2)} + \sum_{n_1>n_2>0} \frac{z^{n_1}}{n_1(n_2-n_1)}.$$

Applying the Mellin transform to both sides above, we have

$$\begin{aligned}
&\sum_{n=1}^{\infty} \frac{1}{n^2(n-\lambda)} \\
&= \sum_{n_1>n_2>0} \frac{1}{n_1(n_1-n_2)(n_2-\lambda)} + \sum_{n_1>n_2>0} \frac{1}{n_1(n_2-n_1)(n_1-\lambda)} \\
&= \sum_{n_1>n_2>0} \frac{1}{n_1(n_1-\lambda)(n_2-\lambda)}.
\end{aligned}$$

The Taylor expansion of the both sides above at $\lambda = 0$ reads

$$\sum_{l=0}^{\infty} \zeta(3+l)\lambda^l = \sum_{l=0}^{\infty} \left\{ \sum_{\substack{c_1+c_2=l \\ c_1,c_2\geq 0}} \zeta(2+c_1, 1+c_2) \right\} \lambda^l,$$

which yields the sum formula for MZVs of the depth 2;

$$\zeta(3+l) = \sum_{\substack{c_1+c_2=l \\ c_1,c_2\geq 0}} \zeta(2+c_1, 1+c_2). \tag{4.8}$$

Now we consider the general case. What we have to show is

Lemma 6 (cf. [OU04]). For $1 \leq j \leq m$,

$$\sum_{n_1>\ldots>n_m>0} \frac{z^{n_j}}{n_1 \prod_{i\neq j}(n_i - n_j)} = - \sum_{\substack{\mathbf{c} \\ \text{weight } m \\ \text{length } m-j+1}} \mathrm{Li}_{\mathbf{c}}\left(\frac{z}{z-1}\right). \tag{4.9}$$

Proof. We prove this by induction on m. For $m=1$, it is obvious. Suppose that it holds for $m-1$. Let $j \neq 1, m$. Then we have

$$\begin{aligned}
&\frac{d}{dz}\,(\text{the LHS of (4.9)}) \\
&= \sum_{n_1>\cdots>n_m>0} \frac{n_j z^{n_j-1}}{n_1(n_1-n_j)\cdots(n_{j-1}-n_j)\cdot(n_{j+1}-n_j)\cdots(n_m-n_j)}
\end{aligned} \tag{$\clubsuit$}$$

Putting $n_i = l_i + \cdots + l_m \quad (1 \leq i \leq m)$, we have

$$\begin{aligned}
(\clubsuit) &= \sum_{l_1,\ldots,l_m=1}^{\infty} \left\{ \frac{1}{l_1+\cdots+l_{j-1}} - \frac{1}{l_1+\cdots+l_m} \right\} \times \\
&\qquad\qquad \times \frac{(-1)^{m-j} z^{l_j+\cdots+l_m-1}}{(l_2+\cdots+l_{j-1})\cdots l_{j-1}\cdot l_j \cdots (l_j+\cdots+l_{m-1})} \\
&= \sum_{l_2,\ldots,l_m=1}^{\infty} \left\{ \sum_{l_1=1}^{l_j+\cdots+l_m} \frac{1}{l_1+\cdots+l_{j-1}} \right\} \times \\
&\qquad\qquad \times \frac{(-1)^{m-j} z^{l_j+\cdots+l_m-1}}{(l_2+\cdots+l_{j-1})\cdots l_{j-1}\cdot l_j \cdots (l_j+\cdots+l_{m-1})}
\end{aligned}$$

$$\begin{aligned}
&= \sum_{l_2,\ldots,l_{m-1}=1}^{\infty} \left\{ \sum_{l_1=1}^{l_j+\cdots+l_{m-1}} \sum_{l_m=1}^{\infty} + \sum_{l_1=l_j+\cdots+l_{m-1}+1}^{\infty} \cdot \sum_{l_m=l_1-(l_j+\cdots+l_{m-1})}^{\infty} \right\} \times \\
&\quad \times \frac{(-1)^{m-j} z^{l_j+\cdots+l_m-1}}{(l_1+\cdots+l_{j-1})(l_2+\cdots+l_{j-1})\cdots l_{j-1}\cdot l_j \cdots (l_j+\cdots+l_{m-1})}
\end{aligned}$$

$$= \frac{1}{1-z} \sum_{l_1,\ldots,l_{m-1}=1}^{\infty} \sum_{l_1=1}^{l_j+\cdots+l_{m-1}} \frac{(-1)^{m-j} z^{l_j+\cdots+l_{m-1}}}{\{\text{the same denominator as above}\}}$$

$$+ \frac{1}{1-z} \sum_{l_1,\ldots,l_{m-1}=1}^{\infty} \sum_{l_1=l_j+\cdots+l_{m-1}+1}^{\infty} \frac{(-1)^{m-j} z^{l_1-1}}{\{\text{the same denominator as above}\}}$$

$$= \frac{1}{1-z} \sum_{l_1,\ldots,l_{m-1}=1}^{\infty} \left\{ \frac{1}{l_1+\cdots+l_{j-1}} - \frac{1}{l_1+\cdots+l_{m-1}} \right\} \times$$

$$\times \frac{(-1)^{m-j} z^{l_j+\cdots+l_{m-1}}}{(l_2+\cdots+l_{j-1})\cdots l_{j-1}\cdot l_j \cdots (l_j+\cdots+l_{m-1})}$$

$$+ \frac{1}{1-z} \sum_{l_1,\ldots,l_{m-1}=1}^{\infty} \frac{(-1)^{m-j} z^{l_j+\cdots+l_m-1}}{(l_2+\cdots+l_m)(l_2+\cdots+l_{j-1})\cdots l_{j-1}} \times$$

$$\times \frac{1}{l_j \cdots (l_j+\cdots+l_{m-1})}$$

$$= \frac{1}{1-z} \sum_{l_1,\ldots,l_{m-1}=1}^{\infty} \frac{(-1)^{m-j} z^{l_j+\cdots+l_{m-1}}}{(l_1+\cdots+l_{m-1})(l_1+\cdots+l_{j-1})\cdots l_{j-1}} \times$$

$$\times \frac{1}{l_j \cdots (l_j+\cdots+l_{m-2})}$$

$$+ \frac{1}{z(1-z)} \sum_{l_1,\ldots,l_{m-1}=1}^{\infty} \frac{(-1)^{m-j} z^{l_{j-1}+\cdots+l_{m-1}}}{(l_1+\cdots+l_{m-1})(l_1+\cdots+l_{j-2})\cdots l_{j-2}} \times$$

$$\times \frac{1}{l_{j-1} \cdots (l_{j-1}+\cdots+l_{m-2})}$$

(putting $n_i = l_i + \cdots + l_{m-1} \quad (1 \le i \le m-1)$)

$$= -\frac{1}{1-z} \sum_{n_1>\cdots>n_{m-1}>0} \frac{z^{n_j}}{n_1(n_1-n_j)\cdots(n_{j-1}-n_j)} \times$$

$$\times \frac{1}{(n_{j+1}-n_j)\cdots(n_{m-1}-n_j)}$$

$$+ \frac{1}{z(1-z)} \sum_{n_1>\cdots>n_{m-1}>0} \frac{z^{n_{j-1}}}{n_1(n_1-n_{j-1})\cdots(n_{j-2}-n_{j-1})} \times$$

$$\times \frac{1}{(n_j-n_{j-1})\cdots(n_{m-1}-n_{j-1})}$$

(by the induction hypothesis)

$$= \frac{1}{1-z} \sum_{\substack{\mathbf{c} \\ \text{weight}\, m-1 \\ \text{length}\, m-j}} \mathrm{Li}_{\mathbf{c}}\left(\frac{z}{z-1}\right) - \frac{1}{z(1-z)} \sum_{\substack{\mathbf{c} \\ \text{weight}\, m-1 \\ \text{length}\, m-j+1}} \mathrm{Li}_{\mathbf{c}}\left(\frac{z}{z-1}\right).$$

Using the differential relation,

$$\frac{d}{dz}\mathrm{Li}_{k_1,\ldots,k_m}\left(\frac{z}{z-1}\right) = \begin{cases} \dfrac{1}{z(1-z)}\mathrm{Li}_{k_1-1,k_2,\ldots,k_m}\left(\dfrac{z}{z-1}\right) & \text{if} \quad k_1 \geq 2, \\[2ex] -\dfrac{1}{1-z}\mathrm{Li}_{k_2,\ldots,k_m}\left(\dfrac{z}{z-1}\right) & \text{if} \quad k_1 = 1, \end{cases}$$

we obtain (4.9) for $j \neq 1, m$. The case for $j = 1, m$ can be shown in the same way. □

From the Landen formula (4.6), we have

$$\sum_{n=1}^{\infty} \frac{z^n}{n^m} = \sum_{j=1}^{m} \sum_{n_1 > \cdots > n_m > 0} \frac{z^{n_j}}{n_1 \prod_{i \neq j}(n_i - n_j)}.$$

The Mellin transform of the above reads

$$\sum_{n=1}^{\infty} \frac{1}{n^m(n-\lambda)} = \sum_{j=1}^{m} \sum_{n_1 > \cdots > n_m > 0} \frac{1}{n_1 \prod_{i \neq j}(n_i - n_j)(n_j - \lambda)}.$$

The Taylor expansion of the both sides yields the sum formula (4.5).

5. Knizhnik-Zamolodchikov equation over the configuration space $X_3(\mathbb{C})$

Let $\mathfrak{P}_n = \mathbb{C}\langle\langle X_{ij} \rangle\rangle_{1 \leq i \neq j \leq n}$ be an algebra with the defining relations

$$\begin{cases} X_{ij} = X_{ji}, & \\ [X_{ij}, X_{kl}] = 0, & (i,j,k,l \text{ distinct}) \\ [X_{ij}, X_{ik} + X_{kj}] = 0. & (i,j,k \text{ distinct}) \end{cases} \tag{5.1}$$

Putting $z_{ij} := z_i - z_j$, we consider the following system of differential equations:

$$dW = \left(\sum_{i<j} X_{ij} d\log z_{ij}\right) W. \tag{KZ$_n$}$$

This system is integrable because of (5.1) (cf. [Kas95]).

In what follows, we consider only the case of $n = 3$. We set $T = X_{12} + X_{13} + X_{23}$ which belongs to the center of $\mathfrak{P}_3$.

Proposition 7. Solutions to (KZ_3) satisfying the following asymptotic behavior exist,

$$W_{(ij)k} \sim z_{ji}^{X_{ij}} z_{ki}^{X_{ik}+X_{jk}} \qquad (|z_{ji}| << |z_{ki}|), \tag{5.2}$$

$$W_{i(jk)} \sim z_{kj}^{X_{jk}} z_{ki}^{X_{ij}+X_{ik}} \qquad (|z_{kj}| << |z_{ki}|), \tag{5.3}$$

and are expressed in terms of the solutions G_0 and G_1 of (KZ) as follows:

$$W_{(ij)k}(z_1, z_2, z_3) = G_0\left(X_{ij}, -X_{jk}; \frac{z_{ji}}{z_{ki}}\right) \times z_{ki}^{T}, \tag{5.4}$$

$$W_{i(jk)}(z_1, z_2, z_3) = G_1\left(X_{ij}, -X_{jk}; \frac{z_{ji}}{z_{ki}}\right) \times z_{ki}^{T}. \tag{5.5}$$

Proof. We set

$$W(z_1, z_2, z_3) = G\left(\frac{z_{ji}}{z_{ki}}\right) z_{ki}^{T}.$$

Then G satisfies

$$dG\left(\frac{z_{ji}}{z_{ki}}\right) z_{ki}^{T} + G\left(\frac{z_{ji}}{z_{ki}}\right) z_{ki}^{T} T d\log z_{ki} = \left(\sum_{p<q} X_{pq} d\log z_{pq}\right) G\left(\frac{z_{ji}}{z_{ki}}\right) z_{ki}^{T},$$

so that we have

$$dG\left(\frac{z_{ji}}{z_{ki}}\right) = \left(X_{ij} d\log\frac{z_{ji}}{z_{ki}} + X_{jk} d\log\left(1 - \frac{z_{ji}}{z_{ki}}\right)\right) G\left(\frac{z_{ji}}{z_{ki}}\right). \tag{5.6}$$

Taking into account (5.2), we obtain the formula (5.4). □

Proposition 8. The solutions above satisfy the connection formulas

$$\begin{aligned}
&W_{i(jk)}(z_1,z_2,z_3)\times\varphi_{\mathrm{KZ}}(X_{ij},-X_{jk}) \\
&\qquad = W_{(ij)k}(z_1,z_2,z_3), && (5.7)\\
&W_{(ji)k}(z_1,z_2,z_3)\times \exp(\pm X_{ij}\pi i) \\
&\qquad = W_{(ij)k}(z_1,z_2,z_3) \qquad \frac{z_{ji}}{z_{ki}}\in\mathbf{H}_\pm, && (5.8)\\
&W_{i(kj)}(z_1,z_2,z_3)\times \exp(\pm X_{jk}\pi i) \\
&\qquad = W_{i(jk)}(z_1,z_2,z_3) \qquad \frac{z_{ji}}{z_{ki}}\in\mathbf{H}_\mp, && (5.9)\\
&W_{k(ij)}(z_1,z_2,z_3)\times \exp(\pm(X_{ik}+X_{jk})\pi i) \\
&\qquad = W_{(ij)k}(z_1,z_2,z_3) \qquad \frac{z_{ji}}{z_{ki}}\in\mathbf{H}_\mp. && (5.10)\\
&W_{(jk)i}(z_1,z_2,z_3)\times \exp(\pm(X_{ik}+X_{jk})\pi i) \\
&\qquad = W_{i(jk)}(z_1,z_2,z_3) \qquad \frac{z_{ji}}{z_{ki}}\in\mathbf{H}_\pm. && (5.11)
\end{aligned}$$

Here in each equation, $\frac{z_{ji}}{z_{ki}}\in\mathbf{H}_\pm$ corresponds to the analytic continuation of the paths Figure 1-4:

Proof. Proof of (5.7). We have

$$W_{(ij)k}(z_1,z_2,z_3) = G_0\left(X_{ij},-X_{jk};\frac{z_{ji}}{z_{ki}}\right)\times z_{ki}^T,$$
$$W_{i(jk)}(z_1,z_2,z_3) = G_1\left(X_{ij},-X_{jk};\frac{z_{ji}}{z_{ki}}\right)\times z_{ki}^T$$

Hence we have

$$\begin{aligned}
W_{(ij)k}(z_1,z_2,z_3) &= G_0\left(X_{ij},-X_{jk};\frac{z_{ji}}{z_{ki}}\right)\times z_{ki}^T\\
&= G_1\left(X_{ij},-X_{jk};\frac{z_{ji}}{z_{ki}}\right)\times\varphi_{\mathrm{KZ}}(X_{ij},-X_{jk})\times z_{ki}^T\\
&= W_{i(jk)}\times\varphi_{\mathrm{KZ}}(X_{ij},-X_{jk}).
\end{aligned}$$

Thus we have (5.7).

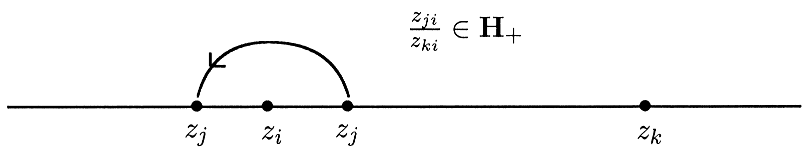

Figure 1. z_j goes around z_i by counter-clockwise

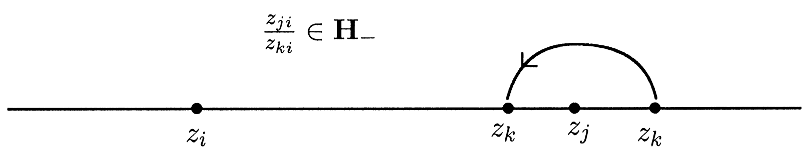

Figure 2. z_k goes around z_j by counter-clockwise

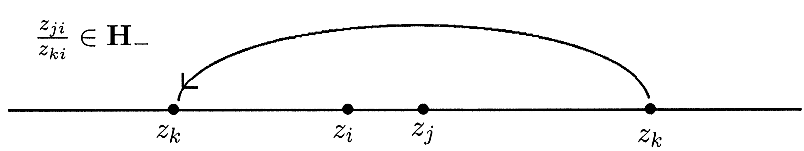

Figure 3. z_k goes around z_i and z_j by counter-clockwise

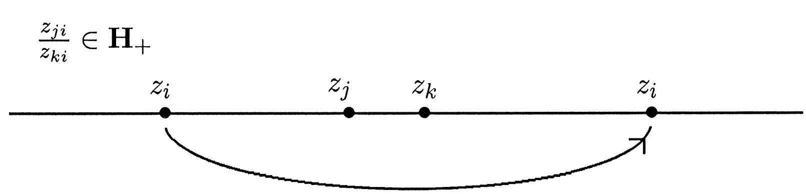

Figure 4. z_i goes around z_j and z_k by counter-clockwise

Proof of (5.8). We have

$$
\begin{aligned}
&W_{(ji)k}(z_1, z_2, z_3)\\
&= G_0\left(X_{ji}, -X_{ik}; \frac{z_{ij}}{z_{kj}}\right) \times z_{kj}^T\\
&= G_0\left(X_{ij}, -X_{ik}; \frac{z_{ji}/z_{ki}}{z_{ji}/z_{ki} - 1}\right) \times z_{kj}^T\\
&= \left(\frac{z}{z-1}\right)_* \circ \pi\left(\frac{z}{z-1}\right)\left(G_0\left(X_{ij}, -X_{ik}; \frac{z_{ji}}{z_{ki}}\right)\right) \times z_{kj}^T\\
&= \left(\frac{z}{z-1}\right)_*\left(G_0\left(X_{ij}, -X_{ik}; \frac{z_{ji}}{z_{ki}}\right) \times \exp(\mp X_{ij}\pi i)\right) \times z_{kj}^T\\
&= G_0\left(X_{ij}, X_{ij} + X_{ik}; \frac{z_{ji}}{z_{ki}}\right) \times \exp(\mp X_{ij}\pi i) \times z_{kj}^T\\
&= \left(\frac{z_{kj}}{z_{ki}}\right)^{-X_{ij}-X_{ik}} \overline{G}_0\left(X_{ij}, X_{ij} + X_{ik}; \frac{z_{ji}}{z_{ki}}\right)\left(\frac{z_{ji}}{z_{kj}}\right)^{X_{ij}}\\
&\quad \times \exp(\mp X_{ij}\pi i) \times z_{kj}^T.
\end{aligned}
$$

Because $\sum_W wW$ is exponential of Lie series, $\overline{G}_0$ is also exponential of Lie series w.r.t. X and Y. So adding any central element of Lie algebra to X or Y does not change $\overline{G}_0$, in particular

$$
\begin{aligned}
\overline{G}_0\left(X_{ij}, X_{ij} + X_{ik}; \frac{z_{ji}}{z_{ki}}\right) &= \overline{G}_0\left(X_{ij}, X_{ij} + X_{ik} - T; \frac{z_{ji}}{z_{ki}}\right)\\
&= \overline{G}_0\left(X_{ij}, -X_{jk}; \frac{z_{ji}}{z_{ki}}\right).
\end{aligned}
$$

Using this equation we obtain

$$
\begin{aligned}
&W_{(ji)k}(z_1, z_2, z_3)\\
&= \left(\frac{z_{kj}}{z_{ki}}\right)^{X_{jk}} \overline{G}_0\left(X_{ij}, -X_{jk}; \frac{z_{ji}}{z_{ki}}\right)\left(\frac{z_{ji}}{z_{kj}}\right)^{X_{ij}} \times z_{ki}^T \times \exp(\mp X_{ij}\pi i)\\
&= W_{(ij)k}(z_1, z_2, z_3) \times \exp(\mp X_{ij}\pi i),
\end{aligned}
$$

where $\frac{z_{ji}}{z_{ki}} \in \mathbf{H}_{\pm}$. Thus we have (5.8).

Proof of (5.9). We have

$$
\begin{aligned}
&W_{i(kj)}(z_1,z_2,z_3)\\
&= G_1\left(X_{ik},-X_{kj};\frac{z_{ki}}{z_{ji}}\right)\times z_{ji}^T\\
&= G_0\left(X_{ik},-X_{kj};\frac{1}{z_{ji}/z_{ki}}\right)\times \varphi_{\mathrm{KZ}}(X_{ik},-X_{kj})^{-1}\times z_{ji}^T\\
&= \left(\frac{1}{z}\right)_*\circ\pi\left(\frac{1}{z}\right)\left(G_0\left(X_{ik},-X_{kj};\frac{z_{ji}}{z_{ki}}\right)\right)\times \varphi_{\mathrm{KZ}}(X_{ik},-X_{kj})^{-1}\times z_{ji}^T\\
&= \left(\frac{1}{z}\right)_*\left(G_0\left(X,Y;\frac{z_{ji}}{z_{ki}}\right)\varphi_{\mathrm{KZ}}(X,Y)^{-1}\exp(\mp Y\pi i)\right.\\
&\qquad\qquad\qquad\left.\left.\times\,\varphi_{\mathrm{KZ}}(-Y,X-Y)^{-1}\right)\right|_{\substack{X=X_{ik}\\ Y=-X_{kj}}}\\
&\qquad\qquad\qquad\qquad\times\,\varphi_{\mathrm{KZ}}(X_{ik},-X_{kj})^{-1}\times z_{ji}^T\\
&= G_0\left(-X+Y,Y;\frac{z_{ji}}{z_{ki}}\right)\varphi_{\mathrm{KZ}}(-X+Y,Y)^{-1}\exp(\mp Y\pi i)\\
&\qquad\qquad\qquad\left.\times\,\varphi_{\mathrm{KZ}}(-Y,-X)^{-1}\right|_{\substack{X=X_{ik}\\ Y=-X_{kj}}}\\
&\qquad\qquad\qquad\qquad\times\,\varphi_{\mathrm{KZ}}(X_{ik},-X_{kj})^{-1}\times z_{ji}^T\\
&= G_0\left(-X_{ik}-X_{kj},-X_{kj};\frac{z_{ji}}{z_{ki}}\right)\varphi_{\mathrm{KZ}}(X_{ij},-X_{kj})^{-1}\times z_{ji}^T\times\exp(\pm X_{kj}\pi i)
\end{aligned}
$$

(in the same way as above)

$$
\begin{aligned}
&= G_0\left(X_{ij},-X_{kj};\frac{z_{ji}}{z_{ki}}\right)\varphi_{\mathrm{KZ}}(X_{ij},-X_{kj})^{-1}\times z_{ki}^T\times\exp(\pm X_{kj}\pi i)\\
&= G_1\left(X_{ij},-X_{kj};\frac{z_{ji}}{z_{ki}}\right)\times z_{ki}^T\times\exp(\pm X_{kj}\pi i)\\
&= W_{i(jk)}(z_1,z_2,z_3)\times\exp(\pm X_{jk}\pi i)
\end{aligned}
$$

where $\frac{z_{ji}}{z_{ki}}\in\mathbf{H}_\pm$. Thus we have (5.9)

Proof of (5.10). We have

$$
\begin{aligned}
&W_{(ij)k}(z_1, z_2, z_3)\\
&= G_0\left(X_{ij}, -X_{jk}; \frac{z_{ji}}{z_{ki}}\right) \times z_{ki}^T\\
&= G_0\left(X_{ij}, -X_{jk}; \frac{\frac{z_{ik}}{z_{jk}} - 1}{\frac{z_{ik}}{z_{jk}}}\right) \times z_{ki}^T\\
&= \left(\frac{z-1}{z}\right)_* \circ \pi\left(\frac{1}{1-z}\right)\left(G_0\left(X_{ij}, -X_{jk}; \frac{z_{ik}}{z_{jk}}\right)\right) \times z_{ki}^T\\
&= \left(\frac{z-1}{z}\right)_* \left(G_1\left(X_{ij}, -X_{jk}; \frac{z_{ik}}{z_{jk}}\right) \times \exp(\pm X_{jk}\pi i)\right) \times z_{ki}^T\\
&= G_1\left(-X_{ij} - X_{jk}, -X_{ij}; \frac{z_{ik}}{z_{jk}}\right) \times \exp(\pm X_{ij}\pi i) \times z_{ki}^T\\
&= \left(\frac{z_{ji}}{z_{jk}}\right)^{X_{ij}} \overline{G}_1\left(X_{ki}, -X_{ij}; \frac{z_{ik}}{z_{jk}}\right)\left(\frac{z_{ji}}{z_{jk}}\right)^{-X_{ij}-X_{jk}}\\
&\qquad\qquad \times \exp(\pm X_{ij}\pi i) \times \left(\frac{z_{ki}}{z_{jk}}\right)^T \times z_{jk}^T.
\end{aligned}
$$

Here we introduce $\overline{G}_1$ by

$$G_1(X, Y; z) = z^X \times \overline{G}_1(X, Y; z) \times (1-z)^{-Y}.$$

$\overline{G}_1$ is also exponential of Lie series, in the same way above, we get

$$
\begin{aligned}
&W_{(ij)k}(z_1, z_2, z_3)\\
&= \left(\frac{z_{ji}}{z_{jk}}\right)^{X_{ij}} \overline{G}_1\left(X_{ki}, -X_{ij}; \frac{z_{ik}}{z_{jk}}\right)\left(\frac{z_{ji}}{z_{jk}}\right)^{X_{ik}} \times z_{jk}^T\\
&\quad \times \exp(\mp(X_{ik} + X_{jk})\pi i)\\
&= W_{k(ij)}(z_1, z_2, z_3) \times \exp(\mp(X_{ik} + X_{jk})\pi i).
\end{aligned}
$$

where $\frac{z_{ji}}{z_{ki}} \in \mathbf{H}_\pm$. Thus we have (5.10).

The last equation in the proposition can be shown as follows:

$$
\begin{aligned}
&W_{i(jk)}(z_1, z_2, z_3)\\
&= G_1\left(X_{ij}, -X_{jk}; \frac{z_{ji}}{z_{ki}}\right) \times z_{ki}^T\\
&= G_0\left(X_{ij}, -X_{jk}; \frac{z_{ji}}{z_{ki}}\right) \times \varphi_{\mathrm{KZ}}(X_{ij}, -X_{jk})^{-1} \times z_{ki}^T\\
&= \left(\frac{1}{1-z}\right)_* \circ \pi\left(\frac{z-1}{z}\right)\left(G_0\left(X_{ij}, -X_{jk}; \frac{z_{kj}}{z_{ij}}\right)\right)\\
&\qquad\qquad\qquad \times \varphi_{\mathrm{KZ}}(X_{ij}, -X_{jk})^{-1} \times z_{ki}^T\\
&= \left(\frac{1}{1-z}\right)_* \left(G_\infty\left(X_{ij}, -X_{jk}; \frac{z_{kj}}{z_{ij}}\right) \times \exp(\pm(-X_{ij} - X_{jk})\pi i)\right)\\
&\qquad\qquad\qquad \times \varphi_{\mathrm{KZ}}(X_{ij}, -X_{jk})^{-1} \times z_{ki}^T\\
&= G_\infty\left(X_{jk}, X_{ij} + X_{jk}; \frac{z_{kj}}{z_{ij}}\right) \times \exp(\pm X_{ij}\pi i)\\
&\qquad\qquad\qquad \times \varphi_{\mathrm{KZ}}(X_{ij}, -X_{jk})^{-1} \times z_{ki}^T\\
&= G_0\left(X_{jk}, X_{ij} + X_{jk}; \frac{z_{kj}}{z_{ij}}\right) \exp(\mp X_{jk}\pi i)\\
&\quad \times \varphi_{\mathrm{KZ}}(X_{jk}, -X_{ij})^{-1} \exp(\mp X_{ij}\pi i) \times \exp(\pm X_{ij}\pi i)\\
&\quad \times \varphi_{\mathrm{KZ}}(X_{ij}, -X_{jk})^{-1} \times z_{ki}^T\\
&= G_0\left(X_{jk}, X_{ij} + X_{jk}; \frac{z_{kj}}{z_{ij}}\right) \times \exp(\mp X_{jk}\pi i) \times z_{ki}^T\\
&= G_0\left(X_{jk}, -X_{ki}; \frac{z_{kj}}{z_{ij}}\right) \times z_{ij}^T \times \exp(\mp(-X_{ij} - X_{ik})\pi i)\\
&= W_{(jk)i}(z_1, z_2, z_3) \times \exp(\pm(X_{ij} + X_{ik}))\pi i),
\end{aligned}
$$

where $\frac{z_{ji}}{z_{ki}} \in \mathbf{H}_\pm$.

□

From this proposition, by comparing two ways to analytic continuation as in [Kas95], we obtain so called hexagon relation for the Drinfel′d associator

By substituting φ satisfy

$$
\begin{aligned}
&\exp((X_{ik} + X_{jk})\pi i)\\
&= \varphi_{\mathrm{KZ}}(X_{ik}, X_{ij}) \exp(X_{ik}\pi i) \varphi_{\mathrm{KZ}}(X_{ik}, X_{jk})^{-1} \exp(X_{jk}\pi i) \varphi_{\mathrm{KZ}}(X_{ij}, X_{jk}),\\
&\exp((X_{ij} + X_{ik})\pi i)\\
&= \varphi_{\mathrm{KZ}}(X_{jk}, X_{ik})^{-1} \exp(X_{ik}\pi i) \varphi_{\mathrm{KZ}}(X_{ij}, X_{ik}) \exp(X_{ij}\pi i) \varphi_{\mathrm{KZ}}(X_{ij}, X_{jk})^{-1}.
\end{aligned}
$$

Thus using Landen and Euler connection formulas, we obtain the hexagon relations.

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ZETA FUNCTIONS OVER ZEROS OF GENERAL ZETA AND L-FUNCTIONS

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We describe in detail three distinct families of generalized zeta functions built over the nontrivial zeros of a rather general arithmetic zeta or L-function, extending the scope of two earlier works that treated the Riemann zeros only. Explicit properties are also displayed more clearly than before. Several tables of formulae cover the simplest concrete cases: L-functions for real primitive Dirichlet characters, and Dedekind zeta functions.

1. Generalities

This text is a partial expansion of our oral presentation, which surveyed an earlier paper [27] on zeta functions over the Riemann zeros: these were Dirichlet series built out of the nontrivial zeros of a "primary" zeta function, Riemann's $\zeta(x)$, thus defining newer or "secondary" [5] zeta functions. Here we will fully develop the argument of [27, Sec. 5.5], which indicated how the primary function can actually be taken more general than just $\zeta(x)$; we also incorporate and extend subsequent work [28]. Accordingly, we can now reword the formalism to accommodate *three* distinct kinds of generalized zeta functions built over the nontrivial zeros of a fairly arbitrary number-theoretic zeta or L-function. The resulting explicit special values are presented in seven Tables.

Earlier *explicit* descriptions of such zeta functions, i.e., over zeros more general than Riemann's, hardly exist in the literature. We set apart the

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zeros of Selberg zeta functions: these zeros correspond to eigenvalues of Laplacians, and zeta functions over them have been analyzed by spectral methods [21, 24, 4, 26]: in the cocompact case, they are particular instances of Minakshisundaram–Pleijel zeta functions. Otherwise, only Dedekind zeta functions get some mention [19, 14]; already the works on L-series [17, 16, 9, 15] do not discuss zeta functions *per se* over the zeros, but exclusively Cramér functions $V(t) \approx \sum_{\{\operatorname{Im}\rho\geq 0\}} \mathrm{e}^{\rho t}$, which are somewhat related to those zeta functions but no such link gets any mention either. Broader references are more fully listed in our previous articles [27, 28].

As for notations, we basically follow [1, 10, 6]:

$$\begin{array}{ll} B_n : \text{Bernoulli numbers;} & B_n(\cdot) : \text{Bernoulli polynomials;} \\ E_n : \text{Euler numbers;} & \gamma : \text{Euler's constant;} \end{array} \tag{1.1}$$

$$\beta(s) \stackrel{\text{def}}{=} \sum_{k=0}^{\infty} (-1)^k (2k+1)^{-s} \ : \text{ a specific Dirichlet } L\text{-function,} \tag{1.2}$$

$$\text{with} \quad \beta(-n) = \tfrac{1}{2} E_n \ (n \in \mathbb{N}) \ \ (e.g., \ \beta(0) = \tfrac{1}{2}),$$

$$\beta'(0) = -\tfrac{3}{2}\log 2 - \log \pi + 2 \log \Gamma(\tfrac{1}{4});$$

$$\zeta(s, w) \stackrel{\text{def}}{=} \sum_{k=0}^{\infty} (k+w)^{-s} \ : \text{ the Hurwitz zeta function.} \tag{1.3}$$

For fixed w, $\zeta(s,w)$ has a single pole at $s = 1$, simple and of residue $= 1$, and the special values [10, Sec. 1.10]

$$\zeta(-n, w) = -B_{n+1}(w)/(n{+}1) \ \ (n \in \mathbb{N}), \ \ (e.g., \ \zeta(0, w) = \tfrac{1}{2} - w) \tag{1.4}$$

$$\mathrm{FP}_{s=1}\, \zeta(s, w) = -\Gamma'(w)/\Gamma(w) \qquad (\mathrm{FP} \stackrel{\text{def}}{=} \text{finite part at a pole}) \tag{1.5}$$

$$\zeta'(0, w) = \log\left[\Gamma(w)/(2\pi)^{1/2}\right] ; \tag{1.6}$$

upon parametric zeta functions as in (1.6) and (1.12–1.14) below, $'$ will always mean differentiation with respect to the *first* variable: the exponent, s or σ.

Our notations (otherwise consistent with [28]) are now generic: objects relative to the primary zeta or L-function which we denote $L(x)$ will obviously depend on it, usually without mention.

1.1 The primary functions $L(x)$

For the sake of definiteness, we confine interest here to situations still fairly close to the "Riemann case" $L(x) = \zeta(x)$; namely, to primary functions $L(x)$:

meromorphic in $\mathbb{C}$ with at most one pole: $x = 1$ (of order $q = 0$ or 1); (1.7)

nonvanishing in $\{\mathrm{Re}\, x > 1\}$, with the normalized asymptotic behavior

$$(\log L)^{(n)}(x) = O(x^{-\infty}) \quad \text{for } x \to +\infty \quad (\forall n \in \mathbb{N}); \tag{1.8}$$

obeying a functional equation of the same type as $\zeta(x)$,

$$\Xi(x) \equiv \Xi(1-x), \quad \Xi(x) \stackrel{\text{def}}{=} \mathbf{G}^{-1}(x)(x-1)^q L(x), \tag{1.9}$$

where both $\Xi(x)$ and $\mathbf{G}(x)$ are *entire functions of order* $\mu_0 = 1$. $\mathbf{G}(x)$ is a *fully explicit* factor, a product mainly of inverse-Gamma factors, which endows $L(x)$ with explicit ("trivial") zeros $x_k \in \{\mathrm{Re}\, x \le 0\}$. $\Xi(x)$ supplies the remaining (nontrivial) zeros of $L(x)$, which lie in symmetrical pairs within the strip $\{0 < \mathrm{Re}\, x < 1\}$ and can be labeled as

$$\{\rho = \tfrac{1}{2} \pm \mathrm{i}\tau_k\}_{k=1,2,\ldots}, \qquad \text{with } \mathrm{Re}\,\tau_k > 0 \text{ and non-decreasing;} \tag{1.10}$$

for simplicity, here we exclude the exceptional occurrence of real zeros ρ. Note: all zeros are systematically counted with multiplicities.

A special notation will be sometimes useful for this Taylor series at $x = 1$,

$$\log\left[(x-1)^q L(x)\right] \equiv \sum_{n=0}^{\infty} \frac{(-1)^{n-1}}{n!}\, g_n^{\mathrm{c}}\{L\}\,(x-1)^n. \tag{1.11}$$

The coefficients $g_n^{\mathrm{c}}\{L\}$ qualify as *generalized Stieltjes cumulants*: in the case $L(x) = \zeta(x)$, $q = 1$, then $g_n^{\mathrm{c}} = n\gamma_{n-1}^{\mathrm{c}}$ where $\{\gamma_{n-1}^{\mathrm{c}}\}$ constitutes a cumulant sequence for the *Stieltjes constants* γ_{n-1}, in the notation of [27]; cf. also the η_{n-1} in [3, Sec. 4]. We now prefer the labeling g_n^{c} (then n is the degree).

1.2 Three zeta families

We can then describe three (inequivalent) parametric zeta functions over the nontrivial zeros $\{\rho\}$ of a generic L satisfying the above conditions (1.7–1.9):

$$\mathscr{Z}(s,x) \stackrel{\text{def}}{=} \sum_\rho (x-\rho)^{-s} \equiv \sum_\rho (\rho + x - 1)^{-s} \quad (\mathrm{Re}\, s > 1) \tag{1.12}$$

definable for $(x-\rho) \notin \mathbb{R}^-$ $(\forall \rho)$, cf. [8, 22, 28] for the Riemann case;

$$\mathcal{Z}(\sigma, v) \stackrel{\text{def}}{=} \sum_{k=1}^{\infty} ({\tau_k}^2 + v)^{-\sigma} \qquad (\mathrm{Re}\,\sigma > \tfrac{1}{2}) \tag{1.13}$$

definable for $({\tau_k}^2 + v) \notin \mathbb{R}^-$ $(\forall k)$, cf. [11, 7, 19, 27] for the Riemann case;

$$\mathfrak{Z}(\sigma, y) \stackrel{\text{def}}{=} \sum_{k=1}^{\infty} (\tau_k + y)^{-2\sigma} \qquad (\operatorname{Re}\sigma > \tfrac{1}{2}) \tag{1.14}$$

definable for $(\tau_k + y) \notin \mathbb{R}^-$ $(\forall k)$, cf. [27, 14] for the Riemann case, with shorthand names for interesting special parameter values:

$$\mathscr{Z}(s) \stackrel{\text{def}}{=} \mathscr{Z}(s,1), \ \mathcal{Z}(\sigma) \stackrel{\text{def}}{=} \mathcal{Z}(\sigma, 0) \text{ (and, in [27]: } Z(\sigma) \stackrel{\text{def}}{=} \mathcal{Z}(\sigma, \tfrac{1}{4})). \tag{1.15}$$

Each family is a generalized zeta function *à la* Hurwitz, cf. eq.(1.3); its analytic structure mainly interests us in the exponent variable (s, or σ); the translation variable (x, v, or y) serves to generate a parametric family in its specified range of values.

The families $\{\mathscr{Z}\}$ and $\{\mathcal{Z}\}$ share a single function, through the relation

$$\mathcal{Z}(\sigma) \ (\equiv \mathcal{Z}(\sigma, 0)) \equiv (2\cos\pi\sigma)^{-1} \mathscr{Z}(2\sigma, \tfrac{1}{2}). \tag{1.16}$$

The family $\{\mathscr{Z}\}$ can be generated from the family $\{\mathfrak{Z}\}$ (but not vice-versa), thanks to the identity (for, e.g., $\operatorname{Re} t > 0$):

$$\mathscr{Z}\big(s, \tfrac{1}{2} + t\big) \equiv \big[\mathrm{e}^{\mathrm{i}\pi s/2} \mathfrak{Z}\big(\tfrac{1}{2}s, \mathrm{i}t\big) + \mathrm{e}^{-\mathrm{i}\pi s/2} \mathfrak{Z}\big(\tfrac{1}{2}s, -\mathrm{i}t\big)\big]. \tag{1.17}$$

The families $\{\mathscr{Z}\}$ and $\{\mathcal{Z}\}$ are built by summations over all zeros $\big(\tfrac{1}{2} \pm \mathrm{i}\tau_k\big)$ symmetrically; due to resulting cancellations, they will be better behaved overall than the third family $\{\mathfrak{Z}\}$ based on the zeros with only one sign – this type is dubbed "half zeta function" in [14]. Indeed, the first two families are formally expressible by "explicit formulae" *à la* Weil with suitably chosen test functions [13]; however, these formulae strictly *diverge* outside of clear-cut parameter domains: $\{\operatorname{Re} x > 1\}$ for $\{\mathscr{Z}(s, x)\}$, resp. $\{\operatorname{Re} v^{1/2} > \tfrac{1}{2}\}$ for $\{\mathcal{Z}(\sigma, v)\}$, and that excludes the most interesting special cases for us: $x = \tfrac{1}{2}$ and 1, resp. $v = 0$ and $\tfrac{1}{4}$. So, better adapted analytical schemes are still needed. On the basis of all the algorithms used in [27, 28], we see as the most efficient approach to fully describe the family $\{\mathscr{Z}\}$ first, then to derive the remaining algebraic properties through expansion formulae in the auxiliary parameter, and the transcendental properties from zeta-regularized factorizations of L. Thus, within the same basic framework as before, we will get broader results in fewer steps. Only for the full mathematical justifications must we still invoke [27, 28].

1.3 Range of application, and examples

Some of the restrictions made above are just convenient to keep the paper short and close to concrete cases, and can probably be weakened.

For instance, zeta functions over zeros of Selberg zeta functions have yielded results comparable to the Riemann case earlier [21, 24, 19, 4], while they correspond to $\mu_0 = 2$ (**G** contains a Barnes G-function), $q = -1$. Other extensions, e.g., to Hecke L-functions as achieved upon their Cramér functions [15], are equally conceivable. Currently, the assumptions are meant to closely fit two basic classes of examples; the most explicit properties of the zeta functions over their zeros will be listed in a concluding section.

- Dirichlet L-functions for real primitive Dirichlet characters: a *Dirichlet L-function* is associated with a character χ of a multiplicative group of integers mod d ($d \in \mathbb{N}^*$ is called the *modulus* or *conductor*), as [10, 6]

$$L_\chi(x) \stackrel{\text{def}}{=} \sum_{k=1}^{\infty} \chi(k)\, k^{-x} \equiv \prod_{\{\text{primes}\}} \left(1 - \chi(p)\, p^{-x}\right)^{-1} \qquad (\operatorname{Re} x > 1). \quad (1.18)$$

Such a character is either even or odd, with a parity index a defined by

$$a = 0 \text{ or } 1, \quad \text{according to} \quad \chi(-1) = (-1)^a. \qquad (1.19)$$

$L_\chi(x)$ always satisfies conditions (1.7–1.8) above. We now restrict to *primitive* characters [6], and $d > 1$ to exclude the case $\chi \equiv 1$, $L_\chi(x) \equiv \zeta(x)$, which more readily fits our next class of examples. Then, $L_\chi(x)$ is *entire*, and the following functional equation holds:

$$\Xi_\chi(x) \equiv W_\chi\, \Xi_{\overline{\chi}}(1 - x), \qquad (1.20)$$

$$\text{with} \quad \Xi_\chi(x) \stackrel{\text{def}}{=} (d/\pi)^{x/2} \Gamma\big(\tfrac{1}{2}(x + a)\big)\, L_\chi(x), \qquad (1.21)$$

$$W_\chi = (-\mathrm{i})^a d^{-1/2} \sum_{n \bmod d} \chi(n) \mathrm{e}^{2\pi \mathrm{i} n/d}\,; \qquad (1.22)$$

the latter sum is called the *Gaussian sum* for χ. The *real* ($\overline{\chi} = \chi$) primitive characters (mod d) are given by Kronecker symbols for quadratic number fields of discriminant $\pm d$; their Gaussian sums are explicitly known [12, thm 164], implying $W_\chi \equiv +1$ always; by way of consequence, the functional equation for their L-functions reduces to eq.(1.9), with

$$q \equiv 0; \quad \mathbf{G}(x) \equiv (\pi/d)^{x/2} / \Gamma\big(\tfrac{1}{2}(x{+}a)\big), \quad a = \begin{cases} 0 & \text{for } \chi \text{ even} \\ 1 & \text{for } \chi \text{ odd.} \end{cases} \qquad (1.23)$$

- Dedekind ζ-functions: for any algebraic number field K, its zeta function is defined as [12]

$$\zeta_K(x) \stackrel{\text{def}}{=} \sum_{\mathfrak{a}} N(\mathfrak{a})^{-x} \equiv \prod_{\mathfrak{p}} \left(1 - N(\mathfrak{p})^{-x}\right)^{-1} \qquad (\operatorname{Re} x > 1) \qquad (1.24)$$

where $\mathfrak{a}$ (resp. $\mathfrak{p}$) runs over all integral (resp. prime) ideals of K and $N(\mathfrak{a})$ is the norm of $\mathfrak{a}$. Then $L(x) = \zeta_K(x)$ satisfies all conditions (1.7–1.9) above, with

$$q \equiv 1, \qquad \mathbf{G}(x) \equiv \frac{\left(4^{r_2}\pi^{n_K}/|d_K|\right)^{x/2}}{x\Gamma(x/2)^{r_1}\Gamma(x)^{r_2}}, \tag{1.25}$$

where r_1 (resp. $2r_2$) is the number of real (resp. complex) conjugate fields of K, n_K ($\equiv r_1 + 2r_2$) the degree of K, and d_K ($\gtrless 0$) its discriminant [12, Sec. 42], [23]. For $K = \mathbb{Q}$, having $r_1 = 1$, $r_2 = 0$ and $d_K = 1$, Riemann's $\zeta(s)$ and its classic functional equation are recovered, with $q = 1$ and $\mathbf{G}(x) \equiv \pi^{x/2}\left[x\Gamma(x/2)\right]^{-1}$ in eq.(1.9).

2. The first family $\{\mathscr{Z}(s,x)\}$

2.1 The zeta function over the trivial zeros

We know [27, 28] that a key role must be played by the zeta function wholly analogous to $\mathscr{Z}(s,x)$ but built on the trivial zeros of $L(x)$,

$$\mathbf{Z}(s,x) \stackrel{\text{def}}{=} \sum_k (x - x_k)^{-s} \qquad (\operatorname{Re} s > 1) \tag{2.1}$$

(which we call the shadow zeta function of $\mathscr{Z}(s,x)$). Here this function and its special values should be taken as completely known, just like the trivial zeros themselves: in our concrete examples, $\mathbf{Z}(s,x)$ will be expressed in terms of the Hurwitz zeta function (1.3). It is also necessary to relate $\mathbf{Z}(s,x)$ and $\mathbf{G}(x)$ as fully as possible. We specially want the results *to include formulae for the special values* $\mathrm{FP}_{s=1}\mathbf{Z}(s,x)$ *and* $\mathrm{FP}_{s=1}\mathscr{Z}(s,x)$, *resp.* $\mathbf{Z}'(0,x)$ *and* $\mathscr{Z}'(0,x)$, because comparable formulae for the Hurwitz zeta function are quite important: eqs.(1.5), resp. (1.6). Then, the original normalization of the trivial factor proves awkward: it is better to rewrite $L(x)$ as a product of either Weierstrass-like factors (as in [27]) or zeta-regularized factors (as in [28]); we follow the latter course here.

We recall some off-the-shelf rules on zeta-regularization for suitable infinite products of order $\mu_0 = 1$, of the form $\Delta(x) = \mathrm{e}^{B_1 x + B_0}\prod_k[(1 - x/y_k)\mathrm{e}^{x/y_k}]$ ([28] and refs. therein); the rules will be valid for $\mathbf{G}(x)$ and $\Xi(x)$. Actually, eqs.(2.2) and (2.5) will also serve with $\mu_0 < 1$ in Sec. 3: they specifically are worded for general $0 < \mu_0 \le 1$. A key further requirement is an *asymptotic* "generalized Stirling" [16] *expansion for*

$\log \Delta(x)$ $(x \to +\infty)$, of the form

$$\log \Delta(x) \sim \widetilde{a}_1 x(\log x - 1) + b_1 x + \widetilde{a}_0 \log x + b_0 \quad \left[+ \sum_{\{\mu_k\} \setminus \{0,1\}} a_{\mu_k} x^{\mu_k} \right] \quad (2.2)$$

for some sequence $(1 \geq)\ \mu_0 > \mu_1 > \cdots > \mu_n \downarrow -\infty$, and indefinitely differentiable term by term. Here, the terms designated by coefficients a_μ or $\widetilde{a}_\mu$ are those *allowed* in a *zeta-regularized* product; any *extra* terms with a pure x^1 or x^0 dependence (more generally: $b_n x^n$, $n \in \mathbb{N}$) are *banned*. A generalized zeta function is also introduced, as $Z(s,x) = \sum_k (x - y_k)^{-s}$ if $\operatorname{Re} s > \mu_0$. Then:

- the zeta-regularized form $D(x)$ of a product $\Delta(x)$ is explicitly obtained just by removing any "banned" portion present in the large-x expansion of $\log \Delta(x)$: specifically here,

$$D(x) \stackrel{\text{def}}{=} \mathrm{e}^{-Z'(0,x)} \equiv \mathrm{e}^{-(b_1 x + b_0)} \Delta(x); \quad (2.3)$$

- the logarithmic derivatives of the zeta-regularized product yield

$$(\log D)'(x) \equiv \mathrm{FP}_{s=1} Z(s,x), \quad (2.4)$$

$$\frac{(-1)^{m-1}}{(m-1)!} (\log D)^{(m)}(x) \equiv Z(m,x) \quad \text{for integer } m > \mu_0 \quad (2.5)$$

(we will also use this last formula once with $\mu_0 = \frac{1}{2}$, in Sec. 3);

- the results carry over to non-integer s as Mellin-transform formulae:

$$\begin{aligned} Z(s,x) &= \frac{\sin \pi s}{\pi(1-s)} I(s,x), \\ I(s,x) &\stackrel{\text{def}}{=} \int_0^\infty Z(2, x+y)\, y^{1-s}\, \mathrm{d}y \quad (1 < \operatorname{Re} s < 2); \end{aligned} \quad (2.6)$$

then, $I(s,x)$ extends to a meromorphic function in the whole s-plane through repeated integrations by parts, and its polar structure is fully encoded in the $(y \to +\infty)$ expansion of $Z(2, x+y)$, itself computable – see next example.

We now specialize the above results first to the trivial factor $\mathbf{G}(x)$. Consisting mainly of inverse Gamma factors, $\mathbf{G}(x)$ has a *computable* Stirling expansion (for $x \to +\infty$) which can be reorganized in the form

$$-\log \mathbf{G}(x) \sim \widetilde{a}_1 x(\log x - 1) + b_1 x + \widetilde{a}_0 \log x + b_0 \ + \sum_{n=1}^{\infty} a_{-n} x^{-n}, \quad (2.7)$$

and which also governs $[\log \Xi(x) - q \log(x-1)]$, by eqs.(1.8) and (1.9). Equation (2.3) then implies that the zeta-regularized forms for $\mathbf{G}(x)$ and $\Xi(x)$ are

$$\mathbf{D}(x) \stackrel{\text{def}}{=} \mathrm{e}^{-\mathbf{Z}'(0,x)} \equiv \mathrm{e}^{+b_1 x + b_0} \mathbf{G}(x), \tag{2.8}$$

$$\mathscr{D}(x) \stackrel{\text{def}}{=} \mathrm{e}^{-\mathscr{Z}'(0,x)} \equiv \mathrm{e}^{-b_1 x - b_0} \Xi(x), \tag{2.9}$$

which in turn entail a zeta-regularized decomposition of $L(x)$, as

$$(x-1)^q L(x) \equiv \mathbf{D}(x) \mathscr{D}(x). \tag{2.10}$$

Concretely here, using eq.(2.8) and $\mu_0 = 1$, eqs.(2.4) and (2.5) translate to

$$\mathrm{FP}_{s=1} \mathbf{Z}(s,x) \equiv (\log \mathbf{G})'(x) + b_1, \tag{2.11}$$

$$\mathbf{Z}(m,x) \equiv \frac{(-1)^{m-1}}{(m-1)!} (\log \mathbf{G})^{(m)}(x) \quad \text{for } m = 2, 3, \ldots . \tag{2.12}$$

The substitution of the Stirling series (2.7) into eq.(2.12) with $m = 2$ leads to the ($y \to +\infty$) expansion of $\mathbf{Z}(2, x+y)$ in the simple form $\sum_{n \ge -1} c_{-n}(x) y^{-n-2}$ (the $c_{-n}(x)$ are polynomials). It follows that eq.(2.6), written for $Z = \mathbf{Z}$, yields an $I(s,x)$ with poles at $s = -n$, $n = -1$, 0, 1, 2, ..., all simple and of residues $c_{-n}(x)$. As consequences for $\mathbf{Z}(s,x)$, restated in fully explicit form:

- $\mathbf{Z}(s,x)$ extends to a meromorphic function in the whole s-plane, with

$$\text{the single pole } s = 1, \text{ simple, of residue } \widetilde{a}_1 \quad \text{(independent of } x\text{)}. \tag{2.13}$$

- the values $\mathbf{Z}(-n,x)$, $n \in \mathbb{N}$ are given by *closed polynomial formulae* ("trace identities" in a spectral setting), as

$$\mathbf{Z}(-n,x) = -\frac{\widetilde{a}_1}{n+1} x^{n+1} - \widetilde{a}_0 x^n + n \sum_{j=1}^{n} (-1)^j \binom{n-1}{j-1} a_{-j} x^{n-j},$$
$$e.g., \quad \mathbf{Z}(0,x) = -\widetilde{a}_1 x - \widetilde{a}_0 \,. \tag{2.14}$$

Then, the same formulae overall hold with $\mathbf{D}$, $\mathbf{Z}$, $\mathbf{G}$ replaced by the (less explicit) $\mathscr{D}$, $\mathscr{Z}$, Ξ respectively, and with suitably changed coefficients.

2.2 The main result

As a generalization of eq.(42) in [28], $\mathscr{Z}(s,x)$ admits an integral representation valid in the half-plane $\{\mathrm{Re}\, s < 1\}$ and for any eligible value of the parameter x avoiding the cut $(-\infty, +1]$:

$$\mathscr{Z}(s,x) = -\mathbf{Z}(s,x) + \frac{q}{(x-1)^s} + \frac{\sin \pi s}{\pi} \mathscr{J}(s,x), \tag{2.15}$$

$$\mathscr{J}(s,x) \stackrel{\text{def}}{=} \int_0^\infty \frac{L'}{L}(x+y)\, y^{-s}\, \mathrm{d}y \quad (\operatorname{Re} s < 1); \tag{2.16}$$

here, $(x-1)^s$ is given its standard determination for $x \in \mathbb{C} \setminus (-\infty, +1]$; its discontinuity across the real axis, as well as those of $-\mathbf{Z}(s,x)$, are precisely cancelled through corresponding jumps of $\mathscr{J}(s,x)$ so that only the *nontrivial* zeros of $L(x)$ induce genuine x-plane discontinuities in $\mathscr{Z}(s,x)$; this can be checked by comparing computations of the right-hand side with small imaginary parts $(\pm \mathrm{i}0)$ added to x.

Eq.(2.15) easily takes real forms; a simple one valid for $x > 0$ (at least) is

$$\mathscr{Z}(s,x) = -\mathbf{Z}(s,x) + \frac{\sin \pi s}{\pi} \int_0^\infty \Big[\frac{L'}{L}(x+y) + \frac{q}{x+y-1}\Big] y^{-s}\, \mathrm{d}y \tag{2.17}$$
$$(0 < \operatorname{Re} s < 1);$$

this form only converges in a strip of the s-plane, but unlike (2.15), it remains well defined as $x \to +1$:

$$\mathscr{Z}(s,1) = -\mathbf{Z}(s,1) + \frac{\sin \pi s}{\pi} \int_0^\infty \Big[\frac{L'}{L}(1+y) + \frac{q}{y}\Big] y^{-s}\, \mathrm{d}y. \tag{2.18}$$

The proof is now a simple application of the general formulae above: the second logarithmic derivative of eq.(2.10) (or (1.9)) gives $[\mathscr{Z}+\mathbf{Z}](2,x) = q(x-1)^{-2} - (L'/L)'(x)$, using eq.(2.5) for $D = \Xi\, \mathbf{G}$ and $m = 2$; upon this, for $x \notin (-\infty, +1]$ the Mellin formula (2.6) yields

$$[\mathscr{Z} + \mathbf{Z}](s,x) \equiv \frac{\sin \pi s}{\pi(1-s)} \int_0^\infty \Big[\frac{q}{(x+y-1)^2} - \Big(\frac{L'}{L}\Big)'(x+y)\Big]\, y^{1-s}\, \mathrm{d}y. \tag{2.19}$$

Now, moreover, *this* integral is convergent and analytic in $\{0 < \operatorname{Re} s < 2\}$: indeed the integrand is regular, bounded for $y \to +0$, and $O(y^{-2})$ for $y \to +\infty$ by eq.(1.8). Then, splitting the integral in two, the first term evaluates explicitly to $q(x-1)^{-s}$, and upon restricting to $0 < \operatorname{Re} s < 1$, the second term transforms to $\pi^{-1} \sin \pi s\, \mathscr{J}(s,x)$ through an integration by parts; hence the result (2.15). – The same integration by parts upon the whole integral yields eq.(2.17) instead.

2.3 Explicit consequences for the family $\{\mathscr{Z}(s,x)\}$

The subsequent statements refer to s as variable, with x fixed.

Eq.(2.15) is a true analog for $\mathscr{Z}(s,x)$ of the Joncquière–Lerch functional relation for $\zeta(s,w)$ [10, Sec. 1.11 eq.(16)]. First of all, it gives an explicit one-step analytical continuation of $\mathscr{Z}(s,x)$ to the half-plane $\{\operatorname{Re} s < 1\}$. It also implies its *meromorphic continuation in* s to all of $\mathbb{C}$, since a Mellin transform like $\mathscr{J}(s,x)$ has a well understood meromorphic structure: repeated integrations by parts on eq.(2.16), invoking the asymptotic formula (1.8), show that $\mathscr{J}(s,x)$ is meromorphic in the whole s-plane, and has only simple poles at $s = 1, 2, \ldots$, with residues

$$\operatorname{Res}_{s=n} \mathscr{J}(s,x) = -(\log|L|)^{(n)}(x)/(n-1)! \qquad (n = 1, 2, \ldots). \tag{2.20}$$

It then follows from eq.(2.15) that $\mathscr{Z}(s,x)$ precisely inherits the polar structure of $-\mathbf{Z}(s,x)$, namely (cf. eq.(2.13)):

$$\mathscr{Z}(s,x) \text{ has the single pole } s = 1, \text{ simple, of residue } -\widetilde{a}_1. \tag{2.21}$$

If $L(x)$ admits an Euler product, as in the examples (1.18) and (1.24), then the substitution of its logarithmic derivative into eq.(2.16), followed by integration term by term, yields an *asymptotic* ($s \to -\infty$) *expansion* for $\mathscr{J}(s,x)$, and thereby for $\mathscr{Z}(s,x)$, just as in the Riemann case [28, eq.(52)].

Finally, almost all the *special values* of $\mathscr{Z}(s,x)$ (at integer s) are explicitly readable off eq.(2.15) thanks to its vanishing factor $(\sin \pi s)$. On general grounds [27, Sec. 4], the $\mathscr{Z}(n,x)$ come out *algebraically* for $n \in -\mathbb{N}$ (Table 1, upper part) and, together with $\mathscr{Z}'(0,x)$, *transcendentally* for $n \in \mathbb{N}^*$: for instance, with the help of eqs.(2.8), (2.11) and (2.20), we get

$$\begin{aligned}
\mathscr{Z}'(0,x) &= -\mathbf{Z}'(0,x) - q\log(x-1) + \mathscr{J}(0,x) \\
&= b_1 x + b_0 + \log \mathbf{G}(x) - \log\left[(x-1)^q L(x)\right] \qquad (2.22) \\
\mathrm{FP}_{s=1}\mathscr{Z}(s,x) &= -\mathrm{FP}_{s=1}\mathbf{Z}(s,x) + \frac{q}{x-1} - \operatorname{Res}_{s=1}\mathscr{J}(s,x), \\
&= -b_1 - (\log \mathbf{G})'(x) + \left[\frac{q}{x-1} + \frac{L'}{L}(x)\right], \qquad (2.23)
\end{aligned}$$

and likewise for $\mathscr{Z}(n,x)$, $n \geq 2$. The terms in brackets stay globally continuous for $x \to 1$ (also in eq.(2.25) below); the special values reached at $x = 1$ are displayed later, in eq.(2.31).

However, the values $\mathscr{Z}(n,x)$ for $n \in \mathbb{N}^*$ now *also including* $n = 1$, emerge more simply by differentiating the logarithm of a symmetrical Hadamard product formula, $\Xi(x) \propto \prod_\rho (1 - x/\rho)$ just as in the Riemann

s	$\mathscr{Z}(s,x)=\sum_\rho (x-\rho)^{-s}$
$-n \le 0$	$-\mathbf{Z}(-n,x)+q(x-1)^n$
0	$\widetilde{a}_1 x+\widetilde{a}_0+q$
s-derivative at 0	$\mathscr{Z}'(0,x)=b_1x+b_0-\log\Xi(x)$
finite part at +1	$\mathrm{FP}_{s=1}\mathscr{Z}(s,x)=-b_1+(\log\Xi)'(x)$
$+n \ge 1$	$\dfrac{(-1)^{n-1}}{(n-1)!}(\log\Xi)^{(n)}(x)$

Table 1. Special values of $\mathscr{Z}(s,x)$ (upper part: algebraic, lower part: transcendental [27]) for a general primary zeta function $L(x)$ with a pole of order q at $x=1$. Notations: see eqs.(1.9) for $\Xi(x)$, (2.1) and (2.14) for $\mathbf{Z}(-n,x)$, (2.7) for $\widetilde{a}_j$, b_j; n is an integer.

case [28]:

$$\mathscr{Z}(n,x)$$
$$=\frac{(-1)^{n-1}}{(n-1)!}(\log\Xi)^{(n)}(x) \qquad (n=1,2,\ldots) \tag{2.24}$$
$$=-\mathbf{Z}(n,x)+\left[\frac{q}{(x-1)^n}+\frac{(-1)^{n-1}}{(n-1)!}(\log|L|)^{(n)}(x)\right] \quad (n=2,3,\ldots). \tag{2.25}$$

This is by far the quickest route to these transcendental values, but it altogether misses two others of interest, $\mathscr{Z}'(0,x)$ and $\mathrm{FP}_{s=1}\mathscr{Z}(s,x)$, which the previous method did find in eqs.(2.22) and (2.23) respectively.

For $n=1$, eq.(2.25) cannot hold: $\mathscr{Z}(1,x)$ is finite, being *defined* by eq.(2.24) to be $\sum_\rho (x-\rho)^{-1}$ with the zeros grouped in pairs as usual, whereas $\mathbf{Z}(1,x)$ diverges; at the same time, both functions $\mathscr{Z}(s,x)$ and $\mathbf{Z}(s,x)$ have a polar singularity at $s=1$, in fact only the signs differ ! Now there is a substitute formula to eq.(2.25) for $n=1$: the comparison of eq.(2.24) with eq.(2.23) yields a *fixed anomaly*, or discrepancy between two natural specifications for a finite value at $s=1$,

$$\mathscr{Z}(1,x)-\mathrm{FP}_{s=1}\mathscr{Z}(s,x)=(\log[\Xi/\mathscr{D}])'(x)=b_1 \quad \text{(constant)}. \tag{2.26}$$

Table 1 summarizes the special values obtained for $\mathscr{Z}(s,x)$ at general x, thus extending to general primary functions $L(x)$ formulae previously restricted to $L(x)=\zeta(x)$, cf. Table 2 in [28].

The two sets of linear identities for the values $\mathscr{Z}(n,x)$ in the Riemann case [28, eqs.(61–62)], which are purely induced by the symmetry ($\rho \longleftrightarrow$

$1-\rho$) in eq.(1.12), naturally persist here:

$$\mathscr{Z}(n,x) = (-1)^n \mathscr{Z}(n,1-x) \qquad \text{for } n=1,2,\ldots; \tag{2.27}$$

$$\mathscr{Z}(k,x) = -\frac{1}{2}\sum_{\ell=k+1}^{\infty}\binom{\ell-1}{k-1}(2x-1)^{\ell-k}\mathscr{Z}(\ell,x) \text{ for each } odd\ k \geq 1. \tag{2.28}$$

Under our assumption $\{\rho\}\cap\mathbb{R}=\emptyset$, $\mathscr{Z}(s,x)$ is regular on the real x-axis, and even more explicit formulae result at special x-values such as $x=\frac{1}{2}$ and $x=1$, which respectively correspond (via the functional equation (1.9)) to the symmetry center of $\Xi(x)$ and to the origin in the x-plane. Thus for $x=\frac{1}{2}$, eq.(2.24) simplifies to

$$\mathscr{Z}(n,\tfrac{1}{2}) \equiv 0 \qquad \text{for all } n \geq 1 \text{ odd} \tag{2.29}$$

$$\Longrightarrow \quad \mathrm{FP}_{s=1}\mathscr{Z}(s,\tfrac{1}{2}) = -b_1 \quad \text{by eq.(2.26)}; \tag{2.30}$$

in combination with eqs.(2.25) and (2.23), these amount to the explicit values $(\log|L|)^{(2m+1)}(\frac{1}{2}) = (\log\mathbf{G})^{(2m+1)}(\frac{1}{2}) + 2^{2m+1}q\,(2m)!$ ($\forall m\in\mathbb{N}$), also directly readable off the functional equation (1.9). Now for $x=1$, that same formula (2.24) brings in the Taylor series (1.11), to yield

$$\begin{aligned} &\mathscr{Z}(1,1) = -(\log\mathbf{G})'(1) + g_1^{\mathrm{c}}\{L\},\\ &\mathscr{Z}(n,1) = -\mathbf{Z}(n,1) + g_n^{\mathrm{c}}\{L\}/(n-1)! \quad (n=2,3,\ldots); \\ \text{also,}\quad &\mathscr{Z}'(0,1) = -\mathbf{Z}'(0,1) + g_0^{\mathrm{c}}\{L\}. \end{aligned} \tag{2.31}$$

Case by case, $\mathbf{Z}(s,x)$ can itself be made explicit for $x=\frac{1}{2}$ or 1, just as when $L(x)=\zeta(x)$ [28, Sec. 3.3]; in our selected examples (1.18) and (1.24) it will then turn into combinations of the two fixed Dirichlet series $\zeta(s)$ and $\beta(s)$ of eq.(1.2). The resulting fully reduced special values of $\mathscr{Z}(s,\frac{1}{2})$ and $\mathscr{Z}(s,1)\equiv\mathscr{Z}(s)$ are tabulated in the concluding Sec. 5.

3. The second family $\{\mathcal{Z}(\sigma,v)\}$

The main starting tool is the relation (1.16), which allows a one-to-one transfer of the previous results for $\mathscr{Z}(s,\frac{1}{2})$ onto one particular member, $\mathcal{Z}(\sigma)\equiv\mathcal{Z}(\sigma,v=0)$, of the second family.

3.1 The basic case $v=0$

The identity (1.16) shows that $\mathcal{Z}(\sigma)$ is meromorphic in all of $\mathbb{C}$ with a double pole at $\sigma=\frac{1}{2}$, simple poles at $\sigma=\frac{1}{2}-m$ ($m=1,2,\ldots$), and polar parts:

$$
\begin{aligned}
&\mathcal{Z}(\tfrac{1}{2}+\varepsilon)\\
&= -\mathrm{Res}_{s=1}\mathscr{Z}(s,\tfrac{1}{2})\frac{1}{4\pi\varepsilon^2} - \mathrm{FP}_{s=1}\mathscr{Z}(s,\tfrac{1}{2})\frac{1}{2\pi\varepsilon} + O(1)_{\varepsilon\to 0}\\
&= \frac{\widetilde{a}_1}{4\pi\varepsilon^2} + \frac{b_1}{2\pi\varepsilon} + O(1)_{\varepsilon\to 0}\ ; \qquad (3.1)\\
&\mathcal{Z}(\tfrac{1}{2}-m+\varepsilon)\\
&= \frac{(-1)^{m+1}}{2\pi\varepsilon}\mathscr{Z}(1-2m,\tfrac{1}{2}) + O(1)_{\varepsilon\to 0} \qquad \text{for } m=1,2,\ldots,
\end{aligned}
$$

$$
\text{i.e., } \mathcal{R}_m \overset{\text{def}}{=} \mathrm{Res}_{\sigma=\frac{1}{2}-m}\mathcal{Z}(\sigma) = \frac{(-1)^m}{2\pi}\left[\mathbf{Z}(1-2m,\tfrac{1}{2}) + q\,2^{1-2m}\right]; \quad (3.2)
$$

eq.(3.1) follows from eqs.(2.21) and (2.30), and $\mathcal{R}_m$ from Table 1.

That relation also yields an integral representation for $\mathcal{Z}(\sigma)$ ([27, eq.(72)] for the Riemann case), just by specializing eq.(2.15) to $x=\frac{1}{2}\pm\mathrm{i}0$. Finally, it delivers all the special values of $\mathcal{Z}(\sigma)$ as

$$
\mathcal{Z}(m) = \tfrac{1}{2}(-1)^m\mathscr{Z}(2m,\tfrac{1}{2}) \quad \text{for } m\in\mathbb{Z}, \qquad \mathcal{Z}'(0) = \mathscr{Z}'(0,\tfrac{1}{2}), \quad (3.3)
$$

which become fully explicit using Table 1. The problem is then to extend all those results to general values of the parameter v.

3.2 Algebraic results for general v

Our best tool here is a straightforward expansion of $\mathcal{Z}(\sigma,v)$ around $v=0$ [27], convergent for $|v|<\min_k\{|\tau_k|^2\}$:

$$
\mathcal{Z}(\sigma,v) = \sum_{k=0}^{\infty}({\tau_k}^2)^{-\sigma}\Big(1+\frac{v}{{\tau_k}^2}\Big)^{-\sigma} = \sum_{\ell=0}^{\infty}\frac{\Gamma(1-\sigma)}{\ell!\,\Gamma(1-\sigma-\ell)}\mathcal{Z}(\sigma+\ell)\,v^\ell. \quad (3.4)
$$

This first provides the meromorphic continuation of $\mathcal{Z}(\sigma,v)$ at fixed $v\neq 0$ to the whole complex σ-plane, now with *double poles* at all $\sigma=-m+\frac{1}{2}$, $m\in\mathbb{N}$. More precisely, the polar part of $\mathcal{Z}(\sigma,v)$ at each pole only depends on a *finite* stretch of the series (3.4),

$$
\mathcal{Z}(-m+\tfrac{1}{2}+\varepsilon,v) = \sum_{\ell=0}^{m}\frac{\Gamma(\frac{1}{2}+m-\varepsilon)}{\ell!\,\Gamma(\frac{1}{2}+m-\ell-\varepsilon)}\mathcal{Z}(-m+\ell+\tfrac{1}{2}+\varepsilon)\,v^\ell + O(1)_{\varepsilon\to 0}\ ; \quad (3.5)
$$

upon importing the polar structure of $\mathcal{Z}(\sigma)$ from eqs.(3.1–3.2), this yields

$$\mathcal{Z}(-m+\tfrac{1}{2}+\varepsilon, v) = \frac{\widetilde{a}_1}{4\pi}\frac{\Gamma(m+\frac{1}{2})}{m!\Gamma(\frac{1}{2})} v^m\, \varepsilon^{-2} + \mathcal{R}_m(v)\,\varepsilon^{-1} \;+ O(1)_{\varepsilon\to 0}\ ,$$

$$\mathcal{R}_m(v) = -\frac{\Gamma(m+\frac{1}{2})}{m!\Gamma(\frac{1}{2})}\Big[\frac{\widetilde{a}_1}{2\pi}\sum_{j=1}^{m}\frac{1}{2j-1} - \frac{b_1}{2\pi}\Big] v^m + \sum_{j=1}^{m}\frac{\Gamma(\frac{1}{2}+m)}{(m-j)!\Gamma(\frac{1}{2}+j)}\mathcal{R}_j\, v^{m-j}. \tag{3.6}$$

Here, the polar part of order 2 at every $(-m+\frac{1}{2})$ clearly comes from the single double pole of $\mathcal{Z}(\sigma)$ (at $\sigma=\frac{1}{2}$); whereas each residue $\mathcal{R}_m(v)$ has contributions from all the residues of $\mathcal{Z}(\sigma)$ at $\sigma = -j+\frac{1}{2} \geq -m+\frac{1}{2}$, specified by eqs.(3.1) for $j=0$ and (3.2) for $j\geq 1$. For the leading pole $s=\frac{1}{2}$, eq.(3.6) boils down to eq.(3.1), i.e., *this* full polar part is independent of v.

For the special values $\mathcal{Z}(-m,v)$, $m\in\mathbb{N}$, the series (3.4) also terminates:

$$\mathcal{Z}(-m,v) \equiv \sum_{\ell=0}^{m}\binom{m}{\ell}\mathcal{Z}(-m+\ell)\, v^{\ell} \qquad (m\in\mathbb{N}), \tag{3.7}$$

where the values $\mathcal{Z}(-m+\ell)$ are explicit from eq.(3.3) and Table 1; e.g.,

$$\mathcal{Z}(0,v) \equiv \tfrac{1}{2}\big[-\mathbf{Z}(0,\tfrac{1}{2})+q\big] \equiv \tfrac{1}{2}(\tfrac{1}{2}\widetilde{a}_1+\widetilde{a}_0+q) \qquad \text{(independent of } v\text{)}. \tag{3.8}$$

In the end, all the polar terms of $\mathcal{Z}(\sigma,v)$, and the special values $\mathcal{Z}(-m,v)$, $m\in\mathbb{N}$ (Table 2, upper half), are *computable polynomials* in v.

3.3 Transcendental values for general v

Now an optimal tool is a variant of the factorization (2.10), using the alternative zeta-regularized factor

$$\mathcal{D}(v) \stackrel{\text{def}}{=} \mathrm{e}^{-\mathcal{Z}'(0,v)} \tag{3.9}$$

instead of $\mathscr{D}(x)$. The main point here is the replacement of x by $v = (x-\frac{1}{2})^2$ as basic variable: then, in contrast to $\mathscr{D}(x)$ of eq.(2.10), this zeta-regularization of $\Xi(x)$ *preserves the symmetry* $(x \longleftrightarrow 1-x)$.

Rewritten in the variable $v \to +\infty$, the Stirling formula (2.7) for $[\log \Xi(x) - q \log(x-1)]$ becomes of order $\frac{1}{2} < 1$, yielding

$$\log \Xi(\sqrt{v} + \tfrac{1}{2}) \sim \tfrac{1}{2}\widetilde{a}_1 v^{\frac{1}{2}} \log v + (b_1 - \widetilde{a}_1) v^{\frac{1}{2}} + \tfrac{1}{2}\big(\tfrac{1}{2}\widetilde{a}_1 + \widetilde{a}_0 + q\big) \log v \\ + \big(\tfrac{1}{2} b_1 + b_0\big)\ [+O(v^{-\frac{1}{2}})]; \tag{3.10}$$

as "banned" terms (cf. Sec. 2.1), only constants ($b_0 v^0$) can now occur ($v^\mu \log v$ are allowed if $\mu \notin \mathbb{N}$, they just induce *double* poles in the zeta functions [27]); here this results in

$$\mathcal{D}(v) \equiv \mathrm{e}^{-(b_0 + b_1/2)} \Xi(\tfrac{1}{2} + v^{1/2}) \equiv \mathrm{e}^{b_1 v^{1/2}} \mathscr{D}(\tfrac{1}{2} + v^{1/2}) \tag{3.11}$$

and in the modified decomposition (cf. [28, eq.(41)] for the Riemann case)

$$(x-1)^q L(x) \equiv \mathrm{e}^{-b_1(x-1/2)} \mathbf{D}(x) \mathcal{D}(v), \qquad v \stackrel{\text{def}}{=} (x - \tfrac{1}{2})^2. \tag{3.12}$$

All transcendental special values of $\mathcal{Z}(\sigma, v)$ immediately follow, just as in the Riemann case [27]: first, $\mathcal{Z}'(0, v) \equiv -\log \mathcal{D}(v)$ expresses in terms of $\log \Xi(\frac{1}{2} \pm v^{1/2})$, and thereby of $\log L(\frac{1}{2} \pm v^{1/2})$, using eq.(3.11); then eq.(2.5), now applied to $\mathcal{D}$ and $\mathcal{Z}$ with v as variable giving $\mu_0 = \frac{1}{2}$, yields

$$\mathcal{Z}(m, v) = \frac{(-1)^{m-1}}{(m-1)!} \frac{\mathrm{d}^m}{\mathrm{d}v^m} \log \Xi(\tfrac{1}{2} \pm v^{1/2}), \qquad m = 1, 2, \ldots. \tag{3.13}$$

By the chain rule, this right-hand side must simplify to a finite linear combination of derivatives $(\log \Xi)^{(\ell)}(x)$ at $x = \frac{1}{2} \pm v^{1/2}$, and thereby of values $\mathscr{Z}(\ell, x)$ by eq.(2.24), but it is unclear how to carry through this nonlinear change of variables for general m and v directly. Instead, setting $v \equiv (x - \frac{1}{2})^2$ and $\rho \equiv \frac{1}{2} + \mathrm{i}\tau$ throughout here, we may start from the identity

$$\Big(1 - \frac{s}{x - \rho}\Big)\Big(1 - \frac{s}{x - 1 + \rho}\Big) \equiv 1 - \frac{s(2x - 1 - s)}{\tau^2 + v}, \tag{3.14}$$

expand the logarithms of both sides, and identify like powers of s to get a triangular sequence (for $n = 1, 2, \ldots$) of linear identities,

$$\frac{(x-\rho)^{-n} + (x-1+\rho)^{-n}}{n} \equiv \sum_{0 \le \ell \le n/2} (-1)^\ell \binom{n-\ell}{\ell} (2x-1)^{n-2\ell} \frac{(\tau^2+v)^{-n+\ell}}{n-\ell}. \tag{3.15}$$

Then, on the one hand, summing this over (half) the zeros yields the identities

$$\frac{\mathscr{Z}(n,x)}{n} \equiv \sum_{0\le\ell\le n/2} (-1)^\ell \binom{n-\ell}{\ell} (2x-1)^{n-2\ell}\, \frac{\mathcal{Z}(n-\ell,v)}{n-\ell} \quad \text{for } n=1,2,\ldots, \tag{3.16}$$

which clearly generalize eqs.(2.29) for n odd, and (3.3) for n even, away from $x=\frac{1}{2}$. On the other hand, eqs.(3.15) invert into finite linear relations of the same form (if $x \neq \frac{1}{2}$): $(\tau^2+v)^{-m} \equiv \sum_{n=1}^{m} V_{m,n}(x)[(x-\rho)^{-n}+(x-1+\rho)^{-n}]$. At this point we can identify $V_{m,n}(x)$: it has to be the coefficient of $(x-\rho)^{-n}$ in the Laurent series of $(\tau^2+v)^{-m} = (x-\rho)^{-m}[2x-1-(x-\rho)]^{-m}$ in powers of $(x-\rho)$, hence $V_{m,n}(x) = \binom{2m-n-1}{m-1}(2x-1)^{n-2m}$. Then, upon summing the above expression for $(\tau^2+v)^{-m}$ over half the zeros, we finally get

$$\mathcal{Z}(m,v) \equiv \sum_{\ell=0}^{m-1} \binom{m+\ell-1}{m-1} (2x-1)^{-m-\ell}\, \mathscr{Z}(m-\ell,x) \tag{3.17}$$

$$\text{for } v \equiv (x-\tfrac{1}{2})^2 \neq 0 \text{ and } m=1,2,\ldots,$$

whereas $\mathcal{Z}(m,0) \equiv \frac{1}{2}(-1)^m \mathscr{Z}(2m,\frac{1}{2})$, by eq.(3.3). Remark: the pair of mutually inverse relations (3.16) and (3.17) are clearly similar to the identities (2.28) and have the same origin. They extend to all primary functions L and all v-values previous results written only for the Riemann case and $v=\frac{1}{4}$ [20, 27].

The resulting values of $\mathcal{Z}(\sigma,v)$ for general v are listed in Table 2 (lower half). This Table improves upon Table 1 of [28] in two independent ways: it is valid for zeros of a general primary function $L(x)$, not just $\zeta(x)$, and it specifies $\mathcal{Z}(+m,v)$ more explicitly.

In the particular case $v=\frac{1}{4}$, the transcendental special values of $\mathcal{Z}(\sigma,\frac{1}{4})$ involve those of $\mathscr{Z}(s,1)$ by eq.(3.17), hence they will likewise end up expressed in terms of the generalized Stieltjes cumulants (1.11), cf. Tables 3, 4, 6 below.

4. The third family $\{\mathfrak{Z}(\sigma,y)\}$

As with the preceding case, a starting point is the knowledge of one particular member of the family, now through the obvious identity $\mathfrak{Z}(\sigma,0) \equiv \mathcal{Z}(\sigma,0)$. All results of Sec. 3.1 then cover this case as well.

The generic $\mathfrak{Z}(\sigma,y)$ (with $y \neq 0$) is built on a *desymmetrized* set of zeros, say $(\frac{1}{2}+\mathrm{i}\tau_k)$ only, hence it will be harder to describe explicitly than

σ	$\mathscr{Z}(\sigma, v) = \sum_{k=1}^{\infty} ({\tau_k}^2 + v)^{-\sigma}$
$-m \le 0$	$\frac{1}{2}\Big[-\sum_{j=0}^{m} {m \atop j} (-1)^j \mathbf{Z}(-2j, \frac{1}{2}) v^{m-j} + q(v - \frac{1}{4})^m\Big]$
0	$\frac{1}{2}(\frac{1}{2}\widetilde{a}_1 + \widetilde{a}_0 + q)$
σ-derivative at 0	$\mathscr{Z}'(0, v) = \frac{1}{2}\, b_1 + b_0 - \log \Xi(\frac{1}{2} \pm v^{1/2})$
$+m \ge 1$	$\begin{cases} -\sum_{\ell=0}^{m-1} {m+\ell-1 \atop m-1} \frac{(\mp 2v^{1/2})^{-m-\ell}}{(m-\ell-1)!} (\log \Xi)^{(m-\ell)}(x)\big\vert_{x=\frac{1}{2}\pm v^{1/2}} & (v \neq 0) \\ \dfrac{(-1)^{m+1}}{2(2m-1)!} (\log \Xi)^{(2m)}(\frac{1}{2}) & (v = 0) \end{cases}$

Table 2. Special values of $\mathscr{Z}(\sigma, v)$ (upper half: algebraic, lower half: transcendental [27]) for a general primary zeta function $L(x)$ with a pole of order q at $x = 1$. Notations: see eqs.(1.9) for $\Xi(x)$, (2.1) and (2.14) for $\mathbf{Z}(-n, x)$, (2.7) for $\widetilde{a}_j$, b_j; m is an integer.

the other two families. Still, its polar structure can be drawn directly from an expansion in $\{|y| < \min_k\{|\tau_k|\}\}$ similar to eq.(3.4) for $\mathscr{Z}(\sigma, v)$, see also [14]:

$$\mathfrak{Z}(\sigma, y) = \sum_{k=0}^{\infty} {\tau_k}^{-2\sigma}\Big(1 + \frac{y}{\tau_k}\Big)^{-2\sigma} = \sum_{\ell=0}^{\infty} \frac{\Gamma(1-2\sigma)}{\ell!\Gamma(1-2\sigma-\ell)} \mathscr{Z}(\sigma + \tfrac{1}{2}\ell)\, y^\ell. \quad (4.1)$$

This formula generates a pole for $\mathfrak{Z}(\sigma, y)$ now at every *integer or half-integer* $\frac{1}{2}(1-n)$, $n \in \mathbb{N}$, according to:

$$\mathfrak{Z}(\tfrac{1}{2}(1-n) + \varepsilon, y) = \sum_{\ell=0}^{n} \frac{\Gamma(n-2\varepsilon)}{\ell!\Gamma(n-\ell-2\varepsilon)} \mathscr{Z}(\tfrac{1}{2}(1-n+\ell) + \varepsilon)\, y^\ell + \begin{cases} O(1) & \text{for } n = 0 \\ O(\varepsilon) & \text{for } n = 1, 2, \ldots \end{cases} \quad (4.2)$$

Concrete differences with eq.(3.5) arise from the factor $\Gamma(n-2\varepsilon)/\Gamma(n-\ell-2\varepsilon)$ vanishing whenever $\ell \ge n > 0$. Only the polar part at $\sigma = \frac{1}{2}$ remains the same as for $\mathscr{Z}(\sigma, v)$, of order $r = 2$ and independent of y, given by eq.(3.1); all other poles $\frac{1}{2}(1-n)$ of $\mathfrak{Z}(\sigma, y)$ are now *simple*, of residues

$$r_n(y) = -\frac{\widetilde{a}_1}{2\pi n}\, y^n + \sum_{0<2m\le n} \binom{n-1}{2m-1} \mathcal{R}_m\, y^{n-2m}, \quad n = 1, 2, \ldots, \quad (4.3)$$

in terms of the residues $\mathcal{R}_m$ given by eq.(3.2). Moreover, at $\sigma = 0$ (only), the ε-expansion of eq.(4.2) captures the *finite part* too (cf. eqs.(2.7) and (3.8)):

$$r_1(y) = \mathrm{Res}_{\sigma=0}\mathfrak{Z}(\sigma, y) = -\frac{\widetilde{a}_1}{2\pi}\, y\,;\ \mathrm{FP}_{\sigma=0}\, \mathfrak{Z}(\sigma, y) = \tfrac{1}{4}\widetilde{a}_1 + \tfrac{1}{2}(\widetilde{a}_0 + q) - \frac{b_1}{\pi}\, y. \tag{4.4}$$

On the other hand, while previously we could express infinite products over *all* the zeros such as $\mathscr{D}$, resp. $\mathcal{D}$, in terms of simpler functions like $\mathbf{D}$ and L (through eqs.(2.10), resp. (3.12)), now we lack that ability for a similar infinite product but restricted to *half* the zeros. We thus have no simple formulae for transcendental special values of $\mathfrak{Z}(\sigma, y)$ in the half-plane $\{\mathrm{Re}\,\sigma > 0\}$. Only a sequence of binary relations results by specializing the identity (1.17) to $s \in \mathbb{N}^*$,

$$\left[\mathrm{i}^m \mathfrak{Z}\left(\tfrac{1}{2}m, \mathrm{i}t\right) + \mathrm{i}^{-m}\mathfrak{Z}\left(\tfrac{1}{2}m, -\mathrm{i}t\right)\right] \equiv \mathscr{Z}\left(m, \tfrac{1}{2} + t\right), \quad m = 1, 2, \ldots, \tag{4.5}$$

constituting an obvious result except for $m = 1$: then, *finite parts* are to be taken *on the left-hand side only*.

5. Concrete examples

We finally illustrate the preceding results upon the two classes of primary zeta functions highlighted in Sec. 1.3. As a rule, it suffices to specialize the general formulae as indicated below, and with the order $\mu_0 = 1$. To enhance the practical side of this work, we will further display the most concrete formulae reached when the shift parameters are themselves fixed at interesting particular values. We will mainly show results for $\mathscr{Z}(s, 1)$ [$\equiv \mathscr{Z}(s)$] and $\mathscr{Z}(s, \frac{1}{2})$, as Tables 4–7; these extend Table 3 of [28], which was specific to $L(x) = \zeta(x)$. The analogous special cases for the second family, $\mathcal{Z}(\sigma, 0)$ [$\equiv \mathfrak{Z}(\sigma, 0) \equiv \mathcal{Z}(\sigma)$] and $\mathcal{Z}(\sigma, \frac{1}{4})$, are easily recovered from the preceding ones using Secs. 3.1 and 3.3, and specially the formulae of Table 3; these results extend Table 1 of [27] to general $L(x)$. – We do not further illustrate the third family $\{\mathfrak{Z}(\sigma, y)\}$, knowing none of its specific ($y \neq 0$) values explicitly.

At those special parameter cases, the relevant values of $\mathbf{Z}(s, x)$ will also become more explicit, using

$$\begin{gathered} \zeta(s, 1) \equiv \zeta(s); \quad \zeta(s, \tfrac{1}{2}) \equiv (2^s - 1)\zeta(s); \\ 2^{-2s}\zeta(s, \tfrac{1}{2} \mp \tfrac{1}{4}) \equiv \tfrac{1}{2}[(1 - 2^{-s})\zeta(s) \pm \beta(s)] \end{gathered} \tag{5.1}$$

(cf. eq.(1.2)). So, the Dirichlet series $\zeta(s)$ and $\beta(s) \equiv L_{\chi_4}(s)$ (χ_4 is the real primitive character for the modulus 4) will both occur ubiquitously in these particular special values, for whatever choice of primary Dirichlet series $L(x)$.

σ	$\mathcal{Z}(\sigma,0)=\sum_{k=1}^{\infty}{\tau_k}^{-2\sigma}$	$\mathcal{Z}(\sigma,\frac14)=\sum_{k=1}^{\infty}({\tau_k}^2+\frac14)^{-\sigma}$
$-m\le 0$	$\frac12(-1)^m\mathscr{Z}(-2m,\frac12)$	$\frac12\sum_{j=0}^{m}\binom{m}{j}(-1)^j 2^{-2(m-j)}\mathscr{Z}(-2j,\frac12)$
0	$\frac12\mathscr{Z}(0,\frac12)$	$\frac12\mathscr{Z}(0,\frac12)$
derivative at 0	$\mathcal{Z}'(0,0)=\mathscr{Z}'(0,\frac12)$	$\mathcal{Z}'(0,\frac14)=-\frac12 b_1+\mathscr{Z}'(0,1)$
$+m\ge 1$	$\frac12(-1)^m\mathscr{Z}(2m,\frac12)$	$\sum_{\ell=0}^{m-1}\binom{m+\ell-1}{m-1}\mathscr{Z}(m-\ell,1)$

Table 3. General formulae for the special values of $\mathcal{Z}(\sigma,0)\equiv\mathcal{Z}(\sigma)$ and $\mathcal{Z}(\sigma,\frac14)$, in terms of those for $\mathscr{Z}(s,\frac12)$ and $\mathscr{Z}(s,1)$ (such as provided in the subsequent Tables). Notations: see eq.(2.7) for b_1; m is an integer.

Again, the Riemann case $L(x)=\zeta(x)$, having $q=1$, is more conveniently treated here as a special Dedekind zeta function and not as an L-function.

5.1 L-functions for real primitive Dirichlet characters

According to eq.(1.23), any L-function $L_\chi(x)$ for such a Dirichlet character χ (mod d), with $d>1$ so as to exclude $\zeta(x)$, is handled by the choice

$$q\equiv 0;\quad \mathbf{G}(x)\equiv(\pi/d)^{x/2}/\Gamma\big(\tfrac12(x+a)\big),\quad a=\begin{cases}0 & \text{for } \chi \text{ even}\\ 1 & \text{for } \chi \text{ odd.}\end{cases}\tag{5.2}$$

In turn, the other useful quantities specialize as follows:
- the leading coefficients in the Stirling formula (2.7):

$$\begin{aligned}\widetilde{a}_1&=\tfrac12\,, & \widetilde{a}_0&=\tfrac12(a-1),\\ b_1&=-\tfrac12\log(2\pi/d), & b_0&=\tfrac12\log(2^{2-a}\pi);\end{aligned}\tag{5.3}$$

- the shadow zeta function, eq.(2.1):

$$\mathbf{Z}(s,x)=2^{-s}\zeta\big(s,\tfrac12(x+a)\big);\tag{5.4}$$

- the lowest generalized Stieltjes cumulants, eq.(1.11): $g_0^{\mathrm{c}}\{L_\chi\}\equiv-\log L_\chi(1)$ can always be specified, as well as $g_1^{\mathrm{c}}\{L_\chi\}\equiv[{L_\chi}'/L_\chi](1)$ when $a=1$.

First, the general formula

$$L_\chi(x) \equiv d^{-x} \sum_{n=1}^{d} \chi(n)\, \zeta(x, n/d), \tag{5.5}$$

together with the special values (1.4–1.6) of the Hurwitz zeta function, and using $\chi(d) = 0$ and $\sum\limits_{n=1}^{d} \chi(n) = 0$ throughout, yield these special values for $L_\chi(x)$:

$$L_\chi(0) = -\frac{1}{d} \sum_{n=1}^{d-1} \chi(n)\, n \qquad \text{(algebraic)} \tag{5.6}$$

$$L_\chi(1) = -\frac{1}{d} \sum_{n=1}^{d-1} \chi(n) \frac{\Gamma'(n/d)}{\Gamma(n/d)} \qquad \text{(transcendental)} \tag{5.7}$$

$$L_\chi{}'(0) = -L_\chi(0) \log d + \sum_{n=1}^{d-1} \chi(n) \log \Gamma(n/d) \quad \text{(transcendental).} \tag{5.8}$$

Then, the functional equation (1.9) also implies (we now suppress the χ labels)

$$\text{if } a = 1: \;\; L(1) = \pi d^{-1/2} L(0), \;\; [L'/L](1) = \gamma + \log(2\pi/d) - [L'/L](0); \tag{5.9}$$

$$\text{if } a = 0: \;\; L(1) = 2d^{-1/2} L'(0), \;\; [L'(1) \text{ involves } L''(0), \text{ unknown; ...}]. \tag{5.10}$$

In the $a = 0$ case, moreover: $L(0) \equiv 0$, and with χ being even, eq.(5.8) for $L'(0)$ is simplified using the reflection formula for Γ. The final outcome is:

• when $a = 1$, an algebraic explicit formula for $L(1)$ plus a transcendental one for $[L'/L](1)$ in terms of Gamma values, overall amounting to

$$\begin{aligned} g_0^{\mathrm{c}}\{L_\chi\} &= -\log\Big[-\frac{\pi}{d^{3/2}} \sum_{n=1}^{d-1} \chi(n)\, n\Big], \\ g_1^{\mathrm{c}}\{L_\chi\} &= \gamma + \log(2\pi) + \frac{\sum\limits_{n=1}^{d-1} \chi(n) \log \Gamma\Big(\dfrac{n}{d}\Big)}{\sum\limits_{n=1}^{d-1} \chi(n)\, \dfrac{n}{d}}\,; \end{aligned} \tag{5.11}$$

s	$\mathscr{Z}(s) \stackrel{\text{def}}{=} \mathscr{Z}(s,1) \equiv \sum_{\rho} \rho^{-s} \qquad [x=1]$
$-n<0$	$\Big[(a-1)(2^n-1)+a\,2^n\Big]\dfrac{B_{n+1}}{n+1}$
0	$\frac{1}{2}a$
derivative at 0	$\mathscr{Z}'(0) = \frac{1}{2}\ (1-a)\log 2 + a\log\pi\ + g_0^{\mathrm{c}}\{L_\chi\}$
finite part at +1	$\mathrm{FP}_{s=1}\mathscr{Z}(s) = (a-\frac{1}{2})\log 2 - \frac{1}{2}\gamma + g_1^{\mathrm{c}}\{L_\chi\}$
$+1$	$(a-1)\log 2 - \frac{1}{2}\log(\pi/d) - \frac{1}{2}\gamma + g_1^{\mathrm{c}}\{L_\chi\}$
$+n>1$	$[(a-1)(1-2^{-n}) - a\,2^{-n}]\,\zeta(n) + \dfrac{g_n^{\mathrm{c}}\{L_\chi\}}{(n-1)!}$

Table 4. Special values of the zeta function $\mathscr{Z}(s,1)$ over the nontrivial zeros of an L-function for a real primitive Dirichlet character χ of modulus $d>1$ and parity $a=0$ or 1: cf. eqs.(1.18–1.19). For the g_n^{c}, see eqs.(1.11) and (5.11–5.13). Notations: see eqs.(1.1); n is an integer. In last line, $\zeta(n) \equiv (2\pi)^n|B_n|/(2\,n!)$ when n is even.

s	$\mathscr{Z}(s,\frac{1}{2}) \equiv \sum_{\rho} (\rho-\frac{1}{2})^{-s} \qquad [x=\frac{1}{2}]$
even $-n\le 0$	$2^{-n-1}(a-\frac{1}{2})E_n$
odd $-n<0$	$-\frac{1}{2}(1-2^{-n})\dfrac{B_{n+1}}{n+1}$
0	$\frac{1}{2}(a-\frac{1}{2})$
derivative at 0	$\mathscr{Z}'(0,\frac{1}{2}) = (\frac{3}{4}-a)\log 2 + (a-\frac{1}{2})\log\ \Gamma(\frac{1}{4})^2/\pi\ - \log L_\chi(\frac{1}{2})$
finite part at +1	$\mathrm{FP}_{s=1}\mathscr{Z}(s,\frac{1}{2}) = \frac{1}{2}\log(2\pi/d)$
odd $+n\ge 1$	0
even $+n>1$	$-\frac{1}{2}\ (2^n-1)\,\zeta(n) + (1-2a)\,2^n\beta(n)\ - \dfrac{(\log L_\chi)^{(n)}(\frac{1}{2})}{(n-1)!}$

Table 5. Same as above, but for the zeta function $\mathscr{Z}(s,\frac{1}{2})$. In last line, n being even, $\zeta(n) \equiv (2\pi)^n|B_n|/(2\,n!)$ while $\beta(n)$ (see eq.(1.2)) remains elusive.

• when $a = 0$, just a formula for $L(1)$, transcendental but more elementary than (5.7), and amounting to

$$g_0^{\rm c}\{L_\chi\} = -\log\Big[-\frac{1}{d^{1/2}}\sum_{n=1}^{d-1}\chi(n)\log\sin\frac{\pi n}{d}\Big] \quad [g_1^{\rm c}\{L_\chi\} \text{ not specified}]. \tag{5.12}$$

E.g., for each of $d = 3$ and 4 (the lowest possible values of d), the real primitive character χ_d is unique: $\chi_d(\pm 1 \bmod d) = \pm 1$, else $\chi_d(n) = 0$; in particular, $L_{\chi_4}(x) \equiv \beta(x)$ as in eq.(1.2); both χ_3 and χ_4 are odd, giving

$$\begin{aligned}
d = 3: \quad & g_0^{\rm c}\{L_{\chi_3}\} = -\log(\pi/3^{3/2}), \\
& g_1^{\rm c}\{L_{\chi_3}\} = \log[(2\pi)^4/3^{3/2}] + \gamma - 6\log\Gamma(\tfrac13); \\
d = 4: \quad & g_0^{\rm c}\{L_{\chi_4}\} = -\log(\pi/4), \\
& g_1^{\rm c}\{L_{\chi_4}\} = \log(4\pi^3) + \gamma - 4\log\Gamma(\tfrac14).
\end{aligned} \tag{5.13}$$

In general, whether $a = 0$ or 1, we cannot specify the $g_n^{\rm c}$ any further than stated; we might just relate them, through eq.(5.5), to special cases of the still more general Laurent coefficients $\gamma_n(w)$ of $\zeta(x, w)$ around $x = 1$ [2, 18].

The finally resulting special values of $\mathscr{Z}(s, 1)$ and $\mathscr{Z}(s, \frac12)$, over zeros of a general real primitive Dirichlet character, are presented in Tables 4 and 5 respectively.

5.2 Dedekind zeta functions

Referring back to eq.(1.25), the Dedekind zeta function $\zeta_K(x)$ of any algebraic number field K is handled by the choice

$$q \equiv 1, \qquad \mathbf{G}(x) \equiv \frac{\big(4^{r_2}\pi^{n_K}/|d_K|\big)^{x/2}}{x\Gamma(x/2)^{r_1}\Gamma(x)^{r_2}}. \tag{5.14}$$

In turn, the other useful quantities specialize as follows:
- the leading coefficients in the Stirling formula (2.7):

$$\widetilde{a}_1 = \tfrac12 n_K, \qquad \widetilde{a}_0 = 1 - \tfrac12(r_1 + r_2),$$

$$b_1 = -\tfrac12\big[\log\big((2\pi)^{n_K}/|d_K|\big)\big], \quad b_0 = (r_1 + \tfrac12 r_2)\log 2 + \tfrac12(r_1 + r_2)\log\pi; \tag{5.15}$$

- the shadow zeta function (eq.(2.1)): counting all zeros of $\mathbf{G}(x)$ with their multiplicities, it reads as

$$\mathbf{Z}(s, x) = r_1 2^{-s}\zeta(s, \tfrac12 x) + r_2\zeta(s, x) - x^{-s}; \tag{5.16}$$

s	$\mathscr{Z}(s) \stackrel{\mathrm{def}}{=} \mathscr{Z}(s,1) \equiv \sum_\rho \rho^{-s} \qquad [x=1]$
$-n<0$	$-r_1(2^n-1)+r_2\ \frac{B_{n+1}}{n+1}+1$
0	$\frac{1}{2}r_2+2$
derivative at 0	$\mathscr{Z}'(0)=\frac{1}{2}\ (r_1+r_2)\log 2+r_2\log\pi\ +g_0^{\mathrm{c}}\{\zeta_K\}$
finite part at +1	$\mathrm{FP}_{s=1}\mathscr{Z}(s)=-\frac{1}{2}r_1\log 2+1-\frac{1}{2}n_K\gamma+g_1^{\mathrm{c}}\{\zeta_K\}$
$+1$	$\frac{1}{2}\log\lvert d_K\rvert-(r_1+r_2)\log 2-\frac{1}{2}n_K\log\pi+1-\frac{1}{2}n_K\gamma+g_1^{\mathrm{c}}\{\zeta_K\}$
$+n>1$	$-[r_1(1-2^{-n})+r_2]\,\zeta(n)+1+\frac{g_n^{\mathrm{c}}\{\zeta_K\}}{(n-1)!}$

Table 6. Special values of the zeta function $\mathscr{Z}(s,1)$ over the nontrivial zeros of a Dedekind zeta function for an algebraic number field K: cf. eqs.(1.24–1.25). For the g_n^{c}, see eqs.(1.11) and (5.17–5.18). Notations: see eqs.(1.1); n is an integer. In last line, $\zeta(n)\equiv(2\pi)^n\lvert B_n\rvert/(2\,n!)$ when n is even.

s	$\mathscr{Z}(s,\frac{1}{2}) \equiv \sum_\rho (\rho-\frac{1}{2})^{-s} \qquad [x=\frac{1}{2}]$
even $-n\le 0$	$2^{-n+1}(1-\frac{1}{8}r_1E_n)$
odd $-n<0$	$-\frac{1}{2}n_K(1-2^{-n})\,\frac{B_{n+1}}{n+1}$
0	$2-\frac{1}{4}r_1$
derivative at 0	$\mathscr{Z}'(0,\frac{1}{2})=(2+\frac{3}{4}r_1+\frac{1}{2}r_2)\log 2-\frac{1}{2}r_1\log\ \Gamma(\frac{1}{4})^2/\pi\ -\log\lvert\zeta_K\rvert(\frac{1}{2})$
finite part at +1	$\mathrm{FP}_{s=1}\mathscr{Z}(s,\frac{1}{2})=\frac{1}{2}\ n_K\log(2\pi)-\log\lvert d_K\rvert$
odd $+n\ge 1$	0
even $+n>1$	$-\frac{1}{2}n_K(2^n-1)\,\zeta(n)-\frac{1}{2}r_1\,2^n\beta(n)+2^{n+1}-\frac{(\log\lvert\zeta_K\rvert)^{(n)}(\frac{1}{2})}{(n-1)!}$

Table 7. Same as above, but for the zeta function $\mathscr{Z}(s,\frac{1}{2})$. In last line, n being even, $\zeta(n)\equiv(2\pi)^n\lvert B_n\rvert/(2\,n!)$ while $\beta(n)$ (see eq.(1.2)) remains elusive.

- the lowest generalized Stieltjes cumulants (eq.(1.11)): $g_0^{\rm c}\{\zeta_K\} \equiv -\log \mathbf{r}_K$, where $\mathbf{r}_K > 0$ is the residue of $\zeta_K(x)$ at its only pole $x = 1$, which is *explicitly known* in terms of field invariants [12, thms 121, 124], [23]. Moreover, sometimes at least, $g_1^{\rm c}\{\zeta_K\} \equiv {\mathbf{r}_K}^{-1}\,\mathrm{FP}_{x=1}\zeta_K(x)$ can also be described. First, if $K = \mathbb{Q}$: then $\zeta_K(x) \equiv \zeta(x)$, hence $\mathbf{r}_K = 1$ and

$$g_0^{\rm c}\{\zeta\} = 0, \qquad\qquad g_1^{\rm c}\{\zeta\} = \gamma; \tag{5.17}$$

in turn, other $g_1^{\rm c}\{\zeta_K\}$ will qualify as kinds of generalized Euler's constants. As next example, if K is a *quadratic* number field, then $\zeta_K(x) \equiv \zeta(x)\,L_\chi(x)$, where χ is the real primitive character of modulus $|d_K|$ given by the Kronecker symbol for the discriminant d_K [12, Sec. 49]. Now in general, the zeta functions over the zeros (and their linear invariants) obviously *add up* when their primary functions L are *multiplied*. So, for a quadratic number field,

$$g_0^{\rm c}\{\zeta_K\} = g_0^{\rm c}\{L_\chi\}, \qquad g_1^{\rm c}\{\zeta_K\} = \gamma + g_1^{\rm c}\{L_\chi\} \tag{5.18}$$

referring to the same cumulants for $L_\chi(x)$ that were precisely described under the previous example by eq.(5.11) for χ odd, or (5.12) for χ even. Two basic examples, both with $r_1 = 0$ and $r_2 = 1$, are: $K = \mathbb{Q}(\mathrm{i})$ (for which $d_K = -4$, $\chi = \chi_4$, $L_\chi(x) \equiv \beta(x)$ as in eq.(1.2)), and $K = \mathbb{Q}(\sqrt{-3})$ (for which $d_K = -3$, $\chi = \chi_3$), hence their specific cumulants $g_0^{\rm c}$, $g_1^{\rm c}$ follow from eqs.(5.13) and (5.18).

The finally resulting special values of $\mathscr{Z}(s,1)$ and $\mathscr{Z}(s,\frac12)$, over zeros of a general Dedekind zeta function, are presented in Tables 6 and 7 respectively.

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HOPF ALGEBRAS AND TRANSCENDENTAL NUMBERS

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In dealing with multiple zeta values, the main diophantine challenge is to prove that known dependence relations among them suffice to deduce all algebraic relations. One tool which should be relevant is the structure of Hopf Algebras, which occurs in several disguises in this context. How to use it is not yet clear, but we point out that it already plays a role in transcendental number theory: Stéphane Fischler deduces interpolation lemmas from zero estimates by using a duality involving bicommutative (commutative and cocommutative) Hopf Algebras.

In the first section we state two transcendence results involving values of the exponential function; they are special cases of the linear subgroup Theorem which deals with commutative linear algebraic groups.

In the second section, following S. Fischler, we explain the connection between the data of the linear subgroup Theorem and bicommutative Hopf algebras of finite type.

In the third and last section we introduce non-bicommutative Hopf algebras related to multiple zeta values.

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1. Transcendence, exponential polynomials and commutative linear algebraic groups

We start with two examples of transcendence results; their proofs involve exponential polynomials and they occur as corollaries of a general result on commutative algebraic groups: the linear subgroup Theorem.

In this context, there is duality, which can be explained by means of the Fourier-Borel transform of exponential polynomials. This duality is revisited by S. Fischler from the view point of commutative linear algebraic groups, using Hopf algebras.

1.1 Transcendence results

Here is our first transcendence result ([B] Theorem 2.1).

Theorem 1.1. (Baker). *Let $\beta_0,\ldots,\beta_n$ be algebraic numbers and $\alpha_1,\ldots,\alpha_n$ be non-zero algebraic numbers. For $1\le i\le n$, denote by $\log\alpha_i$ any complex logarithm of α_i. Assume*

$$\beta_0+\beta_1\log\alpha_1+\cdots+\beta_n\log\alpha_n=0.$$

Then it holds that
1. $\beta_0=0$.
2. If $(\beta_1,\ldots,\beta_n)\neq(0,\ldots,0)$, then the numbers $\log\alpha_1,\ldots,\log\alpha_n$ are $\mathbf{Q}$-linearly dependent.
3.If $(\log\alpha_1,\ldots,\log\alpha_n)\neq(0,\ldots,0)$, then the numbers $\beta_1,\ldots,\beta_n$ are $\mathbf{Q}$-linearly dependent.

As is well known this result includes Hermite's result (1873) on the transcendence of e, Lindemann's result (1882) on the transcendence of π and more generally

Corollary 1.2. (Hermite-Lindemann). *If β is a non-zero algebraic number, then e^β is a transcendental number.*
Equivalently, if α is a non-zero algebraic number and if $\log\alpha$ is any non-zero logarithm of α, then $\log\alpha$ is a transcendental number.

This includes the transcendence of numbers like e, π, $e^{\sqrt{2}}$, $\log 2$.

Denote by $\overline{\mathbf{Q}}$ the field of all complex algebraic numbers, which is the algebraic closure of $\mathbf{Q}$ in $\mathbf{C}$ and by $\mathcal{L}=\exp^{-1}(\overline{\mathbf{Q}}^\times)$ the $\mathbf{Q}$-vector space of logarithms of algebraic numbers:

$$\mathcal{L}=\{\lambda\in\mathbf{C}\ ;\ e^\lambda\in\overline{\mathbf{Q}}^\times\}=\{\log\alpha\ ;\ \alpha\in\overline{\mathbf{Q}}^\times\}.$$

Hermite-Lindemann's Theorem asserts that $\mathcal{L}$ does not contain any non-zero algebraic number:

$$\mathcal{L}\cap\overline{\mathbf{Q}}=\{0\}.$$

Another corollary of Baker's Theorem 1.1 is the answer to Hilbert's seventh problem, given by A.O. Gel'fond and Th. Schneider in 1934:

Corollary 1.3. (Gel'fond-Schneider). *If β is an irrational algebraic number, α a non-zero algebraic number and* $\log\alpha$ *a non-zero logarithm of α, then the number*

$$\alpha^\beta = \exp(\beta\log\alpha)$$

is transcendental.

Gel'fond-Schneider's Theorem (Corollary 1.3) asserts that the quotient of two non-zero elements in $\mathcal{L}$ is either rational or else transcendental; Baker's Theorem 1.1 implies more generally that $\mathbf{Q}$-linearly independent elements of $\mathcal{L}$ are $\overline{\mathbf{Q}}$-linearly independent.

Theorem 1.1 also yields the transcendence of numbers like $e^{\sqrt{2}}2^{\sqrt{3}}$,

$$\int_0^1 \frac{dx}{1+x^3} = \frac{1}{3}\left(\log 2 + \frac{\pi}{\sqrt{3}}\right)$$

and more generally (under suitable assumptions – see [B] Theorems 2.2, 2.3 and 2.4) of numbers of the form

$$e^{\beta_0}\alpha_1^{\beta_1}\cdots\alpha_m^{\beta_m} \quad \text{and} \quad \beta_0+\beta_1\log\alpha_1+\cdots+\beta_m\log\alpha_m$$

when the numbers α_i and β_j are algebraic.

It is to be remarked that Baker's Theorem does not include all known transcendence results related to the exponential function: here is an example ([W] p. 386).

Theorem 1.4. (Sharp six exponentials Theorem). *Let x_1, x_2 be two complex numbers which are $\mathbf{Q}$-linearly independent and y_1, y_2, y_3 three complex numbers which are also $\mathbf{Q}$-linearly independent. Further let β_{ij} $(i = 1, 2,\ j = 1, 2, 3)$ be six algebraic numbers. Assume*

$$e^{x_iy_j-\beta_{ij}} \in \overline{\mathbf{Q}} \quad \textit{for} \quad i = 1, 2,\ j = 1, 2, 3.$$

Then $x_iy_j = \beta_{ij}$ for $i = 1, 2,\ j = 1, 2, 3$.

The special case $\beta_{ij} = 0$ for all i, j is known as the six exponentials Theorem (due to Lang and Ramachandra in the 60's – see references in [W], § 1.3): *if x_1, x_2 are $\mathbf{Q}$-linearly independent and y_1, y_2, y_3 are also $\mathbf{Q}$-linearly independent, then at least one of the six numbers*

$$e^{x_iy_j} \quad (i = 1, 2,\ j = 1, 2, 3)$$

is transcendental.

The four exponentials Conjecture ([W] Conjecture 1.13) asserts that two values for y should suffice: *if x_1, x_2 are $\mathbf{Q}$-linearly independent and y_1, y_2 are also $\mathbf{Q}$-linearly independent, then at least one of the four numbers*

$$e^{x_i y_j} \quad (i = 1, 2,\ j = 1, 2)$$

is transcendental.

A sharper result is expected, which we call here the *sharp four exponentials Conjecture*: under the same assumptions as in the four exponentials Conjecture, *if β_{ij} $(i = 1, 2,\ j = 1, 2)$ are four algebraic numbers such that*

$$e^{x_i y_j - \beta_{ij}} \in \overline{\mathbf{Q}} \quad \textit{for} \quad i = 1, 2,\ j = 1, 2,$$

then one should have $x_i y_j = \beta_{ij}$ for $i = 1, 2,\ j = 1, 2$.

Conjecture 1.5. (Sharp five exponentials Conjecture). *If x_1, x_2 are $\mathbf{Q}$-linearly independent, if y_1, y_2 are $\mathbf{Q}$-linearly independent and if α, β_{11}, β_{12}, β_{21}, β_{22}, γ are six algebraic numbers such that*

$$e^{x_1 y_1 - \beta_{11}},\ e^{x_1 y_2 - \beta_{12}},\ e^{x_2 y_1 - \beta_{21}},\ e^{x_2 y_2 - \beta_{22}},\ e^{(\gamma x_2 / x_1) - \alpha}$$

are algebraic, then $x_i y_j = \beta_{ij}$ for $i = 1, 2,\ j = 1, 2$ and furthermore $\gamma x_2 = \alpha x_1$.

The case $\beta_{ij} = 0$ of Conjecture 1.5 is an easy consequence of the sharp six exponentials Theorem 1.4: this is the five exponentials Theorem ([W] p. 385): *If x_1, x_2 are $\mathbf{Q}$-linearly independent, if y_1, y_2 are $\mathbf{Q}$-linearly independent and if γ is a non-zero algebraic, then at least one of the five numbers*

$$e^{x_1 y_1},\ e^{x_1 y_2},\ e^{x_2 y_1},\ e^{x_2 y_2},\ e^{\gamma x_2 / x_1}$$

is transcendental.

Moreover, in the special case where the three numbers y_1, y_2 and γ / x_1 are $\mathbf{Q}$-linearly independent, the sharp five exponentials Conjecture 1.5 follows from the sharp six exponentials Theorem 1.4 by setting

$$y_3 = \gamma / x_1, \quad \beta_{13} = \gamma, \quad \beta_{23} = \alpha,$$

so that

$$x_1 y_3 - \beta_{13} = 0 \quad \text{and} \quad x_2 y_3 - \beta_{23} = (\gamma x_2 / x_1) - \alpha.$$

In the case where the three numbers y_1, y_2 and γ / x_1 are linearly dependent over $\mathbf{Q}$, the conjecture is open. A consequence of the sharp five exponentials Conjecture 1.5 is the transcendence of the number e^{π^2}: take

$$x_1 = y_1 = \gamma = 1,\ x_2 = y_2 = i\pi,\ \alpha = 0,\ \beta_{11} = 1,\ \beta_{ij} = 0 \quad \text{for} \quad (i, j) \neq (1, 1).$$

So far, we only know (W.D. Brownawell and the author) that at least one of the two statements holds:

- e^{π^2} *is transcendental.*
- *The two numbers* e *and* π *are algebraically independent.*

In the same way, setting

$$x_1 = y_1 = \gamma = 1,\ x_2 = y_2 = \lambda,\ \alpha = 0,\ \beta_{11} = 1,\ \beta_{ij} = 0 \quad \text{for} \quad (i,j) \neq (1,1),$$

we deduce from Conjecture 1.5 the transcendence of e^{λ^2} when λ is a non-zero logarithm of an algebraic number. Writing $\alpha = e^{\lambda}$ or $\lambda = \log \alpha$, we have

$$e^{\lambda^2} = \alpha^{\log \alpha}.$$

Only the following weaker statement is known: *at least one of the two numbers*

$$e^{\lambda^2} = \alpha^{\log \alpha},\ e^{\lambda^3} = \alpha^{(\log \alpha)^2}$$

is transcendental, which was proved initially by W.D. Brownawell and the author as a consequence of a result of algebraic independence; however it is also a consequence of the sharp six exponentials Theorem 1.4 with

$$x_1 = y_1 = 1,\ x_2 = y_2 = \lambda,\ y_3 = \lambda^2,\ \beta_{11} = 1,\ \beta_{ij} = 0 \quad \text{for} \quad (i,j) \neq (1,1).$$

The sharpest known result on this subject is the *strong six exponentials Theorem* due to D. Roy ([W] Corollary 11.16). Denote by $\widetilde{\mathcal{L}}$ the $\overline{\mathbf{Q}}$-vector space spanned by 1 and $\mathcal{L}$: hence $\widetilde{\mathcal{L}}$ is nothing else than the set of complex numbers of the form

$$\beta_0 + \sum_{i=1}^{n} \beta_i \log \alpha_i,$$

with $n \geq 0$, β_j algebraic numbers, α_i non-zero algebraic numbers and all values of their logarithm are considered. The strong six exponentials Theorem states that *if* x_1, x_2 *are* $\overline{\mathbf{Q}}$*-linearly independent and if* y_1, y_2, y_3 *are* $\overline{\mathbf{Q}}$*-linearly independent, then at least one of the six numbers*

$$x_i y_j \quad (i = 1, 2,\ j = 1, 2, 3)$$

is not in $\widetilde{\mathcal{L}}$.

The strong four exponentials Conjecture ([W] Conjecture 11.17) claims that the same should hold with only two values y_1, y_2 in place of three.

1.2 Exponential polynomials

The proofs of both Theorems 1.1 and 1.4 involve exponential polynomials. Here are basic facts on them.

For the proof of Baker's Theorem 1.1, assume

$$\beta_0 + \beta_1 \log \alpha_1 + \cdots + \beta_{n-1} \log \alpha_{n-1} = \log \alpha_n.$$

In *Gel'fond–Baker's Method* (B_1), we consider the following $n+1$ functions

$$z_0,\ e^{z_1},\ \ldots,\ e^{z_{n-1}},\ e^{\beta_0 z_0 + \beta_1 z_1 + \cdots + \beta_{n-1} z_{n-1}}$$

of n variables $z_0, \ldots, z_{n-1}$. At the points $\mathbf{Z}(1, \log \alpha_1, \ldots, \log \alpha_{n-1}) \in \mathbf{C}^n$, all these functions take algebraic values. Moreover we also get algebraic numbers by taking derivatives with respect to the operators $\partial/\partial z_i$, $(0 \le i \le n-1)$.

Notice that there are n variables, $n+1$ functions, 1 point (together with its multiples) and n derivations (together with their compositions).

In *Generalized Schneider's Method* (B_2), we consider the $n+1$ functions: $z_0,\ z_1,\ \ldots, z_{n-1}$ and

$$e^{z_0} \alpha_1^{z_1} \cdots \alpha_{n-1}^{z_{n-1}} = \exp\{z_0 + z_1 \log \alpha_1 + \cdots + z_{n-1} \log \alpha_{n-1}\}$$

at the points: $\{0\} \times \mathbf{Z}^{n-1} + \mathbf{Z}(\beta_0, , \ldots, \beta_{n-1}) \in \mathbf{C}^n$. Only one derivation yields algebraic numbers, namely $\partial/\partial z_0$.

In this alternative approach there are again n variables and $n+1$ functions, but a single derivation, while the points form a group of $\mathbf{Z}$-rank n.

1.3 Data for the proof of Theorem 1.4

Here are the main data for the proof of Theorem 1.4.

Assume $x_1, \ldots, x_a$ are $\mathbf{Q}$-linearly independent, $y_1, \ldots, y_b$ are $\mathbf{Q}$-linearly independent, β_{ij} are algebraic numbers and λ_{ij} are elements in $\mathcal{L}$ such that

$$\lambda_{ij} = x_i y_j - \beta_{ij} \quad \text{for} \quad i = 1, \ldots, a,\ j = 1, \ldots, b$$

with $ab > a + b$.

For Theorem 1.4 it would be sufficient to restrict to $a = 2$, $b = 3$, but it will be useful to introduce these two parameters a and b so that the situation becomes symmetric. As we shall see, we should assume $ab > a + b$, which means either $a \ge 2$ and $b \ge 3$ or else $a \ge 3$ and $b \ge 2$.

Consider the functions:

$$z_i,\ e^{(x_i/x_1)(z_{a+1} + z_1) - z_i} \quad (1 \le i \le a)$$

at the points of the subgroup in $\mathbf{C}$ spanned by

$$(\beta_{1j},\ldots,\beta_{aj},\lambda_{1j})\in\mathbf{C}^{a+1}\quad(1\leq j\leq b).$$

These values are algebraic and the same holds for the values at the same points of the derivatives of these functions with respect to the differential operators $\partial/\partial z_i$ $(2\leq i\leq a)$ and $\partial/\partial z_{a+1}-\partial/\partial z_1$.

Hence we are dealing with $2a$ functions in $a+1$ variables, b points (linearly independent) and a derivations.

1.4 Commutative linear algebraic groups

Theorems 1.1 and 1.4 are special cases of the linear subgroup Theorem. Consider a commutative linear algebraic group, say $G=\mathbf{G}_a^{d_0}\times\mathbf{G}_m^{d_1}$ (where $\mathbf{G}_a$ denotes the additive group and $\mathbf{G}_m$ the multiplicative group), over the field $\overline{\mathbf{Q}}$ of algebraic numbers. Its dimension is $d=d_0+d_1$. Let $\mathcal{W}\subset T_e(G)$ be a $\mathbf{C}$-subspace which is rational over $\overline{\mathbf{Q}}$. Denote by ℓ_0 its dimension. Let $Y\subset T_e(G)$ be a finitely generated subgroup such that $\Gamma=\exp(Y)$ is contained in $G(\overline{\mathbf{Q}})=\overline{\mathbf{Q}}^{d_0}\times(\overline{\mathbf{Q}}^{\times})^{d_1}$. Let ℓ_1 be the $\mathbf{Z}$-rank of Γ. Finally let $\mathcal{V}\subset T_e(G)$ be a $\mathbf{C}$-subspace containing both $\mathcal{W}$ and Y. Let n be the dimension of $\mathcal{V}$.

The conclusion of the linear subgroup Theorem below ([W] Theorem 11.5) is non-trivial only when

$$n(\ell_1+d_1)<\ell_1d_1+\ell_0d_1+\ell_1d_0.\tag{1.6}$$

For each connected algebraic subgroup G^* of G, defined over $\overline{\mathbf{Q}}$, we define

$$Y^*=Y\cap T_e(G^*),\quad \mathcal{V}^*=\mathcal{V}\cap T_e(G^*),\quad \mathcal{W}^*=\mathcal{W}\cap T_e(G^*)$$

and

$$d^*=\dim(G^*),\quad \ell_1^*=\mathrm{rank}_{\mathbf{Z}}(Y^*),\quad n^*=\dim_{\mathbf{C}}(\mathcal{V}^*),\quad \ell_0^*=\dim_{\mathbf{C}}(\mathcal{W}^*).$$

We may write $G^*=G_0^*\times G_1^*$ where G_0^* is an algebraic subgroup of G_0 and G_1^* is an algebraic subgroup of G_1. Define

$$d_0^*=\dim(G_0^*),\quad d_1^*=\dim(G_1^*),$$

so that $d^*=d_0^*+d_1^*$.

If we set

$$G_0'=\frac{G_0}{G_0^*},\quad G_1'=\frac{G_1}{G_1^*},\quad G'=\frac{G}{G^*}=G_0'\times G_1',$$

$$Y' = \frac{Y}{Y^*}, \quad \mathcal{V}' = \frac{\mathcal{V}}{\mathcal{V}^*}, \quad \mathcal{W}' = \frac{\mathcal{W}}{\mathcal{W}^*},$$

and

$$d_0' = \dim(G_0'), \quad d_1' = \dim(G_1'), \quad d' = \dim(G'),$$
$$\ell_1' = \mathrm{rank}_{\mathbf{Z}}(Y'), \quad n' = \dim_{\mathbf{C}}(\mathcal{V}'), \quad \ell_0' = \dim_{\mathbf{C}}(\mathcal{W}'),$$

then

$$d_0 = d_0^* + d_0', \quad d_1 = d_1^* + d_1', \quad d = d^* + d',$$
$$\ell_1 = \ell_1^* + \ell_1', \quad n = n^* + n', \quad \ell_0 = \ell_0^* + \ell_0'.$$

Theorem 1.7. (Linear subgroup Theorem).
(1) Assume $d > n$. Then there exists a connected algebraic subgroup G^* of G such that

$$d' > \ell_0' \quad \textit{and} \quad \frac{\ell_1' + d_1'}{d' - \ell_0'} \leq \frac{d_1}{d - n}.$$

(1') Assume $\ell_1 > 0$. Then there is a G^* for which

$$(d_1^*, \ell_1^*) \neq (0,0) \quad \textit{and} \quad \frac{d^* - \ell_0^*}{d_1^* + \ell_1^*} \leq \frac{n - \ell_0}{\ell_1}.$$

(2) Assume $d > n$ and $\ell_1 > 0$. Assume further that for any G^* for which $Y^* \neq \{0\}$, we have

$$\frac{n^* - \ell_0^*}{\ell_1^*} \geq \frac{n - \ell_0}{\ell_1}.$$

Assume also that there is no G^* for which the three conditions $\ell_1' = 0$, $n' = \ell_0'$ and $d' > 0$ simultaneously hold. Then

$$d_1 > 0 \quad \textit{and} \quad \ell_1(d - n) \leq d_1(n - \ell_0).$$

(2') Assume $d > n$ and $\ell_1 > 0$. Assume further that for any G^* for which $d' > n'$, we have

$$\frac{d_1}{d - n} \leq \frac{d_1'}{d' - n'}.$$

Assume also that there is no G^* for which the three conditions $d_1^* = 0$, $d^* = n^*$ and $d^* > 0$ simultaneously hold. Then

$$n > \ell_0 \quad \textit{and} \quad \ell_1(d - n) \leq d_1(n - \ell_0).$$

(3) Assume $\ell_1 > 0$. Then the family of G^* for which $\ell_1^* \neq 0$ and $(n^* - \ell_0^*)/\ell_1^*$ is minimal is not empty. Let G^* be such an element for which d^* is minimal. Then either $d^* = n^*$ or else

$$d_1^* > 0 \quad \textit{and} \quad \frac{n - \ell_0}{\ell_1} \geq \frac{n^* - \ell_0^*}{\ell_1^*} \geq \frac{d^* - n^*}{d_1^*}.$$

(3') Assume $d > n$. Then the family of G^* for which $d' > n'$ and $d'_1/(d' - n')$ is minimal is not empty. Let G^* be such an element for which d' is minimal. Then either $\ell'_1 = 0$ or else

$$n' > \ell'_0 \quad \textit{and} \quad \frac{d_1}{d-n} \geq \frac{d'_1}{d'-n'} \geq \frac{\ell'_1}{n'-\ell'_0}.$$

1.5 Fourier-Borel duality

Unifying the notation of §1.2 involving exponential polynomials, we let $d_0 + d_1$ be the number of functions, d_0 of which are linear and d_1 are exponential, ℓ_0 the number of derivations, ℓ_1 the number of points and n the number of variables.

	d_0	d_1	ℓ_0	ℓ_1	n
Baker B_1	1	n	n	1	n
Baker B_2	n	1	1	n	n
Sharp six exponentials	a	a	a	b	$a+1$

The inequality (1.6)

$$n(\ell_1 + d_1) < \ell_1 d_1 + \ell_0 d_1 + \ell_1 d_0.$$

is satisfied in the case of Baker's Theorem 1.1 since

$$n(\ell_1 + d_1) = n^2 + n, \qquad \ell_1 d_1 + \ell_0 d_1 + \ell_1 d_0 = n^2 + n + 1.$$

For Theorem 1.4 the condition $a + b < ab$ is required:

$$n(\ell_1 + d_1) = a^2 + ab + a + b, \qquad \ell_1 d_1 + \ell_0 d_1 + \ell_1 d_0 = a^2 + 2ab.$$

There is a duality in each two cases: it consists in permuting

$$(d_0, d_1, \ell_0, \ell_1) \longleftrightarrow (\ell_0, \ell_1, d_0, d_1)$$

For Baker's Theorem 1.1 it permutes methods B_1 and B_2. As pointed out to me by S. Fischler, for Theorem 1.4 it is not a mere permutation of a and b. Indeed the proof in § 1.3 involved the parameters

$$d_0 = d_1 = \ell_0 = a, \quad \ell_1 = b, \quad n = a + 1,$$

henceforth the dual proof will involve the parameters

$$\ell_0 = \ell_1 = d_0 = a, \quad d_1 = b, \quad n = a + 1.$$

In the dual proof there are $d_0 + d_1 = a + b$ functions, namely $z_1 - z_{a+1}, z_2, \ldots, z_a$ together with

$$e^{\beta_{1j}z_1+\cdots+\beta_{aj}z_a+\lambda_{1j}z_{a+1}} \quad (1 \le j \le b),$$

the derivative operators are $\partial/\partial z_i \quad (1 \le i \le a)$ and the points are $(0, \ldots, 0, 1)$ together with

$$(x_i/x_1, -\delta_{i2}, \ldots, -\delta_{ia}, x_i/x_1) \quad (2 \le i \le a)$$

where δ_{ij} is Kronecker's symbol.

This duality rests on the analytic formula

$$\left(\frac{d}{dz}\right)^s \left(z^t e^{xz}\right)_{z=y} = \left(\frac{d}{dz}\right)^t \left(z^s e^{yz}\right)_{z=x}. \tag{1.8}$$

This formula (1.8) is related to the Fourier-Borel transform as follows. For s a non-negative integer and y a complex number, consider the analytic functional

$$\mathsf{L}_{sy} : f \longmapsto \left(\frac{d}{dz}\right)^s f(y).$$

Its Fourier-Borel transform is the analytic function $\mathsf{L}_{sy}(f_\zeta)$ of $\zeta \in \mathbf{C}$ which is the transform of the function $f_\zeta : z \mapsto e^{z\zeta}$:

$$f_\zeta(z) = e^{z\zeta}, \qquad \mathsf{L}_{sy}(f_\zeta) = \zeta^s e^{y\zeta}.$$

This yields (1.8) for $t = 0$. The general case follows from

$$\mathsf{L}_{sy}(z^t f_\zeta) = \left(\frac{d}{d\zeta}\right)^t \mathsf{L}_{sy}(f_\zeta).$$

Formula (1.8) extends to the higher dimensional case (that is when $n > 1$). For $\underline{v} = (v_1, \ldots, v_n) \in \mathbf{C}^n$, set

$$D_{\underline{v}} = v_1 \frac{\partial}{\partial z_1} + \cdots + v_n \frac{\partial}{\partial z_n}.$$

Let $\underline{w}_1, \ldots, \underline{w}_{\ell_0}, \underline{u}_1, \ldots, \underline{u}_{d_0}, \underline{\xi}$ and $\underline{\eta}$ in $\mathbf{C}^n$, $\underline{t} \in \mathbf{N}^{d_0}$ and $\underline{s} \in \mathbf{N}^{\ell_0}$. For $\underline{z} \in \mathbf{C}^n$, write

$$(\mathbf{u}\underline{z})^{\underline{t}} = (\underline{u}_1\underline{z})^{t_1} \cdots (\underline{u}_{d_0}\underline{z})^{t_{d_0}} \quad \text{and} \quad D_{\mathbf{w}}^{\underline{s}} = D_{\underline{w}_1}^{s_1} \cdots D_{\underline{w}_{\ell_0}}^{s_{\ell_0}}.$$

Then

$$D_{\mathbf{w}}^{\underline{s}}\left((\mathbf{u}\underline{z})^{\underline{t}} e^{\underline{\xi}\underline{z}}\right)\Big|_{\underline{z}=\underline{\eta}} = D_{\mathbf{u}}^{\underline{t}}\left((\mathbf{w}\underline{z})^{\underline{s}} e^{\underline{\eta}\underline{z}}\right)\Big|_{\underline{z}=\underline{\xi}}. \tag{1.9}$$

Example. In the proof of the sharp six exponentials Theorem 1.4 given in § 1.3 where $d_0 = d_1 = \ell_0 = a$, $\ell_1 = b$ and $n = a + 1$,

$$\underline{u}_i = (\delta_{i1}, \ldots, \delta_{ia}, 0) \quad (1 \leq i \leq a),$$

$\underline{w}_1 = (1, 0, \ldots, 0, -1)$ and

$$\underline{w}_i = (0, \delta_{i2}, \ldots, \delta_{ia}, 0) \quad (2 \leq i \leq a),$$

$\underline{\xi}$ is a linear combination of $\underline{\xi}_1, \ldots, \underline{\xi}_a$ with $\underline{\xi}_1 = (0, \ldots, 0, 1)$ and

$$\underline{\xi}_i = (x_i/x_1, -\delta_{i2}, \ldots, -\delta_{ia}, x_i/x_1) \quad (2 \leq i \leq a)$$

while $\underline{\eta}$ is a linear combination of $\underline{\eta}_1, \ldots, \underline{\eta}_b$ with

$$\underline{\eta}_j = (\beta_{1j}, \ldots, \beta_{aj}, \lambda_{1j}) \quad (1 \leq j \leq b).$$

Remark. The Fourier-Borel duality is not the same as the duality introduced by D. Roy in [Ro] which relates (1) and (1'), (2) and (2'), (3) and (3').

2. Bicommutative Hopf algebras

We consider commutative and cocommutative Hopf algebras (also called bicommutative Hopf algebras) over a field k of characteristic zero.

As the first example, the algebra of polynomials in one variable $H = k[X]$ is endowed with a Hopf algebra structure with the coproduct Δ, the co-unit ϵ and the antipode S defined as the algebra morphisms for which

$$\Delta(X) = X \otimes 1 + 1 \otimes X, \quad \epsilon(X) = 0 \quad \text{and} \quad S(X) = -X.$$

If we identify $k[X] \otimes k[X]$ with $k[T_1, T_2]$ by mapping $X \otimes 1$ to T_1 and $1 \otimes X$ to T_2, then

$$\Delta P(X) = P(T_1 + T_2), \quad \epsilon P(X) = P(0), \quad SP(X) = P(-X).$$

Since $\mathbf{G}_a(K) = \mathrm{Hom}_k(k[X], K)$ and $k[\mathbf{G}_a] = k[X]$, it follows that $k[\mathbf{G}_a]$ *is a bicommutative Hopf algebra of finite type.*

Our next example is the algebra of Laurent polynomials $H = k[Y, Y^{-1}]$ which becomes a Hopf algebra with the coproduct Δ satisfying $\Delta(Y) = Y \otimes Y$, the co-unit ϵ for which $\epsilon(Y) = 1$ and the antipode S with $S(Y) = Y^{-1}$. The algebra isomorphism between $H \otimes H$ and $k[T_1, T_1^{-1}, T_2, T_2^{-1}]$ defined by

$$Y \otimes 1 \mapsto T_1, \quad 1 \otimes Y \mapsto T_2$$

gives

$$\Delta P(Y) = P(T_1T_2), \quad \epsilon P(Y) = P(1), \quad SP(Y) = P(Y^{-1}).$$

Since $\mathbf{G}_m(K) = \mathrm{Hom}_k(k[Y, Y^{-1}], K)$, we have $k[\mathbf{G}_m] = k[Y, Y^{-1}]$ and again $k[\mathbf{G}_m]$ is a *bicommutative Hopf algebra of finite type.*

Combining these two examples, one gets a whole family of Hopf algebras. Indeed let $d_0 \geq 0$ and $d_1 \geq 0$ be two integers with $d = d_0 + d_1 > 0$. The Hopf algebra

$$k[X]^{\otimes d_0} \otimes k[Y, Y^{-1}]^{\otimes d_1}$$

is isomorphic to

$$H = k[X_1, \ldots, X_{d_0}, Y_1, Y_1^{-1}, \ldots, Y_{d_1}, Y_{d_1}^{-1}],$$

hence is isomorphic to $k[G]$ with $G = \mathbf{G}_a^{d_0} \times \mathbf{G}_m^{d_1}$.

According to [A] Chap. 4 (p. 163), the category of k-linear algebraic groups is anti-equivalent to the category of commutative k-Hopf algebras of finite type. Hence *the category of commutative linear algebraic groups over k is anti-equivalent to the category of bicommutative Hopf algebras of finite type over k.*

The commutative and connected linear algebraic groups over an algebraically closed fields are the groups $\mathbf{G}_a^{d_0} \times \mathbf{G}_m^{d_1}$ and the Hopf algebras $k[\mathbf{G}_a^{d_0} \times \mathbf{G}_m^{d_1}]$ are the bicommutative Hopf algebras of finite type over k without zero divisors. In $k[\mathbf{G}_a^{d_0} \times \mathbf{G}_m^{d_1}]$ the k-vector space of primitive elements has dimension d_0, while the rank of group-like elements is d_1.

We exhausted the list of examples of bicommutative Hopf algebras without zero divisors and of finite type. However this is not the end of the story: let W be a k-vector space of dimension ℓ_0. Then the symmetric algebra $\mathrm{Sym}(W)$ on W has a natural structure of bicommutative Hopf algebra of finite type [H3]. If $\partial_1, \ldots, \partial_{\ell_0}$ is a basis of W over k, then $\mathrm{Sym}(W)$ is isomorphic to $k[\partial_1, \ldots, \partial_{\ell_0}]$, hence to $k[\mathbf{G}_a^{\ell_0}]$.

If Γ is a free $\mathbf{Z}$-module of finite type and rank ℓ_1, then the group algebra $k\Gamma$ is a bicommutative Hopf algebra of finite type isomorphic to $k[\mathbf{G}_m^{\ell_1}]$.

Therefore *the category of bicommutative Hopf algebras without zero divisors and of finite type over k is equivalent to the category of pairs (W, Γ) where W is a k-vector space of finite dimension and Γ a free $\mathbf{Z}$-module of finite type.* In

$$H \simeq \mathrm{Sym}(W) \otimes k\Gamma,$$

the space of primitive elements has dimension $\ell_0 = \dim W$, while the group-like elements have rank $\ell_1 = \mathrm{rank}\Gamma$.

We now take $k = \overline{\mathbf{Q}}$. S. Fischler [F1] further introduces two more categories.

Let $\mathfrak{C}_1$ be the category whose objects are the triples (G, W, Γ) with $G = \mathbf{G}_a^{d_0} \times \mathbf{G}_m^{d_1}$ a commutative linear algebraic group over $\overline{\mathbf{Q}}$, $W \subset T_e(G)$ a subspace which is rational over $\overline{\mathbf{Q}}$ and $\Gamma \subset G(\overline{\mathbf{Q}})$ a torsion free finitely generated subgroup; moreover G is *minimal* for these properties: no algebraic subgroup G^* other than G itself satisfies $W \subset T_e(G^*)$ and $\Gamma \subset G^*(\overline{\mathbf{Q}})$.

We denote by ℓ_0 the dimension of W and by ℓ_1 the rank of Γ.

The morphisms $f : (G_1, W_1, \Gamma_1) \to (G_2, W_2, \Gamma_2)$ are given by a morphism $f : G_1 \to G_2$ of algebraic groups such that $f(\Gamma_1) \subset \Gamma_2$ such that the linear tangent map to f

$$df : T_e(G_1) \longrightarrow T_e(G_2)$$

satisfies $df(W_1) \subset W_2$.

The definition of the category $\mathfrak{C}_2$ requires the following additional data. Let H be an bicommutative Hopf algebra of finite type over $\overline{\mathbf{Q}}$ and without zero divisors. Denote by d_0 the dimension of the $\overline{\mathbf{Q}}$-vector space spanned by the primitive elements and by d_1 the rank of the group-like elements. Let H' be also a Hopf algebra, which is again bicommutative, without zero divisors and of finite type over $\overline{\mathbf{Q}}$. The dimension of the $\overline{\mathbf{Q}}$-vector space spanned by the primitive elements in H' is denoted by ℓ_0 while ℓ_1 is the rank of the group-like elements in H'. Let $\langle\cdot\rangle : H \times H' \longrightarrow \overline{\mathbf{Q}}$ be a bilinear map such that

$$\langle x, yy' \rangle = \langle \Delta x, y \otimes y' \rangle \quad \text{and} \quad \langle xx', y \rangle = \langle x \otimes x', \Delta y \rangle. \tag{2.1}$$

We used the notation

$$\langle \alpha \otimes \beta, \gamma \otimes \delta \rangle = \langle \alpha, \gamma \rangle \langle \beta, \delta \rangle.$$

The objects of the category $\mathfrak{C}_2$ are the triples $(H, H', \langle\cdot\rangle)$ given by two bicommutative Hopf algebras, without zero divisors and of finite type over $\overline{\mathbf{Q}}$, and a bilinear product satisfying (2.1). The morphisms are the pairs $(f, g) : (H_1, H_1', \langle\cdot\rangle_1) \to (H_2, H_2', \langle\cdot\rangle_2)$ where $f : H_1 \to H_2$ and $g : H_2' \to H_1'$ are Hopf algebra morphisms such that

$$\langle x_1, g(x_2') \rangle_1 = \langle f(x_1), x_2' \rangle_2.$$

One composes two morphisms $(f_1, g_1) : (H_1, H_1', \langle\cdot\rangle_1) \to (H_2, H_2', \langle\cdot\rangle_2)$ and $(f_2, g_2) : (H_2, H_2', \langle\cdot\rangle_2) \to (H_3, H_3', \langle\cdot\rangle_3)$ as

$$(f_2 \circ f_1, g_1 \circ g_2) : (H_1, H_1', \langle\cdot\rangle_1) \to (H_3, H_3', \langle\cdot\rangle_3).$$

Stéphane Fischler [F1] proves:

Theorem 2.2. (S. Fischler). *Both categories $\mathfrak{C}_1$ and $\mathfrak{C}_2$ are equivalent. This equivalence preserves the parameters d_0, d_1, ℓ_0, ℓ_1.*

The category $\mathfrak{C}_2$ has a natural contravariant involution which consists in permuting H and H'. The corresponding involution in the category $\mathfrak{C}_1$ is the Fourier-Borel duality (1.9) we discussed above, which exchanges (d_0, d_1) and (ℓ_0, ℓ_1) in Theorem 1.7.

The main goal in [F1] is to establish new *interpolation lemmas.* Theorem 2.2 enables Fischler to obtain them by duality, starting from known *zero estimates.*

Roughly speaking, a zero estimate (see for instance [W] § 2.1) is a lower bound for the degree of a polynomial vanishing at a given finite set of points (multiplicities may be considered). An interpolation lemma provides a lower bound for an integer D with the following property: given a finite set of points (maybe with multiplicities), there is a polynomial of degree at most D taking given values at these points. In terms of matrices, the zero estimates states that a matrix, whose entries are the values of monomials at the given points, has maximal rank, if only there are enough monomials (hence the matrix is sufficiently rectangular), while the interpolation lemma states that such a matrix has maximal rank once there are enough points (again this means that the matrix is sufficiently rectangular, but in the other direction).

This method using a duality to deduce interpolation lemmas from zero estimates works only for *linear* commutative algebraic groups. Zero estimates are known more generally for commutative algebraic groups (hence for abelian and semi-abelian varieties), but duality does not extend to the non-linear case. Fischler [F2] uses other arguments to obtain interpolation lemmas for non-linear commutative algebraic groups.

3. Hopf algebras and multiple zeta values

Let $\mathfrak{S}$ denote the set of sequences $\underline{s} = (s_1, \ldots, s_k) \in \mathbf{N}^k$ with $k \geq 0$, $s_1 \geq 2$, $s_i \geq 1$ $(2 \leq i \leq k)$.

The *weight* $|\underline{s}|$ of $\underline{s}$ is $s_1 + \cdots + s_k$, while k is the *depth of* $\underline{s}$.

For $\underline{s} \in \mathfrak{S}$ set

$$\zeta(\underline{s}) = \sum_{n_1 > \cdots > n_k \geq 1} n_1^{-s_1} \cdots n_k^{-s_k}.$$

When $\underline{s}$ is the empty sequence (of weight and depth 0), we require $\zeta(\underline{s}) = 1$.

3.1 Goncharov's Conjecture

Denote by $\mathfrak{Z}$ the $\mathbf{Q}$-vector subspace of $\mathbf{C}$ spanned by the numbers

$$(2i\pi)^{-|s|}\zeta(\underline{s}) \quad (\underline{s} \in \mathfrak{S}).$$

As is well known (and as we shall see), for $\underline{s}$ and $\underline{s}'$ in $\mathfrak{S}$, the product $\zeta(\underline{s})\zeta(\underline{s}')$ is *in two ways* a linear combination with positive coefficients of numbers $\zeta(\underline{s}'')$.

Hence $\mathfrak{Z}$ is a $\mathbf{Q}$-sub-algebra of $\mathbf{C}$ with a double filtration by weight and depth.

For a graded Lie algebra $C_\bullet$ denote by $\mathfrak{U}C_\bullet$ its universal envelopping algebra and by

$$\mathfrak{U}C_\bullet^\vee = \bigoplus_{n\geq 0}(\mathfrak{U}C)_n^\vee$$

its graded dual, which is a commutative Hopf algebra.

Conjecture 3.1. (Goncharov [G]). *There exists a graded Lie algebra $C_\bullet$ and an isomorphism*

$$\mathfrak{Z} \simeq \mathfrak{U}C_\bullet^\vee$$

of bifiltered algebras, by the weight on the left and by the depth on the right.

Hopf algebras also occur in this theory in a non-conjectural way. They are used to describe the above mentioned quadratic relations expressing the product of two multiple zeta values as a linear combination of multiple zeta values.

3.2 The concatenation Hopf algebra

Let $X = \{x_0, x_1\}$ be an alphabet with two letters. The free monoid (of words) on X is

$$X^* = \{x_{\epsilon_1}\cdots x_{\epsilon_k}\ ;\ \epsilon_i \in \{0,1\},\ (1\leq i\leq k),\ \ k\geq 0\}$$

whose product is concatenation, and its unity is the empty word e.

Let $\mathfrak{H}$ denote the free algebra $\overline{\mathbf{Q}}\langle X\rangle$ on X. An element $P\in\mathfrak{H}$ is written

$$P = \sum_{w\in X^*}\langle P|w\rangle w$$

with coefficients $\langle P|w\rangle \in \overline{\mathbf{Q}}$.

The *concatenation Hopf algebra* is $(\mathfrak{H}, \cdot, e, \Delta, \epsilon, S)$ where the coproduct is

$$\Delta P = P(x_0\otimes 1 + 1\otimes x_0, x_1\otimes 1 + 1\otimes x_1),$$

the co-unit $\epsilon(P) = \langle P \mid e\rangle$ and the antipode

$$S(x_1 \cdots x_n) = (-1)^n x_n \cdots x_1$$

for $n \geq 1$ and $x_1, \ldots, x_n$ in X.

It is a cocommutative, not commutative Hopf algebra.

3.3 The shuffle Hopf algebra

The shuffle product $ш : \mathfrak{H} \times \mathfrak{H} \to \mathfrak{H}$ is defined inductively by the conditions

$$uшe = eшu = u \quad \text{and} \quad xuшyv = x(uшyv) + y(xuшv)$$

for x and y in X, u and v in X^*. It endows $\mathfrak{H}$ with a structure of commutative algebra $\mathfrak{H}_ш$.

According to [Re] Theorem 3.1, for $P \in \mathfrak{H}$,

$$\Delta P = \sum_{u,v\in X^*} (P|uшv) u \otimes v. \tag{3.2}$$

The *shuffle Hopf algebra* is the commutative (not cocommutative) Hopf algebra $(\mathfrak{H}, ш, e, \Phi, \epsilon, S)$, with $\Phi : \mathfrak{H} \to \mathfrak{H} \otimes \mathfrak{H}$ defined by

$$\langle \Phi(w) \mid u \otimes v\rangle = \langle uv \mid w\rangle.$$

Hence

$$\Phi(w) = \sum_{\substack{u,v\in X^*\\ uv=w}} u \otimes v.$$

From (3.2) it follows that the shuffle Hopf algebra is the graded dual of the concatenation Hopf algebra (see [Re] Chap. 1).

We need to consider subalgebras of $\mathfrak{H}$.

For $s \geq 1$ define $y_s = x_0^{s-1}x_1$. The subalgebra $\mathfrak{H}^1$ of $\mathfrak{H}$ spanned by $\{y_1, y_2, \ldots\}$ is free, and so is the subalgebra $\mathfrak{H}^0$ of $\mathfrak{H}^1$ spanned by $\{y_2, y_3, \ldots\}$. Also $\mathfrak{H}^1$ is the $\overline{\mathbf{Q}}$-vector space $\overline{\mathbf{Q}}e + \mathfrak{H}x_1$ spanned by $\{e\} \cup X^*x_1$, while $\mathfrak{H}^0$ is the $\overline{\mathbf{Q}}$-vector space $\overline{\mathbf{Q}}e + x_0\mathfrak{H}x_1$ spanned by $\{e\} \cup x_0X^*x_1$.

The shuffle ш makes $\mathfrak{H}^0$ and $\mathfrak{H}^1$ subalgebras of $\mathfrak{H}_ш$:

$$\mathfrak{H}^0_ш \subset \mathfrak{H}^1_ш \subset \mathfrak{H}_ш.$$

Define a mapping $\hat{\zeta} : x_0X^*x_1 \to \mathbf{C}$ as follows. Each element w in $x_0X^*x_1$ can be written in a unique way $y_{s_1} \cdots y_{s_k}$ with $\underline{s} = (s_1, \ldots, s_k) \in \mathfrak{S}$. The number of letters x_1 in w is the depth k of, while the total number of letters of w is the weight $s_1 + \cdots + s_k$ of $\underline{s}$. Define

$$\hat{\zeta}(y_{s_1} \cdots y_{s_k}) = \zeta(s_1, \ldots, s_k).$$

By $\overline{\mathbf{Q}}$-linearity one extends $\hat{\zeta}$ to a map from $\mathfrak{H}^0$ to $\mathbf{C}$ with $\hat{\zeta}(e) = 1$. Using the representation of $\hat{\zeta}$ as Chen iterated integrals, namely ([K], § XIX.11), for $w \in x_0X^*x_1$,

$$\hat{\zeta}(x_{\epsilon_1} \cdots x_{\epsilon_p}) = \int_{1>t_1>\cdots>t_p>0} \omega_{\epsilon_1}(t_1) \cdots \omega_{\epsilon_p}(t_p)$$

with $\epsilon_i \in \{0,1\}$ $(1 \le i \le p)$, $\epsilon_0 = 0$, $\epsilon_p = 1$,

$$\omega_0(t) = \frac{dt}{t} \quad \text{and} \quad \omega_1(t) = \frac{dt}{1-t},$$

one checks that $\hat{\zeta}$ *is a commutative algebra morphism of* $\mathfrak{H}^0_{ш}$ *into* $\mathbf{C}$.

The structure of the commutative algebra $\mathfrak{H}_{ш}$ is given by *Radford Theorem* [Re] Chap. 6. Consider the lexicographic order on X^* with $x_0 < x_1$. A *Lyndon word* is a word $w \in X^*$ such that, for each decomposition $w = uv$ with $u \ne e$ and $v \ne e$, the inequality $w < v$ holds. Examples of Lyndon words are x_0, x_1, $x_0x_1^k$ $(k \ge 0)$, $x_0^\ell x_1$ $(\ell \ge 0)$, $x_0^2x_1^2$. Denote by L the set of Lyndon words. Then the three shuffle algebras are (commutative) polynomial algebras

$$\mathfrak{H}_{ш} = K[\mathsf{L}]_{ш}, \quad \mathfrak{H}^1_{ш} = K\big[\mathsf{L} \setminus \{x_0\}\big]_{ш} \quad \text{and } \mathfrak{H}^0_{ш} = K\big[\mathsf{L} \setminus \{x_0, x_1\}\big]_{ш}.$$

Therefore

$$\mathfrak{H}_{ш} = \mathfrak{H}^1_{ш}[x_0]_{ш} = \mathfrak{H}^0_{ш}[x_0, x_1]_{ш} \quad \text{and } \mathfrak{H}^1_{ш} = \mathfrak{H}^0_{ш}[x_1]_{ш}. \tag{3.3}$$

3.4 Harmonic algebra

There is another product being shuffle-like law on $\mathfrak{H}$, called *harmonic product* by M. Hoffman ([H1], [H2]) and *stuffle* by other authors [BBBL], denoted with a star, which also gives rise to subalgebras

$$\mathfrak{H}^0_\star \subset \mathfrak{H}^1_\star \subset \mathfrak{H}_\star.$$

It is defined as follows. First on X^*, the map $\star : X^* \times X^* \to \mathfrak{H}$ is defined by induction, starting with

$$x_0^n \star w = w \star x_0^n = wx_0^n$$

for any $w \in X^*$ and any $n \ge 0$ (for $n = 0$ it means $e \star w = w \star e = w$ for all $w \in X^*$) and then

$$y_su \star y_tv = y_s(u \star y_tv) + y_t(y_su \star v) + y_{s+t}(u \star v)$$

for u and v in X^*, s and t positive integers.

The harmonic product is an efficient way of writing the quadratic relations among multiple zeta values arising from the expression of $\zeta(\underline{s})$ as series: $\hat{\zeta}$ *is a commutative algebra morphism of* $\mathfrak{H}^0_\star$ *into* $\mathbf{C}$.

Hoffman [H1] gives the structure of the quasi-harmonic algebra $\mathfrak{H}_\star$ as well as of its subalgebras $\mathfrak{H}^1_\star$ and $\mathfrak{H}^0_\star$: they are again polynomial algebras on Lyndon words:

$$\mathfrak{H}_\star = K[\mathsf{L}]_\star, \quad \mathfrak{H}^0_\star = K\big[\mathsf{L} \setminus \{x_0\}\big]_\star \quad \text{and} \quad \mathfrak{H}^1_\star = K\big[\mathsf{L} \setminus \{x_0, x_1\}\big]_\star.$$

Hence

$$\mathfrak{H}_\star = \mathfrak{H}^1_\star[x_0]_\star = \mathfrak{H}^0_\star[x_0, x_1]_\star \quad \text{and} \quad \mathfrak{H}^1_\star = \mathfrak{H}^0_\star[x_1]_\star. \tag{3.4}$$

The *quasi-shuffle* Hopf algebra is the commutative algebra $\mathfrak{H}^1_\star$ with the coproduct Δ defined by the conditions

$$\Delta(y_i) = y_i \otimes e + e \otimes y_i$$

for $i \geq 1$, the co-unit

$$\epsilon(P) = \langle P \mid e \rangle$$

and the antipode

$$S(y_{s_1} \cdots y_{s_k}) = (-1)^k y_{s_k} \cdots y_{s_1}.$$

This quasi-shuffle Hopf algebra is isomorphic to the Hopf algebra of non-commutative symmetric series, whose graded dual is the Hopf algebra of quasi-symmetric series (see [H2] and [H3]) .

3.5 Regularized double shuffle relations

As we have seen the map $\hat{\zeta}$ is a commutative algebra morphism of $\mathfrak{H}^0_ш$ into $\mathbf{C}$ and also of $\mathfrak{H}^0_\star$ into $\mathbf{C}$. Hence the kernel of $\hat{\zeta}$ in $\mathfrak{H}^0$ is an ideal for the two algebra structures ш and $\star$. A fundamental question (cf. Goncharov's Conjecture 3.1) is to describe this kernel.

The relations

$$\hat{\zeta}(u ш v) = \hat{\zeta}(u)\hat{\zeta}(v) \quad \text{and} \quad \hat{\zeta}(u \star v) = \hat{\zeta}(u)\hat{\zeta}(v) \quad \text{for } u \text{ and } v \text{ in } \mathfrak{H}^0$$

show that, for any u and v in $\mathfrak{H}^0$, $u ш v - u \star v$ belongs to the kernel of $\hat{\zeta}$. The equations

$$\hat{\zeta}(u ш v - u \star v) = 0 \quad \text{for } u \text{ and } v \text{ in } \mathfrak{H}^0 \tag{3.5}$$

are called *the standard linear relations among multiple zeta values.*

Other elements belong to the kernel of $\hat{\zeta}$: *Hoffman's relations* (see for instance [Z]) are

$$\hat{\zeta}(x_1 ш v - x_1 \star v) = 0 \quad \text{for } v \text{ in } \mathfrak{H}^0. \tag{3.6}$$

Notice that $x_1 ш v - x_1 \star v \in \mathfrak{H}^0$ for $v \in \mathfrak{H}^0$. The simplest example

$$x_1 ш y_2 - x_1 \star y_2 \in \ker \hat{\zeta}$$

yields the relation $\zeta(2,1) = \zeta(3)$ known by Euler.

It was conjectured in [MJOP] that the elements

$$u ш v - u \star v \quad \text{and} \quad x_1 ш v - x_1 \star v,$$

when u and v range over the set $\mathfrak{H}^0$, span the $\mathbf{Q}$ vector space $\ker \hat{\zeta}$. This conjecture is not yet disproved, but there is a little doubt about it for the following reason.

From (3.3) and (3.4) it follows that there are two uniquely determined algebra morphisms

$$\hat{Z}_ш : \mathfrak{H}^1_ш \longrightarrow \mathbf{R}[T] \quad \text{and} \quad \hat{Z}_\star : \mathfrak{H}^1_\star \longrightarrow \mathbf{R}[T]$$

which extend $\hat{\zeta}$ and map x_1 to T. According to [C], the next result is due to Boutet de Monvel and Zagier (see also [I-K]).

Proposition 3.7. *There is a* $\mathbf{R}$*-linear isomorphism* $\varrho : \mathbf{R}[T] \to \mathbf{R}[T]$ *which makes the following diagram commutative:*

$$\begin{tikzcd} \mathfrak{H}^1 \arrow[r, "\hat{Z}_\star"] \arrow[d, equal] & \mathbf{R}[T] \arrow[d, "\varrho"] \\ \mathfrak{H}^1 \arrow[r, "\hat{Z}_ш"] & \mathbf{R}[T] \end{tikzcd}$$

An explicit formula for ϱ *is given by means of the generating series*

$$\sum_{\ell \geq 0} \varrho(T^\ell) \frac{t^\ell}{\ell!} = \exp\left(Tt + \sum_{n=2}^{\infty} (-1)^n \frac{\zeta(n)}{n} t^n \right). \tag{3.8}$$

It is instructive to compare the right hand side of (3.8) with the formula giving the expansion of the logarithm of Euler Gamma function:

$$\Gamma(1+t) = \exp\left(-\gamma t + \sum_{n=2}^{\infty} (-1)^n \frac{\zeta(n)}{n} t^n \right).$$

Accordingly, ϱ may be viewed as the differential operator of infinite order

$$\exp\left(\sum_{n=2}^{\infty} (-1)^n \frac{\zeta(n)}{n} \left(\frac{\partial}{\partial T} \right)^n \right)$$

(just consider the image of e^{tT}).

In [I-K] Ihara and Kaneko propose a regularization of the divergent multiple zeta values as follows.

Recall that $\mathfrak{H}_{ш} = \mathfrak{H}^0[x_0, x_1]_{ш}$. Denote by $\mathrm{reg}_{ш}$ the $\mathbf{Q}$-linear map $\mathfrak{H} \to \mathfrak{H}^0$ which maps $w \in \mathfrak{H}$ to its constant term in its expansion as a polynomial in x_0, x_1 in the shuffle algebra $\mathfrak{H}^0[x_0, x_1]_{ш}$. Then $\mathrm{reg}_{ш}$ is an algebra morphism $\mathfrak{H}_{ш} \to \mathfrak{H}^0_{ш}$. Clearly for $w \in \mathfrak{H}^0$ we have

$$\mathrm{reg}_{ш}(w) = w.$$

Theorem 3.9. (Ihara, Kaneko). *Let w be any word in X^*. Write $w = x_1^m w_0 x_0^n$ with $w_0 \in \mathfrak{H}^0$, $m \geq 0$ and $n \geq 0$. Then*

$$\mathrm{reg}_{ш}(w) = \sum_{i=0}^{m} \sum_{j=0}^{n} (-1)^{i+j} x_1^i ш (x_1^{m-i} w_0 x_0^{n-j}) ш x_0^j.$$

Special cases are:

$$\mathrm{reg}_{ш}(x_1^m) = \mathrm{reg}_{ш}(x_0^n) = 0 \quad \text{for} \quad m \geq 1 \quad \text{and} \quad n \geq 1.$$

$$\mathrm{reg}_{ш}(x_1^m x_0^n) = (-1)^{m+n-1} x_0^n x_1^m \quad \text{for} \quad m \geq 1 \quad \text{and} \quad n \geq 1.$$

$$\mathrm{reg}_{ш}(x_1^m x_0 u) = (-1)^m x_0 (x_1^m ш u) \quad \text{for} \quad m \geq 0 \quad \text{and} \quad u \in X^* x_1.$$

$$\mathrm{reg}_{ш}(u x_1 x_0^n) = (-1)^n (u ш x_0^n) x_1 \quad \text{for} \quad n \geq 0 \quad \text{and} \quad u \in x_0 X^*.$$

Moreover there is an explicit expression for w as a polynomial in x_0 and x_1 in the algebra $\mathfrak{H}^0[x_0, x_1]_{ш}$:

$$w = \sum_{i=0}^{m} \sum_{j=0}^{n} \mathrm{reg}_{ш}(x_1^{m-i} w_0 x_0^{n-j}) ш x_1^i ш x_0^j.$$

The *regularized double shuffle relations* of Ihara and Kaneko in [I-K] produce a number of linear relations among multiple zeta values:

Theorem 3.10. (Ihara, Kaneko). *For $w \in \mathfrak{H}^1$ and $w_0 \in \mathfrak{H}^0$,*

$$\mathrm{reg}_{ш}(w ш w_0 - w \star w_0) \in \ker \hat{\zeta}. \tag{3.11}$$

Special cases of (3.11) – for which no regularization is required – are the standard relations (3.5) which correspond to $w \in \mathfrak{H}^0$ and Hoffman's relations (3.6) which correspond to $w = x_1$.

An example of u and v in $\mathfrak{H}^1$ for which $u ш v - u \star v \in \mathfrak{H}^0$ but $\hat{\zeta}(u ш v - u \star v) \neq 0$ is $u = v = x_1$.

3.6 The main diophantine Conjecture

The main diophantine Conjecture arose after the works of several mathematicians, including D. Zagier, A.B. Goncharov, M. Kontsevich, M. Hoffman, M. Petitot and Hoang Ngoc Minh, K. Ihara and M. Kaneko, J. Écalle, P. Cartier (see [C]).

Conjecture 3.12. The kernel of $\hat{\zeta}$ is spanned by the elements

$$\mathrm{reg}_{ш}(w ш w_0 - w \star w_0)$$

where w ranges over $\mathfrak{H}^1$ and w_0 over $\mathfrak{H}^0$.

Conjecture 3.12 means that the ideal of algebraic relations among multiple zeta values is generated by the double shuffle relations of Ihara and Kaneko in Theorem 3.10.

More precisely, we introduce independent variables Z_u, where u ranges over the set $X^* x_1$. For $v = \sum_u c_u u$ in $\mathfrak{H}^1$, we set

$$Z_v = \sum_u c_u Z_u$$

where $Z_e = 1$. In particular, for u_1 and u_2 in $x_0 X^* x_1$, $Z_{u_1 ш u_2}$ and $Z_{u_1 \star u_2}$ are linear forms in Z_u, $u \in x_0 X^* x_1$. Also, for $v \in x_0 \mathfrak{H} x_1$, $Z_{x_1 ш v - x_1 \star v}$ is a linear form in Z_u, $u \in x_0 X^* x_1$.

Denote by $\mathfrak{R}$ the ring of polynomials with coefficients in $\overline{\mathbf{Q}}$ in the variables Z_u, where u ranges over the set of words in $x_0 X^* x_1$ which start with x_0 and end with x_1. Further, denote by $\mathfrak{I}$ the ideal of $\mathfrak{R}$ consisting of all polynomials which vanish under the specialization map $\mathfrak{R} \to \mathbf{R}$ which is the $\overline{\mathbf{Q}}$-algebra morphism defined by

$$Z_u \mapsto \hat{\zeta}(u) \quad (u \in x_0 X^* x_1).$$

The $\overline{\mathbf{Q}}$-sub-algebra in $\mathbf{C}$ of multiple zeta values (up to the normalization with powers of $2\pi i$, this is the algebra $\mathfrak{Z}$ of Goncharov's Conjecture 3.1) is isomorphic to the quotient $\mathfrak{R}/\mathfrak{I}$.

Let $\mathfrak{J}$ be the ideal of $\mathfrak{R}$ generated by the polynomials

$$Z_u Z_v - Z_{u ш v} \quad \text{and} \quad Z_r \quad \text{with} \quad r = \mathrm{reg}_{ш}(w ш w_0 - w \star w_0),$$

where u, v, w_0 range over $\mathfrak{H}^0$ and w over $\mathfrak{H}^1$.

Theorem 3.10 can be written $\mathfrak{J} \subset \mathfrak{I}$ and Conjecture 3.12 means $\mathfrak{J} = \mathfrak{I}$.

The ideal of $\mathfrak{R}$ associated to the above mentioned conjecture of [MJOP] (see § 3.5) is the ideal, contained in $\mathfrak{J}$, generated by the polynomials

$$Z_u Z_v - Z_{u ш v}, \quad Z_u Z_v - Z_{u \star v} \quad \text{and} \quad Z_{x_1 ш u - x_1 \star u},$$

where u and v range over the set of elements in $x_0 X^* x_1$.

The structure of the quotient of $\mathfrak{R}/\mathfrak{J}$ is being studied by Jean Écalle [E].

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