

# PROOF OF THE ZIG-ZAG CONJECTURE

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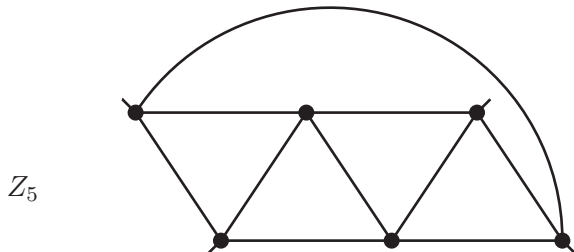
ABSTRACT. A long-standing conjecture in quantum field theory due to Broadhurst and Kreimer states that the amplitudes of the zig-zag graphs are a certain explicit rational multiple of the odd values of the Riemann zeta function. In this paper we prove this conjecture by constructing a certain family of single-valued multiple polylogarithms. The zig-zag graphs therefore provide the only infinite family of primitive graphs in  $\phi_4^4$  theory (in fact, in any renormalisable quantum field theory in four dimensions) whose amplitudes are now known.

To David Broadhurst, a pioneer, for his 65th birthday

## 1. INTRODUCTION

In 1995 Broadhurst and Kreimer [4] conjectured a formula for the amplitudes of a well-known family of graphs in  $\phi^4$  theory called the zig-zag graphs. We give a proof of this conjecture using the second author's theory of graphical functions [22] (see also [12]) and a variant of the first author's theory of single-valued multiple polylogarithms [5]. The proof makes use of a recent theorem due to Zagier [26, 19] on the evaluation of the multiple zeta values  $\zeta(2, \dots, 2, 3, 2, \dots, 2)$  in terms of the numbers  $\zeta(2m + 1)\pi^{2k}$ .

**1.1. Statement of the theorem.** For  $n \geq 3$ , let  $Z_n$  denote the zig-zag graph with  $n$  loops (and zero external momenta), pictured below.



Its scheme independent contribution to the beta function in  $\phi_4^4$  theory (a period in the sense of [17]), can be written in parametric space as follows. Number the edges of  $Z_n$  from 1 to  $2n$ , and to each edge  $e$  associate a variable  $\alpha_e$ . The period of  $Z_n$  is given by the convergent integral in projective space [24]:

$$(1.1) \quad I_{Z_n} = \int_{\Delta} \frac{\Omega_{2n-1}}{\Psi_{Z_n}^2} \in \mathbb{R}$$

where  $\Delta = \{(\alpha_1 : \dots : \alpha_{2n}) : \alpha_i \geq 0\} \subset \mathbb{P}^{2n-1}(\mathbb{R})$  is the standard coordinate simplex,

$$\Omega_{2n-1} = \sum_{i=1}^{2n} (-1)^i \alpha_i d\alpha_1 \wedge \dots \wedge \widehat{d\alpha_i} \dots \wedge d\alpha_{2n},$$

and  $\Psi_{Z_n} \in \mathbb{Z}[\alpha_1, \dots, \alpha_{2n}]$  is the graph, or Kirchhoff [15], polynomial of  $Z_n$ . It is defined more generally for any graph  $G$  by the formula

$$\Psi_G = \sum_{T \subset G} \prod_{e \notin T} \alpha_e$$

where the sum is over all spanning trees  $T$  of  $G$ . Since the degree of  $\Psi_{Z_n}$  is equal to  $n$ , it follows that the integrand of (1.1) is a homogeneous  $2n - 1$ -form on the complement of the graph hypersurface  $V(\Psi_G)$  in  $\mathbb{P}^{2n-1}$ .

For  $n = 3, 4$  the zig-zag graphs  $Z_n$  are isomorphic to the wheels with  $n$  spokes  $W_n$ , whose periods are known for all  $n$  by Gegenbauer polynomial techniques [3]. For  $n \geq 5$ , the graphs  $W_n$  are unphysical, and different from the  $Z_n$ . The period for  $Z_5$  was computed by Kazakov in 1983 [14], for  $Z_6$  by Broadhurst in 1985 [2] (see also [23]), and the cases  $Z_n$  for  $n \leq 12$  can now be obtained by computer [22] using single-valued multiple polylogarithms [5]. The period of  $Z_n$  is *a priori* known to be a multiple zeta value of weight  $2n - 3$  either by this method, or by the general method of parametric integration of [6]. The precise formula for its period was conjectured in [4].

**Theorem 1.1.** (*Zig-zag conjecture* [4]). *The period of the graph  $Z_n$  is given by*

$$(1.2) \quad I_{Z_n} = 4 \frac{(2n-2)!}{n!(n-1)!} \left(1 - \frac{1 - (-1)^n}{2^{2n-3}}\right) \zeta(2n-3)$$

Using the well-known fact that the period of a two-vertex join of a family of graphs is the product of their periods, we immediately deduce:

**Corollary 1.2.** *Any product of odd zeta values  $\prod_{i=1}^N \zeta(2n_i + 1)$ , for  $n_i \geq 1$ , occurs as the period of a primitive logarithmically-divergent graph in  $\phi_4^4$  theory.*

The strategy of our proof is to compute the amplitude of the zig-zag graphs in position space by direct integration. At each integration step, one has to solve a unipotent differential equation in  $\partial/\partial z$  and  $\partial/\partial \bar{z}$  on  $\mathbb{P}^1 \setminus \{0, 1, \infty\}(\mathbb{C})$ , whose solution is necessarily single-valued. Such a method was first introduced by Davidychev and Ussyukina in [11] for a family of ladder diagrams. The functions they obtained are single-valued versions of the classical polylogarithms  $\text{Li}_n(z) = \sum_{k \geq 1} \frac{z^k}{k^n}$ . A broad generalisation of this method was recently found independently by Schnetz [22] and Drummond [12], and works for a large class of graphs. It uses the fact that any unipotent differential equation on  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$  can be solved using the single-valued multiple polylogarithms constructed in [5]. Unfortunately, the definition of these functions is complicated and not completely explicit, so the best one can presently do by this method is to prove the zig-zag conjecture modulo products of multiple zeta values [21], [22]. Therefore this approach fails to predict the most important property of the zig-zag periods, which is that they reduce to a single Riemann zeta value. Experimental evidence suggests that the zig-zags may be the only  $\phi^4$  periods with this property [20].

In this paper we take a different approach, and modify the construction of the single-valued polylogarithms of [5] to write down a specific family of single-valued functions which are tailor-made for the zig-zag graphs. It does not generalise to all multiple polylogarithms, although we expect that some extensions of the present method are possible. The construction relies on some special properties of the Hoffman multiple zeta values  $\zeta(2, \dots, 2, 3, 2, \dots, 2)$  and uses a factorization of various non-commutative generating series into a ‘pure odd zeta’ and ‘pure even zeta’ part.

**1.2. Two families of single-valued multiple polylogarithms.** Most of the paper (§3 and §4) is devoted to constructing the following explicit families of functions. Recall that  $\mathbb{R}\langle\langle x_0, x_1 \rangle\rangle$  denotes the ring of formal power series in two non-commuting

variables  $x_0$  and  $x_1$ . For any element  $S \in \mathbb{R}\langle\langle x_0, x_1 \rangle\rangle$ , let  $\widetilde{S}$  denote the series obtained by reversing the letters in every word which occurs in  $S$ . For any word  $w \in \{x_0, x_1\}^\times$ , let  $L_w(z)$  denote the multiple polylogarithm in one variable, defined by the equations

$$\frac{d}{dz} L_{wx_i}(z) = \frac{L_w(z)}{z-i} \quad \text{for all } i = 0, 1,$$

and the condition  $L_w(z) \sim 0$  as  $z \rightarrow 0$  for all words  $w$  not of the form  $x_0^n$ , and  $L_{x_0^n}(z) = \frac{1}{n!} \log^n(z)$ . The  $L_w(z)$  are multi-valued functions on  $\mathbb{P}^1 \setminus \{0, 1, \infty\}(\mathbb{C})$ .

**Definition 1.3.** Define a formal power series  $\mathcal{S} \in \mathbb{R}\langle\langle x_0, x_1 \rangle\rangle$  by

$$\mathcal{S} = 1 + \mathcal{S}_{0,0}^0 + \mathcal{S}_{0,1}^1 + \mathcal{S}_{1,0}^1 + \mathcal{S}_{0,0}^1,$$

where  $\mathcal{S}_{0,1}^1 = \widetilde{\mathcal{S}_{1,0}^1}$ , and

$$\begin{aligned} (1.3) \quad \mathcal{S}_{0,0}^0 &= -4 \sum_{n \geq 1} \zeta(2n+1) (x_0 x_1)^n x_0 \\ \mathcal{S}_{1,0}^1 &= -4 \sum_{m \geq 1, n \geq 0} \binom{2m+2n}{2m} \zeta(2m+2n+1) (x_1 x_0)^m x_0 (x_1 x_0)^n \\ \mathcal{S}_{0,0}^1 &= \frac{1}{2} (\mathcal{S}_{0,0}^0 \mathcal{S}_{0,0}^0 + \mathcal{S}_{0,0}^0 \mathcal{S}_{1,0}^1 + \mathcal{S}_{0,1}^1 \mathcal{S}_{0,0}^0). \end{aligned}$$

For all  $w \in \{x_0, x_1\}^\times$ , let  $\mathcal{S}_w$  be the coefficient of  $w$  in  $\mathcal{S}$ . It is either an integer multiple of an odd single zeta value  $\zeta(2n+1)$ ,  $n \geq 1$ , or an integral linear combination of products of two odd single zeta values  $\zeta(2n+1)\zeta(2m+1)$ , for  $m, n \geq 1$ .

Let  $\mathcal{B}^0$  denote the set of words  $w \in \{x_0, x_1\}^\times$  which contain no subsequences of the form  $x_1 x_1$  or  $x_0 x_0 x_0$ , and have at most one subsequence of the form  $x_0 x_0$ . These properties are clearly stable under reversing the letters in a word, or taking a subsequence. For every  $w \in \mathcal{B}^0$ , define a series

$$(1.4) \quad F_w(z) = \sum_{w=u_1 u_2 u_3} L_{\widetilde{u}_1}(\bar{z}) \mathcal{S}_{u_2} L_{u_3}(z)$$

where  $\widetilde{w}$  denotes a word  $w$  written in reverse order. *A priori*  $F_w(z)$  is a multivalued, real analytic function on  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ . In §3 we prove the following theorem.

**Theorem 1.4.** *If  $w \in \mathcal{B}^0$ , the function  $F_w(z)$  is single-valued, and satisfies*

$$F_w(z) = F_{\widetilde{w}}(\bar{z}).$$

Let  $i, j \in \{0, 1\}$ . If  $x_i w x_j \in \mathcal{B}^0$ , then

$$(1.5) \quad \frac{\partial^2}{\partial z \partial \bar{z}} F_{x_i w x_j}(z) = \frac{F_w(z)}{(\bar{z}-i)(z-j)}.$$

The second family of functions is defined as follows.

**Definition 1.5.** Define a formal power series  $\hat{\mathcal{S}} \in \mathbb{R}\langle\langle x_0, x_1 \rangle\rangle$  by

$$\hat{\mathcal{S}} = 1 + \hat{\mathcal{S}}_{0,0}^0 + \hat{\mathcal{S}}_{0,1}^1 + \hat{\mathcal{S}}_{1,0}^1 + \hat{\mathcal{S}}_{0,0}^1,$$

where  $\hat{\mathcal{S}}_{0,0}^1 = \mathcal{S}_{0,0}^1$ ,  $\hat{\mathcal{S}}_{0,1}^1 = \widetilde{\hat{\mathcal{S}}_{1,0}^1}$ , and

$$\begin{aligned} (1.6) \quad \hat{\mathcal{S}}_{1,0}^1 &= -4 \sum_{m \geq 0, n \geq 1} (1 - 2^{-2n-2m}) \binom{2m+2n}{2m+1} \zeta(2m+2n+1) (x_1 x_0)^m x_1 (x_1 x_0)^n \\ \hat{\mathcal{S}}_{0,0}^1 &= \frac{1}{2} (\hat{\mathcal{S}}_{0,0}^0 \hat{\mathcal{S}}_{1,0}^1 + \hat{\mathcal{S}}_{0,1}^1 \hat{\mathcal{S}}_{0,0}^0). \end{aligned}$$

Note that, contrary to the previous case, the coefficients of the odd single zeta values and their products in  $\hat{\mathcal{S}}$  now have large powers of 2 in their denominators.

Now let  $\mathcal{B}^1$  denote the set of words  $w$  obtained from  $\mathcal{B}^0$  by interchanging  $x_0$  and  $x_1$ . Thus words  $w \in \mathcal{B}^1$  contain no  $x_0x_0$ , no  $x_1x_1x_1$  and at most one  $x_1x_1$ . For every  $w \in \mathcal{B}^1$ , define a series

$$(1.7) \quad \hat{F}_w(z) = \sum_{w=u_1u_2u_3} L_{\tilde{u}_1}(\bar{z}) \hat{\mathcal{S}}_{u_2} L_{u_3}(z) .$$

In §4 we prove the following theorem.

**Theorem 1.6.** *If  $w \in \mathcal{B}^1$ , the function  $\hat{F}_w(z)$  is single-valued, and satisfies*

$$(1.8) \quad \hat{F}_w(z) = \hat{F}_{\bar{w}}(\bar{z}) .$$

Let  $i, j \in \{0, 1\}$ . If  $x_iwx_j \in \mathcal{B}^1$ , then

$$(1.9) \quad \frac{\partial^2}{\partial z \partial \bar{z}} \hat{F}_{x_iwx_j}(z) = \frac{\hat{F}_w(z)}{(\bar{z} - i)(z - j)} .$$

*Remark 1.7.* It is worth noting that the definition of  $\mathcal{S}$  in (1.3) is compatible with the definition of  $\hat{\mathcal{S}}$  in (1.6), i.e.,  $\mathcal{S}_w = \hat{\mathcal{S}}_w$  for all  $w \in \mathcal{B}^0 \cap \mathcal{B}^1$ . This means that it is possible to combine the previous theorems into a single generating series

$$F_w(z) = \sum_{w=u_1u_2u_3} L_{\tilde{u}_1}(\bar{z}) \mathcal{T}_{u_2} L_{u_3}(z) ,$$

for  $w \in \mathcal{B}^0 \cup \mathcal{B}^1$ , where  $\mathcal{T} = \mathcal{S} + \hat{\mathcal{S}} - 1 - \mathcal{S}_{0,0}^0$ . However, this ansatz does not give single-valued functions for all words  $w$  in  $\{x_0, x_1\}^\times$ . Since the two previous theorems are rather different in character, and play completely different roles in the zig-zag conjecture, we decided to keep their statement and proofs separate.

The zig-zag conjecture itself is proved in §5 using the two previous theorems to deal with the case when  $n$  is even, or odd, respectively.

**1.3. Some remarks.** All available data suggests [20] that the zig-zag graphs play the same role in  $\phi^4$  theory as the odd single zeta values  $\zeta(2n+1)$  in the theory of multiple zeta values. The latter are the primitive elements in the algebra of motivic multiple zeta values and correspond to the generators of the Lie algebra of the motivic Galois group of mixed Tate motives over  $\mathbb{Z}$ . Corollary 1.2 has the important consequence that the periods of  $\phi^4$  theory are closed under the action of the motivic Galois group, to all known weights [10]. It would therefore be very interesting to prove by motivic methods that  $I_{Z_n}$  is an odd single zeta value. The fact that the multiple zeta values  $\zeta(2, \dots, 2, 3, 2, \dots, 2)$  appear in the analytic calculation may give some insight into a long hoped-for formula for the motivic coaction on  $\phi^4$  amplitudes. At present, this is out of reach, but a small step in this direction was taken in [9], where we gave an explicit formula for the class of the zig-zag graph hypersurfaces  $V(\Psi_{Z_n}) \subset \mathbb{P}^{2n-1}$  in the Grothendieck ring of varieties. It is a polynomial in the Lefschetz motive.

Note that it is known by the work of Rivoal and Ball-Rivoal [1] that the odd zeta values span an infinite dimensional vector space over the field of rational numbers. Thus the same conclusion holds for the periods of primitive graphs in  $\phi^4$  theory. In the early days of quantum field theory, the hope was often expressed that the periods would be rational numbers, so corollary 1.2 forms part of an increasing body of evidence (see also [9]), that this is very far from the truth.

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## 2. PRELIMINARIES

**2.1. Reminders on shuffle algebras and formal power series.** Let  $R$  be a commutative unitary ring. The shuffle algebra  $R\langle x_0, x_1 \rangle$  on two letters is the free  $R$ -module spanned by all words  $w$  in the letters  $x_0, x_1$ , together with the empty word  $1$ . The shuffle product is defined recursively by  $w \# 1 = 1 \# w = w$  and

$$x_i w \# x_j w' = x_i(w \# x_j w') + x_j(x_i w \# w')$$

for all  $i, j \in \{0, 1\}$ , and  $w, w' \in \{x_0, x_1\}^\times$ . The shuffle product, extended linearly to all words, makes  $R\langle x_0, x_1 \rangle$  into a commutative unitary ring. The deconcatenation coproduct is defined to be the linear map

$$\begin{aligned} \Delta : R\langle x_0, x_1 \rangle &\longrightarrow R\langle x_0, x_1 \rangle \otimes_R R\langle x_0, x_1 \rangle \\ \Delta(w) &= \sum_{uv=w} u \otimes v \end{aligned}$$

and the antipode is the linear map defined by  $w \mapsto (-1)^{|w|} \tilde{w}$ , where  $|w| \in \mathbb{N}$  denotes the length of a word  $w$  which defines a grading on  $R\langle x_0, x_1 \rangle$ . With these definitions,  $R\langle x_0, x_1 \rangle$  is a commutative, graded, Hopf algebra over  $R$ .

The dual of  $R\langle x_0, x_1 \rangle$  is the  $R$ -module of non-commutative formal power series

$$R\langle\langle x_0, x_1 \rangle\rangle = \{S = \sum_{w \in \{x_0, x_1\}^\times} S_w w \quad , \quad S_w \in R\}$$

equipped with the concatenation product. It is the completion of  $R\langle x_0, x_1 \rangle$  with respect to the augmentation ideal  $\ker \varepsilon$ , where  $\varepsilon : R\langle x_0, x_1 \rangle \rightarrow R$  is the map which projects onto the empty word. Then  $R\langle\langle x_0, x_1 \rangle\rangle$  is a complete Hopf algebra with respect to the (completed) coproduct

$$\Gamma : R\langle\langle x_0, x_1 \rangle\rangle \longrightarrow R\langle\langle x_0, x_1 \rangle\rangle \widehat{\otimes}_R R\langle\langle x_0, x_1 \rangle\rangle$$

for which the elements  $x_0, x_1$  are primitive:  $\Gamma(x_i) = 1 \otimes x_i + x_i \otimes 1$  for  $i = 0, 1$ . The antipode is as before. Thus  $R\langle\langle x_0, x_1 \rangle\rangle$  is cocommutative but not commutative.

By duality, a series  $S \in R\langle\langle x_0, x_1 \rangle\rangle$  defines an element  $S \in \text{Hom}_{R\text{-mod}}(R\langle x_0, x_1 \rangle, R)$  as follows: to any word  $w$  associate the coefficient  $S_w$  of  $w$  in  $S$ .

An invertible series  $S \in R\langle\langle x_0, x_1 \rangle\rangle^\times$  (i.e., with invertible leading term  $S_1$ ) is group-like if  $\Gamma(S) = S \otimes S$ . Equivalently, the coefficients  $S_w$  of  $S$  define a homomorphism for the shuffle product:  $S_w \# S_{w'} = S_w S_{w'}$  for all  $w, w' \in \{x_0, x_1\}^\times$ , where  $S_\bullet$  is extended by linearity on the left-hand side. By the formula for the antipode, it follows that for such a series  $S = S(x_0, x_1)$ , its inverse is given by

$$(2.1) \quad S(x_0, x_1)^{-1} = \tilde{S}(-x_0, -x_1) .$$

**2.2. Multiple polylogarithms in one variable.** Recall that the generating series of multiple polylogarithms on  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$  is denoted by

$$L(z) = \sum_{w \in \{x_0, x_1\}^\times} L_w(z) .$$

It is the unique solution to the Knizhnik-Zamolodchikov equation [16]

$$(2.2) \quad \frac{d}{dz} L(z) = L(z) \left( \frac{x_0}{z} + \frac{x_1}{z-1} \right) ,$$

which satisfies the asymptotic condition

$$(2.3) \quad L(z) = \exp(x_0 \log(z)) h_0(z)$$

for all  $z$  in the neighbourhood of the origin, where  $h_0(z)$  is a function taking values in  $\mathbb{C}\langle\langle x_0, x_1 \rangle\rangle$  which is holomorphic at 0 and satisfies  $h(0) = 1$ . Note that we use the opposite convention to [5] in this paper: differentiation of  $L_w(z)$  corresponds to deconcatenation of  $w$  on the right. The series  $L(z)$  is a group-like formal power series. In particular, the polylogarithms  $\text{Li}_w(z)$  satisfy the shuffle product formula

$$(2.4) \quad L_{w \amalg w'}(z) = L_w(z)L_{w'}(z) \text{ for all } w, w' \in \{x_0, x_1\}^\times .$$

We have

$$(2.5) \quad -L_{x_1 x_0^{n-1}}(z) = \text{Li}_n(z) = \sum_{k \geq 1} \frac{z^k}{k^n} ,$$

for all  $n \geq 1$ , which expresses the classical polylogarithms as coefficients of  $L(z)$ .

Denote the generating series of (shuffle-regularized) multiple zeta values, or Drinfeld's associator, by

$$\mathcal{Z}(x_0, x_1) = \sum_{w \in \{x_0, x_1\}^\times} \zeta(w) w \in \mathbb{C}\langle\langle x_0, x_1 \rangle\rangle .$$

It is the regularized limit of  $L(z)$  at the point  $z = 1$ . In other words, there exists a function  $h_1(z)$  taking values in series  $\mathbb{C}\langle\langle x_0, x_1 \rangle\rangle$ , which is holomorphic at  $z = 1$  where it takes the value  $h(1) = 1$ , such that

$$(2.6) \quad L(z) = \mathcal{Z}(x_0, x_1) \exp(x_1 \log(z-1)) h_1(z) .$$

The series  $\mathcal{Z}(x_0, x_1)$  is group-like, so in particular we have

$$(2.7) \quad \mathcal{Z}(x_0, x_1)^{-1} = \widetilde{\mathcal{Z}}(-x_0, -x_1) .$$

When no confusion arises, we denote  $\mathcal{Z}(x_0, x_1)$  simply by  $\mathcal{Z}$ . Its coefficients are (shuffle-regularized) iterated integrals

$$\zeta(x_{i_1} \dots x_{i_n}) = \int_0^1 \omega_{i_1} \dots \omega_{i_n} \text{ for all } i_1, \dots, i_n \in \{0, 1\}$$

where the differential forms are integrated starting from the left,  $\omega_0 = \frac{dz}{z}$  and  $\omega_1 = \frac{dz}{z-1}$ .

For  $i \in \{0, 1\}$ , let  $\mathcal{M}_i$  denote analytic continuation around a path winding once around the point  $i$  in the positive direction. The operators  $\mathcal{M}_i$  act on the series  $L(z)$  and  $L(\bar{z})$ , commute with multiplication, and commute with  $\frac{\partial}{\partial z}$  and  $\frac{\partial}{\partial \bar{z}}$ .

**Lemma 2.1.** [18]. *The monodromy operators  $\mathcal{M}_0, \mathcal{M}_1$  act as follows:*

$$(2.8) \quad \begin{aligned} \mathcal{M}_0 L(z) &= e^{2\pi i x_0} L(z) \\ \mathcal{M}_1 L(z) &= \mathcal{Z} e^{2\pi i x_1} \mathcal{Z}^{-1} L(z) . \end{aligned}$$

*Proof.* The formula for the monodromy at the origin follows immediately from (2.3) and the equation  $\mathcal{M}_0 \log(z) = \log z + 2i\pi$ . From (2.6) we obtain

$$(2.9) \quad \begin{aligned} \mathcal{M}_1 L(z) &= \mathcal{M}_1(\mathcal{Z} \exp(x_1 \log(z-1)) h_1(z)) \\ &= \mathcal{Z} \exp(2i\pi x_1) \exp(x_1 \log(z-1)) h_1(z) = \mathcal{Z} \exp(2i\pi x_1) \mathcal{Z}^{-1} L(z) . \end{aligned}$$

□

**2.3. Hoffman multiple zeta values.** We need to consider a certain family of multiple zeta values similar to those first considered by Hoffman [13].

If  $n_1, \dots, n_r \geq 1$ , define the following shuffle-regularized multiple zeta value:

$$\zeta_k(n_1, \dots, n_r) = (-1)^r \zeta(x_0^k x_1 x_0^{n_1-1} \dots x_1 x_0^{n_r-1}) .$$

In the non-singular case  $k = 0, n_r \geq 2$ , it reduces to the multiple zeta value

$$\zeta(n_1, \dots, n_r) = \sum_{0 < k_1 < k_2 < \dots < k_r} \frac{1}{k_1^{n_1} \dots k_r^{n_r}} \in \mathbb{R} ,$$

and we shall drop the subscript  $k$  whenever it is equal to 0. Henceforth, let  $2^{\{n\}}$  denote a sequence  $2, \dots, 2$  of  $n$  two's. Certain families of multiple zeta values will repeatedly play a role in the sequel. The first family corresponds to alternating words of type  $(x_1 x_0)^n$  and reduce to even powers of  $\pi$ :

$$(2.10) \quad \zeta(2^{\{n\}}) = \frac{\pi^{2n}}{(2n+1)!} .$$

The following identity, for words of type  $x_0(x_1 x_0)^n$ , is corollary 3.9 in [7], and is easily proved using standard relations between multiple zeta values:

$$(2.11) \quad \zeta_1(2^{\{n\}}) = 2 \sum_{i=1}^n (-1)^i \zeta(2i+1) \zeta(2^{\{n-i\}}) .$$

Next, define for any  $a, b, r \in \mathbb{N}$ ,

$$(2.12) \quad A_a^r = \binom{2r}{2a+2} \quad \text{and} \quad B_b^r = (1 - 2^{-2r}) \binom{2r}{2b+1} .$$

The following theorem is due to Zagier [26], recently reproved in [19].

**Theorem 2.2.** *Let  $a, b \geq 0$ . Then*

$$(2.13) \quad \zeta(2^{\{a\}} 32^{\{b\}}) = 2 \sum_{r=1}^{a+b+1} (-1)^r (A_a^r - B_b^r) \zeta(2r+1) \zeta(2^{\{a+b+1-r\}}) .$$

We denote the corresponding generating series by:

$$(2.14) \quad \begin{aligned} \mathcal{Z}_\pi &= \sum_{n \geq 0} (-1)^n \zeta(2^{\{n\}}) (x_1 x_0)^n \\ \mathcal{Z}_0 &= \sum_{n \geq 1} (-1)^n \zeta_1(2^{\{n\}}) x_0 (x_1 x_0)^n \\ \mathcal{Z}_H &= \sum_{m, n \geq 0} (-1)^{m+n+1} \zeta(2^{\{m\}} 32^{\{n\}}) (x_1 x_0)^{m+1} x_0 (x_1 x_0)^n \\ \mathcal{Z}_s &= \sum_{m, n \geq 0} (-1)^{m+n+1} \zeta_1(2^{\{m\}} 32^{\{n\}}) x_0 (x_1 x_0)^{m+1} x_0 (x_1 x_0)^n \end{aligned}$$

The coefficients of  $\mathcal{Z}_\pi$  are even powers of  $\pi$  by (2.10), and the coefficients of  $\mathcal{Z}_0$  and  $\mathcal{Z}_H$  are products of odd zeta values with even powers of  $\pi$  by (2.11) and (2.13). However, the values of the ‘singular’ Hoffman elements  $\zeta_1(2^{\{m\}} 32^{\{n\}})$  are not known. Luckily, these numbers will drop out of our proofs.

*Remark 2.3.* It turns out that the Galois coaction on the corresponding motivic multiple zeta values  $\zeta_1^m(2^{\{m\}} 32^{\{n\}})$  can be computed explicitly using the motivic version of theorem 2.2 given in ([7], theorem 4.3), and that they have ‘motivic depth’ at most two. It follows from the method of [8] that the numbers  $\zeta_1(2^{\{m\}} 32^{\{n\}})$  are completely determined up to an unknown rational multiple of  $\pi^{2m+2n+4}$ .

**2.4. Duality relations.** The automorphism  $z \mapsto 1 - z$  of  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$  interchanges the two forms  $\omega_0 = \frac{dz}{z}$  and  $\omega_1 = \frac{dz}{z-1}$ , and reverses the canonical path from 0 to 1. The following well-known ‘duality relation’

$$(2.15) \quad \zeta(x_{i_1} \dots x_{i_n}) = (-1)^n \zeta(x_{1-i_n} \dots x_{1-i_1}) \quad \text{for all } i_1, \dots, i_n \in \{0, 1\}$$

follows from their interpretation as iterated integrals. Some analogous series to (2.14) obtained by summing over sets of words in  $\mathcal{B}^1$ , will appear in §4.3. By (2.15) their coefficients can be expressed in terms of the multiple zeta values considered above.

### 3. PROOF OF THEOREM 1.4

#### 3.1. The coalgebra of 1-Hoffman words.

**Definition 3.1.** Let  $I_H \subset \mathbb{C}\langle x_0, x_1 \rangle$  denote the (complete) ideal generated by

$$w_1 x_1^2 w_2 \quad , \quad w_1 x_0^3 w_2 \quad , \quad w_1 x_0^2 w_2 x_0^2 w_3$$

for all  $w_1, w_2, w_3 \in \mathbb{C}\langle x_0, x_1 \rangle$ .

Likewise, let  $H \subset \mathbb{C}\langle x_0, x_1 \rangle$  denote the subspace spanned by the set  $\mathcal{B}^0$  of words  $w$  which contain no word  $x_1 x_1$ , no word  $x_0 x_0 x_0$  and at most a single subsequence  $x_0 x_0$ . It has an increasing filtration  $F$  given by the number of subsequences  $x_0 x_0$  (called the ‘level’ filtration in [7]) which satisfies  $F_{-1}H = 0$  and  $F_1H = H$ . Thus  $F_0H$  is the complex vector space spanned by the empty word and *alternating words* of the form

$$(3.1) \quad w = \dots x_1 x_0 x_1 x_0 \dots \quad ,$$

(with any initial and final letter) and  $\text{gr}_1^F H$  is isomorphic to the vector space spanned by *1-Hoffman words* of the form

$$(3.2) \quad w = \dots x_1 x_0 x_0 x_1 x_0 \dots \quad ,$$

where the letters denoted by three dots are alternating (again with any initial and final letters). Clearly  $H$  is stable under the deconcatenation coproduct:

$$\Delta : H \rightarrow H \otimes_{\mathbb{C}} H \quad ,$$

and the filtration is compatible with deconcatenation:  $\Delta F_i H \subset \bigoplus_{j+k=i} F_j H \otimes_{\mathbb{C}} F_k H$ , where  $i, j, k \in \{-1, 0, 1\}$ . The coalgebra  $H$  is dual to  $\mathbb{C}\langle x_0, x_1 \rangle / I_H$ .

**Definition 3.2.** Let  $T \subset \mathbb{C}\langle x_0, x_1 \rangle$  denote any non-commutative formal power series  $T = \sum_{w \in \{x_0, x_1\}^*} T_w w$ . For all  $i, j \in \{0, 1\}$ , let  $T_{i,j}$  denote the series

$$(3.3) \quad T_{i,j} = T_{x_i} x_i \delta_{ij} + \sum_{w \in x_i \{x_0, x_1\}^* x_j} T_w w$$

where the sum is over words beginning in  $x_i$  and ending in  $x_j$ . Thus

$$T = T_1 \cdot 1 + T_{0,0} + T_{1,0} + T_{0,1} + T_{1,1}$$

where  $T_1 \in \mathbb{C}$ . Likewise, for  $k = 0$  or  $k = 1$ , let

$$(3.4) \quad T^k = \sum_{w \in \mathcal{B}_k^0} T_w w$$

where  $\mathcal{B}_0^0 \subset \mathcal{B}^0$  is the set of words (3.1), and  $\mathcal{B}_1^0 \subset \mathcal{B}^0$  is the set of words (3.2). Combining (3.3) and (3.4) gives rise to eight series  $T_{i,j}^k$  for all  $i, j, k \in \{0, 1\}$ .



For any series  $T \in \mathbb{C}\langle\langle x_0, x_1 \rangle\rangle$ , we have

$$(3.5) \quad T \equiv T_1 \cdot 1 + \sum_{0 \leq i, j, k \leq 1} T_{j,k}^i \pmod{I_H}$$

Let  $A, B \in \mathbb{C}\langle\langle x_0, x_1 \rangle\rangle$  be any two series. It follows from the definition of  $I_H$  that

$$(3.6) \quad A_{*,*}^1 B_{*,*}^1 \equiv A_{*,0}^1 B_{0,*}^0 \equiv A_{*,0}^0 B_{0,*}^1 \equiv A_{*,1}^* B_{1,*}^* \equiv 0 \pmod{I_H}$$

where a  $*$  denotes any index equal to 0 or 1. We will often use the fact that

$$(3.7) \quad T \equiv 0 \pmod{I_H} \iff T_{j,k}^i = 0 \quad \text{for all } i, j, k \leq 1.$$

The following series plays an important role.

**Definition 3.3.** Let  $V = \mathcal{Z}x_1 \mathcal{Z}^{-1} \in \mathbb{C}\langle\langle x_0, x_1 \rangle\rangle$  and  $V_- = V(-x_0, -x_1)$ .

**3.2. Solutions to (1.5) and their monodromy equations.** We wish to construct functions  $F_w(z)$  satisfying the conditions of theorem 1.4. For this, define a generating series  $F(z) = \sum_{w \in \{x_0, x_1\}^\times} F_w(z)w$  by the ansatz

$$(3.8) \quad F(z) = \tilde{L}(\bar{z})\mathcal{S}L(z),$$

where  $\mathcal{S} \in \mathbb{C}\langle\langle x_0, x_1 \rangle\rangle$  is a constant series which is yet to be determined. It follows immediately from (3.8) and equation (2.2) that

$$\frac{\partial^2}{\partial z \partial \bar{z}} F_{x_i w x_j}(z) = \frac{F_w(z)}{(\bar{z} - i)(z - j)}$$

for all  $i, j \in \{0, 1\}$ , and all words  $w \in \{x_0, x_1\}^\times$ . Note that it is *not* possible to choose  $\mathcal{S}$  in such a way that (3.8) is single-valued in general. However, we are only interested in the coefficients  $F_w(z)$  of  $F$  for words  $w$  which satisfy the conditions of theorem 1.4, i.e., those words which are basis elements of the coalgebra  $H$ . This gives rise to a weaker set of conditions on the series  $\mathcal{S}$  modulo the ideal  $I_H$ , which do admit a solution.

**Proposition 3.4.** *The functions  $F_w(z)$  defined by (3.8) are single-valued and satisfy  $F_w(z) = F_{\bar{w}}(\bar{z})$  for every such word  $w$  if and only if the series  $\mathcal{S}$  satisfies*

- (i)  $[\mathcal{S}, x_0] \equiv 0 \pmod{I_H}$
- (ii)  $V_- \mathcal{S} + \mathcal{S}V \equiv 0 \pmod{I_H}$
- (iii)  $\bar{\mathcal{S}} \equiv \tilde{\mathcal{S}} \pmod{I_H}$ .

Equation (i) implies that  $\mathcal{S}_{1,1}^* = \mathcal{S}_{1,0}^0 = \mathcal{S}_{0,1}^0 = 0$ .

*Proof.* Since the ideal  $I_H$  is the annihilator of the coalgebra  $H$ , it is enough to find conditions on  $\mathcal{S}$  so that the following equations hold

$$(3.9) \quad \begin{aligned} \mathcal{M}_0 F(z) &\equiv F(z) \pmod{I_H} \\ \mathcal{M}_1 F(z) &\equiv F(z) \pmod{I_H}. \end{aligned}$$

For the monodromy at 0, lemma (2.1) yields

$$(3.10) \quad e^{-2i\pi x_0} \mathcal{S} e^{2i\pi x_0} \equiv \mathcal{S} \pmod{I_H}.$$

In particular,  $\mathcal{S}_{1,*} e^{2i\pi x_0} \equiv \mathcal{S}_{1,*} \pmod{I_H}$ . There is an invertible series  $T \in \mathbb{C}\langle\langle x_0, x_1 \rangle\rangle$  such that  $e^{2i\pi x_0} - 1 = x_0 T$ , so we deduce that

$$\mathcal{S}_{1,*} x_0 \equiv 0 \pmod{I_H},$$

which implies that  $(\mathcal{S}x_0)_{1,0}^0 + (\mathcal{S}x_0)_{1,0}^1 = 0$ . Removing the final letter  $x_0$  yields the equations  $\mathcal{S}_{1,0}^0 = \mathcal{S}_{1,1}^0 = \mathcal{S}_{1,1}^1 = 0$ . By symmetry, we also have  $\mathcal{S}_{0,1}^0 = 0$ . Thus the only surviving terms in  $\mathcal{S}$  are of the form

$$(3.11) \quad \mathcal{S} = \mathcal{S}_1 \cdot 1 + \mathcal{S}_{0,0}^0 + \mathcal{S}_{1,0}^1 + \mathcal{S}_{0,1}^1 + \mathcal{S}_{0,0}^1$$

and so  $x_0^2 \mathcal{S} \equiv \mathcal{S} x_0^2 \equiv x_0 \mathcal{S} x_0 \equiv x_0^2 \pmod{I_H}$  by equations (3.6). Expanding out equation (3.10), and using the fact that  $x_0^n \in I_H$  for  $n \geq 3$ , we deduce that

$$x_0 \mathcal{S} \equiv \mathcal{S} x_0 \pmod{I_H}.$$

Conversely, this equation clearly implies (3.10), so they are equivalent.

Now consider the monodromy at 1. Lemma 2.1 and (3.9) yield the equation

$$\widetilde{W} \mathcal{S} W \equiv \mathcal{S} \pmod{I_H},$$

where  $W = \mathcal{Z} e^{2i\pi x_1} \mathcal{Z}^{-1}$ . Since  $x_1^2 \in I_H$ , we have  $W \equiv 1 + 2i\pi V \pmod{I_H}$ , and the previous equation is equivalent to

$$2i\pi(-\widetilde{V} \mathcal{S} + \mathcal{S} V) - (2i\pi)^2 \widetilde{V} \mathcal{S} V \equiv 0 \pmod{I_H},$$

Since  $V^2 \equiv \mathcal{Z}^2 x_1^2 \mathcal{Z}^{-2} \equiv 0 \pmod{I_H}$ , multiplying the previous expression on the right by  $V$  yields  $\widetilde{V} \mathcal{S} V \equiv 0 \pmod{I_H}$ , and it is equivalent to the identity

$$-\widetilde{V} \mathcal{S} + \mathcal{S} V \equiv 0 \pmod{I_H},$$

which gives (ii) by equation (2.1).

Finally, the equivalence of (iii) with the equation  $F_{\widetilde{w}}(\bar{z}) = F_w(z)$  is obvious.  $\square$

We can reduce equation (ii) of the previous proposition further.

**Lemma 3.5.** *If  $\mathcal{S}_{1,1}^* = \mathcal{S}_{1,0}^0 = \mathcal{S}_{0,1}^0 = 0$  and  $\mathcal{S}$  is real, the equation  $V_- \mathcal{S} + \mathcal{S} V \equiv 0 \pmod{I_H}$  is equivalent to three sets of equations:*

$$(3.12) \quad 2V_{0,1}^0 + \mathcal{S}_{0,0}^0 V_{1,1}^0 \equiv 0$$

involving only the alternating part  $\mathcal{S}_{0,0}^0$ , an equation involving  $\mathcal{S}_{0,1}^1, \mathcal{S}_{1,0}^1$ :

$$(3.13) \quad 2V_{1,1}^1 - V_{1,1}^0 \mathcal{S}_{0,1}^1 + \mathcal{S}_{1,0}^1 V_{1,1}^0 \equiv 0$$

and a final set of equations involving  $\mathcal{S}_{0,0}^1$  also:

$$(3.14) \quad \begin{aligned} \{V_{0,1}^0, \mathcal{S}_{0,1}^1\} + \mathcal{S}_{0,0}^0 (V_{0,1}^0 + V_{1,1}^1) &\equiv -\mathcal{S}_{0,0}^1 V_{1,1}^0 \\ V^{\text{sing}} + [\mathcal{S}_{0,0}^0, V_{0,0}^0] - V_{0,0}^0 \mathcal{S}_{1,0}^1 + \mathcal{S}_{0,1}^1 V_{0,0}^0 &\equiv -V_{0,1}^0 \mathcal{S}_{0,0}^1 - \mathcal{S}_{0,0}^1 V_{1,0}^0 \end{aligned}$$

where  $V^{\text{sing}} = 2V_{0,0}^1 - V_{0,1}^1 \mathcal{S}_{0,0}^0 + \mathcal{S}_{0,0}^0 V_{1,0}^1$ ,  $\{x, y\} = xy + yx$  and  $[x, y] = xy - yx$ .

*Proof.* Decompose the four equations  $(V_- \mathcal{S} + \mathcal{S} V)_{i,j} \equiv 0$ , for  $i, j \in \{0, 1\}$  into their parts of odd and even weights. After killing terms using (3.6), this gives eight equations, one of which vanishes, and the remaining seven are exactly the equations listed above together with the three equations

$$\begin{aligned} 2V_{1,0}^0 - V_{1,1}^0 \mathcal{S}_{0,0}^0 &\equiv 0 \\ \{V_{1,0}^0, \mathcal{S}_{1,0}^1\} + (V_{1,0}^0 + V_{1,1}^1) \mathcal{S}_{0,0}^0 &\equiv V_{1,1}^0 \mathcal{S}_{0,0}^1 \\ V_{0,1}^0 \mathcal{S}_{0,0}^0 + \mathcal{S}_{0,0}^0 V_{1,0}^0 &\equiv 0. \end{aligned}$$

The first two of these equations follow from (3.12) and the first equation in (3.14), respectively, upon reflection using  $\widetilde{V} = -V_-$  and  $\widetilde{\mathcal{S}} = \mathcal{S}$ . The last equation is an immediate consequence of the first one and equation (3.12).  $\square$

In the sequel we show that our formula for  $\mathcal{S}_{0,0}^0$  given by equation (1.3) is compatible with (3.12). The non-trivial part is to check that our explicit expression for  $\mathcal{S}_{1,0}^1$  and  $\mathcal{S}_{0,1}^1$  indeed gives a solution to (3.13). Finally, admitting (3.13), the first equation of (3.14) defines  $\mathcal{S}_{0,0}^1$ , and it is a simple matter to verify the second equation of (3.14).

**3.3. Decomposition of  $V$ .** It follows from (3.6) and the inversion relation (2.7) that

$$(3.15) \quad V \equiv (1 + \mathcal{Z}_{0,0}^0 + \mathcal{Z}_{1,0}^0 + \mathcal{Z}_{0,0}^1 + \mathcal{Z}_{1,0}^1) \times_1 \\ (1 - \mathcal{Z}_{0,0}^0 + \mathcal{Z}_{0,1}^0 + \mathcal{Z}_{0,0}^1 - \mathcal{Z}_{0,1}^1) \pmod{I_H}.$$

With the notations from (2.14), we find that

$$\mathcal{Z}_0 = \mathcal{Z}_{0,0}^0, \quad \mathcal{Z}_\pi = 1 + \mathcal{Z}_{1,0}^0, \quad \mathcal{Z}_H = \mathcal{Z}_{1,0}^1, \quad \mathcal{Z}_s = \mathcal{Z}_{0,0}^1$$

and therefore by decomposition (3.15) and  $\widetilde{\mathcal{Z}}_0 = \mathcal{Z}_0$

$$(3.16) \quad V_{0,0}^0 = -\mathcal{Z}_0 \times_1 \mathcal{Z}_0, \quad V_{0,1}^0 = \mathcal{Z}_0 \times_1 \widetilde{\mathcal{Z}}_\pi \\ V_{1,0}^0 = -\mathcal{Z}_\pi \times_1 \mathcal{Z}_0, \quad V_{1,1}^0 = \mathcal{Z}_\pi \times_1 \widetilde{\mathcal{Z}}_\pi$$

for the alternating words, and

$$V_{0,0}^1 = \mathcal{Z}_0 \times_1 \widetilde{\mathcal{Z}}_s - \mathcal{Z}_s \times_1 \mathcal{Z}_0, \quad V_{0,1}^1 = -\mathcal{Z}_0 \times_1 \widetilde{\mathcal{Z}}_H + \mathcal{Z}_s \times_1 \widetilde{\mathcal{Z}}_\pi \\ V_{1,0}^1 = \mathcal{Z}_\pi \times_1 \widetilde{\mathcal{Z}}_s - \mathcal{Z}_H \times_1 \mathcal{Z}_0, \quad V_{1,1}^1 = -\mathcal{Z}_\pi \times_1 \widetilde{\mathcal{Z}}_H + \mathcal{Z}_H \times_1 \widetilde{\mathcal{Z}}_\pi.$$

We now proceed with the verification of the equations of lemma 3.5.

**3.4. Alternating words.** The first task is to separate the elements  $V_{*,*}^0$  into a pure odd zeta part  $\mathcal{S}_{0,0}^0$ , and a pure ‘powers of  $\pi$ ’ part  $V_{1,1}^0$ .

**Lemma 3.6.** *We have*

$$(3.17) \quad 2\mathcal{Z}_0 = -\mathcal{S}_{0,0}^0 \mathcal{Z}_\pi = -\widetilde{\mathcal{Z}}_\pi \mathcal{S}_{0,0}^0.$$

*Proof.* By the definition (2.14) of  $\mathcal{Z}_\pi$  and (1.3) we have

$$-\mathcal{S}_{0,0}^0 \mathcal{Z}_\pi = 4 \sum_{m \geq 1, n \geq 0} (-1)^n \zeta(2m+1) \zeta(2^{\{n\}}) (\times_0 \times_1)^m \times_0 (\times_1 \times_0)^n \\ = 4 \sum_{n=0}^{\infty} \sum_{m=1}^n (-1)^{n-m} \zeta(2m+1) \zeta(2^{\{n-m\}}) (\times_0 \times_1)^n \times_0.$$

The first equation in the lemma follows immediately by (2.11). The second equation follows from the first by reversing the order of the words.  $\square$

**Corollary 3.7.** *All four series  $V^0$  can be reduced to the single series  $V_{1,1}^0$ :*

$$(3.18) \quad 4V_{0,0}^0 = -\mathcal{S}_{0,0}^0 V_{1,1}^0 \mathcal{S}_{0,0}^0 \\ 2V_{0,1}^0 = -\mathcal{S}_{0,0}^0 V_{1,1}^0 \\ 2V_{1,0}^0 = V_{1,1}^0 \mathcal{S}_{0,0}^0.$$

*In particular, equation (3.12) holds.*

*Proof.* Immediate consequence of the formulae for  $V^0$  in §3.3 and lemma 3.6.  $\square$

**3.5. Singular Hoffman part.** The next task is to gather all terms involving the singular Hoffman series  $\mathcal{Z}_s$ , which fortunately drops out of the final calculation.

**Lemma 3.8.** *The following identity holds:*

$$(3.19) \quad 2V^{\text{sing}} = \mathcal{S}_{0,0}^0 V_{1,1}^1 \mathcal{S}_{0,0}^0.$$

*Proof.* Rewrite the elements  $V_{*,*}^1$  using the formulae in §3.3. The left-hand side gives

$$4(\mathcal{Z}_0 \times_1 \widetilde{\mathcal{Z}}_s - \mathcal{Z}_s \times_1 \mathcal{Z}_0) - 2(\mathcal{Z}_s \times_1 \widetilde{\mathcal{Z}}_\pi - \mathcal{Z}_0 \times_1 \widetilde{\mathcal{Z}}_H) \mathcal{S}_{0,0}^0 + 2 \mathcal{S}_{0,0}^0 (\mathcal{Z}_\pi \times_1 \widetilde{\mathcal{Z}}_s - \mathcal{Z}_H \times_1 \mathcal{Z}_0)$$

which is equal to

$$(2\mathcal{Z}_0 + \mathcal{S}_{0,0}^0 \mathcal{Z}_\pi) \times_1 (2\widetilde{\mathcal{Z}}_s + \widetilde{\mathcal{Z}}_H \mathcal{S}_{0,0}^0) - (2\mathcal{Z}_s + \mathcal{S}_{0,0}^0 \mathcal{Z}_H) \times_1 (2\mathcal{Z}_0 + \widetilde{\mathcal{Z}}_\pi \mathcal{S}_{0,0}^0) + \mathcal{S}_{0,0}^0 V_{1,1}^1 \mathcal{S}_{0,0}^0.$$

By equation (3.17) the result follows.  $\square$

**3.6. Hoffman part.** The main part of the calculation is the following separation of  $V_{1,1}^1$  into pure odd zeta and pure even zeta parts.

**Lemma 3.9.** *The following identity holds*

$$(3.20) \quad 2V_{1,1}^1 = V_{1,1}^0 \mathcal{S}_{0,1}^1 - \mathcal{S}_{1,0}^1 V_{1,1}^0.$$

*Proof.* With the definition

$$Y = 2\mathcal{Z}_H + \mathcal{S}_{1,0}^1 \mathcal{Z}_\pi$$

we can rewrite equation (3.20) as

$$Y \times_1 \widetilde{\mathcal{Z}}_\pi = \mathcal{Z}_\pi \times_1 \widetilde{Y}.$$

With definition 1.3 and notation (2.12), we have

$$\begin{aligned} \mathcal{S}_{1,0}^1 \mathcal{Z}_\pi &= -4 \sum_{m \geq 1; n, k \geq 0} A_{m-1}^{m+n} \zeta(2m+2n+1) (-1)^k \zeta(2^{\{k\}}) (\mathbf{x}_1 \mathbf{x}_0)^m \mathbf{x}_0 (\mathbf{x}_1 \mathbf{x}_0)^{n+k} \\ &= -4 \sum_{a \geq 1, b \geq 0} \sum_{r=a}^{a+b} (-1)^{a+b-r} A_{a-1}^r \zeta(2r+1) \zeta(2^{\{a+b-r\}}) (\mathbf{x}_1 \mathbf{x}_0)^a \mathbf{x}_0 (\mathbf{x}_1 \mathbf{x}_0)^b. \end{aligned}$$

Equation (2.13) implies that in  $2\mathcal{Z}_H + \mathcal{S}_{1,0}^1 \mathcal{Z}_\pi$  one binomial cancels

$$Y = -4 \sum_{a \geq 1, b \geq 0} \sum_{r=b+1}^{a+b} (-1)^{a+b-r} B_b^r \zeta(2r+1) \zeta(2^{\{a+b-r\}}) (\mathbf{x}_1 \mathbf{x}_0)^a \mathbf{x}_0 (\mathbf{x}_1 \mathbf{x}_0)^b.$$

Right multiplication by  $\mathbf{x}_1 \widetilde{\mathcal{Z}}_\pi$  gives the following expression for  $-Y \times_1 \widetilde{\mathcal{Z}}_\pi / 4$ :

$$\begin{aligned} &\sum_{a \geq 1, b \geq 0} \sum_{r=b+1}^{a+b} \sum_{s=0}^{\infty} (-1)^{a+b-r+s} B_b^r \zeta(2r+1) \zeta(2^{\{a+b-r\}}) \zeta(2^{\{s\}}) (\mathbf{x}_1 \mathbf{x}_0)^a \mathbf{x}_0 (\mathbf{x}_1 \mathbf{x}_0)^b \mathbf{x}_1 (\mathbf{x}_0 \mathbf{x}_1)^s \\ &= \sum_{\alpha, \beta \geq 1} \sum_{\gamma=0}^{\alpha-1} \sum_{\delta=0}^{\beta-1} (-1)^{\alpha+\beta-\gamma-\delta} B_\delta^{\gamma+\delta+1} \zeta(2\gamma+2\delta+3) \zeta(2^{\{\alpha-\gamma-1\}}) \zeta(2^{\{\beta-\delta-1\}}) \\ &\quad (\mathbf{x}_1 \mathbf{x}_0)^\alpha (\mathbf{x}_0 \mathbf{x}_1)^\beta, \end{aligned}$$

by the change of variables  $(a, b, r, s) = (\alpha, \delta, \gamma + \delta + 1, \beta - \delta - 1)$ . The last expression is evidently invariant under letter reversal which completes the proof.  $\square$

**3.7. Monodromy at zero.** To prove the triviality of the monodromy at zero we need the following lemma.

**Lemma 3.10.**  $[\mathcal{S}, \mathbf{x}_0] = 0$ .

*Proof.* From the shape (3.11) of  $\mathcal{S}$ , we find that  $[\mathcal{S}, \mathbf{x}_0] \equiv 0 \pmod{I_H}$  is equivalent to

$$(3.21) \quad \mathcal{S}_{0,0}^0 \mathbf{x}_0 + \mathcal{S}_{0,1}^1 \mathbf{x}_0 = \mathbf{x}_0 \mathcal{S}_{0,0}^0 + \mathbf{x}_0 \mathcal{S}_{1,0}^1.$$

According to equation (1.3) we decompose

$$\begin{aligned}
(3.22) \quad \mathcal{S}_{0,0}^0 &= \sum_{n \geq 1} \mathcal{S}_{0,0}^0(n) (x_0 x_1)^n x_0, \\
\mathcal{S}_{1,0}^1 &= \sum_{m \geq 1, n \geq 0} \mathcal{S}_{1,0}^1(m, n) (x_1 x_0)^m x_0 (x_1 x_0)^n, \quad \text{and} \\
\mathcal{S}_{0,1}^1 &= \sum_{m \geq 0, n \geq 1} \mathcal{S}_{1,0}^1(n, m) (x_0 x_1)^m x_0 (x_0 x_1)^n.
\end{aligned}$$

Projecting (3.21) onto words of the form  $(x_0 x_1)^a x_0 x_0 (x_1 x_0)^b$  leads to identities between the coefficients which must be verified. The case  $b = 0$  leads to the identity  $\mathcal{S}_{0,0}^0(a) = \mathcal{S}_{1,0}^1(a, 0)$  for all  $a \in \mathbb{N}$ . For  $a, b > 0$  we obtain  $\mathcal{S}_{1,0}^1(a, b) = \mathcal{S}_{1,0}^1(b, a)$ . Both equations hold trivially by (1.3). The case  $a = 0$  holds by reflection symmetry.  $\square$

**3.8. Proof of single-valuedness.** To prove property (ii) of proposition 3.4 we need to show that equation (3.14) holds. The proofs are straightforward applications of (3.18), (3.19), and (3.20) to write all  $V$ 's in terms of  $V_{1,1}^0$ , and reduce to the definition of  $\mathcal{S}_{0,0}^1$  in (1.3). Property (i) is lemma 3.10, and property (iii) is immediately obvious from the definition of  $\mathcal{S}$ . This completes the proof of theorem 1.4.

#### 4. PROOF OF THEOREM 1.6

This section proves the analogue of theorem 1.4 where zeros and ones are interchanged. It parallels to a large extent §3.

##### 4.1. The coalgebra of dual 1-Hoffman words.

**Definition 4.1.** Let  $I_{\hat{H}} \subset \mathbb{C}\langle x_0, x_1 \rangle$  denote the (complete) ideal generated by

$$w_1 x_0^2 w_2 \quad , \quad w_1 x_1^3 w_2 \quad , \quad w_1 x_1^2 w_2 x_1^2 w_3$$

for all  $w_1, w_2, w_3 \in \mathbb{C}\langle x_0, x_1 \rangle$ .

Likewise, let  $\hat{H} \subset \mathbb{C}\langle x_0, x_1 \rangle$  denote the subspace spanned by words  $w$  which contain no word  $x_0 x_0$  and at most a single subsequence  $x_1 x_1$ . The filtration and the notation will be the same as in §3 except that we use hat variables for quantities that live in  $\hat{H}$ .

**4.2. Solutions to (1.9) and their monodromy equations.** We again construct functions  $\hat{F}_w(z)$  by a generating series

$$(4.1) \quad \hat{F}(z) = \tilde{L}(\bar{z}) \hat{S} L(z) .$$

The analogue of proposition 3.4 is

**Proposition 4.2.** *Let  $\hat{S}$  be real. The functions  $\hat{F}_w(z)$  defined by (4.1) are single-valued and satisfy  $\hat{F}_w(z) = \hat{F}_{\bar{w}}(\bar{z})$  for every word  $w$  in  $\mathcal{B}^1$  if and only if the series  $\hat{S}$  satisfies*

- (i)  $[\hat{S}, x_0] \equiv 0 \pmod{I_{\hat{H}}}$
- (ii)  $V_- \hat{S} + \hat{S} V \equiv 0 \pmod{I_{\hat{H}}}$
- (iii)  $\hat{S} \equiv \tilde{\hat{S}} \pmod{I_{\hat{H}}}$ .

*Proof.* Equation (i) is an immediate consequence of

$$(4.2) \quad e^{-2i\pi x_0} \mathcal{S} e^{2i\pi x_0} \equiv \mathcal{S} \pmod{I_{\hat{H}}} .$$

Considering the monodromy at 1, lemma 2.1 yields the equation

$$\tilde{\hat{W}} \hat{S} \hat{W} \equiv \hat{S} \pmod{I_{\hat{H}}} ,$$

where  $W \equiv 1 + 2i\pi V + \frac{1}{2}(2i\pi)^2 V^2 \pmod{I_{\hat{H}}}$  and  $\widetilde{W} \equiv 1 + 2i\pi V_- + \frac{1}{2}(2i\pi)^2 V_-^2 \pmod{I_{\hat{H}}}$ . Multiplication on the right by  $V^2$  and taking the imaginary part gives  $V_- \hat{S} V^2 \equiv 0 \pmod{I_{\hat{H}}}$ , since  $V^3 \equiv 0 \pmod{I_{\hat{H}}}$ . Likewise  $V_-^2 \hat{S} V \equiv 0 \pmod{I_{\hat{H}}}$ . Expanding and taking real and imaginary parts gives the two equations

$$\begin{aligned} V_- \hat{S} + \hat{S} V &\equiv 0 \\ V_-(V_- \hat{S} + \hat{S} V) + (V_- \hat{S} + \hat{S} V) V &\equiv 0 \end{aligned}$$

which are equivalent to (ii).

The equivalence of (iii) with the equation  $\hat{F}_{\bar{w}}(\bar{z}) = \hat{F}_w(z)$  is obvious.  $\square$

We use the expansions (where the upper index counts the number of  $x_1^2$ 's)

$$V = \sum_{a,b,c \in \{0,1\}} \hat{V}_{b,c}^a$$

in  $\hat{H}$  to reduce equation (ii) of the previous proposition further.

**Lemma 4.3.** *If  $\hat{S}_{1,1}^0 = \hat{S}_{1,1}^1 = \hat{S}_{1,0}^0 = \hat{S}_{0,1}^0 = 0$  and  $\hat{S}$  is real, the equation  $V_- \hat{S} + \hat{S} V \equiv 0 \pmod{I_{\hat{H}}}$  is equivalent to the equations:*

$$(4.3) \quad \begin{aligned} 2\hat{V}_{0,1}^0 + \hat{S}_{0,0}^0 \hat{V}_{1,1}^0 &\equiv 0, \\ 2\hat{V}_{1,1}^1 - \hat{V}_{1,1}^0 \hat{S}_{0,1}^1 + \hat{S}_{1,0}^1 \hat{V}_{1,1}^0 &\equiv 0, \\ \{\hat{V}_{0,1}^0, \hat{S}_{0,1}^1\} + \hat{S}_{0,0}^0 \hat{V}_{1,1}^1 &\equiv -\hat{S}_{0,0}^1 \hat{V}_{1,1}^0 \\ \hat{V}_{0,0}^{\text{sing}} - \hat{V}_{0,0}^0 \hat{S}_{1,0}^1 + \hat{S}_{0,1}^1 \hat{V}_{0,0}^0 &\equiv -\hat{V}_{0,1}^0 \hat{S}_{0,0}^1 - \hat{S}_{0,0}^1 \hat{V}_{1,0}^0 \end{aligned}$$

where  $\hat{V}_{0,0}^{\text{sing}} = 2\hat{V}_{0,0}^1 - \hat{V}_{0,1}^1 \hat{S}_{0,0}^0 + \hat{S}_{0,0}^0 \hat{V}_{1,0}^1$ .

*Proof.* The proof follows the proof of lemma 3.5.  $\square$

Now we show that (4.3) is consistent with  $\hat{S}$ , as given by equation (1.6).

**4.3. Decomposition of  $\hat{V}$ .** The decomposition of  $\hat{V}_{*,*}^*$  into expressions in  $\mathcal{Z}$  differs slightly from the previous case in §3.3. We encounter two new types of series

$$(4.4) \quad \begin{aligned} \mathcal{Z}_{0,1}^0 &= -\zeta_1(1) x_0 x_1 + \zeta_1(2, 1) x_0 x_1 x_0 x_1 + \dots \\ \mathcal{Z}_{1,1}^0 &= \zeta_1(2) x_1 x_0 x_1 - \zeta_1(2, 2) x_1 x_0 x_1 x_0 x_1 + \dots \\ \hat{\mathcal{Z}}_{1,0}^1 &= \zeta(3) x_1 x_1 x_0 - \zeta(2, 3) x_1 x_1 x_0 x_1 x_0 - \zeta(3, 2) x_1 x_0 x_1 x_1 x_0 + \dots \end{aligned}$$

where we used the duality §2.4 to relate  $\mathcal{Z}_{1,1}^0$  to  $\mathcal{Z}_0$  and  $\hat{\mathcal{Z}}_{1,0}^1$  to  $\mathcal{Z}_H$ . A further series  $\hat{\mathcal{Z}}_{0,0}^1$  will only be needed in intermediate steps because it, like  $\mathcal{Z}_s$ , drops out of the final calculation.

The decomposition of  $\hat{V}^0 = V^0$  is unchanged and given by (3.16) whereas the components of  $\hat{V}^1$  are given by (using the fact that  $\widetilde{\mathcal{Z}}_{1,1}^0 = \mathcal{Z}_{1,1}^0$ ):

$$\begin{aligned} \hat{V}_{0,0}^1 &= \mathcal{Z}_0 x_1 \widetilde{\hat{\mathcal{Z}}}_{0,0}^1 - \hat{\mathcal{Z}}_{0,0}^1 x_1 \mathcal{Z}_0 + \mathcal{Z}_0 x_1 \widetilde{\mathcal{Z}}_{0,1}^0 - \mathcal{Z}_{0,1}^0 x_1 \mathcal{Z}_0, \\ \hat{V}_{0,1}^1 &= -\mathcal{Z}_0 x_1 \widetilde{\hat{\mathcal{Z}}}_{1,0}^1 + \hat{\mathcal{Z}}_{0,0}^1 x_1 \widetilde{\mathcal{Z}}_{\pi} - \mathcal{Z}_0 x_1 \mathcal{Z}_{1,1}^0 + \mathcal{Z}_{0,1}^0 x_1 \widetilde{\mathcal{Z}}_{\pi} \\ \hat{V}_{1,0}^1 &= \mathcal{Z}_{\pi} x_1 \widetilde{\hat{\mathcal{Z}}}_{0,0}^1 - \hat{\mathcal{Z}}_{1,0}^1 x_1 \mathcal{Z}_0 + \mathcal{Z}_{\pi} x_1 \widetilde{\mathcal{Z}}_{0,1}^0 - \mathcal{Z}_{1,1}^0 x_1 \mathcal{Z}_0, \\ \hat{V}_{1,1}^1 &= -\mathcal{Z}_{\pi} x_1 \mathcal{Z}_{1,1}^0 + \hat{\mathcal{Z}}_{1,0}^1 x_1 \widetilde{\mathcal{Z}}_{\pi} - \mathcal{Z}_{\pi} x_1 \widetilde{\hat{\mathcal{Z}}}_{1,0}^1 + \mathcal{Z}_{1,1}^0 x_1 \widetilde{\mathcal{Z}}_{\pi}. \end{aligned}$$

We now proceed with the verification of the equations of lemma 4.3.

**4.4. Alternating words.** The first equation in (4.3) is the same as (3.12).

**4.5. Dual singular Hoffman part.** The series of singular zetas  $\hat{\mathcal{Z}}_{0,0}^1$  drops out of the final calculation, by the following lemma.

**Lemma 4.4.** *The following identity holds:*

$$(4.5) \quad 2\hat{V}^{\text{sing}} = \mathcal{S}_{0,0}^0 \hat{V}_{1,1}^1 \mathcal{S}_{0,0}^0 .$$

*Proof.* The calculation follows the proof of lemma 3.8.  $\square$

**4.6. Dual Hoffman part.** Again the most complicated part of the calculation is the verification of the identity for  $V_{1,1}^1$  in (4.3).

**Lemma 4.5.** *The following identity holds*

$$(4.6) \quad 2\hat{V}_{1,1}^1 = V_{1,1}^0 \hat{\mathcal{S}}_{0,1}^1 - \hat{\mathcal{S}}_{1,0}^1 V_{1,1}^0 .$$

*Proof.* With the definition

$$\hat{Y} = 2\hat{\mathcal{Z}}_{1,0}^1 + 2\mathcal{Z}_{1,1}^0 + \hat{\mathcal{S}}_{1,0}^1 \mathcal{Z}_\pi$$

we can rewrite equation (4.6) as

$$\hat{Y}_{x_1} \widetilde{\mathcal{Z}}_\pi = \mathcal{Z}_\pi x_1 \widetilde{\hat{Y}} .$$

With definition 1.5 and notation (2.12), we have

$$\begin{aligned} \hat{\mathcal{S}}_{1,0}^1 \mathcal{Z}_\pi &= -4 \sum_{m,k \geq 0; n \geq 1} B_m^{m+n} \zeta(2m+2n+1) (-1)^k \zeta(2^{\{k\}}) (x_1 x_0)^m x_1 (x_1 x_0)^{n+k} \\ &= -4 \sum_{a \geq 0, b \geq 1} \sum_{r=a}^{a+b} (-1)^{a+b-r} B_a^r \zeta(2r+1) \zeta(2^{\{a+b-r\}}) (x_1 x_0)^a x_1 (x_1 x_0)^b \end{aligned}$$

where we have set  $\zeta(1) = 0$ . Equation (2.13) together with the duality transformation §2.4 implies that in  $2\hat{\mathcal{Z}}_{1,0}^1 + \hat{\mathcal{S}}_{1,0}^1 \mathcal{Z}_\pi$  one binomial cancels

$$2\hat{\mathcal{Z}}_{1,0}^1 + \hat{\mathcal{S}}_{1,0}^1 \mathcal{Z}_\pi = -4 \sum_{a \geq 0, b \geq 1} \sum_{r=b}^{a+b} (-1)^{a+b-r} A_b^r \zeta(2r+1) \zeta(2^{\{a+b-r\}}) (x_1 x_0)^a x_1 (x_1 x_0)^b .$$

The contribution of  $2\mathcal{Z}_{1,1}^0$ , after applying the duality transformation (2.15), is given by (2.11)

$$2\mathcal{Z}_{1,1}^0 = -4 \sum_{a \geq 0} \sum_{r=1}^a (-1)^{a-r} \zeta(2r+1) \zeta(2^{\{a-r\}}) (x_1 x_0)^a x_1 .$$

This equals the  $b = 0$  term in the above sum. Multiplication by  $x_1 \widetilde{\mathcal{Z}}_\pi$  yields for  $-\hat{Y}_{x_1} \widetilde{\mathcal{Z}}_\pi / 4$  the expression

$$\begin{aligned} &\sum_{a,b \geq 0} \sum_{r=b}^{a+b} \sum_{s=0}^{\infty} (-1)^{a+b-r+s} A_{b-1}^r \zeta(2r+1) \zeta(2^{\{a+b-r\}}) \zeta(2^{\{s\}}) (x_1 x_0)^a x_1 (x_1 x_0)^b x_1 (x_0 x_1)^s \\ &= \sum_{\alpha, \beta \geq 0} \sum_{\gamma=0}^{\alpha} \sum_{\delta=0}^{\beta} (-1)^{\alpha+\beta-\gamma-\delta} A_{\delta-1}^{\gamma+\delta} \zeta(2\gamma+2\delta+1) \zeta(2^{\{\alpha-\gamma\}}) \zeta(2^{\{\beta-\delta\}}) x_1 (x_0 x_1)^\alpha (x_1 x_0)^\beta x_1 . \end{aligned}$$

where the change of summation variables is given by  $(a, b, r, s) = (\alpha, \delta, \gamma + \delta, \beta - \delta)$ . The last expression is invariant under letter reversal which completes the proof.  $\square$

4.7. **Monodromy at zero.** As previously, we need the following lemma.

**Lemma 4.6.**  $[\hat{\mathcal{S}}, \mathbf{x}_0] = 0$ .

*Proof.* By the general shape of  $\hat{\mathcal{S}}$  we find that  $[\hat{\mathcal{S}}, \mathbf{x}_0] \equiv 0 \pmod{I_{\hat{H}}}$  is equivalent to

$$(4.7) \quad \hat{\mathcal{S}}_{0,1}^1 \mathbf{x}_0 = \mathbf{x}_0 \hat{\mathcal{S}}_{1,0}^1.$$

According to equation (1.6) we decompose

$$(4.8) \quad \begin{aligned} \hat{\mathcal{S}}_{1,0}^1 &= \sum_{m \geq 0, n \geq 1} \hat{\mathcal{S}}_{1,0}^1(m, n) (\mathbf{x}_1 \mathbf{x}_0)^m \mathbf{x}_1 (\mathbf{x}_1 \mathbf{x}_0)^n, \quad \text{and} \\ \hat{\mathcal{S}}_{0,1}^1 &= \sum_{m \geq 1, n \geq 0} \hat{\mathcal{S}}_{1,0}^1(n, m) (\mathbf{x}_0 \mathbf{x}_1)^m \mathbf{x}_1 (\mathbf{x}_0 \mathbf{x}_1)^n. \end{aligned}$$

Projecting (4.7) onto words of the form  $(\mathbf{x}_0 \mathbf{x}_1)^a (\mathbf{x}_1 \mathbf{x}_0)^b$  for  $a, b > 0$  gives the single condition  $\hat{\mathcal{S}}_{1,0}^1(a-1, b) = \hat{\mathcal{S}}_{1,0}^1(b-1, a)$  which can be verified in equation (1.6).  $\square$

4.8. **Proof of single-valuedness.** To prove property (ii) of proposition 4.2 we need to show that the last two equations in equation (4.3) hold. The proofs are straightforward applications of (3.18), (4.5), and (4.6) to write all  $\hat{V}$ 's in terms of  $V_{1,1}^0$ , and reduce to the definition of  $\hat{\mathcal{S}}_{0,0}^1$  in (1.6). Property (i) is lemma 4.6, and property (iii) is obvious from the definition of  $\hat{\mathcal{S}}$ . This completes the proof of theorem 1.6.

## 5. PROOF OF THE ZIG-ZAG CONJECTURE

We are now ready to prove the zig-zag theorem 1.1.

**Definition 5.1.** With the notation of equations (1.4) and (1.7) we define functions  $f_{a,n}$ , where  $a \in \{0, 1\}$  and  $n$  is a non-negative integer, by

$$(5.1) \quad f_{a,n} = (-1)^n \begin{cases} \frac{F_w(z, \bar{z}) - F_{\bar{w}}(z, \bar{z})}{z - \bar{z}} & \text{if } a+n \text{ is odd,} \\ \frac{\hat{F}_w(z, \bar{z}) - \hat{F}_{\bar{w}}(z, \bar{z})}{z - \bar{z}} & \text{if } a+n \text{ is even,} \end{cases}$$

where

$$w = u \mathbf{x}_0 \mathbf{x}_1 \tilde{u},$$

and

$$u = \underbrace{\mathbf{x}_a \dots \mathbf{x}_0 \mathbf{x}_1 \mathbf{x}_0 \mathbf{x}_1 \dots}_n$$

is the alternating  $n$  letter word starting with  $\mathbf{x}_a$ . For  $n = 0$  we set  $f_0 = f_{0,0} = f_{1,0}$ .

Recall that the Bloch-Wigner dilogarithm (see e.g. [25]) is the single-valued version of the dilogarithm  $\text{Li}_2(z)$  (2.5) defined by:

$$(5.2) \quad D(z) = \text{Im}(\text{Li}_2(z) + \log|z| \log(1-z)).$$

**Proposition 5.2.** *The functions  $f_{a,n}$  are real-valued, symmetric,*

$$f_{a,n}(z, \bar{z}) = f_{a,n}(\bar{z}, z),$$

*single-valued solutions to the system of differential equations*

$$(5.3) \quad -\frac{1}{z - \bar{z}} \frac{\partial^2}{\partial z \partial \bar{z}} (z - \bar{z}) f_{a,n}(z, \bar{z}) = \frac{1}{(z-a)(\bar{z}-a)} f_{1-a, n-1}(z, \bar{z})$$

*for  $n \geq 1$ , with the initial condition*

$$(5.4) \quad f_0(z, \bar{z}) = \frac{2iD(z, \bar{z})}{z - \bar{z}}.$$



*Proof.* From theorems 1.4 and 1.6, all statements except the last one are obvious. To derive equation (5.4) we first observe that

$$(z - \bar{z})f_0(z, \bar{z}) = L_{x_1x_0}(\bar{z}) + L_{x_1}(\bar{z})L_{x_0}(z) + L_{x_0x_1}(z) - L_{x_1x_0}(z) - L_{x_1}(z)L_{x_0}(\bar{z}) - L_{x_0x_1}(\bar{z}).$$

Then one can use the shuffle product (2.4) to convert this expression into the dilogarithm and logarithms via (2.5) yielding (5.4).  $\square$

From the theory of graphical functions [22] and [12], which in turn uses the existence of the single-valued multiple polylogarithms [5], we have the following general theorem:

**Theorem 5.3.** *The system of differential equations (5.3) with initial condition (5.4) admits a unique real, symmetric, and single-valued solution  $f_{a,n}^{\text{graph}}$ . The period of the zig-zag graphs (1.2) is*

$$(5.5) \quad I_{Z_n} = f_{1,n-2}^{\text{graph}}(0).$$

From proposition 5.2 we know that

$$f_{a,n}^{\text{graph}} = f_{a,n}.$$

To prove the zig-zag conjecture we have to determine the (regular) value of  $f_{1,n-2}$  at  $z = \bar{z} = 0$ . If  $g$  is a single-valued function which vanishes at  $z = 0$ , then setting, for example,  $z = i\varepsilon$  and applying L'Hôpital's rule to compute the limit as  $\varepsilon \rightarrow 0$ , gives

$$\lim_{z \rightarrow 0} \frac{g(z, \bar{z})}{z - \bar{z}} = \frac{1}{2} \left( \frac{\partial g}{\partial z} - \frac{\partial g}{\partial \bar{z}} \right).$$

Applying this formula to (5.1) with the word  $w = x_1 v x_1$ , where  $|v| = n - 2$ , we obtain

$$f_{1,n-2}(0) = \begin{cases} -F_{x_1 v}(0) + F_{v x_1}(0) & \text{if } n \text{ is even,} \\ \hat{F}_{x_1 v}(0) - \hat{F}_{v x_1}(0) & \text{if } n \text{ is odd,} \end{cases}$$

where we have used theorems 1.4 and 1.6, and the fact that  $F_{x_1 \bar{v}}$  and  $F_{\bar{v} x_1}$  are complex conjugates of  $F_{v x_1}$  and  $F_{x_1 v}$ , respectively. By theorem 5.3 the value  $f_{1,n-2}(0)$  is well-defined. Hence we may use the regularized value of the multiple polylogarithms at zero to evaluate this expression. Because the regularized value at zero (setting  $\log(0) = 0$ ) of any non-constant multiple polylogarithm  $L_w(z)$ , for  $w \neq 1$ , vanishes, the only non-trivial contribution comes from the constant part in  $F$  or  $\hat{F}$ , which by definition (1.4) or (1.5) is the pure  $\mathcal{S}$  or  $\hat{\mathcal{S}}$  part. Thus

$$I_{Z_n} = \begin{cases} -\mathcal{S}_{x_1 v} + \mathcal{S}_{v x_1} & \text{if } n \text{ is even,} \\ \hat{\mathcal{S}}_{x_1 v} - \hat{\mathcal{S}}_{v x_1} & \text{if } n \text{ is odd.} \end{cases}$$

Now, in the case of even  $n$  we find that  $\mathcal{S}_{x_1 v}$  and  $\mathcal{S}_{v x_1}$  are summands in  $\mathcal{S}_{1,0}^1$  and  $\mathcal{S}_{0,1}^1$ , respectively. With notation (3.22) we have

$$I_{Z_n} = -\mathcal{S}_{1,0}^1 \left( \frac{n-2}{2}, \frac{n-2}{2} \right) + \mathcal{S}_{1,0}^1 \left( \frac{n}{2}, \frac{n-4}{2} \right)$$

which evaluates by (1.3) to

$$-4 \left[ -\binom{2n-4}{n-2} + \binom{2n-4}{n-4} \right] \zeta(2n-3) = 4 \frac{(2n-2)!}{n!(n-1)!} \zeta(2n-3)$$

as in theorem 1.1.

If  $n$  is odd then  $\hat{\mathcal{S}}_{x_1 v}$  and  $\hat{\mathcal{S}}_{v x_1}$  are summands in  $\hat{\mathcal{S}}_{1,0}^1$  and  $\hat{\mathcal{S}}_{0,1}^1$ , respectively. With notation (4.8) we get

$$I_{Z_n} = \hat{\mathcal{S}}_{1,0}^1 \left( \frac{n-1}{2}, \frac{n-3}{2} \right) - \hat{\mathcal{S}}_{1,0}^1 \left( \frac{n-3}{2}, \frac{n-1}{2} \right)$$

which evaluates to

$$4(1 - 2^{-2n+4}) \frac{(2n-2)!}{n!(n-1)!} \zeta(2n-3)$$

by exactly the same calculation. This completes the proof of the zig-zag theorem.

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