THE KASHIWARA-VERGNE CONJECTURE AND DRINFELD'S ASSOCIATORS

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Abstract. The Kashiwara-Vergne (KV) conjecture is a property of the Campbell-Hausdorff series put forward in 1978, in [13]. It has been settled in the positive by E. Meinrenken and the first author in 2006, in [2]. In this paper, we study the uniqueness issue for the KV problem. To this end, we introduce a family of infinite dimensional groups KV_n, and an extension $\widehat{\mathrm{KV}}_2$ of the group KV_2. We show that the group $\widehat{\mathrm{KV}}_2$ contains the Grothendieck-Teichmüller group GRT as a subgroup, and that it acts freely and transitively on the set of solutions of the KV problem $\mathrm{Sol}(\widehat{\mathrm{KV}})$. Furthermore, we prove that $\mathrm{Sol}(\widehat{\mathrm{KV}})$ is isomorphic to a direct product of a line $\mathbb{K}$ ($\mathbb{K}$ being a field of characteristic zero) and the set of solutions of the pentagon equation with values in the group KV_3. The latter contains the set of Drinfeld's associators as a subset. As a by-product of our construction, we obtain a new proof of the Kashiwara-Vergne conjecture based on the Drinfeld's theorem on existence of associators.

1. Introduction

The Kashiwara-Vergne (KV) conjecture is a property of the Campbell-Hausdorff series which was put forward in [13]. The KV conjecture has many implications in Lie theory and harmonic analysis. Let $\mathfrak{g}$ be a finite dimensional Lie algebra over a field of characteristic zero. The KV conjecture implies the Duflo theorem [8] on the isomorphism between the center of the universal enveloping algebra $U\mathfrak{g}$ and the ring of invariant polynomials $(S\mathfrak{g})^{\mathfrak{g}}$. Another corollary of the KV conjecture is a ring isomorphism in cohomology $H(\mathfrak{g}, U\mathfrak{g}) \cong H(\mathfrak{g}, S\mathfrak{g})$ (proved by Shoikhet [20] and by Pevzner-Torossian [17]) for the enveloping and symmetric algebras viewed as $\mathfrak{g}$-modules with respect to the adjoint action. For $\mathbb{K} = \mathbb{R}$, another application of the KV conjecture is the extension of the Duflo theorem to germs of invariant distributions on the Lie algebra $\mathfrak{g}$ and on the corresponding Lie group G (see Proposition 4.1 and Proposition 4.2 in [13] proved in [4] and [5]).

The KV conjecture was established for solvable Lie algebras by Kashiwara and Vergne in [13], for $\mathfrak{g} = \mathrm{sl}(2, \mathbb{R})$ by Rouvière in [19], and for quadratic Lie algebras (that is, Lie algebras equipped with an invariant nondegenerate symmetric bilinear form, *e.g.* the Killing form for $\mathfrak{g}$ semisimple) by Vergne [22]. The general case has been settled by Meinrenken and the first author in [2] based on the previous work of the second author [21] and on the Kontsevich deformation quantization theory [14].

In this paper, we establish a relation between the KV conjecture and the theory of Drinfeld's associators developed in [7]. To this end, we introduce a family of infinite dimensional groups $\mathrm{KV}_n, n = 2, 3, \dots$, and an extension $\widehat{\mathrm{KV}}_2$ of the group KV_2. We show that the set of solutions of the KV conjecture $\mathrm{Sol}(\widehat{\mathrm{KV}})$ carries a free and transitive action of the group $\widehat{\mathrm{KV}}_2$ which contains the Drinfeld's Grothendieck-Teichmüller group GRT as a subgroup. Furthermore, the set $\mathrm{Sol}(\widehat{\mathrm{KV}})$ is isomorphic to a direct product of a line $\mathbb{K}$ and the set of solutions of the pentagon equation with values in the group KV_3. We make use of an involution τ acting on solutions of the KV conjecture to select symmetric solutions of the KV problem, $\mathrm{Sol}^\tau(\widehat{\mathrm{KV}})$. The set $\mathrm{Sol}^\tau(\widehat{\mathrm{KV}})$ is isomorphic to a direct product of a line and the set of associators (joint solutions of the pentagon, hexagon and inversion equations of [7]) with values in the group KV_3. The latter contains the set of Drinfeld's associators as a subset.

In summary, we solve the uniqueness issue for the KV problem in terms of associators with values in the group KV_3. As a by-product, we obtain a new proof of the KV conjecture. Indeed, by Drinfeld's theorem, the set of Drinfeld's associators in non empty. Hence, so is the set of associators with values in the group KV_3, and the set of symmetric solutions of the KV conjecture $\mathrm{Sol}^\tau(\widehat{\mathrm{KV}})$. This new proof is based on the theory of associators rather than on the deformation quantization machine.

An outstanding question which we were not able to resolve is whether or not the symmetry group of the KV problem, $\widehat{\mathrm{KV}}_2$, is isomorphic to a direct product of a line and the Grothendieck-Teichmüller group GRT. A numerical experiment of L. Albert and the second author shows that the corresponding graded Lie algebras coincide up to degree 16! If correct, the isomorphism $\widehat{\mathrm{KV}}_2 \cong \mathbb{K} \times \mathrm{GRT}$ would imply that all solutions of the KV conjecture are symmetric, and that all associators with values in the group KV_3 are Drinfeld's associators.

Below we explain *raison d'être* of the link between the Kashiwara-Vergne and associator theories. One possible formulation of the KV problem is as follows: find an automorphism F of the (degree completion of the) free Lie algebra with generators x and y such that

$$F : x + y \mapsto \mathrm{ch}(x, y), \tag{1}$$

where $\mathrm{ch}(x, y) = x + y + \frac{1}{2}[x, y] + \dots$ is the Campbell-Hausdorff series. The automorphism F should satisfy several other properties which we omit here. Consider a free Lie algebra with three generators x, y, z and define the automorphism $F^{1,2}$ which is equal to F when acting on generators x and y and which preserves the generator z. Similarly, define $F^{2,3}$ acting on generators y and z and preserving x. Furthermore, define $F^{12,3}$ acting on $x+y$ and z, and $F^{1,23}$ acting on x and $y+z$ (for a precise definition see Section 3). The main property of the Campbell-Hausdorff series is the associativity,

$$\mathrm{ch}(x, \mathrm{ch}(y, z)) = \mathrm{ch}(\mathrm{ch}(x, y), z).$$

We use this property to establish the following formula:

$$\begin{aligned} F^{1,2}F^{12,3}(x + y + z) &= F^{1,2}(\mathrm{ch}(x + y, z)) \\ &= \mathrm{ch}(\mathrm{ch}(x, y), z) \\ &= \mathrm{ch}(x, \mathrm{ch}(y, z)) \\ &= F^{2,3}(\mathrm{ch}(x, y + z)) \\ &= F^{2,3}F^{1,23}(x + y + z). \end{aligned}$$

Hence, the combination

$$\Phi = (F^{12,3})^{-1}(F^{1,2})^{-1}F^{2,3}F^{1,23} \tag{2}$$

has the property $\Phi(x+y+z) = x+y+z$ which is one of the defining properties of the group KV_3. Furthermore, as an easy consequence of (1) and (2), the automorphism

Φ satisfies the pentagon equation

$$\Phi^{1,2,3}\Phi^{1,23,4}\Phi^{2,3,4} = \Phi^{12,3,4}\Phi^{1,2,34}. \tag{3}$$

Equation (3) is an algebraic presentation of two sequences of parenthesis redistributions in a product of four objects (a standard example is a tensor product in tensor categories): the left hand side corresponds to a passage $((12)3)4 \to (1(23))4 \to 1((23)4) \to (1(2(34))$, while the right hand side to $((12)3)4 \to ((12)(34)) \to 1(2(34))$. The pentagon equation is the most important element of the Drinfeld's theory of associators. Our main technical result shows that solutions of equation (3) with values in the group KV_3 admit an almost unique decomposition of the form (2), and the corresponding automorphism F is automatically a solution of the KV problem (and, in particular, has the property (1)).

An important object of the Kashiwara-Vergne theory is the Duflo function $J^{1/2}$ which corrects the symmetrization map $\mathrm{sym} : S\mathfrak{g} \to U\mathfrak{g}$ so as it restricts to a ring isomorphism on $\mathrm{ad}_\mathfrak{g}$-invariants. It is more convenient to discuss the logarithm of the Duflo function,

$$f(x) = \frac{1}{2} \ln \left(\frac{e^{x/2} - e^{-x/2}}{x} \right) = \frac{1}{2} \sum_{k=2}^{\infty} \frac{B_k}{k \cdot k!} \, x^k, \tag{4}$$

where B_k are Bernoulli numbers. The function $f(x)$ is even, and it is known that any function $\tilde{f}(x) = f(x) + h(x)$ with $h(x)$ odd still defines a ring isomorphism between $Z(U\mathfrak{g})$ and $(S\mathfrak{g})^\mathfrak{g}$ (in the category of Lie algebras, all these isomorphisms coincide with the Duflo isomorphism). We show that the Drinfeld's generators $\sigma_{2k+1}, k = 1, 2, \dots$ of the Grothendieck-Teichmüller Lie algebra $\mathfrak{grt}$ define flows on the set of solutions of the KV conjecture $\mathrm{Sol}(\widehat{\mathrm{KV}})$, and on the odd parts of Duflo functions such that $(\sigma_{2k+1} \cdot h)(x) = -x^{2k+1}$. Hence, all odd formal power series (the linear term of the Duflo function is not well defined) $h(x)$ can be reached by the action of the group GRT on the symmetric Duflo function (4). This action coincides with the one described in [15] (see Theorem 7).

The plan of the paper is as follows: in Section 2 we introduce a Hochschild-type cohomology theory for free Lie algebras, compute the cohomology in low degrees (Theorem 2.1), and discuss the associativity property of the Campbell-Hausdorff series. In Section 3 we study derivations of free Lie algebras. Again, we define a Hochschild-type cohomology theory, and compute cohomology in low degrees (Theorem 3.1). In Section 4 we introduce a family of Kashiwara-Vergne Lie algebras $\mathfrak{kv}_n$ and the Lie algebra $\widehat{\mathfrak{kv}}_2$, and show that the Grothendieck-Teichmüller Lie algebra $\mathfrak{grt}$ injects into $\widehat{\mathfrak{kv}}_2$ (Theorem 4.1). In Section 5 we give a new formulation of the Kashiwara-Vergne conjecture, and show that it is equivalent to the original statement of [13] (Theorem 5.2). In Section 6 we discuss properties of Duflo functions and show that they can acquire arbitrary odd parts. In Section 7 we establish a link between solutions of the KV problem and solutions of the pentagon equation with values in the group KV_3 (Theorem 7.1). In Section 8 we discuss an involution τ on the set of solutions of the KV problem, and derive the hexagon equations using this involution. Finally, in Section 9 we introduce associators with values in the group KV_3, compare them to Drinfeld's associators, and give a new proof of the KV conjecture (Theorem 9.2).

Acknowledgements: We are indebted to V. Drinfeld for posing us a question on the relation between solutions of the Kashiwara-Vergne conjecture and associators. We are grateful to L. Albert who helped setting up numerical experiments which influenced this project in a significant way. We thank D. Bar-Natan, M. Duflo, A. Joseph, I. Marin, E. Meinrenken and S. Sahi for useful discussions and remarks. Research of A.A. was supported in part by the Swiss National Science Foundation. Research of C.T. was supported by CNRS.

2. Free Lie algebras

2.1. **Lie algebras $\mathfrak{lie}_n$ and the Campbell-Hausdorff series.** Let $\mathbb{K}$ be a field of characteristic zero, and let $\mathfrak{lie}_n = \mathfrak{lie}(x_1, \dots, x_n)$ be the degree completion of the free Lie algebra over $\mathbb{K}$ with generators $x_1, \dots, x_n$. It is a graded Lie algebra

$$\mathfrak{lie}_n = \prod_{k=1}^{\infty} \mathfrak{lie}^k(x_1, \dots, x_n),$$

where $\mathfrak{lie}^k(x_1, \dots, x_n)$ is spanned by Lie words consisting of k letters. In case of $n = 1, 2, 3$ we shall often denote the generators by x, y, z.

The universal enveloping algebra of $\mathfrak{lie}_n$ is the degree completion of the free associative algebra with generators $x_1, \dots, x_n$, $U(\mathfrak{lie}_n) = \mathrm{Ass}_n$. Every element $a \in \mathrm{Ass}_n$ has a unique decomposition

$$a = a_0 + \sum_{k=1}^{n} (\partial_k a) x_k, \tag{5}$$

where $a_0 \in \mathbb{K}$ and $(\partial_k a) \in \mathrm{Ass}_n$.

The Campbell-Hausdorff series is an element of Ass_2 defined by formula $\mathrm{ch}(x, y) = \ln(e^x e^y)$, where $e^x = \sum_{k=0}^{\infty} x^k/k!$ and $\ln(1-a) = -\sum_{k=1}^{\infty} a^k/k$. By Dynkin's theorem [9], $\mathrm{ch}(x, y) \in \mathfrak{lie}_2$ and

$$\mathrm{ch}(x, y) = x + y + \frac{1}{2}[x, y] + \dots,$$

where $\dots$ stands for a series in multiple Lie brackets in x and y. The Campbell-Hausdorff series satisfies the associativity property in $\mathfrak{lie}_3$,

$$\mathrm{ch}(x, \mathrm{ch}(y, z)) = \mathrm{ch}(\mathrm{ch}(x, y), z). \tag{6}$$

One can rescale the Lie bracket of $\mathfrak{lie}_2$ by posing $[\cdot, \cdot]_s = s[\cdot, \cdot]$ for $s \in \mathbb{K}$ to obtain a rescaled Campbell-Hausdorff series,

$$\mathrm{ch}_s(x, y) = x + y + \frac{s}{2}[x, y] + \dots,$$

where elements of $\mathfrak{lie}^k(x, y)$ get a extra factor of s^{k-1}. Note that $\mathrm{ch}_s(x, y) = s^{-1}\,\mathrm{ch}(sx, sy)$ and $\mathrm{ch}_0(x, y) = x + y$. The rescaled Campbell-Hausdorff series $\mathrm{ch}_s(x, y)$ satisfies the associativity equation,

$$\begin{aligned} \mathrm{ch}_s(x, \mathrm{ch}_s(y, z)) &= s^{-1}\,\mathrm{ch}(sx, \mathrm{ch}(sy, sz)) \\ &= s^{-1}\,\mathrm{ch}(\mathrm{ch}(sx, sy), sz) \\ &= \mathrm{ch}_s(\mathrm{ch}_s(x, y), z). \end{aligned}$$

***Remark* 2.1.** Let $\mathfrak{g}$ be a finite dimensional Lie algebra over $\mathbb{K}$. Then, every element $a \in \mathfrak{lie}_n$ defines a formal power series $a_{\mathfrak{g}}$ on $\mathfrak{g}^n$ with values in $\mathfrak{g}$. For instance, the Campbell-Hausdorff series $\mathrm{ch} \in \mathfrak{lie}_2$ defines a formal power series $\mathrm{ch}_{\mathfrak{g}}$ on $\mathfrak{g}^2$ with rational coefficients. For every finite dimensional Lie algebra $\mathfrak{g}$ this formal power series has a finite convergence radius.

2.2. **The vector space $\mathfrak{tr}_n$.** For every n we define a graded vector space $\mathfrak{tr}_n$ as a quotient

$$\mathfrak{tr}_n = \mathrm{Ass}_n^+ / \langle (ab - ba); a, b \in \mathrm{Ass}_n \rangle.$$

Here $\mathrm{Ass}_n^+ = \prod_{k=1}^\infty \mathrm{Ass}^k(x_1, \dots, x_n)$, and $\langle (ab - ba); a, b \in \mathrm{Ass}_n \rangle$ is the subspace of Ass_n^+ spanned by commutators. Product of Ass_n does not descend to $\mathfrak{tr}_n$ which only has a structure of a graded vector space. We shall denote by $\mathrm{tr} : \mathrm{Ass}_n \to \mathfrak{tr}_n$ the natural projection. By definition, we have $\mathrm{tr}(ab) = \mathrm{tr}(ba)$ for all $a, b \in \mathrm{Ass}_n$ imitating the defining property of trace.

***Example* 2.1.** The space $\mathfrak{tr}_1$ is isomorphic to the space of formal power series in one variable without constant term, $\mathfrak{tr}_1 \cong x\mathbb{K}[[x]]$. This isomorphism is given by the following formula,

$$f(x) = \sum_{k=1}^\infty f_k x^k \mapsto \sum_{k=1}^\infty f_k \,\mathrm{tr}(x^k).$$

In general, graded components $\mathfrak{tr}_n^k$ of the space $\mathfrak{tr}_n$ are spanned by words of length k modulo cyclic permutations.

***Example* 2.2.** For $n = 2$, $\mathfrak{tr}_2^1$ is spanned by $\mathrm{tr}(x)$ and $\mathrm{tr}(y)$, $\mathfrak{tr}_2^2$ is spanned by $\mathrm{tr}(x^2), \mathrm{tr}(y^2)$ and $\mathrm{tr}(xy) = \mathrm{tr}(yx)$, $\mathfrak{tr}_2^3$ is spanned by $\mathrm{tr}(x^3)$, $\mathrm{tr}(x^2y)$, $\mathrm{tr}(xy^2)$ and $\mathrm{tr}(y^3)$, $\mathfrak{tr}_2^4$ is spanned by $\mathrm{tr}(x^4)$, $\mathrm{tr}(x^3y)$, $\mathrm{tr}(x^2y^2)$, $\mathrm{tr}(xyxy)$, $\mathrm{tr}(xy^3)$ and $\mathrm{tr}(y^4)$ *etc.*

***Remark* 2.2.** Let $\mathfrak{g}$ be a finite dimensional Lie algebra over $\mathbb{K}$, $\rho : \mathfrak{g} \to \mathrm{End}(V)$ be a finite dimensional representation of $\mathfrak{g}$, and $a = \sum_{k=1}^\infty a_k \in \mathfrak{tr}_n$ an element of $\mathfrak{tr}_n$. We define $\rho(a)$ as a formal power series on $\mathfrak{g}^n$ such that $\rho(\mathfrak{tr}(x_{i_1} \dots x_{i_k})) = \mathrm{Tr}_V(\rho(x_{i_1}) \dots \rho(x_{i_k}))$ for monomials, and this definition extends by linearity to all elements of $\mathfrak{tr}_n$.

2.3. **Cohomology problems in $\mathfrak{lie}_n$ and $\mathfrak{tr}_n$.** For all $n = 1, 2, \dots$ we define an operator $\delta : \mathfrak{lie}_n \to \mathfrak{lie}_{n+1}$ by formula

$$\begin{array}{rcl} (\delta f)(x_1, \dots, x_{n+1}) & = & f(x_2, x_3, \dots, x_{n+1}) \\ & + & \sum_{i=1}^n (-1)^i f(x_1, \dots, x_i + x_{i+1}, \dots, x_{n+1}) \\ & + & (-1)^{n+1} f(x_1, \dots, x_n). \end{array} \tag{7}$$

It is easy to see that $\delta^2 = 0$.

***Example* 2.3.** For $n = 1$ and $f = ax \in \mathfrak{lie}_1 \cong \mathbb{K}$ we have

$$(\delta f)(x, y) = f(x) - f(x + y) + f(y) = 0.$$

For $n = 2$ we get

$$(\delta f)(x, y, z) = f(y, z) - f(x + y, z) + f(x, y + z) - f(x, y).$$

One can also use equation (7) to define a differential on the family for vector spaces $\mathfrak{tr}_n$. By abuse of notations, we denote it by the same letter, $\delta : \mathfrak{tr}_n \to \mathfrak{tr}_{n+1}$.

***Example* 2.4.** For $n = 1$, we have for $f(x) = \mathrm{tr}(x^k)$

$$(\delta f)(x, y) = \mathrm{tr}(x^k + y^k - (x + y)^k).$$

Note that the right hand side vanishes for $k = 1$ and that it is non-vanishing for all other $k = 2, 3 \dots$.

The following theorem gives the cohomology of δ in degrees $n = 1, 2$.

Theorem 2.1.

$$\begin{array}{rcl} H^1(\mathfrak{lie}, \delta) & = & \ker(\delta : \mathfrak{lie}_1 \to \mathfrak{lie}_2) = \mathfrak{lie}_1\,, \\ H^1(\mathfrak{tr}, \delta) & = & \ker(\delta : \mathfrak{tr}_1 \to \mathfrak{tr}_2) \cong \mathbb{K}\ \mathrm{tr}(x)\,, \\ H^2(\mathfrak{lie}, \delta) & \cong & [\mathbb{K}[x,y]\,]\,, \\ H^2(\mathfrak{tr}, \delta) & = & 0\,. \end{array}$$

Proof. The first statement is obvious since $\mathfrak{lie}_1 = \mathbb{K}x$ and $\delta(x) = x-(x+y)+y = 0$. The second statement follows from the calculation of Example 2.4.

For computing the second cohomology, let f be a solution of degree $n \geq 2$ of equation

$$f(y,z) - f(x+y,z) + f(x,y+z) - f(x,y) = 0. \tag{8}$$

By putting $x \mapsto sx, y \mapsto x, z \mapsto z$ we obtain

$$f(sx,x) + f((1+s)x,z) - f(sx,x+z) - f(x,z) = 0.$$

In a similar fashion, putting $x \mapsto x, y \mapsto z, z \mapsto sz$ yields

$$f(x,z) + f(x+z,sz) - f(x,(1+s)z) - f(sz,z) = 0.$$

Subtracting the first equation from the second one and differentiating the result in s gives

$$\begin{array}{rcl} nf(x,z) & = & \frac{d}{ds}\left(f((1+s)x,z) + f(x,(1+s)z)\right)|_{s=0} \\ & = & \frac{d}{ds}\left(f(sx,x+z) + f(x+z,sz) - f(sx,x) - f(sz,z)\right)|_{s=0}. \end{array} \tag{9}$$

First, we solve equation (9) for $f \in \mathfrak{lie}_2$. In this case, $f(sx,x) = f(sz,z) = 0$ and we obtain

$$f(x,z) = \mathrm{ad}_{x+z}^{n-1}(\alpha x + \beta z)$$

for some $\alpha, \beta \in \mathbb{K}$. For $n = 2$, this yields $f(x,z) = (\beta - \alpha)[x,z]$. It is easy to check that this is a solution of equation (8).

For $n \geq 3$, consider equation (8) and first put $y = -z$ to get $f(x,z) = -f(x-z,z)$, and then put $y = -x$ to obtain $f(x,z) = -f(-x,x+z)$. Hence,

$$f(x,z) = (\alpha - \beta)\,\mathrm{ad}_x^{n-1}\, z = (\alpha - \beta)\,\mathrm{ad}_z^{n-1}\, x$$

which implies $f(x,z) = 0$. Finally, for $n = 1$ we put $f(x,y) = \alpha x + \beta y$ to obtain $\delta f = \alpha x - \beta z$. In conclusion, $\delta f = 0$ implies that f is of degree two, and $f(x,y) = \alpha[x,y]$ for $\alpha \in \mathbb{K}$.

For $f \in \mathfrak{tr}_2$ equation (9) gives

$$f(x,z) = \mathrm{tr}\,\left((\alpha x + \beta z)(x+z)^{n-1} - \alpha x^n - \beta z^n\right)\,,$$

for some $\alpha, \beta \in \mathbb{K}$. For $n = 1$, it implies $f(x,z) = 0$. For $n = 2$, we get

$$f(x,z) = (\alpha + \beta)\,\mathrm{tr}(xz) = -\,\frac{\alpha+\beta}{2}\delta(\mathrm{tr}(x^2))\,.$$

For $n \geq 3$, we have

$$\delta f = (\beta - \alpha)\,\mathrm{tr}\ y((x+y)^{n-1} + (y+z)^{n-1} - (x+y+z)^{n-1} - y^{n-1})\,.$$

The coefficient in front of $\mathrm{tr}(y^{n-2}xz)$ in this expression is equal to $(\beta - \alpha)(n-2)$, and it vanishes if and only if $\beta = \alpha$. In this case, $f(x,z) = -\alpha\delta(\mathrm{tr}(x^n))$. Hence, $\delta f = 0$ implies the existence of $g \in \mathfrak{tr}_1$ such that $\delta g = f$, and the second cohomology $H^2(\mathfrak{tr}, \delta)$ vanishes. $\square$

***Remark* 2.3.** In the proof of Theorem 2.1 we have shown that $\ker(\delta : \mathfrak{lie}_2 \to \mathfrak{lie}_3) = \mathbb{K}[x,y]$. That is, the only solution of equation (8) is $f(x,y) = \alpha[x,y]$. Equation (8) has been previously considered in the proof of Proposition 5.7 in [7]. There it is stated that equation (8) has no nontrivial symmetric, $f(x,y) = f(y,x)$, solutions in $\mathfrak{lie}_2$.

2.4. **Applications.** In this section we collect two simple applications of the cohomology computations of Section 2.3.

Proposition 2.1. *Let $s \in \mathbb{K}$ and let $\chi \in \mathfrak{lie}_2$ be a Lie series of the form $\chi(x,y) = x + y + \frac{s}{2}[x,y] + \dots$, where $\dots$ stand for a series in multibrackets. Assume that χ is associative, that is*

$$\chi(x, \chi(y,z)) = \chi(\chi(x,y), z) \in \mathfrak{lie}_3 \ .$$

Then, χ coincides with the rescaled Campbell-Hausdorff series, $\chi(x,y) = \mathrm{ch}_s(x,y)$.

Proof. The Lie series χ and ch_s coincide up to degree 2. Assume that they coincide up to degree $n-1$, and let $\chi = \sum_{n=1}^{\infty} \chi_n$ with $\chi_n(x,y)$ a Lie polynomial of degree n. The associativity equation implies the following equation for χ_n:

$$\chi_n(x, y+z) + \chi_n(y,z) - \chi_n(x,y) - \chi_n(x+y, z) = \mathcal{F}(\chi_1(x,y), \dots, \chi_{n-1}(x,y)),$$

where $\mathcal{F}$ is a certain (nonlinear) function of the lower degree terms. By the induction hypothesis, the lower degree terms of χ and ch_s coincide. And the equation for χ_n has a unique solution since the only solution of the corresponding homogeneous equation $\delta\chi_n = 0$ for $n \geq 3$ is $\chi_n = 0$. Hence, $\chi_n = (\mathrm{ch}_s)_n$ and $\chi = \mathrm{ch}_s$. □

Similar to the differential δ, we introduce another differential $\tilde{\delta}$ acting on $\mathfrak{lie}_n$ and $\mathfrak{tr}_n$:

$$\begin{array}{rcl} (\tilde{\delta} f)(x_1, \dots, x_{n+1}) & = & f(x_2, x_3, \dots, x_{n+1}) \\ & + & \sum_{i=1}^{n} (-1)^i f(x_1, \dots, \mathrm{ch}(x_i, x_{i+1}), \dots, x_{n+1}) \\ & + & (-1)^{n+1} f(x_1, \dots, x_n). \end{array} \tag{10}$$

Again, $\tilde{\delta}^2 = 0$, but in contrast to δ, $\tilde{\delta}$ does not preserve the degree. In the following proposition we compute the cohomology of $\tilde{\delta}$ for $n = 1, 2$.

Proposition 2.2.

$$\begin{array}{rcl} H^1(\mathfrak{lie}, \tilde{\delta}) & = & 0\,, \\ H^1(\mathfrak{tr}, \delta) & = & \ker(\tilde{\delta} : \mathfrak{tr}_1 \to \mathfrak{tr}_2) \cong \mathbb{K}\ \mathrm{tr}(x)\,, \\ H^2(\mathfrak{lie}, \delta) & = & 0\,, \\ H^2(\mathfrak{tr}, \delta) & = & 0\,. \end{array}$$

Proof. For $H^1(\mathfrak{lie}, \tilde{\delta})$ we consider $\tilde{\delta}(x) = x + y - \mathrm{ch}(x,y) \neq 0$ which implies $H^1(\mathfrak{lie}, \tilde{\delta}) = \ker(\tilde{\delta} : \mathfrak{lie}_1 \to \mathfrak{lie}_2) = 0$. To compute $H^1(\mathfrak{tr}, \delta)$, observe that $\tilde{\delta}(\mathrm{tr}(x)) = \mathrm{tr}(x + y - \mathrm{ch}(x,y)) = 0$ (here we used that $\mathrm{tr}(a) = 0$ for all $a \in \mathfrak{lie}_n$ of degree greater or equal to two), and $\tilde{\delta}\,\mathrm{tr}(x^k) = \delta\,\mathrm{tr}(x^k) + \cdots \neq 0$ for $k \geq 2$ (here $\dots$ stand for the terms of degree greater than k).

In order to compute the second cohomology, let $f = \sum_{n=k}^{\infty} f_n$, where f_n is homogeneous of degree n, and $f_k \neq 0$. Then, $\tilde{\delta} f = \delta f_k + \text{terms of degree} > k$, and $\tilde{\delta} f = 0$ implies $\delta f_k = 0$.

First, consider $f \in \mathfrak{lie}_2$. In this case, $\delta f_k = 0$ implies $f_k = 0$ for all k except $k = 2$. For $k = 2$, we have $f_2(x,y) = \frac{\alpha}{2}[x,y]$ for some $\alpha \in \mathbb{K}$. Define $g = f + \alpha(\tilde{\delta} x) =$

$f + \alpha(x + y - \mathrm{ch}(x, y))$. We have $\tilde{\delta} g = \tilde{\delta} f + \alpha \tilde{\delta}^2 x = 0$, and $g_2(x, y) = 0$. Hence, $g = 0$ and $f = -\alpha(x + y - \mathrm{ch}(x, y)) = \tilde{\delta}(-\alpha x)$.

For $f \in \mathfrak{tr}_2$, equation $\delta f_k = 0$ implies $f_k = \delta h_k$ for some $h_k \in \mathfrak{tr}_1$. Consider $g = f - \tilde{\delta} h_k$. It satisfies $\tilde{\delta} g = 0$, and $g = \sum_{n=k+1}^{\infty} g_k$. In this way, we inductively construct $h \in \mathfrak{tr}_1$ such that $g = \tilde{\delta} h$. □

***Remark* 2.4.** For every $s \in \mathbb{K}$ one can introduce a differential $\tilde{\delta}_s$ by replacing $\mathrm{ch}(x, y)$ with $\mathrm{ch}_s(x, y)$ in formula (10). We have $\tilde{\delta}_1 = \tilde{\delta}$ and $\tilde{\delta}_0 = \delta$. Proposition 2.2 applies to all $s \neq 0$. Note that $H^1(\mathfrak{tr}, \tilde{\delta}_s) = \mathbb{K}\,\mathrm{tr}(x)$ and $H^2(\mathfrak{tr}, \tilde{\delta}_s) = 0$ for all $s \in \mathbb{K}$ (including $s = 0$).

3. Derivations of free Lie algebras

3.1. **Tangential and special derivations.** We shall denote by $\mathfrak{der}_n$ the Lie algebra of derivations of $\mathfrak{lie}_n$. An element $u \in \mathfrak{der}_n$ is completely determined by its values on the generators, $u(x_1), \ldots, u(x_n) \in \mathfrak{lie}_n$. The Lie algebra $\mathfrak{der}_n$ carries a grading induced by the one of $\mathfrak{lie}_n$.

Definition 3.1. A derivation $u \in \mathfrak{der}_n$ is called *tangential* if there exist $a_i \in \mathfrak{lie}_n, i = 1, \ldots, n$ such that $u(x_i) = [x_i, a_i]$.

Another way to define tangential derivations is as follows: for each $i = 1, \ldots, n$ there exists an inner derivation u_i such that $(u - u_i)(x_i) = 0$. We denote the subspace of tangential derivations by $\mathfrak{tder}_n \subset \mathfrak{der}_n$.

***Remark* 3.1.** Let $p_k : \mathfrak{lie}_n \to \mathbb{K}$ be a projection which assigns to an element $a = \sum_{k=1}^{n} \lambda_k x_k + \ldots$, where $\ldots$ stand for multibrackets, the coefficient $\lambda_k \in \mathbb{K}$. Elements of $\mathfrak{tder}_n$ are in one-to-one correspondence with n-tuples of elements of $\mathfrak{lie}_n$, $(a_1, \ldots, a_n)$, which satisfy the condition $p_k(a_k) = 0$ for all k. Indeed, the kernel of the operator $\mathrm{ad}_{x_k} : a \mapsto [x_k, a]$ is exactly $\mathbb{K}x_k$. Hence, an n-tuple $(a_1, \ldots, a_n)$ defines a vanishing derivation $u(x_k) = [x_k, a_k] = 0$ if and only if $a_k \in \mathbb{K}x_k$ for all k. By abuse of notations, we shall often write $u = (a_1, \ldots, a_n)$.

Proposition 3.1. *Tangential derivations form a Lie subalgebra of* $\mathfrak{der}_n$.

Proof. Let $u = (a_1, \ldots, a_n)$ and $v = (b_1, \ldots, b_n)$. We have

$$\begin{aligned} [u, v](x_k) &= u([x_k, b_k]) - v([x_k, a_k]) \\ &= [[x_k, a_k], b_k] + [x_k, u(b_k)] - [[x_k, b_k], a_k] - [x_k, v(a_k)] \\ &= [x_k, u(b_k) - v(a_k) + [a_k, b_k]] \end{aligned}$$

which shows $[u, v] \in \mathfrak{tder}_n$. □

One can transport the Lie bracket of $\mathfrak{tder}_n$ to the set of n-tuples $(a_1, \ldots, a_n)$ which satisfy the condition $p_k(a_k) = 0$. Indeed, put the kth component of the new n-tuple equal to $u(b_k) - v(a_k) + [a_k, b_k]$. This expression does not contain linear terms, and in particular it is in the kernel of p_k.

Definition 3.2. A derivation $u \in \mathfrak{tder}_n$ is called *special* if $u(x) = 0$ for $x = \sum_{i=1}^{n} x_i$.

We shall denote the space of special derivations of $\mathfrak{lie}_n$ by $\mathfrak{sder}_n$. It is obvious that $\mathfrak{sder}_n \subset \mathfrak{tder}_n$ is a Lie subalgebra. Indeed, for $u, v \in \mathfrak{sder}_n$ we have $[u, v](x) = u(v(x)) - v(u(x)) = 0$ and, hence, $[u, v] \in \mathfrak{sder}_n$.

***Remark* 3.2.** Ihara [11] calls elements of $\mathfrak{sder}_n$ normalized special derivations.

***Example* 3.1.** Consider $r = (y, 0) \in \mathfrak{tder}_2$. By definition, $r(x) = [x, y], r(y) = 0$. Note that $r(x+y) = [x, y] \neq 0$ and $r \notin \mathfrak{sder}_2$. Consider another element $t = (y, x) \in \mathfrak{tder}_2$. We have $t(x) = [x, y], t(y) = [y, x]$ and $t(x + y) = [x, y] + [y, x] = 0$. Hence, $t \in \mathfrak{sder}_2$.

3.2. **Simplicial and coproduct maps.** We shall need a number of Lie algebra homomorphisms mapping $\mathfrak{tder}_{n-1}$ to $\mathfrak{tder}_n$. First, observe that the permutation group S_n acts on $\mathfrak{lie}_n$ by Lie algebra automorphisms. For $\sigma \in S_n$, we have $a \mapsto a^\sigma = a(x_{\sigma(1)}, \ldots, x_{\sigma(n)})$. The induced action on $\mathfrak{tder}_n$ is given by formula,

$$u = (a_1, \ldots, a_n) \mapsto u^\sigma = (a_{\sigma^{-1}(1)}(x_{\sigma(1)}, \ldots, x_{\sigma(n)}), \ldots, a_{\sigma^{-1}(n)}(x_{\sigma(1)}, \ldots, x_{\sigma(n)})).$$

***Example* 3.2.** For $u = (a(x, y), b(x, y)) \in \mathfrak{tder}_2$ we have $u^{2,1} = (b(y, x), a(y, x))$, where $\sigma = (21)$ is the nontrivial element of S_2. In the same fashion, for $u = (a(x, y, z), b(x, y, z), c(x, y, z)) \in \mathfrak{tder}_3$ we have $u^{3,1,2} = (b(z, x, y), c(z, x, y), a(z, x, y))$.

We define *simplicial maps* by the following property. For $u = (a_1, \ldots, a_{n-1}) \in \mathfrak{tder}_{n-1}$ define $u^{1,2,\ldots,n-1} = (a_1, \ldots, a_{n-1}, 0) \in \mathfrak{tder}_n$. It is clear that the map $u \mapsto u^{1,2,\ldots,n-1}$ is a Lie algebra homomorphism. We obtain other simplicial maps by composing with the action of S_n on $\mathfrak{tder}_n$. Simplicial maps restrict to special derivations. Indeed, for $u \in \mathfrak{sder}_{n-1}$ and $x = \sum_{i=1}^n x_i$ we compute

$$u^{1,2,\ldots,n-1}(x) = \sum_{i=1}^{n-1} [x_i, a_i] = 0$$

which implies $u^{1,2,\ldots,n-1} \in \mathfrak{sder}_n$.

***Example* 3.3.** For $u = (a(x, y), b(x, y)) \in \mathfrak{tder}_2$ we have $u^{1,2} = (a(x, y), b(x, y), 0) \in \mathfrak{tder}_3$ and $u^{2,3} = (0, a(y, z), b(y, z))$. For instance, for $r = (y, 0)$ we obtain $r^{1,2} = (y, 0, 0), r^{2,3} = (0, z, 0), r^{1,3} = (z, 0, 0)$.

Proposition 3.2. *The element $r = (y, 0) \in \mathfrak{tder}_2$ satisfies the classical Yang-Baxter equation,*

$$[r^{1,2}, r^{1,3}] + [r^{1,2}, r^{2,3}] + [r^{1,3}, r^{2,3}] = 0.$$

Proof. We compute,

$$[r^{1,2}, r^{1,3}] = [(y, 0, 0), (z, 0, 0)] = ([y, z], 0, 0),$$
$$[r^{1,2}, r^{2,3}] = [(y, 0, 0), (0, z, 0)] = -([y, z], 0, 0),$$
$$[r^{1,3}, r^{2,3}] = [(z, 0, 0), (0, z, 0)] = 0.$$

Adding these expressions gives zero, as required. □

Next, consider $t = (y, x) \in \mathfrak{sder}_2$. By composing various simplicial maps we obtain $n(n-1)/2$ elements of $t^{i,j} = t^{j,i} \in \mathfrak{tder}_n$ with non-vanishing components x_i at the jth place and x_j at the ith place.

Proposition 3.3. *Elements $t^{i,j} \in \mathfrak{sder}_n$ span a Lie subalgebra isomorphic to the quotient of the free Lie algebra with $n(n-1)/2$ generators by the following relations,*

$$[t^{i,j}, t^{k,l}] = 0 \tag{11}$$

for $k, l \neq i, j$, and

$$[t^{i,j} + t^{i,k}, t^{j,k}] = 0 \tag{12}$$

for all triples of distinct indices i, j, k.

***Remark* 3.3.** We denote by $\mathfrak{t}_n$ the Lie algebra defined by relations (11) and (12). Note that $c = \sum_{i<j} t^{i,j}$ is a central element of $\mathfrak{t}_n$. Indeed, $[t^{i,j}, c] = \sum_{k \neq i, k \neq j} [t^{i,j}, t^{i,k} + t^{j,k}] = 0$. It is known (see Section 5 of [7]) that

$$\mathfrak{t}_n \cong \mathfrak{t}_{n-1} \oplus \mathfrak{lie}(t^{1,n}, \ldots, t^{n-1,n}),$$

where the free Lie algebra $\mathfrak{lie}(t^{1,n}, \ldots, t^{n-1,n})$ is an ideal in $\mathfrak{t}_n$ and $\mathfrak{t}_{n-1} \subset \mathfrak{t}_n$ is a complementary Lie subalgebra spanned by $t^{i,j}$ with $i, j < n$. In particular, $\mathfrak{t}_2 = \mathbb{K}t^{1,2}$ is an abelian Lie algebra with one generator, and $\mathfrak{t}_3 \cong \mathfrak{t}_2 \oplus \mathfrak{lie}(t^{1,3}, t^{2,3})$. In fact, $\mathrm{ad}_{t^{1,2}}$ is an inner derivation of $\mathfrak{lie}(t^{1,3}, t^{2,3})$,

$$[t^{1,2}, a] = [t^{1,2} - c, a] = -[t^{1,3} + t^{2,3}, a],$$

and $\mathfrak{t}_3 \cong \mathbb{K}c \oplus \mathfrak{lie}(t^{1,3}, t^{2,3})$.

Proof. First, we verify the relations (11) and (12). The first one is obvious since the derivations $t^{i,j}$ and $t^{k,l}$ act on different generators of $\mathfrak{lie}_n$. For the second one, we choose $n = 3$ and compute $[t^{1,2} + t^{1,3}, t^{2,3}]$:

$$[t^{1,2}, t^{2,3}] = [(y, x, 0), (0, z, y)] = (-[y, z], [x, z], [y, x]),$$
$$[t^{1,3}, t^{2,3}] = [(z, 0, x), (0, z, y)] = (-[z, y], [z, x], [x, y]).$$

Adding these expressions gives zero, as required. We obtain the relation (12) for other values of i, j, k by applying the S_n action to replace $1, 2, 3$ by i, j, k. Hence, the expressions $t^{i,j}$ define a Lie algebra homomorphism from $\mathfrak{t}_n$ to $\mathfrak{sder}_n$. We prove that it is injective by induction. Clearly, the map $\mathfrak{t}_2 = \mathbb{K}t^{1,2} \to \mathfrak{sder}_2$ is injective. Assume that the Lie homomorphism $\mathfrak{t}_{n-1} \to \mathfrak{tder}_{n-1}$ is injective. Let $a \in \mathfrak{t}_n$, $a = a' + a''$, where $a' \in \mathfrak{t}_{n-1}$ and $a'' \in \mathfrak{lie}(t^{1,n}, \ldots, t^{n-1,n})$. We denote by A' and A'' their images in $\mathfrak{sder}_n$. Observe that $A'(x_n) = 0$ since A' is a derivation acting only on generators $x_1, \ldots, x_{n-1}$. It is easy to check that $A''(x_n) = [x_n, a''(x_1, \ldots, x_{n-1})]$, where $a''(x_1, \ldots, x_{n-1})$ is obtained by replacing the generators $t^{i,n}$ by x_i in $a''(t^{1,n}, \ldots, t^{n-1,n})$. Assuming $A = A' + A'' = 0$, we have $A(x_n) = 0$ which implies $A''(x_n) = 0$ and $a'' = 0$. Then, $a = a' \in \mathfrak{t}_{n-1}$ and $A = 0$ implies $a = 0$ by the induction hypothesis. □

Proposition 3.4. *The element $c = \sum_{i<j} t^{i,j}$ belongs to the center of $\mathfrak{sder}_n$.*

Proof. First, note that $c(x_i) = \sum_{j \neq i} [x_i, x_j] = [x_i, x]$ for $x = \sum_{j=1}^n x_j$. Hence, c is an inner derivation, and for any $a \in \mathfrak{lie}_n$ we have $c(a) = [a, x]$. Let $u = (a_1, \ldots, a_k) \in \mathfrak{sder}_n$ and compute the kth component of the bracket $[c, u]$:

$$\begin{aligned} c(a_k) - u(\textstyle\sum_{i \neq k} x_i) + \sum_{i \neq k} [x_i, a_k] &= [a_k, x] + u(x_k) + \textstyle\sum_{i \neq k} [x_i, a_k] \\ &= [a_k, x] + [x_k, a_k] + \textstyle\sum_{i \neq k} [x_i, a_k] \\ &= [a_k, x] + [x, a_k] = 0. \end{aligned}$$

Here we have used that $u(x) = 0$ for $u \in \mathfrak{sder}_n$. □

Another family of Lie algebra homomorphisms $\mathfrak{tder}_{n-1} \to \mathfrak{tder}_n$ is given by *coproduct maps.* For $u = (a_1, \ldots, a_{n-1}) \in \mathfrak{tder}_{n-1}$ we define

$$\begin{aligned} u^{12,3,\ldots,n} = \; &(a_1(x_1 + x_2, x_3, \ldots, x_n), \\ &a_1(x_1 + x_2, x_3, \ldots, x_n), \\ &a_2(x_1 + x_2, x_3, \ldots, x_n), \\ &\ldots, \\ &a_{n-1}(x_1 + x_2, x_3, \ldots, x_n)). \end{aligned}$$

Other coproduct maps are obtained by using the action of the permutation groups on $\mathfrak{tder}_{n-1}$ and on $\mathfrak{tder}_n$.

***Example* 3.4.** For $n = 2$ and $u = (a(x,y), b(x,y))$ we have $u^{12,3} = (a(x+y,z), a(x+y,z), b(x+y,z))$ and $u^{1,23} = (a(x,y+z), b(x,y+z), b(x,y+z))$.

Coproduct maps $\mathfrak{tder}_{n-1} \to \mathfrak{tder}_n$ are Lie algebra homomorphisms. Let $u = (a,b) \in \mathfrak{tder}_2$ and compute $u^{12,3}(x+y) = [x+y, a(x+y,z)]$ and $u^{12,3}(z) = [z, b(x+y,z)]$. Hence, for any $f \in \mathfrak{lie}_2$ we obtain $u^{12,3}(f(x+y,z)) = (u(f))(x+y,z)$. For $u = (a_1, b_1), v = (a_2, b_2) \in \mathfrak{tder}_2$ we compute $[u^{12,3}, v^{12,3}] = (c_1, c_2, c_3)$ where

$$\begin{aligned} c_1 = c_2 &= u^{12,3}(a_2(x+y,z)) - v^{12,3}(a_1(x+y,z)) + [a_1(x+y,z), a_2(x+y,z)] \\ &= (u(a_2) - v(a_1) + [a_1,a_2])(x+y,z), \\ c_3 &= u^{12,3}(b_2(x+y,z)) - v^{12,3}(b_1(x+y,z)) + [b_1(x+y,z), b_2(x+y,z)] \\ &= (u(b_2) - v(b_1) + [b_1,b_2])(x+y,z). \end{aligned}$$

Hence, $[u^{12,3}, v^{12,3}] = [u,v]^{12,3}$. Coproduct maps restrict to Lie subalgebras of special derivations. For $u \in \mathfrak{sder}_{n-1}$ and $x = \sum_{i=1}^n x_i$ we compute

$$u^{12,3,\ldots,n}(x) = [x_1 + x_2, a_1(x_1+x_2,\ldots,x_n)] + \cdots + [x_n, a_{n-1}(x_1+x_2,\ldots,x_n)] = 0$$

which implies $u^{12,3,\ldots,n} \in \mathfrak{sder}_n$.

***Example* 3.5.** For $r = (y, 0) \in \mathfrak{tder}_2$ we have $r^{12,3} = (z,z,0) = r^{1,3} + r^{2,3}$ and $r^{1,23} = (y+z,0,0) = r^{1,2} + r^{1,3}$. Similarly, for $t = (y,x) \in \mathfrak{tder}_2$ we have $t^{12,3} = (z,z,x+y) = t^{1,3} + t^{2,3}$ and $t^{1,23} = (y+z,x,x) = t^{1,2} + t^{1,3}$.

Let $u = (a_1,b_1) \in \mathfrak{sder}_2$ and $v = (a_2,b_2) \in \mathfrak{tder}_2$. Then, $[u^{1,2}, v^{12,3}] = 0$. Indeed, note that $u^{1,2}$ acts by zero on $\mathfrak{lie}(x+y,z)$ and $v^{12,3}$ acts as an inner derivation with generator $a_2(x+y,z)$ on $\mathfrak{lie}(x,y)$. We compute

$$\begin{aligned} [u^{1,2}, v^{12,3}](x) &= u^{1,2}([x, a_2(x+y,z)]) - v^{12,3}([x, a_1(x,y)]) \\ &= [[x, a_1(x,y)], a_2(x+y,z)] - [[x,a_1(x,y)], a_2(x+y,z)] = 0, \end{aligned}$$

and similarly $[u^{1,2}, v^{12,3}](y) = 0$. Finally, $[u^{1,2}, v^{12,3}](z) = u^{1,2}([z, b_2(x+y,z)]) = 0$. In general, for $u \in \mathfrak{sder}_n, v \in \mathfrak{tder}_{m+1}$ we have $[u^{1,2,\ldots,n}, v^{12\ldots n, n+1,\ldots,n+m}] = 0$.

3.3. Cohomology.

We define a differential $\mathrm{d} : \mathfrak{tder}_n \to \mathfrak{tder}_{n+1}$ by formula,

$$\mathrm{d}u = u^{2,3,\ldots,n+1} - u^{12,\ldots,(n-1),n} + \cdots + (-1)^n u^{1,2,\ldots,(n-1)n} + (-1)^{n+1} u^{1,2,\ldots,n}.$$

It is easy to check that d squares to zero, $\mathrm{d}^2 = 0$.

***Example* 3.6.** For $u \in \mathfrak{tder}_2$ we get $\mathrm{d}u = u^{2,3} - u^{12,3} + u^{1,23} - u^{1,2}$. For $u \in \mathfrak{tder}_3$ we obtain $\mathrm{d}u = u^{2,3,4} - u^{12,3,4} + u^{1,23,4} - u^{1,2,34} + u^{1,2,3}$.

We shall compute the cohomology groups

$$H^n(\mathfrak{tder}, \mathrm{d}) = \ker(\mathrm{d} : \mathfrak{tder}_n \to \mathfrak{tder}_{n+1}) / \mathrm{im}(\mathrm{d} : \mathfrak{tder}_{n-1} \to \mathfrak{tder}_n)$$

for $n = 2, 3$.

Theorem 3.1.

$$\begin{aligned} H^2(\mathfrak{tder}, \mathrm{d}) &= \ker(\mathrm{d} : \mathfrak{tder}_2 \to \mathfrak{tder}_3) = \mathbb{K}r \oplus \mathbb{K}t, \\ H^3(\mathfrak{tder}, \mathrm{d}) &\cong \mathbb{K}[(0,[z,x],0)], \end{aligned}$$

where $r = (y,0), t = (y,x)$.

Proof. Since $\mathfrak{tder}_1 = 0$, we have $H^2(\mathfrak{tder}, \mathrm{d}) = \ker(\mathrm{d} : \mathfrak{tder}_2 \to \mathfrak{tder}_3)$. Let $u = (a, b) \in \mathfrak{tder}_2$, and consider $\mathrm{d}u = u^{2,3} - u^{12,3} + u^{1,23} - u^{1,2}$. Equation $\mathrm{d}u = 0$ reads

$$\begin{array}{rcrcrcrcl} & - & a(x+y,z) & + & a(x,y+z) & - & a(x,y) & = & 0, \\ a(y,z) & - & a(x+y,z) & + & b(x,y+z) & - & b(x,y) & = & 0, \\ b(y,z) & - & b(x+y,z) & + & b(x,y+z) & & & = & 0. \end{array}$$

Put $x = 0$ in the first equation to get $a(y,z) = a(0, y+z) - a(0, y) = \alpha z$. In the same way, put $z = 0$ in the third equation to obtain $b(x,y) = b(x+y, 0) - b(y) = \beta x$. All three equations are satisfied by $u = (\alpha y, \beta x) = (\alpha - \beta)r + \beta t$ for all $\alpha, \beta \in \mathbb{K}$. Hence, $\ker(\mathrm{d} : \mathfrak{tder}_2 \to \mathfrak{tder}_3) = \mathbb{K}r \oplus \mathbb{K}t$

In order to compute $H^3(\mathfrak{tder}, \mathrm{d})$ we put $u = (a, b, c) \in \mathfrak{tder}_3$ and write $\mathrm{d}u = u^{2,3,4} - u^{12,3,4} + u^{1,23,4} - u^{1,2,34} + u^{1,2,3}$. Equation $\mathrm{d}u = 0$ yields

$$\begin{array}{rrrrrcl} & -a(x+y,z,w) & +a(x,y+z,w) & -a(x,y,z+w) & +a(x,y,z) & = & 0, \\ a(y,z,w) & -a(x+y,z,w) & +b(x,y+z,w) & -b(x,y,z+w) & +b(x,y,z) & = & 0, \\ b(y,z,w) & -b(x+y,z,w) & +b(x,y+z,w) & -c(x,y,z+w) & +c(x,y,z) & = & 0, \\ c(y,z,w) & -c(x+y,z,w) & +c(x,y+z,w) & -c(x,y,z+w) & & = & 0, \end{array}$$

Make a substitution $x \mapsto x, y \mapsto -x, z \mapsto x+y, w \mapsto z$ in the first equation to get

$$a(x,y,z) = a(x, -x, x+y+z) - a(x, -x, x+y) + a(0, x+y, z).$$

Let $f(x,y) = -a(x, -x, x+y)$ and $k(x,y) = a(0,x,y) - f(x,y)$ to get the following expression for a,

$$a(x,y,z) = f(x,y) - f(x, y+z) + f(x+y, z) + k(x+y, z).$$

In the same fashion, putting $x \mapsto y, y \mapsto z+w, z \mapsto -w, w \mapsto w$ in the forth equation gives

$$c(y,z,w) = c(y+z+w, -w, w) - c(z+w, -w, w) + c(y, z+w, 0).$$

By letting $g(z,w) = -c(z+w, -w, w)$ and $l(z,w) = c(z,w,0) + g(z,w)$ we obtain

$$c(y,z,w) = -g(y, z+w) + g(y+z, w) - g(z,w) + l(y, z+w).$$

Consider $\tilde{u} = (\tilde{a}, \tilde{b}, \tilde{c}) = u + \mathrm{d}(f, g)$. It satisfies $\mathrm{d}\tilde{u} = 0$ and it has $\tilde{a}(x,y,z) = k(x+y, z)$ and $\tilde{c}(x,y,z) = l(x, y+z)$. The first equation (for $\tilde{a}$) implies $k(x+y, z) = k(x+y, z+w)$ which forces $k = 0$ (since $\tilde{a}$ does not contain terms linear in x). In the same way, the forth equation yields $l(x+y, z+w) = l(y, z+w)$ which implies $l = 0$. Hence, $\tilde{u} = (0, \tilde{b}, 0)$. Denote $h(x,y) = \tilde{b}(x, 0, y)$ and first put $y = 0$ in the third equation to get $\tilde{b}(x,z,w) = h(x, z+w) - h(x,z)$, then put $z = 0$ to obtain $\tilde{b}(x,y,w) = h(x+y, w) - h(y,w)$. These two equations imply

$$h(x,y) - h(x, y+w) + h(x+y, w) - h(y,w) = 0,$$

and, by Theorem 2.1, $h(x,y) = \gamma[x,y]$ for some $\gamma \in \mathbb{K}$. This implies $\tilde{b}(x,y,z) = \gamma[x, y+z] - \gamma[x,y] = \gamma[x,z]$. It is easy to check that $\tilde{u} = (0, \gamma[x,z], 0)$ verifies $\mathrm{d}\tilde{u} = 0$. Finally, in degree two, $\mathrm{im}(\mathrm{d} : \mathfrak{tder}_2 \to \mathfrak{tder}_3)$ is spanned by

$$\mathrm{d}(\alpha[x,y], \beta[x,y]) = (-\alpha[y,z], (\alpha - \beta)[z,x], \beta[x,y]),$$

and $(0, \gamma[x,z], 0) \notin \mathrm{im}(\mathrm{d} : \mathfrak{tder}_2 \to \mathfrak{tder}_3)$ for $\gamma \neq 0$. $\square$

3.4. **Cocycles in $\mathfrak{tr}_n$.** The action of $\mathfrak{der}_n$ extends from $\mathfrak{lie}_n$ to Ass_n and descends to the graded vector space $\mathfrak{tr}_n$. For $u \in \mathfrak{der}_n$ and $a \in \mathfrak{tr}_n$ we denote this action by $u \cdot a \in \mathfrak{tr}_n$.

***Example* 3.7.** Let $r = (y, 0) \in \mathfrak{tder}_2$, and $a = \mathrm{tr}(xy) \in \mathfrak{tr}_2$. We compute $r \cdot a = \mathrm{tr}(r(x)y + xr(y)) = \mathrm{tr}([x, y]y) = \mathrm{tr}((xy - yx)y) = 0$.

We shall be interested in 1-cocycles on the subalgebra $\mathfrak{tder}_n$ with values in $\mathfrak{tr}_n$. That is, we are looking for linear maps $\alpha : \mathfrak{tder}_n \to \mathfrak{tr}_n$ such that

$$u \cdot \alpha(v) - v \cdot \alpha(u) - \alpha([u, v]) = 0$$

for all $u, v \in \mathfrak{tder}_n$.

Proposition 3.5. *For all $k = 1, \dots, n$ the map $\alpha : u = (a_1, \dots, a_n) \mapsto \mathrm{tr}(a_k)$ is a 1-cocycle.*

Proof. Note that α vanishes on all elements of degree greater or equal to two. Hence, $\alpha([u, v]) = 0$ for all $u, v \in \mathfrak{tder}_n$. Let $u = (a_1, \dots, a_n)$ and $v = (b_1, \dots, b_n)$. Then, $u \cdot \alpha(v) = u \cdot \mathrm{tr}(b_k) = \mathrm{tr}(u(b_k)) = 0$ since $u(b_k)$ is of degree at least two, and similarly $v \cdot \alpha(u) = \mathrm{tr}(v(a_k)) = 0$. □

Proposition 3.6. *The map* $\mathrm{div} : u = (a_1, \dots, a_n) \mapsto \sum_{k=1}^n \mathrm{tr}(x_k(\partial_k a_k))$ *is a 1-cocycle.*

Proof. On the one hand, we get

$$\begin{array}{rcl} u \cdot \mathrm{div}(v) - v \cdot \mathrm{div}(u) & = & \sum_{k=1}^n \mathrm{tr}\left(u(x_k(\partial_k b_k)) - v(x_k(\partial_k a_k))\right) \\ & = & \sum_{k=1}^n \mathrm{tr}([x_k, a_k](\partial_k b_k) + x_k u(\partial_k b_k) \\ & - & [x_k, b_k](\partial_k a_k) - x_k v(\partial_k a_k)). \end{array}$$

On the other hand, we obtain,

$$\begin{array}{rcl} \mathrm{div}([u, v]) & = & \sum_{k=1}^n \mathrm{tr}(x_k \partial_k (u(b_k) - v(a_k) + [a_k, b_k])) \\ & = & \sum_{k=0}^n \mathrm{tr}(x_k \partial_k (u(\sum_{i=1}^n (\partial_i b_k) x_i) - v(\sum_{j=1}^n (\partial_j a_k) x_j) + [a_k, b_k])) \\ & = & \sum_{k=0}^n \mathrm{tr}(x_k \partial_k (\sum_{i=1}^n (u(\partial_i b_k) x_i + (\partial_i b_k)[x_i, a_i]) \\ & - & \sum_{j=1}^n (v(\partial_j a_k) x_j + (\partial_j a_k)[x_j, a_j]) + [a_k, b_k])) \\ & = & \sum_{k=0}^n \mathrm{tr}(x_k (u(\partial_k b_k) - (\partial_k b_k) a_k + \sum_{i=1}^n (\partial_i b_k) x_i (\partial_k a_i) \\ & - & v(\partial_k a_k) + (\partial_k a_k) b_k - \sum_{j=1}^n (\partial_j a_k) x_j (\partial_k b_j) + a_k(\partial_k b_k) - b_k(\partial_k a_k))) \\ & = & \sum_{k=1}^n \mathrm{tr}(x_k (u(\partial_k b_k) - (\partial_k b_k) a_k - v(\partial_k a_k) \\ & + & (\partial_k a_k) b_k + a_k(\partial_k b_k) - b_k(\partial_k a_k))) \\ & = & u \cdot \mathrm{div}(v) - v \cdot \mathrm{div}(u). \end{array}$$

proving the cocycle condition. Here we have used the definition of ∂_k operators (see equation (5)) and the fact that $a_k = \sum_{j=1}^n (\partial_j a_k) x_j$ and $b_k = \sum_{i=1}^n (\partial_i b_k) x_i$. □

The *divergence cocycle* transforms in a nice way under simplicial and coproduct maps. For $u = (a_1, \dots, a_n) \in \mathfrak{tder}_n$ we have $\mathrm{div}(u^{1,2,\dots,n}) = \sum_{i=1}^n \mathrm{tr}(x_i(\partial_i a_i)) = \mathrm{div}(u)(x_1, \dots, x_n)$. For $\mathrm{div}(u^{12,\dots,n+1})$ we compute

$$\begin{array}{rcl} \mathrm{div}(u^{12,\dots,n+1}) & = & \mathrm{tr}(x_1(\partial_1 a_1(x_1 + x_2, \dots)) + x_2(\partial_2 a_1(x_1 + x_2, \dots))) \\ & + & \sum_{k=3}^{n+1} \mathrm{tr}(x_k(\partial_k a_{k-1}(x_1 + x_2, \dots))) \\ & = & \mathrm{tr}((x_1 + x_2)(\partial_1 a_1)(x_1 + x_2, \dots) \\ & + & \sum_{k=2}^n x_{k+1}(\partial_k a_k)(x_1 + x_2, \dots)) \\ & = & (\mathrm{div}(u))(x_1 + x_2, x_3, \dots, x_{n+1}). \end{array}$$

Proposition 3.7. $\mathrm{div}(du) = \delta(\mathrm{div}(u))$.

Proof. We compute,

$$\begin{aligned}
\mathrm{div}(\mathrm{d}u) &= \mathrm{div}(u^{2,\dots,n+1}) - \mathrm{div}(u^{12,\dots,n+1}) + \dots + (-1)^{n+1}\mathrm{div}(u^{1,2,\dots,n}) \\
&= \mathrm{div}(u)(x_2,\dots,x_{n+1}) - \mathrm{div}(u)(x_1+x_2,\dots,x_{n+1}) + \dots \\
&+ (-1)^{n+1}\mathrm{div}(x_1,\dots,x_n) \\
&= \delta(\mathrm{div}(u)).
\end{aligned}$$

□

4. Kashiwara-Vergne Lie algebras

4.1. **Definitions.** In this section we introduce a family of subalgebras of $\mathfrak{sder}_n$ called *Kashiwara-Vergne* Lie algebras.

Definition 4.1. The Kashiwara-Vergne Lie algebra $\mathfrak{kv}_n$ is a Lie subalgebra of special derivations spanned by elements with vanishing divergence.

Note that $\mathfrak{kv}_n$ is indeed a Lie subalgebra of $\mathfrak{sder}_n$. For two derivations $u, v \in \mathfrak{kv}_n$ the cocycle property for divergence implies $\mathrm{div}([u,v]) = u \cdot \mathrm{div}(v) - v \cdot \mathrm{div}(u) = 0$, as required.

***Example* 4.1.** The element $t = (y, x) \in \mathfrak{sder}_2$ is contained in $\mathfrak{kv}_2$. Indeed, we have $a(x,y) = y, b(x,y) = x$ and $\partial_x a = \partial_y b = 0$ which implies $\mathrm{div}(t) = 0$.

Simplicial and coproduct maps restrict to $\mathfrak{kv}_n$ subalgebras. Indeed, for $u \in \mathfrak{sder}_n$ the condition $\mathrm{div}(u) = 0$ implies $\mathrm{div}(u^{1,2,\dots,n}) = 0$ and $\mathrm{div}(u^{12,3,\dots,n+1}) = 0$.

***Example* 4.2.** Since $t \in \mathfrak{kv}_2$, we have $t^{1,2}, t^{1,3}, t^{2,3} \in \mathfrak{kv}_3$ and $[t^{1,3}, t^{2,3}] = ([y,z],[z,x],[x,y]) \in \mathfrak{kv}_3$.

In the case of $n = 2$ we introduce an extension of $\mathfrak{kv}_2$,

$$\widehat{\mathfrak{kv}}_2 := \{u \in \mathfrak{sder}_2, \mathrm{div}(u) \in \ker(\delta)\}.$$

Recall that $\ker(\delta : \mathfrak{tr}_2 \to \mathfrak{tr}_3) = \mathrm{im}(\delta : \mathfrak{tr}_1 \to \mathfrak{tr}_2)$. Hence, for $u \in \widehat{\mathfrak{kv}}_2$ there exists an element $f \in \mathfrak{tr}_1$ such that $\mathrm{div}(u) = \mathrm{tr}(f(x) - f(x+y) + f(y))$. By Theorem 2.1, such an element is unique if we choose it in the form $f(x) = \sum_{k=2}^{\infty} f_k x^k$. By abuse of notations we denote by f the map $f : u \mapsto f$, and by f_k the maps $f_k : u \mapsto f_k$.

The subspace $\widehat{\mathfrak{kv}}_2$ is a Lie subalgebra of $\mathfrak{sder}_2$. Indeed, for two derivations $u, v \in \widehat{\mathfrak{kv}}_2$ we compute $\mathrm{div}([u,v]) = u \cdot \mathrm{div}(v) - v \cdot \mathrm{div}(u)$. We have $\mathrm{div}(v) = \delta f = \mathrm{tr}(f(x) - f(x+y) + f(y))$ with $f \in x^2\mathbb{K}[[x]]$. Note that $u \cdot \mathrm{tr}(f(x+y)) = 0$ since $u(x+y) = 0$ and $u \cdot \mathrm{tr}(f(x)) = \mathrm{tr}([x,a]f'(x)) = \mathrm{tr}([xf'(x), a]) = 0$, where $u(x) = [x,a]$. Hence, $u \cdot \mathrm{div}(v) = 0$, and similarly $v \cdot \mathrm{div}(u) = 0$. In fact, we proved $[\widehat{\mathfrak{kv}}_2, \widehat{\mathfrak{kv}}_2] \subset \mathfrak{kv}_2$.

Proposition 4.1. *Let $u \in \widehat{\mathfrak{kv}}_2$. Then, $f(u)$ is odd, and Taylor coefficients $f_k, k = 3, 5, \dots$ are characters of $\widehat{\mathfrak{kv}}_2$.*

Proof. Let $u \in \widehat{\mathfrak{kv}}_2$ with divergence $\mathrm{div}(u) = \mathrm{tr}(f(x) - f(x+y) + f(y))$, where $f(x) = \sum_{k=2}^{\infty} f_k x^k$. Note that the coefficient in front of $\mathfrak{tr}(xy^{n-1})$ in $\mathrm{div}(u)$ is equal to $-nf_n$. Since $u = (a,b) \in \widehat{\mathfrak{kv}}_2$, we have $u(x+y) = [x,a] + [y,b] = 0$. Consider terms linear in x in both a and b. First, observe that b does not contain terms of the form $\mathrm{ad}_y^m(x)$ for $m \geq 1$ since $\mathrm{ad}_y^{m+1}(x) \notin \mathrm{im}(\mathrm{ad}_x)$. In particular, this applies to all m odd. Next, note that a does not contain terms of the form $\mathrm{ad}_y^m(x)$ for m odd since in this case $[x, \mathrm{ad}_y^m(x)] \notin \mathrm{im}(\mathrm{ad}_y)$. Hence, $\mathrm{div}(u) = \mathrm{tr}(x\partial_x a + y\partial_y b)$ does not contain terms of the form $\mathrm{tr}(xy^m)$ for m odd, and $f_k = 0$ for all $k = m+1$ even. Finally, Taylor coefficients of f are characters of $\widehat{\mathfrak{kv}}_2$ since they vanish on $\mathfrak{kv}_2$, and on $[\widehat{\mathfrak{kv}}_2, \widehat{\mathfrak{kv}}_2] \subset \mathfrak{kv}_2$. □

4.2. **The Grothendieck-Teichmüller Lie algebra.** Recall that the Grothendieck-Teichmüller Lie algebra $\mathfrak{grt}$ was defined by Drinfeld [7] in the following way. It is spanned by derivations $(0, \psi) \in \mathfrak{tder}_2$ which satisfy the following three relations

$$\psi(x, y) = -\psi(y, x), \tag{13}$$

$$\psi(x, y) + \psi(y, z) + \psi(z, x) = 0 \tag{14}$$

for $x + y + z = 0$ (that is, one can put $z = -x - y$),

$$\psi(t^{1,2}, t^{2,34}) + \psi(t^{12,3}, t^{3,4}) = \psi(t^{2,3}, t^{3,4}) + \psi(t^{1,23}, t^{23,4}) + \psi(t^{1,2}, t^{2,3}), \tag{15}$$

where the last equation takes values in the Lie algebra $\mathfrak{t}_4$ and $t^{1,23} = t^{1,2} + t^{1,3}$ *etc.* Note that defining equations of $\mathfrak{grt}$ have no solutions in degrees one and two. The Lie bracket induced on solutions of (13), (14),(15) is called Ihara bracket,

$$[\psi_1, \psi_2]_{\mathrm{Ih}} = (0, \psi_1)(\psi_2) - (0, \psi_2)(\psi_1) + [\psi_1, \psi_2].$$

Theorem 4.1. *The map $\nu : \psi \mapsto (\psi(-x-y, x), \psi(-x-y, y))$ is an injective Lie algebra homomorphism mapping $\mathfrak{grt}$ to $\widehat{\mathfrak{kv}}_2$.*

We split the proof of Theorem 4.1 into several steps.

Proposition 4.2. *Let $\psi \in \mathfrak{grt}$. Then, $\Psi = \nu(\psi)$ verifies*

$$\mathrm{d}\Psi = \psi(t^{1,2}, t^{2,3}). \tag{16}$$

We defer the proof of this proposition to Appendix.

Proposition 4.3. $\mathrm{im}(\nu) \subset \widehat{\mathfrak{kv}}_2$.

Proof. Using equation (16) we compute

$$\delta(\Psi(x+y)) = (\mathrm{d}\Psi)(x+y+z) = \psi(t^{1,2}, t^{2,3})(x+y+z) = 0$$

because $t^{1,2}, t^{2,3} \in \mathfrak{sder}_3$. Since $\Psi \in \mathfrak{tder}_2$ is of degree at least three, $\Psi(x+y)$ is of degree at least four, and by Theorem 2.1 this implies $\Psi(x+y) = 0$ and $\Psi \in \mathfrak{sder}_2$.

Similarly, we compute

$$\delta(\mathrm{div}(\Psi)) = \mathrm{div}(\mathrm{d}\Psi) = \mathrm{div}(\psi(t^{1,2}, t^{2,3})) = 0$$

since $t^{1,2}, t^{2,3} \in \mathfrak{kv}_3$. By Theorem 2.1, this implies $\mathrm{div}(\Psi) \in \mathrm{im}(\delta)$ and $\Psi \in \widehat{\mathfrak{kv}}_2$. □

Proposition 4.4. *$\nu : \mathfrak{grt} \to \widehat{\mathfrak{kv}}_2$ is a Lie algebra homomorphism.*

Proof. Let $\psi_1, \psi_2 \in \mathfrak{grt}$ and compute $(a, b) = [\nu(\psi_1), \nu(\psi_2)]$,

$$\begin{array}{rcl} a(x,y) & = & \nu(\psi_1)(\psi_2(-x-y,x)) - \nu(\psi_2)(\psi_1(-x-y,x) \\ & + & [\psi_1(-x-y,x), \psi_2(-x-y,x)] \\ & = & ((0,\psi_1)(\psi_2) - (0,\psi_2)(\psi_1) + [\psi_1,\psi_2])\,(-x-y,x), \end{array}$$

where we used that $\nu(\psi_1), \nu(\psi_2) \in \mathfrak{sder}_2$. Similarly, we have

$$\begin{array}{rcl} b(x,y) & = & \nu(\psi_1)(\psi_2(-x-y,y)) - \nu(\psi_2)(\psi_1(-x-y,y) \\ & + & [\psi_1(-x-y,y), \psi_2(-x-y,y)] \\ & = & ((0,\psi_1)(\psi_2) - (0,\psi_2)(\psi_1) + [\psi_1,\psi_2])\,(-x-y,y). \end{array}$$

In conclusion, $[\nu(\psi_1), \nu(\psi_2)] = \nu([\psi_1, \psi_2]_{\mathrm{Ih}})$, as required. □

This observation completes the proof of Theorem 4.1.

It is known [11, 7] that there exit elements $\sigma_{2n+1} \in \mathfrak{grt}$ of degree $2n+1$ for all $n = 1, 2, \dots$ Modulo the double commutator ideal $[[\mathfrak{lie}_2, \mathfrak{lie}_2], [\mathfrak{lie}_2, \mathfrak{lie}_2]]$, σ_{2n+1} has the following form,

$$\sigma_{2n+1} = \sum_{k=1}^{2n} \frac{(2n+1)!}{k!(2n+1-k)!} \operatorname{ad}_x^{k-1} \operatorname{ad}_y^{2n-k} [x, y]. \tag{17}$$

Proposition 4.5. $f \circ \nu(\sigma_{2n+1}) = -x^{2n+1}$.

Proof. Equation (17) implies that the linear in x part of $a(x, y) = \sigma(-x-y, x)$ is equal to $(2n+1) \operatorname{ad}_y^{2n} x$, and the linear in x part of $b(x, y) = \sigma(-x-y, y)$ vanishes. Hence, the coefficient in front of $\operatorname{tr}(xy^{2n})$ in $\operatorname{div}(\nu(\sigma_{2n+1}))$ is equal to $(2n+1)$, and

$$\operatorname{div}(\nu(\sigma_{2n+1})) = -\operatorname{tr}(x^{2n+1} - (x+y)^{2n+1} + y^{2n+1}) = -\delta \operatorname{tr}(x^{2n+1}),$$

which implies $f(\nu(\sigma_{2n+1})) = -x^{2n+1}$. □

Theorem 4.1 shows that $\widehat{\mathfrak{kv}}_2$ is infinite dimensional, and Proposition 4.5 implies that characters $f_k, k = 3, 5, \dots$ are surjective. The Lie algebra $\widehat{\mathfrak{kv}}_2$ contains a central one dimensional Lie subalgebra $\mathbb{K}t$ for $t = (y, x)$, and a Lie subalgebra isomorphic to the Lie algebra $\mathfrak{grt}$. This observation suggests the following conjecture on the structure of $\widehat{\mathfrak{kv}}_2$.

Conjecture. The Lie algebra $\widehat{\mathfrak{kv}}_2$ is isomorphic to a direct sum of the Grothendieck-Teichmüller Lie algebra $\mathfrak{grt}$ and a one dimensional Lie algebra with generator in degree one, $\widehat{\mathfrak{kv}}_2 \cong \mathbb{K}t \oplus \mathfrak{grt}$.

***Remark* 4.1.** The Deligne-Drinfeld conjecture (see Section 6, [7]) states that $\mathfrak{grt}$ is a free Lie algebra with generators σ_{2n+1}. In [18], Racinet introduced a graded Lie algebra $\mathfrak{dmr}_0$ related to combinatorics of multiple zeta values. A numerical experiment of [10] shows that up to degree 19 the Lie algebra $\mathfrak{dmr}_0$ is freely generated by σ_{2k+1}, and that $\mathfrak{dmr}_0 \subset \mathfrak{grt}$. A numerical computation by Albert and the second author [1] shows that up to degree 16 the dimensions of graded components of $\widehat{\mathfrak{kv}}_2$ coincide with those of $\mathbb{K}t \oplus \mathfrak{lie}(\sigma_3, \sigma_5, \dots)$ (up to degree 7, the computation has been done by Podkopaeva [16]) . Since $\mathbb{K}t \oplus \nu(\mathfrak{grt}) \subset \widehat{\mathfrak{kv}}_2$, we conclude that the Conjecture stated above and the Deligne-Drinfeld conjecture are verified up to degree 16.

5. The Kashiwara-Vergne problem

5.1. **Automorphisms of free Lie algebras.** Recall that one can associate a group G to a positively graded Lie algebra $\mathfrak{g} = \prod_{k=1}^{\infty} \mathfrak{g}_k$ with all graded components of finite dimension. G coincides with $\mathfrak{g}$ as a set, and the group multiplication is defined by the Campbell-Hausdorff formula. If $\mathfrak{g}$ is finite dimensional, G is the connected and simply connected Lie group with Lie algebra $\mathfrak{g}$. Even for $\mathfrak{g}$ infinite dimensional we shall denote the map identifying $\mathfrak{g}$ and G by $\exp : \mathfrak{g} \to G$ and its inverse by $\ln : G \to \mathfrak{g}$. Then, the definition of the group multiplication in G reads: $\exp(u)\exp(v) = \exp(\operatorname{ch}(u, v))$.

Lie algebras $\mathfrak{tder}_n, \mathfrak{sder}_n, \mathfrak{kv}_n$ and $\widehat{\mathfrak{kv}}_2$ introduced in the previous Section are positively graded, and all their graded components are finite dimensional. Hence, they integrate to groups. We shall denote these groups by $\mathrm{TAut}_n, \mathrm{SAut}_n, \mathrm{KV}_n$ and $\widehat{\mathrm{KV}}_2$, respectively. The natural actions of $\mathfrak{tder}_n, \mathfrak{sder}_n, \mathfrak{kv}_n$ and $\widehat{\mathfrak{kv}}_2$ on $\mathfrak{lie}_n$ and on $\mathfrak{tr}_n$ lift to actions of the corresponding groups given by formula

$$\exp(u)(a) := \sum_{n=0}^{\infty} u^n(a),$$

where $u^n(a)$ is the n-tuple action of the derivation u on a. Note that the group TAut_n consists of automorphisms g of $\mathfrak{lie}_n$ with the property that for each $i = 1, \ldots, n$ there is an inner automorphism g_i such that $g(x_i) = g_i(x_i)$. Furthermore, the group SAut_n is a subgroup of TAut_n singled out by the condition $g(x) = x$ for $x = \sum_{i=1}^n x_i$.

In order to discuss the groups KV_n and $\widehat{\mathrm{KV}}_2$ we introduce a Lie group 1-cocycle $j : \mathrm{TAut}_n \to \mathfrak{tr}_n$ which integrates the Lie algebra 1-cocycle $\mathrm{div} : \mathfrak{tder}_n \to \mathfrak{tr}_n$.

Proposition 5.1. *There is a unique map $j : \mathrm{TAut}_n \to \mathfrak{tr}_n$ which satisfies the group cocycle condition*

$$j(gh) = j(g) + g \cdot j(h), \tag{18}$$

and has the property

$$\frac{d}{ds} j(\exp(su))|_{s=0} = \mathrm{div}(u). \tag{19}$$

Proof. Let $\mathfrak{g}$ be a semi-direct sum of $\mathfrak{tder}_n$ and $\mathfrak{tr}_n$. The cocycle property of the divergence implies that the map $\mathfrak{tder}_n \to \mathfrak{g}$ defined by formula $u \mapsto u + \mathrm{div}(u)$ is a Lie algebra homomorphism. Define $j(\exp(u))$ by formula $\exp(u + \mathrm{div}(u)) = \exp(j(\exp(u)))\exp(u)$. For $g = \exp(u)$ and $h = \exp(v)$ we have

$$\exp(j(gh))gh = (\exp(j(g))g)(\exp(j(h))h) = \exp(j(g) + g \cdot j(h))gh$$

which implies (18).

Equations (18) and (19) imply the following differential equation for j:

$$\frac{d}{ds} j(\exp(su)) = \mathrm{div}(u) + u \cdot j(\exp(su)).$$

Given the initial condition $j(e) = 0$, this equation admits a unique solution,

$$j(\exp(u)) = \frac{e^u - 1}{u} \cdot \mathrm{div}(u)$$

which proves uniqueness of the cocycle j. $\square$

***Remark* 5.1.** Equation (18) for $h = g^{-1}$ implies $j(g^{-1}) = -g^{-1} \cdot j(g)$.

Proposition 5.2. *The group KV_n is isomorphic to a subgroup of SAut_n singled out by the condition $j(g) = 0$.*

Proof. Let $u \in \mathfrak{kv}_n$. Then, $\mathrm{div}(u) = 0$ implies $j(\exp(u)) = 0$ and $\exp(u) \in \mathrm{KV}_n$. In the other direction, $j(g) = 0$ for $g = \exp(u)$ implies $\mathrm{div}(u) = u/(e^u - 1) \cdot j(g) = 0$, and $u \in \mathfrak{kv}_n$. $\square$

Proposition 5.3. *Let $g \in \widehat{\mathrm{KV}}_2$. Then, $j(g) \in \mathrm{im}(\delta)$.*

Proof. Let $u \in \widehat{\mathfrak{kv}}_2$. Then, $\mathrm{div}(u) = \mathrm{tr}(f(x) + f(y) - f(x+y))$ with $f \in x^2\mathbb{K}[[x]]$. Note that $u \cdot \mathrm{tr}(f(x)) = u \cdot \mathrm{tr}(f(y)) = 0$ since u acts as an inner derivation on x and as a (different) inner derivation on y. Furthermore, $u \cdot \mathrm{tr}(f(x+y)) = 0$ because $u(x+y) = 0$. Hence, $u \cdot \mathrm{div}(u) = 0$, and $j(\exp(u)) = (e^u - 1)/u \cdot \mathrm{div}(u) = \mathrm{div}(u) \in \mathrm{im}(\delta)$. $\square$

5.2. **Scaling transformations.** For $0 \neq s \in \mathbb{K}$ consider an automorphism A_s of the free Lie algebra $\mathfrak{lie}_n$ such that $A_s : x_i \mapsto sx_i$ for all $i = 1, \dots, n$. We have $A_{s_1}A_{s_2} = A_{s_1+s_2}$, $(A_s)^{-1} = A_{s^{-1}}$, and $A_1 = e$. For example, we compute

$$A_s(\mathrm{ch}(x,y)) = \mathrm{ch}(sx, sy) = s\,\mathrm{ch}_s(x,y).$$

Note that for $g \in \mathrm{TAut}_n$ an automorphism $g_s = A_s g A_s^{-1}$ is also an element of TAut_n. Indeed, $g(x_i) = g_i(x_i) = e^a x_i e^{-a}$, where g_i is an inner automorphism of $\mathfrak{lie}_n$ given by conjugation by e^a for $a \in \mathfrak{lie}_n$. Then,

$$g_s(x_i) = A_s g A_s^{-1}(x_i) = s^{-1} A_s g(x_i) = e^{A_s(a)} x_i e^{-A_s(a)}$$

proving $g_s \in \mathrm{TAut}_n$. Moreover, since $a_s = A_s(a)$ is analytic in s with $a_0 = 0$, we conclude that g_s is also analytic in s with $g_0 = e$. We shall denote the derivative of g_s with respect to the scaling parameter s by $\dot{g}_s$.

Proposition 5.4. *Let $g \in \mathrm{TAut}_n$. Then, $u_s := \dot{g}_s g_s^{-1}$ has the property $u_s = s^{-1} A_s u A_s^{-1}$, where $u = u_1$.*

Proof. Let l be a derivation of $\mathfrak{lie}_n$ defined by the property $l(x_i) = x_i$ for all i. We have, $\dot{A}_s A_s^{-1} = s^{-1} l$, and

$$u_s = \dot{g}_s g_s^{-1} = s^{-1}(l - g_s l g_s^{-1}) = s^{-1} A_s (l - g l g^{-1}) A_s^{-1}.$$

Hence, $u = u_1 = l - glg^{-1}$ and $u_s = s^{-1} A_s u A_s^{-1}$ as required. □

Note that $u_s = s^{-1}(a_1(sx_1, sx_2, \dots), \dots)$ is analytic in s with u_0 given by the degree one component of u. For $g \in \mathrm{TAut}_n$ we denote by $\kappa_s : \mathrm{TAut}_n \to \mathfrak{tder}_n$ the map $\kappa_s : g \mapsto u_s = s^{-1} A_s (l - glg^{-1}) A_s^{-1}$, and we put $\kappa = \kappa_1$. Similarly, let $u \in \mathfrak{tder}_n$, set $u_s = s^{-1} A_s u A_s^{-1}$ and denote by $E_s : \mathfrak{tder}_n \to \mathrm{TAut}_n$ the map $E_s : u \mapsto g_s$ defined as a unique solution of the ordinary differential equation $\dot{g}_s g_s^{-1} = u_s$ with initial condition $g_0 = e$. We denote $E = E_1$.

Proposition 5.5. *The maps E and κ are inverse to each other.*

Proof. Let $g \in \mathrm{TAut}_n$ and consider $u = \kappa(g)$. Then, $u_s = s^{-1} A_s u A_s^{-1} = \kappa_s(g)$ and $g_s = A_s g A_s^{-1}$ is a solution of the ordinary differential equation (ODE) $\dot{g}_s = u_s g_s$ with initial condition $g_0 = e$. But so does $E_s(u)$. Hence, by the uniqueness property for solutions of ODEs, we have $g = E(u) = E(\kappa(g))$. In the other direction, let $u \in \mathfrak{tder}_n$ and consider $g = E(u)$. Then, $g_s = A_s g A_s^{-1} = E_s(u)$ and $\kappa_s(g) = \dot{g}_s g_s^{-1} = u_s$. Hence, $\kappa(E(u)) = u$ as required. □

Automorphisms A_s extend from $\mathfrak{lie}_n$ to Ass_n and to $\mathfrak{tr}_n$. Note that for $u \in \mathfrak{tder}_n$ and $u_s = s^{-1} A_s u A_s^{-1}$ we have $\mathrm{div}(u_s) = s^{-1} A_s \cdot \mathrm{div}(u)$. Similarly, for $g \in \mathrm{TAut}_n$ and $g_s = A_s g A_s^{-1}$ we obtain $j(g_s) = A_s \cdot j(g)$.

Proposition 5.6. *Let $g \in \mathrm{TAut}_n$ and $u = \kappa(g)$. Then,*

$$\frac{dj(g_s)}{ds} = u_s \cdot j(g_s) + \mathrm{div}(u_s). \tag{20}$$

Proof. We compute

$$j(g_q) = j(g_q g_s^{-1} g_s) = j(g_q g_s^{-1}) + (g_q g_s^{-1}) \cdot j(g_s).$$

Taking a derivative with respect to q and putting $q = s$ yields the equation (20), as required. □

For $g = E(u)$, equation (20) at $s = 1$ implies the following relation between $j(g)$ and $\mathrm{div}(u)$: $l \cdot j(g) = u \cdot j(g) + \mathrm{div}(u)$. By using equation $u = l - glg^{-1}$ we obtain $glg^{-1} \cdot j(g) = \mathrm{div}(u)$.

5.3. **The generalized Kashiwara-Vergne problem.** The generalized Kashiwara-Vergne (KV) problem is the following question:

Generalized KV problem: Find an element $F \in \mathrm{TAut}_2$ with the properties

$$F(x+y) = \mathrm{ch}(x,y), \tag{21}$$

and

$$j(F) \in \mathrm{im}(\tilde{\delta}). \tag{22}$$

We shall denote the set of solutions of the generalized KV problem by $\mathrm{Sol}(\widehat{\mathrm{KV}})$. For any $s \in \mathbb{K}$ one can introduce rescaled versions of equations (21) and (22) as $F(x+y) = \mathrm{ch}_s(x,y)$ and $j(F) \in \mathrm{im}(\tilde{\delta}_s)$. We shall denote the corresponding set of solutions by $\mathrm{Sol}_s(\widehat{\mathrm{KV}})$. For $s = 0$, $\mathrm{Sol}_0(\widehat{\mathrm{KV}}) = \widehat{\mathrm{KV}}_2$. For all $s \neq 0$, $\mathrm{Sol}_s(\widehat{\mathrm{KV}}) \cong \mathrm{Sol}(\widehat{\mathrm{KV}})$ with isomorphism given by the scaling transformation $F \mapsto F_s = A_s F A_s^{-1}$.

Proposition 5.7. *Let $F \in \mathrm{Sol}(\widehat{\mathrm{KV}})$ and $a \in \mathfrak{tr}_1$. Then, $\tilde{\delta} a = F \cdot (\delta a)$.*

Proof. We have, $a = \mathrm{tr}(f(x))$ for some formal power series f. We compute

$$\begin{aligned} F \cdot (\delta a) &= F \cdot \mathrm{tr}(f(x) - f(x+y) + f(y)) \\ &= \mathrm{tr}(f(x) - f(\mathrm{ch}(x,y)) + f(y)) = \tilde{\delta} a. \end{aligned}$$

Here we used that $F \cdot \mathrm{tr}(f(x)) = \mathrm{tr}(f(x))$ and $F \cdot \mathrm{tr}(f(y)) = \mathrm{tr}(f(y))$ since F acts as an inner automorphism on x and as a (different) inner automorphism on y. We also used that $F \cdot \mathrm{tr}(f(x+y)) = \mathrm{tr}(f(\mathrm{ch}(x,y)))$ because $F(x+y) = \mathrm{ch}(x,y)$. □

The fact that $\mathrm{Sol}(\widehat{\mathrm{KV}})$ is non empty has been proved in [2]. We shall give an alternative proof in the end of the paper. In order to preserve the logic of the presentation, we shall not be using the existence of solutions of the KV problem until we prove it.

Theorem 5.1. *Assume that $\mathrm{Sol}(\widehat{\mathrm{KV}})$ is nonempty. Then, the group $\widehat{\mathrm{KV}}_2$ acts on $\mathrm{Sol}(\widehat{\mathrm{KV}})$ by multiplications on the right. This action is free and transitive.*

Proof. Let $F \in \mathrm{Sol}(\widehat{\mathrm{KV}})$ and $g \in \widehat{\mathrm{KV}}_2$. Then, $(Fg)(x+y) = F(g(x+y)) = F(x+y) = \mathrm{ch}(x,y)$ and $j(Fg) = j(F) + F \cdot j(g)$. Note that $j(F) \in \mathrm{im}(\tilde{\delta})$ and, by Proposition 5.3, $j(g) \in \mathrm{im}(\delta)$. Hence, $F \cdot j(g) \in \mathrm{im}(\tilde{\delta})$ and $j(Fg) \in \mathrm{im}(\tilde{\delta})$. In conclusion, $\widehat{\mathrm{KV}}_2$ acts on the set $\mathrm{Sol}(\widehat{\mathrm{KV}})$ by right multiplications. This action is free since the multiplication on the right is.

Let $F_1, F_2 \in \mathrm{Sol}(\widehat{\mathrm{KV}})$ and put $g = F_1^{-1} F_2$. We have, $g(x+y) = F_1^{-1}(F_2(x+y)) = F_1^{-1}(\mathrm{ch}(x,y)) = x + y$ and $j(g) = j(F_1^{-1}) + F_1^{-1} \cdot j(F_2) = F_1^{-1} \cdot (j(F_2) - j(F_1))$. Since $j(F_1), j(F_2) \in \mathrm{im}(\tilde{\delta})$, we have $F_1^{-1} \cdot (j(F_2) - j(F_1)) \in \mathrm{im}(\delta)$ and $g \in \widehat{\mathrm{KV}}_2$. Hence, the action of $\widehat{\mathrm{KV}}_2$ on $\mathrm{Sol}(\widehat{\mathrm{KV}})$ is transitive. □

The Kashiwara-Vergne problem was stated in [13] in somewhat different terms. We shall now establish a relation between our approach and the original formulation of the KV problem (KV conjecture).

Theorem 5.2. *An element $F \in \mathrm{TAut}_2$ is a solution of the generalized KV problem if and only if $u = \kappa(F) = (A(x,y), B(x,y))$ satisfies the following two properties,*

$$x + y - \mathrm{ch}(y,x) = (1 - \exp(-\mathrm{ad}_x))A(x,y) + (\exp(\mathrm{ad}_y) - 1)B(x,y), \tag{23}$$

and

$$\mathrm{div}(u) \in \mathrm{im}(\tilde{\delta}). \tag{24}$$

Proof. First, we show that equation $F(x+y) = \mathrm{ch}(x,y)$ is equivalent to equation $(d/ds - u_s)\,\mathrm{ch}_s(x,y) = 0$. Indeed, we have

$$F_s(x+y) = A_s F A_s^{-1}(x+y) = s^{-1}A_s F(x+y) = s^{-1}A_s\,\mathrm{ch}(x,y) = \mathrm{ch}_s(x,y)$$

and

$$u_s(\mathrm{ch}_s(x,y)) = \dot{F}_s F_s^{-1}(\mathrm{ch}_s(x,y)) = \dot{F}_s(x+y) = \frac{d}{ds}\,(F_s(x+y)) = \frac{d\,\mathrm{ch}_s(x,y)}{ds}.$$

In the other direction,

$$\frac{d}{ds}\,F_s^{-1}(\mathrm{ch}_s(x,y)) = F_s^{-1}\left(\frac{d}{ds} - u_s\right)\mathrm{ch}_s(x,y) = 0$$

implies that $F_s^{-1}(\mathrm{ch}_s(x,y))$ is independent of s, and comparison with the value at $s=0$ gives $F_s^{-1}(\mathrm{ch}_s(x,y)) = x + y$ or $F_s(x+y) = \mathrm{ch}_s(x,y)$.

A straightforward calculation (see Lemma 3.2 of [13]) shows that equation $(d/ds - u_s)\,\mathrm{ch}_s(x,y) = 0$ is equivalent to (23).

Finally, we compare equations (22) and (24). Let $F \in \mathrm{Sol}(\widehat{\mathrm{KV}})$, $j(F) = \tilde{\delta}(\mathrm{tr}(f(x)))$. We compute,

$$\begin{aligned}
\mathrm{div}(u) = FlF^{-1}\cdot j(F) &= FlF^{-1}\cdot \mathrm{tr}(f(x) - f(\mathrm{ch}(x,y)) + f(y)) \\
&= Fl\cdot \mathrm{tr}(f(x) - f(x+y) + f(y)) \\
&= F\cdot \mathrm{tr}(\phi(x) - \phi(x+y) + \phi(y)) \\
&= \mathrm{tr}(\phi(x) - \phi(\mathrm{ch}(x,y)) + \phi(y)) \in \mathrm{im}(\tilde{\delta}),
\end{aligned}$$

where $\phi = xf'(x)$ results from the action of the derivation $l : x^n \mapsto nx^n$. In the other direction, assume $\mathrm{div}(u) \in \mathrm{im}(\tilde{\delta})$. Then, for $u_s = s^{-1}A_s u A_s^{-1}$ we have $\mathrm{div}(u_s) \in \mathrm{im}(\tilde{\delta}_s)$. Equation $(d/ds - u_s)j(F_s) = \mathrm{div}(u_s)$ implies $d/ds(F_s^{-1}\cdot j(F_s)) = F_s^{-1}\cdot \mathrm{div}(u_s) \in \mathrm{im}(\delta)$. Hence, $F_s^{-1}\cdot j(F_s) \in \mathrm{im}(\delta)$ and $j(F_s) \in \mathrm{im}(\tilde{\delta}_s)$. □

***Remark* 5.2.** Let $\mathfrak{g}$ be a finite dimensional Lie algebra over $\mathbb{K}$. Then, $A, B \in \mathfrak{lie}_2$ define a pair of formal power series on $\mathfrak{g}\times\mathfrak{g}$ with values in $\mathfrak{g}$ which satisfy equation (23). By applying the adjoint representation to the equation $\mathrm{div}(u) = \tilde{\delta}(\phi)$ we obtain an equality in formal power series on $\mathfrak{g}\times\mathfrak{g}$ with values in $\mathbb{K}$,

$$\mathrm{Tr}(\mathrm{ad}_x \circ d_x A + \mathrm{ad}_y \circ d_y B) = \mathrm{Tr}(\phi(x) + \phi(y) - \phi(\mathrm{ch}(x,y))). \tag{25}$$

Here $(d_xA)(z) = dA(x+tz,y)/dt|_{t=0}$ and $(d_yB)(z) = dB(x, y+tz)/dt|_{t=0}$. Indeed, for $A \in \mathfrak{lie}_2$ consider $U(x,y,z) = dA(x+tz,y)/dt|_{t=0} \in \mathfrak{lie}_3$. It has the form $U = \mathrm{ad}_a(z)$ for some $a \in \mathrm{Ass}_2$. We compute (see equation (5)),

$$a = \partial_z U(x,y,z) = \left(\frac{d}{dt}\,\partial_z A(x+tz,y)\right)|_{t=0} = \partial_x A$$

showing $\mathrm{ad}(\partial_x A) = d_x A$. Similarly, $\mathrm{ad}(\partial_y B) = d_y B$.

6. Duflo functions

Let $F \in \mathrm{Sol}(\widehat{\mathrm{KV}})$. Then, $j(F) = \mathrm{tr}(f(x) - f(\mathrm{ch}(x,y)) + f(y))$, and $\mathrm{div}(\kappa(F)) = \mathrm{tr}(\phi(x) - \phi(\mathrm{ch}(x,y)) + \phi(y))$ for $f, \phi \in x^2\mathbb{K}[[x]]$. We shall call $f(x)$ a Duflo function of F. In this Section, we describe the set of formal power series which may arise as Duflo functions associated to solutions of the KV problem.

Proposition 6.1. *Let $u \in \mathfrak{tder}_2$ and assume that it satisfies equations* (23) *and* (24) *with* $\mathrm{div}(u) = \tilde{\delta}(\mathrm{tr}(\phi(x)))$. *Then, the even part of the formal power series ϕ is given by the following formula*

$$\phi_{even}(x) = \frac{1}{2}\left(\phi(x) + \phi(-x)\right) = \frac{1}{2}\sum_{k=2}^{\infty} \frac{B_n}{n!}\, x^n = \frac{1}{2}\left(\frac{x}{e^x - 1} - 1 + \frac{x}{2}\right),$$

where B_n are Bernoulli numbers.

Proof. We follow [3] (see Remark 4.3). Write $A(x,y) = \alpha(\mathrm{ad}_x)y + \ldots, B(x,y) = bx + \beta(\mathrm{ad}_x)y + \ldots$, where $b \in \mathbb{K}, \alpha, \beta \in \mathbb{K}[[x]]$, and $\ldots$ stand for the terms containing at least two y's. Replace $y \mapsto sy$ in equation (23), and compute the first and second derivatives in s at $s = 0$. The first derivative yields

$$y - \frac{\mathrm{ad}_x}{e^{\mathrm{ad}_x} - 1}\, y = (1 - e^{-\mathrm{ad}_x})\alpha(\mathrm{ad}_x)y - b[x,y],$$

and we obtain

$$\alpha(t) = b\,\frac{t}{1 - e^{-t}} - \frac{t}{(e^t - 1)(1 - e^{-t})} + \frac{1}{1 - e^{-t}}.$$

Note that elements of $\mathfrak{lie}_2$ quadratic in the generator y are in bijection with skew-symmetric formal power series in two variables,

$$a(u,v) = \sum_{i,j=0}^{\infty} a_{i,j} u^i v^j \mapsto \sum_{i,j=0}^{\infty} a_{i,j} [\mathrm{ad}_x^i\, y, \mathrm{ad}_x^j\, y]$$

The second derivative of (23) gives the following equality in formal power series,

$$\frac{1}{2}\,\frac{(u+v)(e^u - e^v) - (u-v)(e^{u+v} - 1)}{(e^{u+v} - 1)(e^u - 1)(e^v - 1)} = (1 - e^{-(u+v)})a_2(u,v) + \frac{b}{2}(u - v) + (\beta(v) - \beta(u)),$$

where the left hand side corresponds to the second derivative of the Campbell-Hausdorff series $-\mathrm{ch}(sy, x)$, and $a_2(u,v)$ represents the second derivative of $A(x, sy)$. By putting $v = -u$ in the last equation we obtain,

$$\beta_{odd}(t) = \frac{b}{2}\,t - \frac{1}{2}\,\frac{t}{(e^t - 1)(1 - e^{-t})} + \frac{1}{4}\,\frac{e^t + 1}{e^t - 1}\,.$$

Here $\beta_{odd}(t) = (\beta(t) - \beta(-t))/2$.

Finally, consider equation (25) and compute the contribution linear in y (that is, of the form $\mathrm{tr}(f(x)y)$) on the left hand side and on the right hand side. Since we only control the odd part of the function $\beta(t)$, we obtain an equation in odd formal power series,

$$\beta_{odd}(t) - \alpha_{odd}(t) = -(\phi'(t))_{odd} = -(\phi_{even})'(t)$$

which implies

$$\phi_{even}(t) = \frac{1}{2}\left(\frac{t}{e^t - 1} - 1 + \frac{t}{2}\right),$$

as required. □

Proposition 6.2. *Let $F \in \mathrm{Sol}(\widehat{\mathrm{KV}})$ and $f \in x^2\mathbb{K}[[x]]$ such that $j(F) = \tilde{\delta}(\mathrm{tr}(f(x)))$. Then, the even part of $f(x)$ coincides with the function $f_{even}(x) = \frac{1}{2}\ln(e^{x/2} - e^{-x/2})/x)$, and for every odd formal power series $f_{odd}(x) = \sum_{k=1}^{\infty} f_{2k+1}x^{2k+1}$ there is an element $F \in \mathrm{Sol}(\widehat{\mathrm{KV}})$ such that $j(F) = \tilde{\delta}(\mathrm{tr}(f_{even}(x) + f_{odd}(x)))$.*

Proof. Let f and ϕ be the power series in $j(F) = \tilde{\delta}(\mathrm{tr}(f(x)))$ and $\mathrm{div}(u) = \tilde{\delta}(\mathrm{tr}(\phi(x)))$ for $u = \kappa(F)$. Then, we have (see the proof of Theorem 5.2) $\phi(s) = sf'(s)$. By Proposition 6.1, we obtain

$$f_{even} = \int \frac{\phi_{even}(s)}{s}\, ds = \frac{1}{2}\sum_{k=2}^{\infty} \frac{B_k}{k \cdot k!}\, s^k = \frac{1}{2}\ln\left(\frac{e^{s/2} - e^{-s/2}}{s}\right).$$

Let $F \in \mathrm{Sol}(\widehat{\mathrm{KV}})$ with $j(F) = \tilde{\delta}(\mathrm{tr}(f(x)))$, and $g \in \widehat{\mathrm{KV}}_2$ with $j(g) = \delta(\mathrm{tr}(h(x)))$. Then, $Fg \in \mathrm{Sol}(\widehat{\mathrm{KV}})$ and

$$j(Fg) = j(F) + F \cdot j(g) = \tilde{\delta}(\mathrm{tr}(f(x) + h(x))).$$

Put $g = \exp(u)$ for $u \in \widehat{\mathfrak{kv}}_2$, and compute $j(g) = (e^u - 1)/u \cdot \mathrm{div}(u) = \mathrm{div}(u)$. By choosing $u = -\sum_{k=1}^{\infty} h_{2k+1}\nu(\sigma_{2k+1})$ we obtain $j(g) = \mathrm{div}(u) = \delta(\mathrm{tr}(h(x)))$ for $h(x) = \sum_{k=1}^{\infty} h_{2k+1}x^{2k+1}$. Hence, by an appropriate choice of $g \in \widehat{\mathrm{KV}}_2$, one can make the odd part of the linear combination $f(x) + h(x)$ equal to any given odd power series without linear term. □

***Remark* 6.1.** The group $\widehat{\mathrm{KV}}_2$ acts on $\mathrm{Sol}(\widehat{\mathrm{KV}})$, and this action descends to the space of formal power series $x^2\mathbb{K}[[x]]$ along the map $f : \mathrm{Sol}(\widehat{\mathrm{KV}}) \to x^2\mathbb{K}[[x]]$. In Proposition 6.2 we have used this action to change the odd part of $f(F)$. Previously, this action (for the Grothendieck-Teichmüller subgroup $\mathrm{GRT} \subset \widehat{\mathrm{KV}}_2$) on the Duflo functions has been described in [15] (see Theorem 7).

Proposition 6.3. *Let $F = \exp(u) \in \mathrm{Sol}(\widehat{\mathrm{KV}})$ with $u = (a, b) \in \mathfrak{tder}_2$ such that*

$$\begin{aligned} a(x,y) &= a_0 y + \alpha(\mathrm{ad}_y)x + \dots \\ b(x,y) &= b_0 x + \beta(\mathrm{ad}_y)x + \dots, \end{aligned}$$

where $a_0, b_0 \in \mathbb{K}$, $\alpha, \beta \in s\mathbb{K}[[s]]$, and $\dots$ stand for terms which contain at least two x. Then, the Duflo function associated to F satisfies equation $f' = \beta - \alpha$.

Proof. Consider the part of $j(F) = \mathrm{tr}(f(x) - f(\mathrm{ch}(x, y)) + f(y))$ linear in the generator x. On the one hand, we have

$$j(F)_{x-lin} = \mathrm{tr}(f(x) - f(\mathrm{ch}(x, y)) + f(y))_{x-lin} = -\,\mathrm{tr}(f'(y)x).$$

On the other hand, we obtain

$$j(F)_{x-lin} = \left(\frac{e^u - 1}{u} \cdot \mathrm{div}(u)\right)_{x-lin} = \mathrm{div}(u)_{x-lin}.$$

Here we used the fact that linear in x terms cannot arise under the action of elements of $\mathfrak{tder}_2$ on $\mathfrak{tr}_2$. Indeed, such a term would be of the form $\mathrm{tr}(h(y)[x, y])$ for some formal power series h, and $\mathrm{tr}(h(y)[x, y]) = \mathrm{tr}(h(y)yx - h(y)xy) = 0$.

Finally, we compute

$$\mathrm{div}(u)_{x-lin} = \mathrm{tr}(x(\partial_x a) + y(\partial_y b))_{x-lin} = \mathrm{tr}(x\alpha(y) - \beta(y)x) = \mathrm{tr}((\alpha(y) - \beta(y))x).$$

Comparison with the first equation yields $f'(y) = \beta(y) - \alpha(y)$, as required. □

In the original formulation of the Kashiwara-Vergne problem the Duflo function f was assumed to be even.

KV problem: Find an element $F \in \mathrm{TAut}_2$ such that $F(x+y) = \mathrm{ch}(x,y)$ and $j(F) = \frac{1}{2}\sum_{k=2}^{\infty} \frac{B_k x^k}{k \cdot k!} = \frac{1}{2}\ln((e^{x/2} - e^{-x/2})/x)$.

We shall denote the set of solutions of the KV problem by Sol(KV). Note that the KV problem is equivalent to finding an element $u = (A, B) \in \mathfrak{tder}_2$ which satisfies equation (23) and the identity $\mathrm{div}(u) = \tilde{\delta}\left(\frac{1}{2}\,\mathrm{tr}\sum_{k=2}^{\infty}\frac{B_k x^k}{k!}\right)$.

***Remark* 6.2.** The group KV_2 acts on Sol(KV) by right multiplications. This action is free and transitive. The proof of this statement is completely analogous to the proof of Theorem 5.1.

7. Pentagon equation

In this Section we establish a relation between the Kashiwara-Vergne problem and the pentagon equation introduced in [7]. Let $\Phi \in \mathrm{TAut}_3$. We say that Φ satisfies the pentagon equation if

$$\Phi^{12,3,4}\Phi^{1,2,34} = \Phi^{1,2,3}\Phi^{1,23,4}\Phi^{2,3,4}. \tag{26}$$

Proposition 7.1. *Let* $F \in \mathrm{Sol}(\widehat{\mathrm{KV}})$. *Then,*

$$\Phi = (F^{12,3})^{-1}(F^{1,2})^{-1}F^{2,3}F^{1,23} \tag{27}$$

is an element of KV_3*, and it satisfies the pentagon equation.*

Proof. First, we compute

$$\begin{array}{rcl}\Phi(x+y+z) & = & (F^{12,3})^{-1}(F^{1,2})^{-1}F^{2,3}F^{1,23}(x+y+z) \\ & = & (F^{12,3})^{-1}(F^{1,2})^{-1}F^{2,3}(\mathrm{ch}(x, y+z)) \\ & = & (F^{12,3})^{-1}(F^{1,2})^{-1}(\mathrm{ch}(x, \mathrm{ch}(y,z))) \\ & = & (F^{12,3})^{-1}(\mathrm{ch}(x+y, z)) \\ & = & x+y+z.\end{array}$$

Hence, $\Phi \in \mathrm{SAut}_3$. Next, we rewrite the defining equation for Φ as $F^{1,2}F^{12,3}\Phi = F^{2,3}F^{1,23}$ and apply the cocycle j to both sides to get

$$j(F^{1,2}) + F^{1,2}\cdot j(F^{12,3}) + (F^{1,2}F^{12,3})\cdot j(\Phi) = j(F^{2,3}) + F^{2,3}\cdot j(F^{1,23}).$$

Since $j(F) = \mathrm{tr}(f(x) - f(\mathrm{ch}(x,y)) + f(y))$, we have

$$\begin{array}{rcl} j(F^{1,2}) + F^{1,2}\cdot j(F^{12,3}) & = & \mathrm{tr}(f(x) + f(y) - f(\mathrm{ch}(x,y))) \\ & + & F^{1,2}\cdot \mathrm{tr}(f(x+y) - f(\mathrm{ch}(x+y), z) + f(z)) \\ & = & \mathrm{tr}(f(x) + f(y) + f(z) - f(\mathrm{ch}(\mathrm{ch}(x,y), z)))\end{array}$$

Similarly, we obtain

$$\begin{array}{rcl} j(F^{2,3}) + F^{2,3}\cdot j(F^{1,23}) & = & \mathrm{tr}(f(y) - f(\mathrm{ch}(y,z)) + f(z)) \\ & + & F^{2,3}\cdot \mathrm{tr}(f(x) - f(\mathrm{ch}(x, y+z)) + f(y+z)) \\ & = & \mathrm{tr}(f(x) + f(y) + f(z) - f(\mathrm{ch}(x, \mathrm{ch}(y,z)))).\end{array}$$

We conclude $(F^{1,2}F^{12,3})\cdot j(\Phi) = 0$, $j(\Phi) = 0$ and $\Phi \in \mathrm{KV}_3$.

The pentagon equation is satisfied by substituting the expression for Φ into the equation, and by using that for $\Phi \in \mathrm{KV}_3 \subset \mathrm{SAut}_3$ we have $F^{123,4}\Phi^{1,2,3} = \Phi^{1,2,3}F^{123,4}$ and $F^{1,234}\Phi^{2,3,4} = \Phi^{2,3,4}F^{1,234}$. □

Let $F_1 \in \mathrm{Sol}(\widehat{\mathrm{KV}})$ and Φ_1 be the corresponding solution of the pentagon equation. Consider another element $F_2 \in \mathrm{Sol}(\widehat{\mathrm{KV}})$. By Theorem 5.1, $F_2 = F_1 g$ for some $g \in \widehat{\mathrm{KV}}_2$. The corresponding solution of the pentagon equation reads

$$\begin{aligned} \Phi_2 &= (F_2^{12,3})^{-1}(F_2^{1,2})^{-1}F_2^{2,3}F_2^{1,23} \\ &= (g^{12,3})^{-1}(F_1^{12,3})^{-1}(g^{1,2})^{-1}(F_1^{1,2})^{-1}F_1^{2,3}g^{2,3}F_1^{1.23}g^{1,23} \\ &= (g^{12,3})^{-1}(g^{1,2})^{-1}\Phi_1 g^{2,3}g^{1,23}. \end{aligned} \tag{28}$$

Equation (28) defines an action of $\widehat{\mathrm{KV}}_2$ on solutions of the pentagon equation with values in KV_3. Actions of this type are called *Drinfeld twists*.

Proposition 7.2. *Let $F_1, F_2 \in \mathrm{Sol}(\widehat{\mathrm{KV}})$ and assume that they give rise to the same solution Φ of the pentagon equation. Then, $F_2 = F_1 \exp(\lambda t)$ for some $\lambda \in \mathbb{K}$.*

Proof. First, note that for $g = \exp(\lambda t)$ we have for all $\Phi \in \mathrm{KV}_3$

$$(g^{12,3})^{-1}(g^{1,2})^{-1}\Phi g^{2,3}g^{1,23} = e^{-\lambda c}\Phi e^{\lambda c} = \Phi,$$

where $c = t^{1,2} + t^{1,3} + t^{2,3}$ is a central element in $\mathfrak{sder}_3$ and in $\mathfrak{kv}_3$.

The degree one component of $\widehat{\mathfrak{kv}}_2$ is spanned by t, and t is central in $\widehat{\mathfrak{kv}}_2$. Hence, one can represent $g = F_1^{-1}F_2$ in the form $g = \exp(\lambda t)\exp(u)$, where $u = \sum_{k=2}^{\infty} u_k \in \widehat{\mathfrak{kv}}_2$. Let Φ be a solution of the pentagon equation which corresponds to both F_1 and F_2. Let k_0 be the lowest degree such that $u_{k_0} \neq 0$. Then, equation $\Phi = (g_2^{12,3})^{-1}(g_2^{1,2})^{-1}\Phi g^{2,3}g^{1,23}$ implies $\mathrm{d}u_{k_0} = 0$, and by Theorem 3.1 we have $u_{k_0} = 0$ which implies $u = 0$ and $g = \exp(\lambda t)$, as required. □

Proposition 7.3. *Let $\Phi = \exp(\phi) \in \mathrm{TAut}_2$ be a solution of the pentagon equation, where $\phi = \sum_{k=1}^{\infty} \phi_k$ with $\phi_k \in \mathfrak{tder}_3$ homogeneous of degree k. Then, $\phi_1 = 0$ and $\phi_2 = (\alpha[y,z], \beta[z,x], \gamma[x,y])$.*

Proof. The degree one component of the pentagon equation reads $\mathrm{d}\phi_1 = 0$. Since the degree one component of $H^3(\mathfrak{tder}, \mathrm{d})$ vanishes, we have $\phi_1 = \mathrm{d}f$ for a degree one element $f \in \mathfrak{tder}_2$. However, the degree one component of $\mathfrak{tder}_2$ is spanned by $r = (0, x)$ and $t = (y, x)$, and both r and t are in the kernel of d. Hence, $\phi_1 = 0$. This implies that the degree two component of the pentagon equation is of the form, $\mathrm{d}\phi_2 = 0$. Then (see the proof of Theorem 3.1), ϕ_2 is expressed as $(\alpha[y,z], \beta[z,x], \gamma[x,y])$ for some $\alpha, \beta, \gamma \in \mathbb{K}$. □

Note that $H^3(\mathfrak{tder}, \mathrm{d})$ is one-dimensional, and the cohomology lies in degree two. One can choose the isomorphism $H^3(\mathfrak{tder}, \mathrm{d}) \cong \mathbb{K}$ in such a way that it is represented by the map $\pi : \phi_2 = (\alpha[y,z], \beta[z,x], \gamma[x,y]) \mapsto \alpha + \beta + \gamma$.

Proposition 7.4. *Let $F = \exp(u)\exp(sr/2)\exp(\alpha t) \in \mathrm{TAut}_2$, where u is an element of $\mathfrak{tder}_2$ of degree greater of equal to two. Assume that the expression $\Phi = (F^{12,3})^{-1}(F^{1,2})^{-1}F^{2,3}F^{1,23}$ is an element of KV_3, and denote $\pi(\phi_2) = \lambda$. Then, $\lambda = s^2/8$ and $F \in \mathrm{Sol}_s(\widehat{\mathrm{KV}})$.*

Proof. Note that the degree two component of $\phi = \ln(\Phi)$ is given by

$$\phi_2 = \mathrm{d}u_2 + \frac{s^2}{8}([r^{2,3}, r^{1,23}] + [r^{12,3}, r^{1,2}]) = \mathrm{d}u_2 + \frac{s^2}{8}[r^{2,3}, r^{1,2}] = \mathrm{d}u_2 + \frac{s^2}{8}([y,z], 0, 0).$$

Here we used the classical Yang-Baxter equation of Proposition 3.2. In conclusion, $\lambda = \pi(\phi_2) = s^2/8$.

Denote $\chi(x,y) = F(x+y) = x + y + \frac{s}{2}[x,y] + \dots$, where $\dots$ stand for elements of degree greater or equal to three. Since $\Phi(x+y+z) = x+y+z$, we have

$$\chi(x, \chi(y,z)) = F^{2,3}F^{1,23}(x+y+z) = F^{1,2}F^{12,3}(x+y+z) = \chi(\chi(x,y),z).$$

By Proposition 2.1, this implies $\chi(x,y) = \mathrm{ch}_s(x,y)$. Denote $b(x,y) = j(F) \in \mathfrak{tr}_2$. By applying j to the equality $F^{2,3}F^{1,23} = F^{1,2}F^{12,3}\Phi$ we obtain,

$$b(y,z) + F^{2,3} \cdot b(x, y+z) = b(x,y) + F^{1,2} \cdot b(x+y, z).$$

Equivalently, $\tilde{\delta}_s(b) = 0$ which implies, by Proposition 2.2, $b \in \mathrm{im}(\tilde{\delta}_s)$ and $F \in \mathrm{Sol}_s(\widehat{\mathrm{KV}})$. □

Theorem 7.1. *Let $\Phi \in \mathrm{KV}_3$ be a solution of the pentagon equation with $\pi(\phi_2) = \lambda$ and let $s \in \mathbb{K}$ be a square root of 8λ, $s^2/8 = \lambda$. Then, there is a unique element $F \in \mathrm{Sol}_s(\widehat{\mathrm{KV}})$ such that $F = \exp(u)\exp(sr/2) \in \mathrm{TAut}_2$, where u is an element of $\mathfrak{tder}_2$ of degree greater of equal to two, and $\Phi = (F^{12,3})^{-1}(F^{1,2})^{-1}F^{2,3}F^{1,23}$.*

Proof. Our task is to find $f = \sum_{k=1}^{\infty} f_k \in \mathfrak{tder}_2$ with the degree one component $f_1 = sr/2$ such that $F = \exp(f)$ solves equation $\Phi = (F^{12,3})^{-1}(F^{1,2})^{-1}F^{2,3}F^{1,23}$. In degree two, it implies,

$$\mathrm{d}f_2 + \frac{s^2}{8}([y,z],0,0) = \phi_2.$$

Recall that $\mathrm{d}\phi_2 = 0$ and $\pi(\phi_2) = \lambda = s^2/8$. Hence, this equation admits a solution, and it is unique since $\mathrm{d} : \mathfrak{tder}_2 \to \mathfrak{tder}_3$ has no kernel in degrees greater than one.

Assume that we found $F_n \in \mathrm{TAut}_2$ such that $\Phi_n = (F_n^{12,3})^{-1}(F_n^{1,2})^{-1}F_n^{2,3}F_n^{1,23}$ is equal to Φ modulo terms of degree greater than n. Then, $F_n^{2,3}F_n^{1,23}(x+y+z) = F_n^{1,2}F_n^{12,3}(x+y+z)$ modulo terms of degree greater than $n+1$, and $F_n(x,y) = \mathrm{ch}_s(x,y)$ modulo terms of degree greater than $n{+}1$. Since $F_n^{123,4}\Phi_n^{1,2,3} = \Phi_n^{1,2,3}F_n^{123,4}$ and $F_n^{1,234}\Phi_n^{2,3,4} = \Phi_n^{2,3,4}F_n^{1,234}$ modulo terms of degree greater than $n+1$, Φ_n satisfies the pentagon equation modulo terms of degree greater than $n+1$. Write $\Phi_n = \exp(\sum_{k=2}^{\infty} \psi_k)$, where $\psi_k = \phi_k$ for $k \leq n$ and denote $\varphi = \phi_{n+1} - \psi_{n+1}$. The pentagon equation for Φ and the pentagon equation modulo terms of degree greater then $n+1$ for Φ_n imply $\mathrm{d}\varphi = 0$. Hence, by Theorem 3.1, $\varphi = \mathrm{d}u$ for a unique element $u \in \mathfrak{tder}_2$ of degree $n+1$. Put $F_{n+1} = F_n \exp(u)$. It satisfies equation $\Phi = (F_{n+1}^{12,3})^{-1}(F_{n+1}^{1,2})^{-1}F_{n+1}^{2,3}F_{n+1}^{1,23}$ modulo terms of degree greater than $n+1$. By induction, we construct a unique F which solves equation $\Phi = (F^{12,3})^{-1}(F^{1,2})^{-1}F^{2,3}F^{1,23}$ and has $f_1 = sr/2$, as required. By Proposition 7.4, the element F solves the KV problem, $F \in \mathrm{Sol}_s(\widehat{\mathrm{KV}})$. □

Theorem 7.1 implies that the Kashiwara-Vergne problem has solutions if an only if the pentagon equation has solutions $\Phi \in \mathrm{KV}_3$ with $\pi(\phi_2) = 1/8$. The next proposition provides a tool extracting the Duflo function of an element $F \in \mathrm{Sol}(\widehat{\mathrm{KV}})$ from the corresponding solution of the pentagon equation.

Proposition 7.5. *Let $\Phi = \exp(\phi) \in \mathrm{KV}_3$ be a solution of the pentagon equation with $\pi(\phi_2) = 1/8$, and let $F \in \mathrm{Sol}(\widehat{\mathrm{KV}})$ be a solution of equation (27). Denote $\phi = (A, B, C)$, and $B(x,0,z)_{x-lin} = h(\mathrm{ad}_z)x$ for $h \in x\mathbb{K}[[x]]$. Then, the Duflo function of F satisfies equation $f'(x) = h(x)$.*

Proof. Let $F = \exp(u)$ with $u = (a, b)$. Put $a(x, y) = a_0 y + \alpha(\mathrm{ad}_y)x + \dots$ and $b(x, y) = b_0 y + \beta(\mathrm{ad}_y)x + \dots$. Then, by Proposition 6, the Duflo function associated to F is a solution of equation $f' = \beta - \alpha$.

Denote

$$\begin{aligned} u^l = u^{1,2} + u^{12,3} &= (a(x,y) + a(x+y,z), b(x,y) + a(x+y,z), b(x+y,z)) \\ u^r = u^{2,3} + u^{1,23} &= (a(x,y+z), a(y,z) + b(x,y+z), b(y,z) + b(x,y+z)), \end{aligned}$$

and observe that $\phi = \mathrm{ch}(-u^l, u^r)$. The contribution of $u^r - u^l$ in $B(x, 0, z)_{x-lin}$ is equal to $\beta(\mathrm{ad}_z)x - \alpha(\mathrm{ad}_z)x$. Note that the linear in z contributions in both u^l and u^r are of the form $(z, z, 0)$. Since

$$[(z, z, 0), (0, h(\mathrm{ad}_z)x, 0)] = (0, h(\mathrm{ad}_z)[x, z] + [z, h(\mathrm{ad}_z)x], 0) = 0,$$

we conclude that the nonlinear terms in the Campbell-Hausdorff series $\mathrm{ch}(-u^l, u^r)$ do not contribute in $B(x, 0, z)_{x-lin}$, and $h(x) = \beta(x) - \alpha(x)$. Hence, $f'(x) = h(x)$, as required. □

8. $\mathbb{Z}_2$-symmetry of the KV problem and hexagon equations

In this Section we introduce an involution on τ the set of solutions of the generalized KV problem, and show that the corresponding solutions of the pentagon equation verify a pair of hexagon equations.

8.1. **The automorphism R and the Yang-Baxter equation.** Let $R \in \mathrm{TAut}_2$ be an automorphism of $\mathfrak{lie}_2$ defined on generators by $R(x) = e^{-\mathrm{ad}_y} x, R(y) = y$. Note that $R = \exp(r)$ for $r = (y, 0) \in \mathfrak{tder}_2$, and

$$R\,(\mathrm{ch}(y, x)) = \mathrm{ch}(y, \exp(-\mathrm{ad}_y)x) = \mathrm{ch}(x, y).$$

Denote by θ the inner derivation of $\mathfrak{lie}_2$ with generator $\mathrm{ch}(x, y)$. That is, for $a \in \mathfrak{lie}_2$ we have $\theta(a) = [a, \mathrm{ch}(x, y)]$. Note that the derivation $t = (y, x) \in \mathfrak{tder}_2$ is an inner derivation of $\mathfrak{lie}_2$ with generator $x + y$. Indeed, $t(x) = [x, y] = [x, x + y]$ and $t(y) = [y, x] = [y, x + y]$. Let $F \in \mathrm{TAut}_2$ be a solution of the first KV equation, $F(x + y) = \mathrm{ch}(x, y)$. Then, $FtF^{-1} = \theta$. Indeed, for $a \in \mathfrak{lie}_2$ we have

$$FtF^{-1}(a) = F([F^{-1}(a), x + y]) = [a, F(x + y)] = [a, \mathrm{ch}(x, y)] = \theta(a).$$

Proposition 8.1. $RR^{2,1} = \exp(\theta)$.

Proof. Note that $R^{2,1}(x) = x$ and $R^{2,1}(y) = e^{-\mathrm{ad}_x} y$. We compute,

$$RR^{2,1}(x) = R(x) = \exp(-\mathrm{ad}_y)x = \exp(-\mathrm{ad}(\mathrm{ch}(x, y)))x,$$

and

$$RR^{2,1}(y) = R(\exp(-\mathrm{ad}_x)y) = \exp(-\mathrm{ad}(\exp(-\mathrm{ad}_y)x))y = \exp(-\mathrm{ch}(x, y))y,$$

as required. □

Proposition 8.2. *The element R satisfies the Yang-Baxter equation,*

$$R^{1,2}R^{1,3}R^{2,3} = R^{2,3}R^{1,3}R^{1,2}.$$

Proof. In components, we have $R^{1,2} = (\exp(-\mathrm{ad}_y), 1, 1), R^{1,3} = (\exp(-\mathrm{ad}_z), 1, 1)$ and $R^{2,3} = (1, \exp(-\mathrm{ad}_z), 1)$. One easily computes both the left hand side and the right hand side of the Yang-Baxter equation on generators y and z, $z \mapsto z$ and $y \mapsto \exp(-\mathrm{ad}_z)y$. We compute the action of the left hand side on x:

$$R^{1,2}R^{1,3}R^{2,3}(x) = R^{1,2}R^{1,3}(x) = R^{1,2}(\exp(-\mathrm{ad}_z)x) = \exp(-\mathrm{ad}_z)\exp(-\mathrm{ad}_y)x,$$

and the action of the right hand side,

$$\begin{aligned} R^{2,3}R^{1,3}R^{1,2}(x) &= R^{2,3}R^{1,3}(\exp(-\operatorname{ad}_y)x) \\ &= R^{2,3}(\exp(-\operatorname{ad}_y)\exp(-\operatorname{ad}_z)x) \\ &= \exp(-\operatorname{ad}_z)\exp(-\operatorname{ad}_y)x \end{aligned}$$

which completes the proof. □

Proposition 8.3. $R^{12,3} = R^{1,3}R^{2,3}$. *Let* $F \in \mathrm{TAut}_2$ *be a solution of equation* $F(x+y) = \mathrm{ch}(x,y)$. *Then,* $F^{2,3}R^{1,23}(F^{2,3})^{-1} = R^{1,2}R^{1,3}$.

Proof. For the first equation, note that both sides are represented by the automorphism $(\exp(-\operatorname{ad}_z), \exp(-\operatorname{ad}_z), 1) \in \mathrm{TAut}_3$.

For the second equation, both the left hand side and the right hand side preserve generators y and z, $y \mapsto y, z \mapsto z$. It remains to compute the action on x:

$$F^{2,3}R^{1,23}(F^{2,3})^{-1}(x) = F^{2,3}R^{1,23}(x) = F^{2,3}(\exp(-\operatorname{ad}_{y+z})x) = \exp(-\mathrm{ch}(y,z))x,$$

and the same for the right hand side

$$R^{1,2}R^{1,3}(x) = R^{1,2}(\exp(-\operatorname{ad}_z)x) = \exp(-\operatorname{ad}_z)\exp(-\operatorname{ad}_y)x = \exp(-\mathrm{ch}(y,z))x,$$

as required. □

8.2. **Involution on** $\mathrm{Sol}(\widehat{\mathrm{KV}})$**.** In this Section we introduce and study a certain involution on the set of solutions of the KV problem.

Proposition 8.4. *Let* $F \in \mathrm{Sol}(\widehat{\mathrm{KV}})$. *Then,* $\tau(F) = RF^{2,1}e^{-t/2}$ *is a solution of the KV problem,* $\tau(F) \in \mathrm{Sol}(\widehat{\mathrm{KV}})$. *The map* τ *is an involution,* $\tau^2 = 1$.

Proof. We compute,

$$\tau(F)(x+y) = RF^{2,1}e^{-t/2}(x+y) = RF^{2,1}(x+y) = R(\mathrm{ch}(y,x)) = \mathrm{ch}(x,y).$$

Furthermore,

$$j(\tau(F)) = j(RF^{2,1}e^{-t/2}) = R \cdot j(F^{2,1}).$$

Here we used that $\mathrm{div}(r) = \mathrm{div}(t) = 0$ and $j(R) = j(\exp(-t/2)) = 0$. Let $f \in x^2\mathbb{K}[[x]]$ such that $j(F) = \mathrm{tr}(f(x) - f(\mathrm{ch}(x,y)) + f(y))$. Then, $j(F^{2,1}) = \mathrm{tr}(f(x) - f(\mathrm{ch}(y,x)) + f(y))$ and $R \cdot j(F^{2,1}) = \mathrm{tr}(f(x) - f(\mathrm{ch}(x,y)) + f(y)) = j(F)$. Hence, $\tau(F)$ is a solution of the KV problem.

Finally,

$$\tau^2(F) = R\tau(F)^{2,1}e^{-t/2} = RR^{2,1}Fe^{-t} = e^{\theta}Fe^{-t} = F,$$

where we used $t^{2,1} = t$, $RR^{2,1} = \exp(\theta)$ and $FtF^{-1} = \theta$. We conclude that $\tau^2 = 1$, and τ defines an involution on $\mathrm{Sol}(\widehat{\mathrm{KV}})$. □

Proposition 8.5. *Let* $F \in \mathrm{Sol}(\widehat{\mathrm{KV}})$ *and let* Φ_F *be the corresponding solution of the pentagon equation. Then,*

$$\Phi_{\tau(F)} = (\Phi_F^{3,2,1})^{-1}.$$

Proof. We compute,

$$\begin{aligned} \Phi_{\tau(F)} &= e^{t^{12,3}/2}(F^{3,21})^{-1}(R^{12,3})^{-1}e^{t^{1,2}/2}(F^{2,1})^{-1}(R^{1,2})^{-1}R^{2,3}F^{3,2}e^{-t^{2,3}/2}R^{1,23}F^{32,1}e^{-t^{1,23}/2} \\ &= e^{c/2}(F^{3,21})^{-1}(R^{12,3})^{-1}(F^{2,1})^{-1}(R^{1,2})^{-1}R^{2,3}F^{3,2}R^{1,23}F^{32,1}e^{-c/2} \\ &= e^{c/2}(F^{3,21})^{-1}(F^{2,1})^{-1}(R^{2,3})^{-1}(R^{1,3})^{-1}(R^{1,2})^{-1}R^{2,3}R^{1,3}R^{1,2}F^{3,2}F^{32,1}e^{-c/2} \\ &= e^{c/2}(F^{3,21})^{-1}(F^{2,1})^{-1}F^{3,2}F^{32,1}e^{-c/2} = e^{c/2}(\Phi^{3,2,1})^{-1}e^{-c/2} = (\Phi^{3,2,1})^{-1}. \end{aligned}$$

Here in passing from the first to the second line we used that $g^{1,2}h^{12,3} = h^{12,3}g^{1,2}$ for $g \in \mathrm{SAut}_2, h \in \mathrm{TAut}_2$, and the definition of the element $c = t^{1,2}+t^{1,3}+t^{2,3} \in \mathfrak{t}_3$; Proposition 8.3 in the passage from the second to the third line; and finally the Yang-Baxter equation (Proposition 8.2) and the fact that c is central in $\mathfrak{kv}_3$ in the passage from the third to the fourth line. □

Proposition 8.6. *Let* $F \in \mathrm{Sol}(\widehat{\mathrm{KV}})$ *and* $\kappa(F) = (A(x,y), B(x,y)) \in \mathfrak{tder}_2$. *Then,*

(29)
$$\kappa(\tau(F)) = \left(e^{\mathrm{ad}_x} B(y,x) + \frac{1}{2}(\mathrm{ch}(x,y) - x), e^{-\mathrm{ad}_y} A(y,x) - \frac{1}{2}(\mathrm{ch}(x,y) - y)\right).$$

Proof. We compute,

$$\kappa(\tau(F)) = \frac{d\tau(F)_s}{ds}|_{s=1}\, \tau(F)^{-1} = r + R\,\frac{dF^{2,1}_s}{ds}|_{s=1}(F^{2,1})^{-1}R^{-1} - \frac{1}{2}RF^{2,1}t(F^{2,1})^{-1}R^{-1},$$

where we used that $dR_sR_s^{-1} = r = (y,0) \in \mathfrak{tder}_2$. In the last term, $F^{2,1}t(F^{2,1})^{-1}$ is the inner derivation with generator $\mathrm{ch}(y,x)$, and $RF^{2,1}t(F^{2,1})^{-1}R^{-1}$ is an inner derivation with generator $\mathrm{ch}(x,y)$. With our normalization condition, it is represented by $(\mathrm{ch}(x,y) - x, \mathrm{ch}(x,y) - y) \in \mathfrak{tder}_2$.

Finally, for the middle term $R\kappa(F)^{2,1}R^{-1}$ we compute,

$$\begin{aligned} R(A,B)^{2,1}R^{-1}(x) &= R(B(y,x), A(y,x))e^{\mathrm{ad}_y}(x) \\ &= R(e^{\mathrm{ad}_y}[x, B(y,x)] + e^{\mathrm{ad}_y}[A(y,x), x] - [A(y,x), e^{\mathrm{ad}_y}(x)]) \\ &= [x, B(y,x) + (e^{-\mathrm{ad}_y} - 1)A(y,x)] \\ &= [x, e^{\mathrm{ad}_x}B(y,x) + \mathrm{ch}(x,y) - x - y]. \end{aligned}$$

Here in the passage to the last line we have used equation (23) (with x and y exchanged). For the action on y we compute,

$$R(A,B)^{2,1}R^{-1}(y) = R(B(y,x)A(y,x))(y) = R([y, A(y,x)]) = [y, e^{-\mathrm{ad}_y}A(y,x)].$$

By adding up all three terms we obtain,

$$\begin{aligned} \kappa(\tau(F)) &= (e^{\mathrm{ad}_x}B(y,x) + \mathrm{ch}(x,y) - x - y, e^{-\mathrm{ad}_y}A(y,x)) \\ &+ (y,0) - \tfrac{1}{2}(\mathrm{ch}(x,y) - x, \mathrm{ch}(x,y) - y) \\ &= (e^{\mathrm{ad}_x}B(y,x) + \tfrac{1}{2}(\mathrm{ch}(x,y) - x), e^{-\mathrm{ad}_y}A(y,x) - \tfrac{1}{2}(\mathrm{ch}(x,y) - y), \end{aligned}$$

as required. □

***Remark* 8.1.** Symmetry (29) has been introduced in [13] (see discussion after Proposition 5.3).

8.3. **Symmetric solutions of the KV problem.**

Definition 8.1. An element $F \in \mathrm{Sol}(\widehat{\mathrm{KV}})$ is called *a symmetric solution* of the generalized Kashiwara-Vergne conjecture if $\tau(F) = F$.

We shall denote the set of symmetric solutions by $\mathrm{Sol}^\tau(\widehat{\mathrm{KV}})$. Since the map $\kappa : \mathrm{TAut}_2 \to \mathfrak{tder}_2$ is a bijection, $\tau(F) = F$ if and only if $\kappa(\tau(F)) = \kappa(F)$. That is, $\kappa(F) = (A(x,y), B(x,y))$ satisfies the (equivalent) linear equations

$$A(x,y) = e^{\mathrm{ad}_x}B(y,x) + \frac{1}{2}(\mathrm{ch}(x,y) - x)\,,\ B(x,y) = e^{-\mathrm{ad}_y}A(y,x) - \frac{1}{2}(\mathrm{ch}(x,y) - y).$$

Since equations (23) and (24) are linear in A and B, one can average an arbitrary solution to obtain a symmetric solution $\tilde{F}$ with $\kappa(\tilde{F}) = (\kappa(F) + \kappa(\tau(F)))/2$.

The involution $u \mapsto u^{2,1}$ acts on the Lie algebra $\widehat{\mathfrak{kv}}_2$, and it lifts to the group $\widehat{\mathrm{KV}}_2$. We shall denote the corresponding invariant subalgebra by $\widehat{\mathfrak{kv}}_2^{sym} \subset \widehat{\mathfrak{kv}}_2$ and the invariant subgroup by $\widehat{\mathrm{KV}}_2^{sym} \subset \widehat{\mathrm{KV}}_2$.

Proposition 8.7. *The group* $\widehat{\mathrm{KV}}_2^{sym}$ *acts on the set* $\mathrm{Sol}^\tau(\widehat{\mathrm{KV}})$ *by multiplications on the right. This action is free and transitive.*

Proof. Let $g \in \widehat{\mathrm{KV}}_2^{sym}$ and $F \in \mathrm{Sol}^\tau(\widehat{\mathrm{KV}})$. By Theorem 5.1, $Fg \in \mathrm{Sol}(\widehat{\mathrm{KV}})$. By applying τ we obtain

$$\tau(Fg) = RF^{2,1}g^{2,1}e^{-t/2} = RF^{2,1}e^{-t/2}g = \tau(F)g = Fg.$$

Hence, $Fg \in \mathrm{Sol}^\tau(\widehat{\mathrm{KV}})$.

Consider two elements $F_1, F_2 \in \mathrm{Sol}^\tau(\widehat{\mathrm{KV}})$. We denote $g = F_1^{-1}F_2$ and compute

$$g^{2,1} = (F_1^{-1}F_2)^{2,1} = (R^{-1}F_1e^{t/2})^{-1}(R^{-1}F_2e^{t/2}) = e^{-t/2}(F_1^{-1}F_2)e^{t/2} = e^{-t/2}ge^{t/2} = g,$$

as required. □

***Remark* 8.2.** Note that the element $t = (y, x)$ as well as the image of the injection $\nu : \mathfrak{grt} \to \widehat{\mathfrak{kv}}_2$ is contained in $\widehat{\mathfrak{kv}}_2^{sym}$. In fact, it is not known whether any non-symmetric elements of $\widehat{\mathfrak{kv}}_2$ exist. If correct, Conjecture stated in the end of Section 4 would imply $\widehat{\mathfrak{kv}}_2 = \widehat{\mathfrak{kv}}_2^{sym}$.

Proposition 8.8. *Let* $F \in \mathrm{Sol}^\tau(\widehat{\mathrm{KV}})$*, and let* $\Phi \in \mathrm{KV}_3$ *be the corresponding solution of the pentagon equation. Then,*

$$\Phi^{1,2,3}\Phi^{3,2,1} = e, \tag{30}$$

$$e^{(t^{1,3}+t^{2,3})/2} = \Phi^{2,1,3}e^{t^{1,3}/2}(\Phi^{2,3,1})^{-1}e^{t^{2,3}/2}\Phi^{3,2,1} \tag{31}$$

and

$$e^{(t^{1,2}+t^{1,3})/2} = (\Phi^{1,3,2})^{-1}e^{t^{1,3}/2}\Phi^{3,1,2}e^{t^{1,2}/2}(\Phi^{3,2,1})^{-1} \tag{32}$$

Proof. Equation (30) follows by Proposition 8.5. In order to prove equation (31) recall that $R^{12,3} = R^{1,3}R^{2,3} = (\exp(-\mathrm{ad}_z), \exp(-\mathrm{ad}_z), 1) \in \mathrm{TAut}_3$. Furthermore, this automorphism commutes with $g^{1,2}$ for any $g \in \mathrm{TAut}_2$. In particular, we have $F^{2,1}R^{12,3}(F^{2,1})^{-1} = R^{1,3}R^{2,3}$. By substituting $R = Fe^{t/2}(F^{2,1})^{-1}$ we obtain,

$$F^{2,1}R^{12,3}(F^{2,1})^{-1} = F^{2,1}F^{21,3}e^{(t^{1,2}+t^{1,3})/2}(F^{3,12})^{-1}(F^{2,1})^{-1},$$

and

$$\begin{aligned} R^{1,3}R^{2,3} &= F^{1,3}e^{t^{1,3}/2}(F^{3,1})^{-1}F^{2,3}e^{t^{2,3}/2}(F^{3,2})^{-1} \\ &= F^{1,3}F^{2,13}e^{t^{1,3}/2}(F^{2,31})^{-1}(F^{3,1})^{-1}F^{2,3}F^{23,1}e^{t^{2,3}/2}(F^{32,1})^{-1}(F^{3,2})^{-1}. \end{aligned}$$

A comparison of these two equations yields equation (31). Equation (32) follows by applying the (13)-permutation to equation (31) and by using the inversion formula (30). □

***Remark* 8.3.** Equations (31) and (32) are called as *hexagon equations*. They were first introduced in [7] (see equations (2.14a) and (2.14b)).

9. Associators

In this Section we consider joint solutions of pentagon and hexagon equations called *associators* (with values in the group KV_3). We show that Drinfeld's associators defined in [7] make part of this set, and we use this fact to give a new proof of the KV conjecture.

9.1. Associators with values in KV_3 and Drinfeld's associators.

Definition 9.1. An element $\Phi \in \mathrm{KV}_3$ is an associator if it satisfies the pentagon equation (26), hexagon equations (31) and (32) and the inversion property (30).

Proposition 9.1. *Let $\Phi = \exp(\phi) \in \mathrm{KV}_3$ be an associator. Then, $\pi(\phi_2) = 1/8$.*

Proof. The degree two component of the hexagon equation (31) reads

$$\frac{1}{8}\,[t^{1,3}, t^{2,3}] + \phi_2^{2,1,3} - \phi_2^{2,3,1} + \phi_2^{3,2,1} = 0.$$

Note that $[t^{1,3}, t^{2,3}] = ([y, z], [z, x], [x, y])$ which implies $\pi([t^{1,3}, t^{2,3}]) = 3$. Also observe that $\pi(\phi_2^{2,3,1}) = \pi(\phi_2)$ and $\pi(\phi_2^{2,1,3}) = \pi(\phi_2^{3,2,1}) = -\pi(\phi_2)$. We conclude that $3\pi(\phi_2) = 3/8$ and $\pi(\phi_2) = 1/8$, as required. □

Proposition 9.2. *Let $\Phi = \exp(\phi) \in \mathrm{KV}_3$ be a solution of equations* (26) *and* (30) *with $\pi(\phi_2) = 1/8$. Then, each $F \in \mathrm{Sol}(\widehat{\mathrm{KV}})$ which verifies equation* (27) *is a symmetric solution of the KV problem, $F \in \mathrm{Sol}^{\tau}(\widehat{\mathrm{KV}})$.*

Proof. Theorem 7.1 implies that equation (27) admits solutions $F \in \mathrm{Sol}(\widehat{\mathrm{KV}})$. By Proposition 8.5, $\Phi_{\tau(F)} = (\Phi_F^{3,2,1})^{-1} = \Phi_F$. Hence, by Proposition 7.2, $\tau(F) = F\exp(\lambda t)$ for some $\lambda \in \mathbb{K}$. The degree one component of this equation reads $r + f_1^{2,1} - t/2 = f_1 + \lambda t$. Since $f_1 = r/2 + \alpha t$ for some $\alpha \in \mathbb{K}$, we have $r + f_1^{2,1} - f_1 = t/2$ and $\lambda = 0$. In conclusion, $\tau(F) = F$, as required. □

Recall that by Proposition 3.3 Lie algebras $\mathfrak{t}_n$ inject into $\mathfrak{kv}_n$. In particular, $\mathfrak{t}_3$ injects into $\mathfrak{kv}_3$, and the corresponding group T_3 is a subgroup of KV_3.

Definition 9.2. An associator $\Phi \in \mathrm{KV}_3$ is called a Drinfeld's associator if $\Phi \in T_3$.

Drinfeld's associators can be defined without referring to the Lie algebras $\mathfrak{tder}_n$ and $\mathfrak{kv}_n$ since both simplicial and coproduct maps restrict to Lie subalgebras $\mathfrak{t}_n$ in a natural way. In [6] Drinfeld proved the following theorem:

Theorem 9.1. *The set of Drinfeld's associators is non empty.*

This implies the following result:

Theorem 9.2. *The set of symmetric solutions of the KV problem $\mathrm{Sol}^{\tau}(\widehat{\mathrm{KV}})$ is non empty.*

Proof. Each Drinfeld's associator $\Phi = \exp(\phi)$ is an associator with values in KV_3 with $\pi(\phi_2) = 1/8$. Then, by Theorem 7.1, there is an element $F = \exp(f) \in \mathrm{TAut}_2$ with $f_1 = r/2$ which solves equation (27). By Proposition 7.4 this automorphism is a solution of the KV problem, and by Proposition 9.2 this solution is symmetric. □

***Remark* 9.1.** The KV problem has been settled in [2]. The solution is based on the Kontsevich deformation quantization scheme [14], and on the earlier work of the second author [21]. Theorem 9.2 gives a new proof of the KV conjecture by reducing it to the existence theorem for Drinfeld's associators.

Proposition 9.3. *Let $\Phi = \exp(\phi) \in T_3$ be a Drinfeld's associator, and let $F \in \mathrm{Sol}(\widehat{\mathrm{KV}})$ be a solution of the KV problem which satisfies equation (27). Write $\phi = h(\mathrm{ad}_{t^{2,3}})t^{1,2} + \dots$, where $h \in x\mathbb{K}[[x]]$, and $\dots$ stand for terms which contain at least two generators $t^{1,2}$. Then, the Duflo function associated to F satisfies equation $f'(x) = h(x)$.*

Proof. By putting $y = 0$ we obtain $t^{1,2} = (y, x, 0) \mapsto (0, x, 0)$ and $t^{2,3} = (0, z, y) \mapsto (0, z, 0)$. Hence,

$$\phi(t^{1,2}, t^{2,3})_{y=0} = (0, \phi(x, z), 0).$$

In particular, for $\phi = (A, B, C)$, we have $B(x, 0, z)_{x-lin} = h(\mathrm{ad}_z)x$. Then, by Proposition 7.5, we obtain $f'(x) = h(x)$, as required. □

***Example* 9.1.** Consider the Knizhnik-Zamolodchikov associator (with values in T_3) constructed in Drinfeld. Equation (2.15) of [7] yields the function $h(x)$:

$$h(x) = -\sum_{n=2}^{\infty} \frac{\zeta(n)}{(2\pi i)^n}\, x^{n-1}.$$

Note that our associators are obtained by taking an inverse of associators the in Drinfeld's paper. The Duflo function corresponding to the Knizhnik-Zamolodchikov associator is given by

$$f(x) = -\sum_{n=2}^{\infty} \frac{\zeta(n)}{n(2\pi i)^n}\, x^n = \frac{\gamma}{2\pi i} x - \ln\left(\Gamma\left(1 - \frac{x}{2\pi i}\right)\right).$$

Here γ is the Euler's constant, and the term $\gamma x/2\pi i$ cancels the linear part in the logarithm of the Γ-function. Formula for $f(x)$ matches (up to a sign change) the expression $\ln(F_{nice}(x))$ in [15].

9.2. **Actions of the group** GRT. Let Lie_n be a group associated to the Lie algebra $\mathfrak{lie}_n$ (such that $a \cdot b = \mathrm{ch}(a, b)$). Then, one can view the Grothendieck-Teichmüller group GRT as a subset of Lie_2 defined by a number of relations (see Section 5 of [7]), and equipped with the new multiplication,

$$(h_1 *_{\mathrm{GRT}}\ h_2)(x, y) = h_1(x, h_2(x, y) y h_2^{-1}(x, y)) h_2(x, y).$$

***Remark* 9.2.** Note that we have chosen to act on the second argument of the function h rather than on the first one (as in [7]).

Let $\psi \in \mathfrak{grt}$ and consider a one parameter subgroup of GRT defined by ψ, $h_s = \exp_{\mathrm{GRT}}(s\psi)$. Write $h_t = h_{t-s} *_{\mathrm{GRT}} h_s$ and differentiate in t at $t = s$ to obtain

$$\frac{dh_s(x, y)}{ds} = \psi(x, h_s(x, y) y h_s(x, y)^{-1}) h_s(x, y).$$

This differential equation together with the initial condition $h_0(x, y) = 1$ defines the exponential function $\exp_{\mathrm{GRT}}$ in a unique way.

Proposition 9.4. *Let $\psi \in \mathfrak{grt}$, $h = \exp_{\mathrm{GRT}}(\psi) \in \mathrm{GRT}$ and $g = \exp(\nu(\psi)) \in \widehat{\mathrm{KV}}_2$. Then,*

$$\hat{g} = (g^{12,3})^{-1} (g^{1,2})^{-1} g^{2,3} g^{1,23} = h(t^{1,2}, t^{2,3}) \in \mathrm{KV}_3\,.$$

Proof. First, observe that for $g \in \mathrm{SAut}_2$, $g^{1,2}$ commutes with $g^{12,3}$, and $g^{2,3}$ commutes with $g^{1,23}$. Hence, the maps $g \mapsto g^l = g^{1,2} g^{12,3}$ and $g \mapsto g^r = g^{2,3} g^{1,23}$ are group homomorphisms mapping SAut_2 to SAut_3.

Next, replace ψ by $s\psi$ and consider the derivative in s of $\hat{g}_s = (g^l_s)^{-1} g^r_s$:

$$\begin{aligned} \frac{d\hat{g}_s}{ds} &= (g^l_s)^{-1} \left(\frac{dg^r_s}{ds} (g^r_s)^{-1} - \frac{dg^l_s}{ds} (g^l_s)^{-1} \right) g^r_s \\ &= (g^l_s)^{-1} (\mathrm{d}\nu(\psi)) g^r_s \\ &= (g^l_s)^{-1} \psi(t^{1,2}, t^{2,3}) g^r_s \\ &= \psi(t^{1,2}, (g^l_s)^{-1} t^{2,3} g^l_s)(g^l_s)^{-1} g^r_s \\ &= \psi(t^{1,2}, (g^l_s)^{-1} g^r_s t^{2,3} (g^r_s)^{-1} g^l_s) \hat{g}_s \\ &= \psi(t^{1,2}, \hat{g}_s t^{2,3} (\hat{g}_s)^{-1}) \hat{g}_s. \end{aligned}$$

Obviously, $\hat{g}_0 = e \in \mathrm{KV}_3$. We conclude that $h(t^{1,2}, t^{2,3})$ and $\hat{g}$ satisfy the same first order linear ordinary differential equation with the same initial condition. Hence, they coincide, as required. □

The Lie algebra homomorphism $\nu : \mathfrak{grt} \to \widehat{\mathfrak{kv}}_2$ gives rise to a subgroup of $\widehat{\mathrm{KV}}_2$ isomorphic to GRT. The group $\widehat{\mathrm{KV}}_2$ acts on the set of solutions of the KV problem, and on the set of associators with values in KV_3 (see equation (28)). In [7] (see Section 5) Drinfeld defines a free and transitive action of the group GRT on the set of associators with values in T_3. This action is given by the following formula,

$$g : \Phi(t^{1,2}, t^{2,3}) \mapsto \Phi(t^{1,2}, g t^{2,3} g^{-1}) g, \tag{33}$$

where $g = \exp_{\mathrm{GRT}}(\psi) \in \mathrm{GRT}$ and $\Phi \in T_3$ are viewed as elements of the group $\mathrm{Lie}_2(t^{1,2}, t^{2,3})$. The following proposition relates these two actions.

Proposition 9.5. *When restricted to the set of Drinfeld's associators, the action of the group* GRT *on associators with values in* KV_3 *coincides with the canonical action* (33).

Proof. Let $g \in \widehat{\mathrm{KV}}_2$ and rewrite the action (28) on $\Phi(t^{1,2}, t^{2,3}) \in T_3$ as follows,

$$\Phi \cdot g = (g^{12,3})^{-1} (g^{1,2})^{-1} \Phi(t^{1,2}, t^{2,3}) g^{2,3} g^{1,23} = \Phi(t^{1,2}, \hat{g} t^{2,3} \hat{g}^{-1}) \hat{g},$$

for $\hat{g} = (g^{12,3})^{-1} (g^{1,2})^{-1} g^{2,3} g^{1,23}$. Let $\psi \in \mathfrak{grt}$ and $g = \exp(\nu(\psi))$. Then, by Proposition 9.4 we have $\hat{g} = (\exp_{\mathrm{GRT}}(\psi))(t^{1,2}, t^{2,3})$, and the action (28) coincides with the canonical action (33). □

***Remark* 9.3.** If Conjecture of Section 4 is correct, we have $\widehat{\mathrm{KV}}_2 \cong \mathbb{K}t \times \nu(\mathrm{GRT})$, where the additive group $\mathbb{K}t$ injects into $\widehat{\mathrm{KV}}_2$ via the exponential map, $\lambda t \mapsto \exp(\lambda t)$. In particular, this implies $\widehat{\mathrm{KV}}_2 = \widehat{\mathrm{KV}}_2^{sym}$ since both $\mathbb{K}t$ and $\nu(\mathrm{GRT})$ are contained in $\widehat{\mathrm{KV}}_2^{sym}$. Note that the action of $\mathbb{K}t$ on associators is trivial, and the action of GRT on the set of Drinfeld's associators is transitive. The action of $\widehat{\mathrm{KV}}_2^{sym}$ on associators with values KV_3 is also transitive, and we conclude that all associators with values in KV_3 are Drinfeld's associators.

***Remark* 9.4.** For Drinfeld's associators, Furusho [12] showed that the hexagon equations (31), (32) and the inversion property (30) follow from the pentagon equation and the normalization condition $\pi(\phi_2) = 1/8$. In the case of associators with values in KV_3, Proposition 9.2 shows that the hexagon equations (31), (32) follow from the pentagon equation, the inversion property and the normalization condition $\pi(\phi_2) = 1/8$. If we assumed $\widehat{\mathrm{KV}}_2 = \widehat{\mathrm{KV}}_2^{sym}$, the inversion property would be automatic, and we would get the analogue of Furusho's result for associators with values in KV_3. If Conjecture of Section 4 holds true, we recover the Furusho's result.

Appendix: proof of Proposition 4.2

In this Appendix we give a proof of Proposition 4.2. It is inspired by the proof of Proposition 5.7 in [7].

Denote $\mathrm{d}\Psi = (a, b, c)$. We have,

$$\begin{array}{rcl} a & = & -\psi(-x-y,x)+\psi(-x-y-z,x)-\psi(-x-y-z,x+y), \\ b & = & -\psi(-x-y,y)+\psi(-x-y-z,y+z)-\psi(-x-y-z,x+y)+\psi(-y-z,y), \\ c & = & \psi(-x-y-z,y+z)-\psi(-x-y-z,z)+\psi(-y-z,z). \end{array}$$

Let $\mathfrak{g}$ be the semi-direct sum of $\mathfrak{tder}_3$ and $\mathfrak{lie}_3$. The following formulas define an injective Lie algebra homomorphism of $\mathfrak{t}_4$ to $\mathfrak{g}$:

$$\begin{array}{lll} t^{1,2} \mapsto (y,x,0) \in \mathfrak{tder}_3, & t^{1,3} \mapsto (z,0,x) \in \mathfrak{tder}_3, & t^{2,3} \mapsto (0,z,y) \in \mathfrak{tder}_3, \\ t^{1,4} \mapsto x \in \mathfrak{lie}_3, & t^{2,4} \mapsto y \in \mathfrak{lie}_3, & t^{3,4} \mapsto z \in \mathfrak{lie}_3\,. \end{array}$$

Indeed, $t^{1,2}, t^{1,3}$ and $t^{2,3}$ span a Lie subalgebra of $\mathfrak{tder}_3$ isomorphic to $\mathfrak{t}_3$, and x, y and z span an ideal of $\mathfrak{t}_4$ isomorphic to a free Lie algebra with three generators. It remains to check the Lie brackets between generators of these two Lie subalgebras. For instance, we compute,

$$[t^{1,2}, t^{3,4}] = t^{1,2}(z) = 0, \;\; [t^{1,2}, t^{2,4}] = t^{1,2}(y) = [y, x] = [t^{2,4}, t^{1,4}],$$

as required.

Note that $(\mathrm{d}\Psi)(x)$ is the image of the following element of $\mathfrak{t}_4$,

$$\begin{array}{rl} & [t^{1,4}, -\psi(-t^{1,4}-t^{2,4}, t^{1,4}) + \psi(-t^{1,4}-t^{2,4}-t^{3,4}, t^{1,4}) \\ - & \psi(-t^{1,4}-t^{2,4}-t^{3,4}, t^{1,4}+t^{2,4})] \\ = & [t^{1,4}, -\psi(t^{1,2}, t^{1,4}) + \psi(t^{1,2}+t^{1,3}+t^{2,3}, t^{1,4}) - \psi(t^{1,2}+t^{1,3}+t^{2,3}, t^{1,4}+t^{2,4})] \\ = & [t^{1,4}, -\psi(t^{1,2}, t^{1,4}) + \psi(t^{1,2}+t^{1,3}, t^{1,4}) - \psi(t^{1,3}+t^{2,3}, t^{1,4}+t^{2,4})] \\ = & [t^{1,4}, -\psi(t^{2,3}, t^{1,2}+t^{2,4}) + \psi(t^{2,3}, t^{1,2})] \\ = & [t^{1,4}, \psi(t^{2,3}, t^{1,2})] = [\psi(t^{1,2}, t^{2,3}), t^{1,4}]. \end{array}$$

Here in passing from the first to the second line we used the properties of central elements in $\mathfrak{t}_3$ and $\mathfrak{t}_4$. For instance, $t^{1,2} + t^{1,4} + t^{2,4}$ is central in the Lie subalgebra (isomorphic to $\mathfrak{t}_3$) spanned by $t^{1,2}, t^{1,4}$ and $t^{2,4}$. In the passage from the second to the third line we used the defining relations of the Lie algebra $\mathfrak{t}_4$. For instance, in the second term we used that $t^{2,3}$ has a vanishing bracket with $t^{1,4}$ and $t^{1,2} + t^{1,3}$. In the passage from the second to the third line we used a (3214) permutation of the equation (15). Finally, in the last passage we again used the defining relations of $\mathfrak{t}_4$, and in particular the fact that $t^{1,4}$ has a vanishing bracket with $t^{2,3}$ and with $t^{1,2} + t^{2,4}$. In conclusion, we have

$$\mathrm{d}\Psi(x) = \psi(t^{1,2}, t^{2,3})(x).$$

Similarly, $(\mathrm{d}\Psi)(y)$ is the image of the following element,

$$\begin{array}{rl} & [t^{2,4}, -\psi(-t^{1,4}-t^{2,4}, t^{2,4}) + \psi(-t^{1,4}-t^{2,4}-t^{3,4}, t^{2,4}+t^{3,4}) \\ - & \psi(-t^{1,4}-t^{2,4}-t^{3,4}, t^{1,4}+t^{2,4}) + \psi(-t^{2,4}-t^{3,4}, t^{2,4})] \\ = & [t^{2,4}, -\psi(t^{1,2}, t^{2,4}) + \psi(t^{1,2}+t^{1,3}+t^{2,3}, t^{2,4}+t^{3,4}) \\ - & \psi(t^{1,2}+t^{1,3}+t^{2,3}, t^{1,4}+t^{2,4}) + \psi(t^{2,3}, t^{2,4})] \\ = & [t^{2,4}, -\psi(t^{1,3}, t^{1,2}+t^{1,4}) + \psi(t^{1,3}, t^{1,2}) + \psi(t^{1,3}, t^{2,3}+t^{3,4}) - \psi(t^{1,3}, t^{2,3})] \\ = & [t^{2,4}, -\psi(t^{1,3}, t^{1,2}+t^{1,4}) + \psi(t^{1,3}, t^{2,3}+t^{3,4}) - \psi(t^{1,2}, t^{2,3})] \\ = & [\psi(t^{1,2}, t^{2,3}), t^{2,4}]. \end{array}$$

Here we used the (1324) and (3124) permutations of equation (15) as well as equation (14) which implies $\psi(t^{1,2}, t^{2,3}) = \psi(t^{1,2}, t^{1,3}) + \psi(t^{1,3}, t^{2,3})$. Again, the conclusion is

$$\mathrm{d}\Psi(y) = \psi(t^{1,2}, t^{2,3})(y).$$

Finally, we represent $(\mathrm{d}\Psi)(z)$ as the image of the element

$$\begin{array}{rl} & [t^{3,4}, \psi(-t^{1,4} - t^{2,4} - t^{3,4}, t^{2,4} + t^{3,4}) - \psi(-t^{1,4} - t^{2,4} - t^{3,4}, t^{3,4}) \\ + & \psi(-t^{2,4} - t^{3,4}, t^{3,4})] \\ = & [t^{3,4}, \psi(t^{1,2} + t^{1,3} + t^{2,3}, t^{2,4} + t^{3,4}) - \psi(t^{1,2} + t^{1,3} + t^{2,3}, t^{3,4}) + \psi(t^{2,3}, t^{3,4})] \\ = & [t^{3,4}, \psi(t^{1,2} + t^{1,3}, t^{2,4} + t^{3,4}) - \psi(t^{1,3} + t^{2,3}, t^{3,4}) + \psi(t^{2,3}, t^{3,4})] \\ = & [t^{3,4}, -\psi(t^{1,2}, t^{2,3}) + \psi(t^{1,2}, t^{2,3} + t^{2,4})] = [\psi(t^{1,2}, t^{2,3}), t^{3,4}], \end{array}$$

where we used the equation (15) (no permutation needed). We conclude

$$\mathrm{d}\Psi(z) = \psi(t^{1,2}, t^{2,3})(z),$$

and $\mathrm{d}\Psi = \psi(t^{1,2}, t^{2,3})$, as required.

References

[1] L. Albert, P. Harinck, C. Torossian, Solution non universelle pour le problème $KV - 78$, preprint arXiv:0802.2049.
[2] A. Alekseev, E. Meinrenken, On the Kashiwara-Vergne conjecture, Invent. math. **164**, 615–634, (2006).
[3] A. Alekseev, E. Petracci, Low Order Terms of the Campbell-Hausdorff Series and the Kashiwara-Vergne Conjecture, J. Lie Theory **16**, no.3, 531–538, (2006); Uniqueness in the Kashiwara-Vergne conjecture, preprint arXiv:math/0508077 (Note that only the arXiv version of this paper contains statements which we are referring to).
[4] M. Andler, A. Dvorsky, S. Sahi, Deformation quantization and invariant distributions, C. R. Acad. Sci. Paris, Sér. I, Math. **330**, 115–120, (2000).
[5] M. Andler, S. Sahi, C. Torossian, Convolutions of invariant distributions: Proof of the Kashiwara-Vergne conjecture, Lett. Math. Phys. **69**, 177–203, (2004).
[6] V.G. Drinfeld, Quasi-Hopf algebras, Leningrad Math. J., vol. **1** no. 6, (1990).
[7] V.G. Drinfeld, On quasi-triangular quasi-Hopf algebras and a group closely connected with $\mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})$, Leningrad Math. J., vol. **2** no. 4, 829–860, (1991).
[8] M. Duflo, Opérateurs différentiels bi-invariants sur un groupe de Lie, Ann. Sci. Éc. Norm. Sur., IV. Sér. **10**, 265–288, (1977).
[9] E. B. Dynkin, Calculation of the coefficients in the Campbell-Hausdorff formula, (Russian) Doklady Akad. Nauk SSSR (N.S.) **57**, 323–326, (1947).
[10] M. Espie, J.-C. Novelli, G. Racinet, Formal computations about multiple zeta values. From combinatorics to dynamical systems, 1–16, IRMA Lect. Math. Theor. Phys., 3, de Gruyter, Berlin, (2003).
[11] Y. Ihara, The Galois representations arising from $\mathbb{P}^1 - \{0, 1, \infty\}$ and Tate twists of even degree, Galois Groups over $\mathbb{Q}$, Math. Sci. Res. Inst. Publ., vol. **16**, Springer-Verlag, Berlin and New York, 199 –313, (1989).
[12] H. Furusho, Pentagon and hexagon equations, preprint arXiv:math/0702128.
[13] M. Kashiwara, M. Vergne, The Campbell-Hausdorff formula and invariant hyperfunctions, Invent. math. **47**, 249–272, (1978).
[14] M. Kontsevich, Deformation quantization of Poisson manifolds, Lett. Math. Phys. **66**, 157–216, (2003).
[15] M. Kontsevich, Operads and Motives in Deformation Quantization, Lett. Math. Phys. **48**, 35–72, (1999).
[16] M. Podkopaeva, private communications
[17] M. Pevzner, C. Torossian, Isomorphisme de Duflo et la cohomologie tangentielle, J. Geom. Phys. **51**, 486–505, (2004).
[18] G. Racinet, Doubles mélanges des polylogarithmes multiples aux racines de l'unité, Publ. Math. Inst. Hautes Études Sci. **95**, 185–231, (2002).

[19] F. Rouvière, Démonstration de la conjecture de Kashiwara-Vergne pour l'algèbre sl(2), C.R. Acad. Sci. Paris, Sér. I, Math. **292**. 657–660, (1981).
[20] B. Shoikhet, Tsygan formality and Duflo formulas, Math. Res. Lett. **10**, 763–775, (2003).
[21] C. Torossian, Sur la conjecture combinatoire de Kashiwara-Vergne, J. Lie Theory **12**, 597–616, (2002).
[22] M. Vergne, Le centre de l'algèbre enveloppante et la formule de Campbell-Hausdoreff, C.R. Acad. Sci. Paris, Sér. I, Math. **329**, 767–772, (1999).

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