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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. It has been settled in the positive by E. Meinrenken and the first author in 2006. In this paper, we study the uniqueness issue for the KV problem. To this end, we introduce a family of infinite-dimensional groups KRV_n^0, and a group KRV_2 which contains KRV_2^0 as a normal subgroup. We show that KRV_2 also contains the Grothendieck-Teichmüller group GRT_1 as a subgroup, and that it acts freely and transitively on the set of solutions of the KV problem SolKV. Furthermore, we prove that SolKV is isomorphic to a direct product of affine line $\mathbb{A}^1$ and the set of solutions of the pentagon equation with values in the group KRV_3^0. 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 [15]. The KV conjecture has many implications in Lie theory and harmonic analysis. Let $\mathfrak{g}$ be a finite-dimensional Lie algebra over a field $\mathbb{K}$ of characteristic zero. The KV conjecture implies the Duflo theorem [9] 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 [23] and by Pevzner-Torossian [18]; see [3, §4.2] for the relation to the KV problem) 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 Propositions 4.1 and 4.2 in [15], proved in [5] and [6]).

The KV conjecture was established for solvable Lie algebras by Kashiwara and Vergne in [15], for $\mathfrak{g} = \mathrm{sl}(2, \mathbb{R})$ by Rouvière in [21], 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 [26]. The general case has been settled by Meinrenken and the first author in [3] based on the previous work of the second author [24] and on the Kontsevich deformation quantization theory [17].

In this paper, we establish a relation between the KV conjecture and the theory of Drinfeld's associators developed in [8]. To this end, we introduce a family of infinite-dimensional groups $\mathrm{KRV}^0{}_n, n = 2, 3, \ldots$, and a group KRV_2. The group KRV_2 contains the Drinfeld's Grothendieck-Teichmüller group GRT_1 as a subgroup and the group $\mathrm{KRV}^0{}_2$ as a normal subgroup. We show that KRV_2 acts freely and transitively on the set of solutions of the KV conjecture SolKV. Furthermore, the set SolKV 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 $\mathrm{KRV}^0{}_3$. We make use of an involution τ acting on solutions of the KV conjecture to select symmetric solutions of the KV problem, SolKV^τ. The set SolKV^τ is isomorphic to a direct product of a line and the set of associators (joint solutions of the pentagon, hexagon, and inversion equations of [8]) with values in the group $\mathrm{KRV}^0{}_3$. 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 $\mathrm{KRV}^0{}_3$. As a by-product, we obtain a new proof of the KV conjecture. Indeed, by Drinfeld's theorem, the set of Drinfeld's associators is nonempty. Hence, the set of associators with values in the group $\mathrm{KRV}^0{}_3$ and the set of symmetric solutions of the KV conjecture SolKV^τ are also nonempty. 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, KRV_2, is isomorphic to a direct product of a line and the Grothendieck-Teichmüller group GRT_1. 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 $\mathrm{KRV}_2 \cong \mathbb{K} \times \mathrm{GRT}_1$ would imply that all solutions of the KV conjecture are symmetric and that all associators with values in the group $\mathrm{KRV}^0{}_3$ are Drinfeld's associators.

Below we explain the *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 $\mathrm{ch}(x, y) = x + y + \frac{1}{2}[x, y] + \ldots$ 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 §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 $\mathrm{KRV}^0{}_3$. 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 $\mathrm{KRV}^0{}_3$ 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 that 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. Consider a formal power series $\tilde{f}(x) = f(x) + h(x)$ with $h(x)$ odd. It is known that replacing $J^{1/2}$ with $\tilde{J}^{1/2}(x) = \exp(\tilde{f}(x))$ in the definition of the Duflo homomorphism preserves its property of being a ring isomorphism between $Z(U\mathfrak{g})$ and $(S\mathfrak{g})^{\mathfrak{g}}$. (In the category of Lie algebras, all these isomorphisms coincide.) We show that Drinfeld's generators $\sigma_{2k+1}, k = 1, 2, \dots$ (see equation (15)) of the Grothendieck-Teichmüller Lie algebra $\mathfrak{grt}_1$ define flows on the set of solutions of the KV conjecture SolKV and on the odd parts of Duflo functions such that $(\sigma_{2k+1} \cdot h)(x) = -x^{2k+1}$ (see Proposition 4.10). 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_1 on the symmetric Duflo function (4). This action coincides with the one described in [16] (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 2.8), 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 3.17). In Section 4 we introduce a family of Kashiwara-Vergne Lie algebras ${\mathfrak{krv}^0}_n$ and the Lie algebra $\mathfrak{krv}_2$ and show that the Grothendieck-Teichmüller Lie algebra $\mathfrak{grt}_1$ injects into $\mathfrak{krv}_2$ (Theorem 4.6). In Section 5 we give a new formulation of the Kashiwara-Vergne conjecture, and we show that it is equivalent to the original statement of [15] (Theorem 5.8). 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 ${\mathrm{KRV}^0}_3$ (Theorem 7.5). 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 study elements of the group ${\mathrm{KRV}^0}_3$ solving the pentagon equation (3). We compare them to Drinfeld's associators and give a new proof of the KV conjecture (Theorem 9.6).

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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 $\mathfrak{lie}_n = \mathfrak{lie}(x_1, \ldots, x_n)$ be the degree completion of the free Lie algebra over $\mathbb{K}$ with generators $x_1, \ldots, x_n$. It is the product

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

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

The completed universal enveloping algebra of $\mathfrak{lie}_n$ is the degree completion of the free associative algebra with generators $x_1, \ldots, x_n$, $U(\mathfrak{lie}_n) = \mathrm{Ass}_n$. 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 the element of Ass_2 defined by the 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 [10], $\mathrm{ch}(x, y) \in \mathfrak{lie}_2$ and

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

where $\ldots$ 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,

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

where elements of $\mathfrak{lie}^k(x, y)$ get an extra factor of s^{k-1}. Note that $\mathrm{ch}_s(x, y) = s^{-1}\,\mathrm{ch}(sx, sy)$ for $s \in \mathbb{K}^*$ 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 power series has a nonvanishing convergence radius (see, e.g., Lemma 9.1 in [2]).

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 $\mathbb{K}$-linear subspace of Ass_n^+ spanned by commutators. One can think of $\mathfrak{tr}_n$ as a $\mathbb{K}$-vector space spanned by cyclic words in letters $x_1, \dots, x_n$. The 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 basic property of trace.

Example 2.2. 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 2.3. 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 $\mathrm{tr}(x^3)$, $\mathrm{tr}(x^2 y)$, $\mathrm{tr}(xy^2)$, and $\mathrm{tr}(y^3)$, $\mathfrak{tr}_2^4$ is spanned by $\mathrm{tr}(x^4)$, $\mathrm{tr}(x^3 y)$, $\mathrm{tr}(x^2 y^2)$, $\mathrm{tr}(xyxy)$, $\mathrm{tr}(xy^3)$, and $\mathrm{tr}(y^4)$, etc.

Remark 2.4. 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 $\rho(\mathrm{tr}(x_{i_1} \dots x_{i_k})) = \mathrm{Tr}_V(\rho(x_{i_1}) \dots \rho(x_{i_k}))$ 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 the formula

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

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

Remark 2.5. The differential δ originates from the fact that $\mathfrak{lie}_n$ (for different n) form a cosimplicial vector space, with coface maps being the terms in (7) and codegeneracy maps s_i for $i = 1, \dots, n$ given by

$$(s_i f)(x_1, \dots, x_{n-1}) = f(x_1, \dots, x_{i-1}, 0, x_{i+1}, \dots, x_{n-1}).$$

Here $f \in \mathfrak{lie}_n$ and $s_i(f) \in \mathfrak{lie}_{n-1}$. In this paper, we do not make use of the codegeneracy maps.

Example 2.6. For $n = 1$ and $f = ax \in \mathfrak{lie}_1 \cong \mathbb{K}$, we have

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

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 2.7. For $n = 1$, we have

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

for $f(x) = \mathrm{tr}(x^k)$. Note that the right-hand side vanishes for $k = 1$ and that it is nonvanishing for all other $k = 2, 3 \ldots$.

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

THEOREM 2.8. *In degrees one and two, the cohomology of complexes* $(\mathfrak{lie}_n, \delta)$ *and* $(\mathfrak{tr}_n, \delta)$ *are given by*

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

The proof of Theorem 2.8 is deferred to Appendix A.

2.4. *Applications.* In this section we collect two simple applications of the cohomology computations of Theorem 2.8.

PROPOSITION 2.9. *Let* $s \in \mathbb{K}$, *and let* $\chi \in \mathfrak{lie}_2$ *be a Lie series of the form* $\chi(x, y) = x + y + \frac{s}{2}[x, y] + \ldots$, *where* $\ldots$ *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:

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

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. Furthermore, 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 $\chi = \mathrm{ch}_s$. $\square$

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

$$
\begin{aligned}
(\tilde{\delta} f)(x_1, \ldots, x_{n+1}) = {} & f(x_2, x_3, \ldots, x_{n+1}) \\
& + \sum_{i=1}^{n} (-1)^i f(x_1, \ldots, \mathrm{ch}(x_i, x_{i+1}), \ldots, x_{n+1}) \\
& + (-1)^{n+1} f(x_1, \ldots, x_n).
\end{aligned} \tag{8}
$$

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 2.10.

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

The proof of this proposition can be found in Appendix A.

Remark 2.11. 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 (8). We have $\tilde{\delta}_1 = \tilde{\delta}$ and $\tilde{\delta}_0 = \delta$. Proposition 2.10 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 $\mathfrak{lie}_n$.

Remark 3.1. Let $\mathfrak{g}$ be a finite-dimensional Lie algebra. Then, to every $u \in \mathfrak{der}_n$ one can associate a formal vector field $u_{\mathfrak{g}}$ on $\mathfrak{g}^n$ such that $u_{\mathfrak{g}}(x_1, \ldots, x_n) = (u(x_1)_{\mathfrak{g}}, \ldots, u(x_n)_{\mathfrak{g}})$. Here $u(x_1), \ldots, u(x_n)$ are elements of $\mathfrak{lie}_n$, $x_1, \ldots, x_n \in \mathfrak{g}$, and we define formal power series $u(x_1)_{\mathfrak{g}}, \ldots, u(x_n)_{\mathfrak{g}}$ on $\mathfrak{g}^n$ with values in $\mathfrak{g}$ as in Remark 2.1. The map $u \mapsto u_{\mathfrak{g}}$ is a Lie homomorphism.

Definition 3.2. 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 3.3. 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 elements of degree greater than one, 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 notation, we shall often write $u = (a_1, \ldots, a_n)$.

Proposition 3.4. *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 3.5. 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 3.6. Ihara [14] calls elements of $\mathfrak{sder}_n$ *normalized special derivations.*

Example 3.7. 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. *Cosimplicial maps and cohomology.* 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 the formula

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

Example 3.8. 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

$$u^{3,1,2} = (b(z,x,y), c(z,x,y), a(z,x,y)).$$

Similar to $\mathfrak{lie}_n$, we define coface 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 Lie homomorphisms maps by composing with the action of S_n on $\mathfrak{tder}_n$. Note that they map special derivations 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 3.9. For $u = (a(x,y), b(x,y)) \in \mathfrak{tder}_2$, we have

$$u^{1,2} = (a(x,y), b(x,y), 0) \in \mathfrak{tder}_3 \quad \text{and} \quad u^{2,3} = (0, a(y,z), b(y,z)).$$

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 3.10. *The element $r = (y,0) \in \mathfrak{tder}_2$ satisfies the classical Yang-Baxter equation in $\mathfrak{tder}_3$,*

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

Proof. We compute

$$\begin{aligned} [r^{1,2}, r^{1,3}] &= [(y,0,0),(z,0,0)] = ([y,z],0,0), \\ [r^{1,2}, r^{2,3}] &= [(y,0,0),(0,z,0)] = -([y,z],0,0), \\ [r^{1,3}, r^{2,3}] &= [(z,0,0),(0,z,0)] = 0. \end{aligned}$$

Adding these expressions gives zero, as required. □

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

PROPOSITION 3.11. *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*:

$$[t^{i,j}, t^{k,l}] = 0 \tag{9}$$

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

$$[t^{i,j} + t^{i,k}, t^{j,k}] = 0 \tag{10}$$

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

Remark 3.12. We denote by $\mathfrak{t}_n$ the (degree completed) Lie algebra with generators $t^{i,j} = t^{j,i}$ with $1 \le i, j \le n$ and $i \ne j$ defined by relations (9) and (10). Note that $c = \sum_{1 \le i < j \le n} t^{i,j}$ is a central element of $\mathfrak{t}_n$. Indeed, $[t^{i,j}, c] = \sum_{k \ne i, k \ne j} [t^{i,j}, t^{i,k} + t^{j,k}] = 0$. It is known (see [8, §5]) that

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

where the free Lie algebra $\mathfrak{lie}(t^{1,n}, \dots, t^{n-1,n})$ 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 $\mathfrak{lie}(t^{1,3}, t^{2,3})$. For any $a \in \mathfrak{lie}(t^{1,3}, t^{2,3})$, we have

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

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

Proof. First, we verify the relations (9) and (10). 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 (10) 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 $a'' \in \mathfrak{lie}(t^{1,n}, \dots, t^{n-1,n})$. 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 $x_1, \dots, x_{n-1}$. It is easy to check that $A''(x_n) = [x_n, a''(x_1, \dots, x_{n-1})]$, where $a''(x_1, \dots, x_{n-1})$ is obtained by replacing the generators $t^{i,n}$ by x_i in $a''(t^{1,n}, \dots, t^{n-1,n})$. 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 3.13. *The element* $c = \sum_{1 \le i<j \le n} t^{i,j}$ *belongs to the center of* $\mathfrak{sder}_n$.

Proof. First, note that $c(x_i) = \sum_{j \ne i}[x_i, x_j] = [x_i, x]$ 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 $u = (a_1, \dots, a_k) \in \mathfrak{sder}_n$ and compute for $1 \le k \le n$ the kth component of the bracket $[c, u]$:

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

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

Another family of coface maps is constructed in the following way. For $u=(a_1, \dots, a_{n-1}) \in \mathfrak{tder}_{n-1}$, we define

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

One uses the action of the permutation groups on $\mathfrak{tder}_{n-1}$ and on $\mathfrak{tder}_n$ to obtain other coface maps.

Example 3.14. 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

$$u^{1,23} = (a(x, y + z), b(x, y + z), b(x, y + z)).$$

These maps 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

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

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

Hence, $[u^{12,3}, v^{12,3}] = [u,v]^{12,3}$. As before, coface maps map special derivations to special derivations. For $u \in \mathfrak{sder}_{n-1}$ and $x = \sum_{i=1}^n x_i$, we compute

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

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

Example 3.15. 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 $[u^{1,2,\dots,n}, v^{12\dots n,n+1,\dots,n+m}] = 0$ in $\mathfrak{tder}_{m+n}$. Here $v^{12\dots n,n+1,\dots,n+m}$ is obtained from v by applying the coface map $(n-1)$ times.

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

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

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

Example 3.16. 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 3.17.

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

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

For the proof of Theorem 3.17 we refer the reader to Appendix A.

3.3. *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 3.18. 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 3.19. *For all $n \geq 2$ and $k = 1, \ldots, n$, the map $\alpha_k : \mathfrak{tder}_n \to \mathfrak{tr}_n$ defined by formula $\alpha_k : u = (a_1, \ldots, a_n) \mapsto \mathrm{tr}(a_k)$ is a 1-cocycle of the Lie algebra $\mathfrak{tder}_n$ with values in $\mathfrak{tr}_n$.*

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

Proposition 3.20. *The map* $\mathrm{div} : \mathfrak{tder}_n \to \mathfrak{tr}_n$ *defined by the formula* $\mathrm{div} : u = (a_1, \ldots, a_n) \mapsto \sum_{k=1}^n \mathrm{tr}(x_k(\partial_k a_k))$ *is a* 1*-cocycle.*

Proof. On the one hand, we get

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

On the other hand, we obtain,

$$\begin{aligned} \mathrm{div}([u, v]) &= \sum_{k=1}^n \mathrm{tr}\Big(x_k \partial_k\big(u(b_k) - v(a_k) + [a_k, b_k]\big)\Big) \\ &= \sum_{k=1}^n \mathrm{tr}\Big(x_k \partial_k\Big(u\Big(\sum_{i=1}^n (\partial_i b_k) x_i\Big) - v\Big(\sum_{j=1}^n (\partial_j a_k) x_j\Big) + [a_k, b_k]\Big)\Big) \\ &= \sum_{k=1}^n \mathrm{tr}\Big(x_k \partial_k\Big(\sum_{i=1}^n \big(u(\partial_i b_k) x_i + (\partial_i b_k)[x_i, a_i]\big) \\ &\qquad - \sum_{j=1}^n \big(v(\partial_j a_k) x_j + (\partial_j a_k)[x_j, b_j]\big) + [a_k, b_k]\Big)\Big) \end{aligned}$$

$$
\begin{aligned}
&= \sum_{k=1}^{n} \operatorname{tr}\Big(x_k\Big(u(\partial_k b_k) - (\partial_k b_k)a_k + \sum_{i=1}^{n}(\partial_i b_k)x_i(\partial_k a_i) \\
&\quad - v(\partial_k a_k) + (\partial_k a_k)b_k - \sum_{j=1}^{n}(\partial_j a_k)x_j(\partial_k b_j) + a_k(\partial_k b_k) - b_k(\partial_k a_k)\Big)\Big) \\
&= \sum_{k=1}^{n} \operatorname{tr}\Big(x_k\Big(u(\partial_k b_k) - (\partial_k b_k)a_k - v(\partial_k a_k) \\
&\quad + (\partial_k a_k)b_k + a_k(\partial_k b_k) - b_k(\partial_k a_k)\Big)\Big) \\
&= u \cdot \operatorname{div}(v) - v \cdot \operatorname{div}(u),
\end{aligned}
$$

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 $u = (a_1, \ldots, a_n) \in \mathfrak{tder}_n$, we have

$$
\operatorname{div}(u^{1,2,\ldots,n}) = \sum_{i=1}^{n} \operatorname{tr}(x_i(\partial_i a_i)) = \operatorname{div}(u)(x_1, \ldots, x_n).
$$

For $\operatorname{div}(u^{12,\ldots,n+1})$, we compute

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

PROPOSITION 3.21. $\operatorname{div}(\mathrm{d}u) = \delta\Big(\operatorname{div}(u)\Big)$.

Proof. We compute

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

□

Remark 3.22. Let $\mathfrak{g}$ be a finite-dimensional Lie algebra, $u \in \mathfrak{tder}_n$ a tangential derivation, $u_{\mathfrak{g}}$ the corresponding formal vector field on $\mathfrak{g}^n$, $\operatorname{div}(u) \in \mathfrak{tr}_n$ the divergence cocycle, $\alpha_k(u) \in \mathfrak{tr}_n$ cocycles of Proposition 3.19, and $\mathrm{ad}(\mathrm{div}(u))$, $\mathrm{ad}(\alpha_k(u))$ formal power series on $\mathfrak{g}^n$ defined by the adjoint representation of $\mathfrak{g}$ (see Remark 2.4). Denote by div the divergence of the vector fields on $\mathfrak{g}^n$ with respect to the Lebesgue measure. Then, it is easy to show that

$$div(u_{\mathfrak{g}}) = \mathrm{ad}\left(\mathrm{div}(u)\right) - \sum_{k=1}^{n} \mathrm{ad}\left(\alpha_k(u)\right).$$

In view of this relation, it would be more logical to call "divergence" the cocycle $\mathrm{div} - \sum_{k=1}^n \alpha_k$, but it would have made notation in the rest of the paper much heavier.

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 ${\mathfrak{krv}^0}_n \subset \mathfrak{sder}_n$ is a Lie subalgebra of special derivations spanned by elements with vanishing divergence. For $n = 1$, we define ${\mathfrak{krv}^0}_1 = \{0\} \subset \mathfrak{sder}_1 = \mathbb{K}$.

Remark 4.2. The divergence cocycle defines an extension $\widehat{\mathfrak{tr}}_n$ of the trivial $\mathfrak{tder}_n$ module by the module $\mathfrak{tr}_n$. As a graded vector space, $\widehat{\mathfrak{tr}}_n = \mathbb{K}c \oplus \mathfrak{tr}_n$, where c is a generator of degree zero. The action of $\mathfrak{tder}_n$ on c is given by $u \cdot c = \mathrm{div}(u)$. By restriction, $\mathfrak{sder}_n$ acts on $\widehat{\mathfrak{tr}}_n$, and ${\mathfrak{krv}^0}_n \subset \mathfrak{sder}_n$ is the stabilizer of c for this action.

Example 4.3. The element $t = (y, x) \in \mathfrak{sder}_2$ is contained in ${\mathfrak{krv}^0}_2$. Indeed, we have $a(x, y) = y, b(x, y) = x$, and $\partial_x a = \partial_y b = 0$, which implies $\mathrm{div}(t) = 0$.

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

Example 4.4. Since $t \in {\mathfrak{krv}^0}_2$, we have $t^{1,2}, t^{1,3}, t^{2,3} \in {\mathfrak{krv}^0}_3$ and

$$[t^{1,3}, t^{2,3}] = ([y, z], [z, x], [x, y]) \in {\mathfrak{krv}^0}_3 \,.$$

Observe that for $n = 2$, the subspace $\ker(\delta) = \mathrm{im}(\delta) \subset \mathfrak{tr}_2$ is annihilated by the action of $\mathfrak{sder}_2$. Indeed, for $u = (a, b) \in \mathfrak{sder}_2$ and $\mathrm{tr}(f) \in \mathfrak{tr}_1$, one has

$$u(\delta\, \mathrm{tr}(f)) = u(\mathrm{tr}(f(x)) + \mathrm{tr}(f(y)) - \mathrm{tr}(f(x+y))) = \mathrm{tr}([f(x), a] + [f(y), b]) = 0.$$

Let $\mathfrak{krv}_2 \subset \mathfrak{sder}_2$ be the normalizer of the subspace $\mathbb{K}c \oplus \ker(\delta)$. That is,

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

Obviously, this is a Lie subalgera of $\mathfrak{sder}_2$ containing ${\mathfrak{krv}^0}_2$. Moreover, for $u, v \in \mathfrak{krv}_2$, one has $\mathrm{div}([u, v]) = u \cdot \mathrm{div}(v) - v \cdot \mathrm{div}(u)$. Hence, $[\mathfrak{krv}_2, \mathfrak{krv}_2] \subset {\mathfrak{krv}^0}_2$.

For every $u \in \mathfrak{krv}_2$ there exists an element $\mathrm{tr}(f) \in \mathfrak{tr}_1$ such that $\mathrm{div}(u) = \mathrm{tr}(f(x) - f(x+y) + f(y))$. By Theorem 2.8, 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 notation, we denote by $f : \mathfrak{krv}_2 \to \mathbb{K}[x]$ the map $f : u \mapsto f$ and by $f_k : \mathfrak{krv}_2 \to \mathbb{K}$ for $k \geq 2$ the maps $f_k : u \mapsto f_k$.

PROPOSITION 4.5. *Let* $u \in \mathfrak{krv}_2$. *Then*, $\mathrm{div}(u) = \delta(f)$ *with*

$$f = \sum_{k=3}^{\infty} f_k \,\mathrm{tr}(x^k)$$

odd, and Taylor coefficients $f_k, k = 3, 5, \ldots$ *are characters of* $\mathfrak{krv}_2$.

Proof. Let $u \in \mathfrak{krv}_2$ with divergence $\mathrm{div}(u) = \mathrm{tr}(f(x) - f(x+y) + f(y))$, where $f(x) = \sum_{k=2}^{\infty} f_k x^k$. Consider the bigrading of $\mathfrak{tr}_2$ by the number of x's and y's in the cyclic word. Then, the degree $(1, n-1)$ component of $\mathfrak{tr}_2$ is one-dimensional, and it is spanned by $\mathrm{tr}(xy^{n-1})$. The corresponding contribution in $\mathrm{div}(u)$ is equal to $-nf_n$. Since $u = (a, b) \in \mathfrak{krv}_2$, we have $u(x+y) = [x, a] + [y, b] = 0$. Consider terms linear in x in both a and b. First, observe that for $m \geq 1$, the degree $(1, m)$ component of b vanishes since $\mathrm{ad}_y^{m+1}(x) \notin \mathrm{im}(\mathrm{ad}_x)$. In particular, this applies to all m odd.

Next, note that for m odd, the degree $(1, m)$ of a vanishes since in this case $[x, \mathrm{ad}_y^m(x)] \notin \mathrm{im}(\mathrm{ad}_y)$. Indeed, let $m = 2s + 1$. The subspace of $\mathfrak{lie}_2$ of bidegree $(2, 2s)$ has a basis $z_{k,2s-k} = [\mathrm{ad}_y^k(x), \mathrm{ad}_y^{2s-k}(x)]$ for $k = 0, \ldots, s-1$. By applying ad_y to an element $\sum_{k=0}^{s-1} \lambda_k z_{k,2s-k}$ we obtain an element $z = \sum_{k=0}^{s} \mu_k z_{k,2s+1-k}$, where $\mu_0 = \lambda_0$, $\mu_k = \lambda_{k-1} + \lambda_k$ for $k = 1, \ldots, s-1$ and $\mu_s = \lambda_{s-1}$. Observe that $\sum_{k=0}^{s} (-1)^k \mu_k = 0$, which is a necessary and sufficient condition for $z \in \mathrm{im}(\mathrm{ad}_y)$. We conclude that $z_{0,2s+1} = [x, \mathrm{ad}_y^m(x)] \notin \mathrm{im}(\mathrm{ad}_y)$, as required.

We conclude that $\mathrm{div}(u) = \mathrm{tr}(x\partial_x a + y\partial_y b)$ does not contain terms in degree $(1, m)$ for m odd, and $f_k = 0$ for all $k = m + 1$ even. Finally, Taylor coefficients of f are characters of $\mathfrak{krv}_2$ since they vanish on ${\mathfrak{krv}^0}_2$ and on $[\mathfrak{krv}_2, \mathfrak{krv}_2] \subset {\mathfrak{krv}^0}_2$. □

4.2. *The Grothendieck-Teichmüller Lie algebra.* Recall that the Grothendieck-Teichmüller Lie algebra $\mathfrak{grt}_1$ was defined by Drinfeld [8] in the following way. It is spanned by derivations $(0, \psi) \in \mathfrak{tder}_2$ which satisfy the following three relations:

$$\psi(x, y) = -\psi(y, x), \tag{11}$$

$$\psi(x, y) + \psi(y, z) + \psi(z, x) = 0 \tag{12}$$

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

$$\psi(t^{1,2}, t^{2,34}) + \psi(t^{12,3}, t^{3,4}) = \psi(t^{2,3}, t^{3,4}) + \psi(t^{1,23}, t^{23,4}) + \psi(t^{1,2}, t^{2,3}), \tag{13}$$

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 $\mathfrak{grt}_1$ have no solutions in degrees one and two. The Lie bracket induced on solutions of (11), (12), and (13) 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 4.6. *The map* $\nu : \psi \mapsto (\psi(-x-y, x), \psi(-x-y, y))$ *is an injective Lie algebra homomorphism mapping* $\mathfrak{grt}_1$ *to* $\mathfrak{krv}_2$.

We split the proof of Theorem 4.6 into several steps.

PROPOSITION 4.7. *Let* $\psi \in \mathfrak{grt}_1$. *Then,* $\Psi = \nu(\psi) \in \mathfrak{tder}_2$ *verifies the following equation in* $\mathfrak{tder}_3$:

$$\mathrm{d}\Psi = \psi(t^{1,2}, t^{2,3}). \tag{14}$$

We defer the proof of this proposition to Appendix B.

PROPOSITION 4.8. $\mathrm{im}(\nu) \subset \mathfrak{krv}_2$.

Proof. Using equation (14) 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 2.8 this implies $\Psi(x+y) = 0$ and $\Psi \in \mathfrak{sder}_2$. Note that this reproduces the result of Proposition 5.7 in [8].

Similarly, we compute

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

since $t^{1,2}, t^{2,3} \in {\mathfrak{krv}^0}_3$. By Theorem 2.8, this implies $\mathrm{div}(\Psi) \in \mathrm{im}(\delta)$ and $\Psi \in \mathfrak{krv}_2$. □

PROPOSITION 4.9. $\nu : \mathfrak{grt}_1 \to \mathfrak{krv}_2$ *is a Lie algebra homomorphism.*

Proof. Let $\psi_1, \psi_2 \in \mathfrak{grt}_1$ and compute $(a, b) = [\nu(\psi_1), \nu(\psi_2)]$:

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

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

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

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

This observation completes the proof of Theorem 4.6.

It is known [14], [8] that there exist elements $\sigma_{2n+1} \in \mathfrak{grt}_1$ 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:

$$\sigma_{2n+1} = \sum_{k=1}^{2n} \frac{(2n+1)!}{k!(2n+1-k)!} \operatorname{ad}_x^{k-1} \operatorname{ad}_y^{2n-k}[x, y]. \tag{15}$$

Proposition 4.10. *For $n \geq 1$, $f \circ \nu(\sigma_{2n+1}) = -x^{2n+1}$.*

Proof. Equation (15) implies that the degree $(1, 2n)$ part of $a(x, y) = \sigma(-x-y, x)$ is equal to $(2n+1) \operatorname{ad}_y^{2n} x$, and the degree $(1, 2n)$ part of $b(x, y) = \sigma(-x-y, y)$ vanishes. Hence, the degree $(1, 2n)$ component of $\operatorname{div}(\nu(\sigma_{2n+1}))$ is equal to $(2n+1) \operatorname{tr}(xy^{2n})$, 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 4.6 shows that $\mathfrak{krv}_2$ is infinite-dimensional, and Proposition 4.10 implies that characters $f_k, k = 3, 5, \dots$ are surjective. The Lie algebra $\mathfrak{krv}_2$ contains a central one-dimensional Lie subalgebra $\mathbb{K}t$ for $t = (y, x)$ and a Lie subalgebra isomorphic to the Lie algebra $\mathfrak{grt}_1$. This observation suggests the following conjecture on the structure of $\mathfrak{krv}_2$.

Conjecture. *The Lie algebra $\mathfrak{krv}_2$ is isomorphic to a direct sum of the Grothendieck-Teichmüller Lie algebra $\mathfrak{grt}_1$ and a one-dimensional Lie algebra with generator in degree one, $\mathfrak{krv}_2 \cong \mathbb{K}t \oplus \mathfrak{grt}_1$.*

Remark 4.11. The Deligne-Drinfeld conjecture (see [8, §6]) states that $\mathfrak{grt}_1$ is a free Lie algebra with generators σ_{2n+1} for $n = 1, 2, \dots$. In [20], Racinet introduced a graded Lie algebra $\mathfrak{dmr}_0$ related to combinatorics of multiple zeta values. A numerical experiment of [11] shows that up to degree 19 the Lie algebra $\mathfrak{dmr}_0$ coincides with $\mathfrak{grt}_1$ and is freely generated by σ_{2k+1}'s. Recently, Furusho showed (see [13]) that there is an injective Lie homomorphism $\mathfrak{grt}_1 \to \mathfrak{dmr}_0$. A numerical computation by Albert and the second author [1] shows that up to degree 16 the dimensions of graded components of $\mathfrak{krv}_2$ 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 [19]). Since $\mathbb{K}t \oplus \nu(\mathfrak{grt}_1) \subset \mathfrak{krv}_2$, we conclude that the conjecture stated above is 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: $\exp(u)\exp(v) = \exp(\mathrm{ch}(u, v))$.

Lie algebras $\mathfrak{tder}_n, \mathfrak{sder}_n, \mathfrak{krv}^0{}_n$, and $\mathfrak{krv}_2$ 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 TAut_n, SAut_n, $\mathrm{KRV}^0{}_n$, and KRV_2, respectively. The natural actions of $\mathfrak{tder}_n$, $\mathfrak{sder}_n$, $\mathfrak{krv}^0{}_n$, and $\mathfrak{krv}_2$ on $\mathfrak{lie}_n$ and on $\mathfrak{tr}_n$ lift to actions of the corresponding groups given by the formula

$$\exp(u)(a) := \sum_{n=0}^{\infty} \frac{1}{n!} \, u^n(a)$$

for $a \in \mathfrak{lie}_n$ or $a \in \mathfrak{tr}_n$, where $u^n(a)$ is the n-uple iterate of the derivation u on a. Note that the group TAut_n consists of automorphisms g of $\mathfrak{lie}_n$ with the property that the action of g preserves conjugacy classes of generators x_i for $i = 1, \ldots, n$. That is, for each $i = 1, \ldots, n$, there exists an element $g_i \in \exp(\mathfrak{lie}_n)$ such that $g(x_i) = g_i^{-1} x_i g_i$. Furthermore, the group SAut_n is the subgroup of TAut_n preserving $x = \sum_{i=1}^n x_i$.

The representation of $\mathfrak{tder}_n$ on $\widehat{\mathfrak{tr}}_n$ defined by the divergence cocycle (see Remark 4.2) lifts to a representation of TAut_n. It defines an additive group cocycle $j : \mathrm{TAut}_n \to \mathfrak{tr}_n$ given by the formula $j(g) = g \cdot c - c$. It verifies the cocycle condition

$$j(gh) = j(g) + g \cdot j(h) \tag{16}$$

and has the property

$$\frac{d}{ds} \, j(\exp(su))|_{s=0} = \mathrm{div}(u). \tag{17}$$

In the case of vector fields on a manifold, a multiplicative cocycle integrating the divergence is called Jacobian. The letter j stands for Jacobian cocycle (more precisely, for the logarithm of the Jacobian cocycle since j is additive). Equation (16) for $h = g^{-1}$ implies $j(g^{-1}) = -g^{-1} \cdot j(g)$. Together, equations (16) and (17) give the following differential equation for j:

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

Given the initial condition $j(e) = 0$, we obtain

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

The action of TAut_n on $\widehat{\mathfrak{tr}}_n$ restricts to an action of SAut_n. The group $\mathrm{KRV}^0{}_n$ is the stabilizer of c for this action. Similarly, the group KRV_2 is the normalizer of the subspace $\mathbb{K}c \oplus \ker(\delta) \subset \widehat{\mathfrak{tr}}_2$. In particular, for $g \in \mathrm{KRV}_2$, we have $j(g) = g \cdot c - c \in \ker(\delta) = \mathrm{im}(\delta) \subset \mathfrak{tr}_2$. Note that for any $g \in \mathrm{SAut}_2$ and $f \in \mathfrak{tr}_1$, we have $g \cdot \delta(f) = \delta(f)$ since the action of g preserves conjugacy classes of x and y and stabilizes $x + y$. Hence, we obtain a more explicit description of

$$\mathrm{KRV}_2 = \{g \in \mathrm{SAut}_2;\ j(g) \in \ker(\delta)\}.$$

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 $\dot{g}_s$. Here $\dot{g}_s$ is understood as a linear operator on $\mathfrak{lie}_n$ given by the derivative in s of the family of linear operators defined by automorphisms g_s. That is, for $z \in \mathfrak{lie}_n$, we have $\dot{g}_s(z) = dg_s(z)/ds$. In general, $\dot{g}_s$ is neither an automorphism nor a derivation of $\mathfrak{lie}_n$. Note, however, that $u_s := \dot{g}_s g_s^{-1}$ is an element of $\mathfrak{tder}_n$.

Proposition 5.1. *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 the unique solution of the ordinary differential equation $\dot{g}_s g_s^{-1} = u_s$ with initial condition $g_0 = e$. We denote $E = E_1$. It is important to note that E_s is not the exponential map for $\mathfrak{tder}_n$. Indeed, for $u \in \mathfrak{tder}_n$, one can define an element $\exp(su)$ as the unique solution of the differential equation $\dot{g}_s g_s^{-1} = u$ (the right-hand side is independent of s!) with initial condition $g_0 = e$.

PROPOSITION 5.2. *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 $j(g_s) = A_s \cdot j(g)$. Indeed, for $g = \exp(u)$ with $u \in \mathfrak{tder}_n$, we have $g_s = A_s \exp(u) A_s^{-1} = \exp(A_s u A_s^{-1})$. Then,

$$\begin{aligned} j(g_s) = j\left(\exp(A_s u A_s^{-1})\right) &= A_s \, \frac{e^u - 1}{u} \, A_s^{-1} \cdot \mathrm{div}\left(A_s u A_s^{-1}\right) \\ &= A_s \, \frac{e^u - 1}{u} \cdot \mathrm{div}(u) = A_s \cdot j(g). \end{aligned}$$

PROPOSITION 5.3. *Let $g \in \mathrm{TAut}_n$ and $u = \kappa(g)$. Then,*

$$\frac{dj(g_s)}{ds} = u_s \cdot j(g_s) + \mathrm{div}(u_s). \tag{18}$$

Proof. We compute

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

Put $q - s = \varepsilon$. Since $\dot{g}_s g_s^{-1} = u_s$, we have $g_q g_s^{-1} = \exp\left(\varepsilon u_s + O(\varepsilon^2)\right)$. Then, taking a derivative of $j(g_q)$ with respect to q and putting $q = s$ yields

$$\begin{aligned} \frac{dj(g_s)}{ds} &= \frac{d}{d\varepsilon}\Big(j\Big(\exp(\varepsilon u_s + O(\varepsilon^2)\Big) + \exp(\varepsilon u_s + O(\varepsilon^2)\Big) \cdot j(g_s)\Big)\Big|_{\varepsilon=0} \\ &= \mathrm{div}(u_s) + u_s \cdot j(g_s), \end{aligned}$$

as required. □

Proposition 5.3 implies the following statement that we shall be using later.

PROPOSITION 5.4. *Let $u \in \mathfrak{tder}_n$ and $g = E(u)$. Then, $glg^{-1} \cdot j(g) = \mathrm{div}(u)$.*

Proof. For $g = E(u)$, equation (18) at $s = 1$ implies the following relation between $j(g)$ and $\mathrm{div}(u)$: $l \cdot j(g) = u \cdot j(g) + \mathrm{div}(u)$. Since $u = l - glg^{-1}$, we obtain $glg^{-1} \cdot j(g) = \mathrm{div}(u)$, as required. □

Remark 5.5. The maps E and κ establish bijections $\mathfrak{sder}_n \to \mathrm{SAut}_n$, ${\mathfrak{krv}^0}_n \to {\mathrm{KRV}^0}_n$ and $\mathfrak{krv}_2 \to \mathrm{KRV}_2$. In order to prove the last statement observe that for $u \in \mathfrak{krv}_2$ we have $\mathrm{div}(u_s) \in \mathrm{im}(\delta)$. Hence, equation (18) implies $j(g_s) \in \mathrm{im}(\delta)$ and $E(u) \in \mathrm{KRV}_2$.

Note that the map E *is not* the exponential map, and the map κ is not the logarithm relating a group of Lie type to the corresponding Lie algebra.

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

$$F(x+y) = \mathrm{ch}(x,y) \tag{19}$$

and

$$j(F) \in \mathrm{im}(\tilde{\delta}). \tag{20}$$

We shall denote the set of solutions of the generalized KV problem by SolKV. For any $s \in \mathbb{K}$, one can introduce rescaled versions of equations (19) and (20) 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 SolKV_s. For $s = 0$, $\mathrm{SolKV}_0 = \mathrm{KRV}_2$. For all $s \neq 0$, $\mathrm{SolKV}_s \cong \mathrm{SolKV}$ with isomorphism given by the scaling transformation $F \mapsto F_s = A_s F A_s^{-1}$.

PROPOSITION 5.6. *Let $F \in$ SolKV 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 Kashiwara-Vergne conjecture has been proved in [3] (see Theorem 3.3). We shall see in this section (see Theorem 5.8) that the original statement of the Kashiwara-Vergne conjecture is equivalent to the fact that the set SolKV is nonempty. We shall give an alternative proof of nonemptiness of SolKV 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 generalized KV problem until we prove it with our methods.

THEOREM 5.7. *Assume that* SolKV *is nonempty. Then, the group* KRV_2 *acts on* SolKV *by multiplications on the right. This action is free and transitive.*

Proof. Let $F \in \mathrm{SolKV}$ and $g \in \mathrm{KRV}_2$. 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 $j(g) \in \mathrm{im}(\delta)$. Hence, $F \cdot j(g) \in \mathrm{im}(\tilde{\delta})$ and by Proposition 5.6 we have $j(Fg) \in \mathrm{im}(\tilde{\delta})$. In conclusion, KRV_2 acts on the set SolKV by right multiplications. This action is free since the multiplication on the right is.

Let $F_1, F_2 \in \mathrm{SolKV}$ 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 $j(F_1), j(F_2) \in \mathrm{im}(\tilde{\delta})$, by Proposition 5.6 we have $F_1^{-1} \cdot (j(F_2) - j(F_1)) \in \mathrm{im}(\delta)$ and $g \in \mathrm{KRV}_2$. Hence, the action of KRV_2 on SolKV is transitive. □

The Kashiwara-Vergne problem was stated in [15] in somewhat different terms. We shall now establish a relation between our approach and the original formulation of the KV problem (KV conjecture).

THEOREM 5.8. *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*:

$$x + y - \mathrm{ch}(y,x) = (1 - \exp(-\mathrm{ad}_x))A(x,y) + (\exp(\mathrm{ad}_y) - 1)B(x,y) \tag{21}$$

and

$$\mathrm{div}(u) \in \mathrm{im}(\tilde{\delta}). \tag{22}$$

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,

$$\begin{aligned}\frac{d}{ds}\,F_s^{-1}\big(\,\mathrm{ch}_s(x,y)\big) &= -F_s^{-1}\dot{F}_s F_s^{-1}\big(\,\mathrm{ch}_s(x,y)\big) + F_s^{-1}\Big(\frac{d}{ds}\,\mathrm{ch}_s(x,y)\Big)\\ &= F_s^{-1}\Big(\frac{d}{ds} - u_s\Big)\,\mathrm{ch}_s(x,y) = 0\end{aligned}$$

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 $F_s(x+y) = \mathrm{ch}_s(x,y)$.

The equivalence of $(d/ds - u_s)\,\mathrm{ch}_s(x,y) = 0$ and equation (21) is shown in Lemma 3.2 of [15]. For completeness of the presentation we reproduce the argument. First, using the formula for the derivative of the exponential map we observe that

$$\begin{aligned}\frac{d}{dt}\,\mathrm{ch}(x+tz,y)\Big|_{t=0} &= \frac{\mathrm{ad}_{\mathrm{ch}(x,y)}}{\exp(\mathrm{ad}_{\mathrm{ch}(x,y)})-1}\,\frac{\exp(\mathrm{ad}_x)-1}{\mathrm{ad}_x}\,z,\\ \frac{d}{dt}\,\mathrm{ch}(x,y+tz)\Big|_{t=0} &= \frac{\mathrm{ad}_{\mathrm{ch}(x,y)}}{1-\exp(-\mathrm{ad}_{\mathrm{ch}(x,y)})}\,\frac{1-\exp(-\mathrm{ad}_y)}{\mathrm{ad}_y}\,z.\end{aligned}$$

Since $\mathrm{ch}_s(x,y) = s^{-1}\,\mathrm{ch}(sx,sy)$ and $u_s(x) = [x,A_s] = s^{-1}[x,A(sx,sy)], u_s(y) = [y,B_s] = s^{-1}[y,B(sx,sy)]$, we obtain

$$\begin{aligned}(d/ds-u_s)\,\mathrm{ch}_s(x,y) &= -s^{-1}\,\mathrm{ch}_s(x,y)\\ &\quad + s^{-1}\frac{\mathrm{ad}_{\mathrm{ch}(sx,sy)}}{\exp(\mathrm{ad}_{\mathrm{ch}(sx,sy)})-1}\,\frac{\exp(s\,\mathrm{ad}_x)-1}{s\,\mathrm{ad}_x}(x-[x,A(sx,sy)])\\ &\quad + s^{-1}\frac{\mathrm{ad}_{\mathrm{ch}(sx,sy)}}{1-\exp(-\mathrm{ad}_{\mathrm{ch}(sx,sy)})}\,\frac{1-\exp(-s\,\mathrm{ad}_y)}{s\,\mathrm{ad}_y}(y-[y,B(sx,sy)]).\end{aligned}$$

Hence, $(d/ds-u_s)\,\mathrm{ch}_s(x,y)=0$ is equivalent to

$$\begin{aligned}\mathrm{ch}_s(x,y) &= \frac{\mathrm{ad}_{\mathrm{ch}(sx,sy)}}{\exp(\mathrm{ad}_{\mathrm{ch}(sx,sy)})-1}\,\Big(x-s^{-1}\big(\exp(s\,\mathrm{ad}_x)-1\big)A(sx,sy)\Big)\\ &\quad + \frac{\mathrm{ad}_{\mathrm{ch}_s(x,y)}}{1-\exp(-\mathrm{ad}_{\mathrm{ch}_s(x,y)})}\,\Big(y-s^{-1}\big(1-\exp(-s\,\mathrm{ad}_y)\big)B(sx,sy)\Big).\end{aligned}$$

Multiplying both the left-hand side and the right-hand side by

$$\exp(-s\,\mathrm{ad}_x)(\exp(\mathrm{ad}_{\mathrm{ch}(sx,sy)})-1)/\,\mathrm{ad}_{\mathrm{ch}(sx,sy)},$$

we obtain

$$\mathrm{ch}_s(y,x) = x - s^{-1}\big(1-\exp(-s\,\mathrm{ad}_x)\big)A(sx,sy) + y - s^{-1}\big(\exp(s\,\mathrm{ad}_y)-1)B(sx,sy).$$

Replacing $x\mapsto s^{-1}x, y\mapsto s^{-1}y$ yields

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

as required.

Finally, we compare equations (20) and (22). Let $F\in\mathrm{SolKV}$, $j(F) = \tilde{\delta}(\mathrm{tr}(f(x)))$. Using Proposition 5.4, 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 $u_s = s^{-1}A_suA_s^{-1}$, we have $\mathrm{div}(u_s)\in\mathrm{im}(\tilde{\delta}_s)$. Equation (18) for F_s gives $(d/ds-u_s)j(F_s) = \mathrm{div}(u_s)$ and 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 $j(F_s) \in \mathrm{im}(\tilde{\delta}_s)$. $\square$

Remark 5.9. Let $\mathfrak{g}$ be a finite-dimensional Lie algebra over $\mathbb{K}$. The adjoint representation is defined on elements of $\mathfrak{g} \subset U\mathfrak{g}$ by the standard formula, $\mathrm{ad}_a(z) = [a, z]$, and it extends by universality to $U\mathfrak{g}$. For instance, $\mathrm{ad}_{ab}(z) = \mathrm{ad}_a\left(\mathrm{ad}_b(z)\right) = abz - azb - bza + zba$ for $a, b \in \mathfrak{g}$.

For $A, B \in \mathfrak{lie}_2$ of Theorem 5.8, define a pair of formal power series on $\mathfrak{g} \times \mathfrak{g}$ with values in $\mathfrak{g}$ which satisfy equation (21). 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 $\mathbb{K}$,

$$\mathrm{Tr}_{\mathfrak{g}}\Big(\mathrm{ad}_x \circ \mathrm{ad}_{\partial_x A} + \mathrm{ad}_y \circ \mathrm{ad}_{\partial_y B}\Big) = \mathrm{Tr}_{\mathfrak{g}}\Big(\phi(\mathrm{ad}_x) + \phi(\mathrm{ad}_y) - \phi(\mathrm{ad}_{\mathrm{ch}(x,y)})\Big). \tag{23}$$

Here $\partial_x A, \partial_y B \in \mathrm{Ass}_2$, and for every Lie algebra $\mathfrak{g}$, they define formal power series on $\mathfrak{g} \times \mathfrak{g}$ with values in $U\mathfrak{g}$.

One can rewrite expressions for the operators $\mathrm{ad}_{\partial_x A}, \mathrm{ad}_{\partial_y B}$ in the following fashion. Let x, y, z be generators of $\mathfrak{lie}_3$ and $t \in \mathbb{K}$. For $A \in \mathfrak{lie}_2$, consider the expression $U(x, y, z) = dA(x + tz, y)/dt|_{t=0} \in \mathfrak{lie}_3$. Since U is linear in z, one can represent it in the form $U = \mathrm{ad}_{a(x,y)}(z)$ for a unique $a \in \mathrm{Ass}_2$. Note that the only term in $U(x, y, z)$ which ends on z is az, and $a = \partial_z U$. Using equation (5) we compute

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

This shows that for $x, y, z \in \mathfrak{g}$ we have $\mathrm{ad}_{\partial_x A(x,y)}\, z = dA(x + tz, y)/dt|_{t=0} =: d_x A(z)$ and similarly $\mathrm{ad}_{\partial_y B(x,y)}\, z = dB(x, y + tz)/dt|_{t=0} =: d_y B(z)$.

By choosing $\phi(x) = \frac{1}{2}\left(\frac{x}{e^x - 1} - 1\right)$ (see §6 for details), we obtain a new form of equation (23):

$$\begin{aligned}\mathrm{Tr}_{\mathfrak{g}}&\Big(\mathrm{ad}_x \circ d_x A + \mathrm{ad}_y \circ d_y B\Big)\\ &= \frac{1}{2}\,\mathrm{Tr}_{\mathfrak{g}}\left(\frac{\mathrm{ad}_x}{\exp(\mathrm{ad}_x) - 1} + \frac{\mathrm{ad}_y}{\exp(\mathrm{ad}_y) - 1} - \frac{\mathrm{ad}_{\mathrm{ch}(x,y)}}{\exp(\mathrm{ad}_{\mathrm{ch}(x,y)}) - 1} - 1\right),\end{aligned}$$

which coincides with the second equation in the original formulation of the Kashiwara-Vergne conjecture (see, e.g., equation (24) in [3]).

6. Duflo functions

Let $F \in \mathrm{SolKV}$. Then, $j(F) = \mathrm{tr}(f(x) - f(\mathrm{ch}(x, y)) + f(y))$ for some $f \in x^2\mathbb{K}[[x]]$. We shall refer to $f(x)$ as to the 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 generalized KV problem. It is convenient to introduce another formal power series $\phi(x) = xf'(x)$.

PROPOSITION 6.1. *Let* $u \in \mathfrak{tder}_2$ *and assume that it satisfies equations* (21) *and* (22) *with* $\operatorname{div}(u) = \tilde{\delta}(\operatorname{tr}(\phi(x)))$. *Then, the even part of the formal power series* ϕ *is given by the following formula*:

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

where B_n *are Bernoulli numbers.*

Proof. We follow [4] (see Remark 4.3). Write $A(x, y) = \alpha(\operatorname{ad}_x)y + \dots$, $B(x, y) = bx + \beta(\operatorname{ad}_x)y + \dots$, where $b \in \mathbb{K}, \alpha, \beta \in \mathbb{K}[[x]]$, and $\dots$ stand for the terms containing at least two y's. Replace $y \mapsto sy$ in equation (21), and compute the first and second derivatives in s at $s = 0$. The first derivative yields

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

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 (that is, homogeneous of $\deg_y = 2$) are in bijection with skew-symmetric (that is, $a(u, v) = -a(v, u)$) formal power series in two variables,

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

The second derivative of (21) 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 $-\operatorname{ch}(sy, x)$, and $a_2(u, v)$ represents the second derivative of $A(x, sy)$ at $s = 0$. By putting $v = -u$ in the last equation, we obtain

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

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

Finally, consider equation (23) and compute the contribution linear in y (that is, of the form $\operatorname{tr}(f(x)y)$) 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,

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

which implies

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

as required. □

Proposition 6.2. *Let* $F \in \mathrm{SolKV}$ *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* $f_{\mathrm{even}}(x) = \frac{1}{2}\ln(e^{x/2} - e^{-x/2})/x)$, *and for every odd formal power series*

$$f_{\mathrm{odd}}(x) = \sum_{k=1}^{\infty} f_{2k+1}x^{2k+1},$$

there is an element $F \in \mathrm{SolKV}$ *such that* $j(F) = \tilde{\delta}(\mathrm{tr}(f_{\mathrm{even}}(x) + f_{\mathrm{odd}}(x)))$.

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 5.8) $\phi(s) = sf'(s)$. By Proposition 6.1, we obtain

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

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

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

Put $g = \exp(u)$ for $u \in \mathfrak{krv}_2$, and compute $j(g) = (e^u - 1)/u \cdot \mathrm{div}(u) = \mathrm{div}(u)$. By choosing g with $u = -\sum_{k=1}^{\infty} h_{2k+1}\nu(\sigma_{2k+1})$ (with $h_{2k+1} \in \mathbb{K}$), 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 $g \in \mathrm{KRV}_2$, 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 6.3. The group KRV_2 acts on SolKV, and this action descends to the space of formal power series $x^2\mathbb{K}[[x]]$ along the map $f : \mathrm{SolKV} \to x^2\mathbb{K}[[x]]$ sending F to $f = j(F)$. In Proposition 6.2 we have used this action to change the odd part of f. Previously, this action (for the Grothendieck-Teichmüller group $\mathrm{GRT}_1 \subset \mathrm{KRV}_2$) on Duflo functions has been described in [16] (see Theorem 7).

Proposition 6.4. *Let* $F = \exp(u) \in \mathrm{SolKV}$ *with* $u = (a, b) \in \mathfrak{tder}_2$ *such that*

$$a(x, y) = a_0 y + \alpha(\mathrm{ad}_y)x + \ldots,$$
$$b(x, y) = b_0 x + \beta(\mathrm{ad}_y)x + \ldots,$$

where $a_0, b_0 \in \mathbb{K}$, $\alpha, \beta \in s\mathbb{K}[[s]]$, *and* $\ldots$ *stand for terms which contain at least two* x. *If* $a_0 = 0$, *then the Duflo function* $f(s)$ *associated to* F *satisfies equation* $f'(s) = \beta(s) - \alpha(s)$.

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

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

On the other hand, for $a_0 = 0$, we obtain

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

Here we used that u is of degree greater than or equal to one in variable x, and all contributions nonlinear in u are of degree at least two in x.

Finally, we compute

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

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

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

The KV *problem.* Find an element $F \in \mathrm{TAut}_2$ such that $F(x+y) = \mathrm{ch}(x,y)$ and $j(F) = \tilde{\delta}(f)$, where

$$f(x) = \frac{1}{2} \sum_{k=2}^{\infty} \frac{B_k x^k}{k \cdot k!} = \frac{1}{2} \ln\big((e^{x/2} - e^{-x/2})/x\big). \tag{24}$$

We shall denote the set of solutions of the KV problem by SolKV^0. Note that the KV problem is equivalent to finding an element $u = (A, B) \in \mathfrak{tder}_2$ which satisfies equation (21) 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 6.5. The group $\mathrm{KRV}^0{}_2$ acts on SolKV^0 by right multiplications. This action is free and transitive. The proof of this statement is completely analogous to the proof of Theorem 5.7.

Remark 6.6. Recall that the Kashiwara-Vergne conjecture implies the following Duflo theorem [9] (see [25] for the detailed account). Let $\mathfrak{g}$ be a finite-dimensional Lie algebra over $\mathbb{K}$. Then, there is an isomorphism $\mathrm{Duf} : (S\mathfrak{g})^{\mathfrak{g}} \to Z\big(U(\mathfrak{g})\big)$, where $(S\mathfrak{g})^{\mathfrak{g}}$ is the ring of invariant polynomials (under the adjoint action), and $Z\big(U(\mathfrak{g})\big)$ is the center of the universal enveloping algebra. In more detail, the Duflo isomorphism $\mathrm{Duf} = \mathrm{Sym} \circ \partial_{J^{1/2}}$ is the composition of the symmetrization map $\mathrm{Sym} : S(\mathfrak{g}) \to U(\mathfrak{g})$ and the (infinite order) constant coefficient differential operator $\partial_{J^{1/2}}$. This differential operator is associated by the Fourier transform to the function $J^{1/2}$ defined on the neighborhood of zero in $\mathfrak{g}$,

$$J^{1/2}(x) = \det\left(\frac{e^{\mathrm{ad}_x/2} - e^{-\mathrm{ad}_x/2}}{\mathrm{ad}_x}\right)^{1/2}.$$

Note that, up to replacing $x \mapsto \mathrm{ad}_x$, the function $J^{1/2}(x)$ is the exponential of the function $f(x)$ in equation (24). This explains the name of "Duflo function" in the title of this section.

7. Pentagon equation

In this section we establish a relation between the Kashiwara-Vergne problem and the pentagon equation introduced in [8]. Let $\Phi \in \mathrm{TAut}_3$. We say that Φ satisfies the pentagon equation if

$$\Phi^{12,3,4}\Phi^{1,2,34} = \Phi^{1,2,3}\Phi^{1,23,4}\Phi^{2,3,4} \tag{25}$$

in TAut_4.

PROPOSITION 7.1. *Let* $F \in \mathrm{SolKV}$. *Then,*

$$\Phi = (F^{12,3})^{-1}(F^{1,2})^{-1}F^{2,3}F^{1,23} \tag{26}$$

is an element of $\mathrm{KRV^0}_3$, *and it satisfies the pentagon equation.*

Proof. First, we compute

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

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

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

Similarly, we obtain

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

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

The pentagon equation is satisfied by substituting the expression for Φ into the equation, and by using the fact that for $\Phi \in \mathrm{KRV}^0{}_3 \subset \mathrm{SAut}_3$, we have $F^{123,4}\Phi^{1,2,3} = \Phi^{1,2,3}F^{123,4}$ and $F^{1,234}\Phi^{2,3,4} = \Phi^{2,3,4}F^{1,234}$. $\square$

Let $F_1 \in \mathrm{SolKV}$ and Φ_1 be the corresponding solution of the pentagon equation. Consider another element $F_2 \in \mathrm{SolKV}$. By Theorem 5.7, $F_2 = F_1 g$ for some $g \in \mathrm{KRV}_2$. The corresponding solution of the pentagon equation reads

$$\begin{aligned} \Phi_2 &= (F_2^{12,3})^{-1}(F_2^{1,2})^{-1}F_2^{2,3}F_2^{1,23} \\ &= (g^{12,3})^{-1}(F_1^{12,3})^{-1}(g^{1,2})^{-1}(F_1^{1,2})^{-1}F_1^{2,3}g^{2,3}F_1^{1,23}g^{1,23} \\ &= (g^{12,3})^{-1}(g^{1,2})^{-1}\Phi_1 g^{2,3}g^{1,23}. \end{aligned} \tag{27}$$

Equation (27) defines an action of KRV_2 on solutions of the pentagon equation with values in $\mathrm{KRV}^0{}_3$. Actions of this type are called *Drinfeld twists* (see [8], equation (1.11)).

Proposition 7.2. *Let $F_1, F_2 \in \mathrm{SolKV}$ 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

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

for all $\Phi \in \mathrm{KRV}^0{}_3$, where $c = t^{1,2} + t^{1,3} + t^{2,3}$ is a central element in $\mathfrak{sder}_3$ and in $\mathfrak{krv}^0{}_3$.

The degree one component of $\mathfrak{krv}_2$ is spanned by t, and t is central in $\mathfrak{krv}_2$. Hence, one can represent $g = F_1^{-1}F_2$ in the form $g = \exp(\lambda t)\exp(u)$, where $u = \sum_{k=2}^\infty u_k \in \mathfrak{krv}_2$. 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 3.17 we have $u_{k_0} = 0$ which implies $u = 0$ and $g = \exp(\lambda t)$, as required. $\square$

Proposition 7.3. *Let $\Phi = \exp(\phi) \in \mathrm{TAut}_3$ 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 $\phi_2 = (\alpha[y,z], \beta[z,x], \gamma[x,y])$ for some $\alpha, \beta, \gamma \in \mathbb{K}$.*

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 3.17) 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* $s, \alpha \in \mathbb{K}$, *and* u *is an element of* $\mathfrak{tder}_2$ *of degree greater than or 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* $\mathrm{KRV}^0{}_3$, *and denote* $\pi(\phi_2) = \lambda$. *Then,* $\lambda = s^2/8$ *and* $F \in \mathrm{SolKV}_s$.

Proof. First note that Φ is independent of α (see the first paragraph in the proof of Proposition 7.2). Hence, without loss of generality one can put $\alpha = 0$.

Let $\phi = \ln(\Phi) = \sum_{k=1}^{\infty} \phi_k$, where ϕ_k is of degree k. We have $\phi_1 = s(dr)/2 = 0$. For the degree two part, we use the Campbell-Hausdorff formula to compute $F^{1,2}F^{12,3}$ and $F^{2,3}F^{1,23}$ up to degree two, and notice that $r^{1,2} + r^{12,3} = r^{12,3} + r^{1,2}$ (since $dr = 0$). This yields

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

Here we used the classical Yang-Baxter equation of Proposition 3.10. In conclusion, $\lambda = \pi(\phi_2) = s^2/8$.

Denote $\chi(x, y) = F(x + y) = x + y + \frac{s}{2}[x, y] + \ldots$, where $\ldots$ stand for elements of degree greater than 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 2.9, 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 $F^{2,3}F^{1,23} = F^{1,2}F^{12,3}\Phi$ (and using $j(\Phi) = 0$), 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 2.10, $b \in \mathrm{im}(\tilde{\delta}_s)$ and $F \in \mathrm{Sol}_s(\mathrm{KRV})$. □

THEOREM 7.5. *Let* $\Phi = \exp\left(\sum_{k=2}^{\infty} \phi_k\right) \in \mathrm{KRV}^0{}_3$ *be a solution of the pentagon equation with* $\pi(\phi_2) = \lambda$, *and assume that* 8λ *admits a square root* $s \in \mathbb{K}$. *Then, there is a unique element* $F \in \mathrm{SolKV}_s$ *such that* $F = \exp(u)\exp(sr/2) \in \mathrm{TAut}_2$, *where* u *is an element of* $\mathfrak{tder}_2$ *of degree greater than or 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 the equation

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

In degree two, this 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 the operator $\mathrm{d} : \mathfrak{tder}_2 \to \mathfrak{tder}_3$ has no kernel in degrees greater than one.

Assume that we found $F_n \in \mathrm{TAut}_2$ such that

$$\Phi_n = \exp\left(\sum_{k=2}^{\infty} \psi_k\right) = (F_n^{12,3})^{-1}(F_n^{1,2})^{-1}F_n^{2,3}F_n^{1,23}$$

and $\psi_k = \phi_k$ for $k \le n$. (We say that Φ_n 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 $n+1$. By the proof of Proposition 2.9, $F_n(x+y) = \mathrm{ch}_s(x,y)$ 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 $n+1$. 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 3.17, $\varphi = \mathrm{d}u$ 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, $F \in \mathrm{SolKV}_s$. □

Remark 7.6. One can also express Theorem 7.5 in the following way. Denote by Pent_λ the set of solutions $\Phi = \exp\left(\sum_{k=2}^{\infty} \phi_k\right) \in \mathrm{KRV}^0{}_3$ of the pentagon equation with $\pi(\phi_2) = \lambda$. Assume that 8λ admits a square root $s \in \mathbb{K}$. Then, the map (26) $F \mapsto \Phi$ defines an isomorphism $\mathrm{Pent}_\lambda \cong \mathrm{SolKV}_s/\mathbb{K}$, where the action of the additive group $\mathbb{K}$ is by $F \mapsto F\exp(\lambda t)$.

In particular, Theorem 7.5 implies that the Kashiwara-Vergne problem has solutions if and only if the pentagon equation admits solutions $\Phi \in \mathrm{KRV}^0{}_3$ with $\pi(\phi_2) = 1/8$.

The next proposition provides a tool for extracting the Duflo function of an element $F \in \mathrm{SolKV}$ from the corresponding solution of the pentagon equation.

PROPOSITION 7.7. *Let $\Phi = \exp(\phi) \in \mathrm{KRV}^0{}_3$ be a solution of the pentagon equation with $\pi(\phi_2) = 1/8$, and let $F \in \mathrm{SolKV}$ be a solution of equation* (26). *Denote $\phi = (A, B, C)$, and $B(x, 0, z)_{x-\mathrm{lin}} = h(\mathrm{ad}_z)x$ for $h \in x\mathbb{K}[[x]]$. Then, the Duflo function $f(x)$ 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 $b(x, y) = b_0 x + \beta(\mathrm{ad}_y)x + \dots$. Choose F in such a way that $a_0 = 0$ (this is always possible by replacing $F \mapsto F\exp(\lambda t)$ if needed). By Proposition 6.4, the Duflo function f associated to F is a solution of equation $f' = \beta - \alpha$.

Put $y = 0$ in all components of $u^{1,2}, u^{12,3}, u^{2,3}, u^{1,23}$. Assumption $a_0 = 0$ implies that all these expressions are of degree greater than or equal to one in the variable x. Hence, for the computation of the degree one in x part of $\phi = \ln\big((F^{12,3})^{-1}(F^{1,2})^{-1}F^{2,3}F^{1,23}\big)$, one can replace it by $u^{1,23} + u^{2,3} - u^{1,2} - u^{12,3}$. This yields $B(x, 0, z)_{x-\mathrm{lin}} = \beta(\mathrm{ad}_z)x - \alpha(\mathrm{ad}_z)x$ and $h(x) = \beta(x) - \alpha(x)$. Hence, $f'(x) = h(x)$, as required. $\square$

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

In this section we introduce an involution τ on 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 the 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 $a \in \mathfrak{lie}_2$,

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

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

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

and

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

as required. $\square$

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

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

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 $y \mapsto \exp(-\operatorname{ad}_z)y$. We compute the action of the left-hand side on x:

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

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, $y \mapsto y$, and $z \mapsto z$. It remains to compute the action on x:

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

and the same for the right-hand side:

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

as required. □

8.2. *Involution on* SolKV. In this section we introduce and study a certain involution on the set of solutions of the KV problem.

PROPOSITION 8.4. *Let $F \in \mathrm{SolKV}$. Then, $\tau(F) = RF^{2,1}e^{-t/2}$ is a solution of the* KV *problem, $\tau(F) \in \mathrm{SolKV}$. 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 $j(F) = \mathrm{tr}(f(x) - f(\mathrm{ch}(x,y)) + f(y))$. Note that $j(F^{2,1}) = j(F)^{2,1})$ (since $\mathrm{div}(u^{2,1}) = \mathrm{div}(u)^{2,1}$ for $u \in \mathfrak{tder}_2$). This implies $j(F^{2,1}) = \mathrm{tr}(f(x) - f(\mathrm{ch}(y,x)) + f(y))$ 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 SolKV. $\square$

Proposition 8.5. *Let $F \in \mathrm{SolKV}$ 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

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

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 $\mathfrak{krv}^0{}_3$ in the passage from the third to the fourth line. $\square$

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

(28)
$$\kappa(\tau(F)) = \Big(e^{\mathrm{ad}_x}B(y,x) + \frac{1}{2}(\mathrm{ch}(x,y) - x), e^{-\mathrm{ad}_y}A(y,x) - \frac{1}{2}(\mathrm{ch}(x,y) - y)\Big).$$

Proof. We compute

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

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 (21) (with x and y exchanged). For the action on y, we compute

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

By adding up all three terms, we obtain

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

as required. ∎

Remark 8.7. Symmetry (28) has been introduced in [15] (see the discussion after Proposition 5.3).

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

Definition 8.8. An element $F\in\mathrm{SolKV}$ is called *a symmetric solution* of the generalized Kashiwara-Vergne conjecture if $\tau(F)=F$.

We shall denote the set of symmetric solutions by SolKV^τ. 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 (21) and (22) 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 $\mathfrak{krv}_2$, and it lifts to the group KRV_2. We shall denote the corresponding invariant subalgebra by $\mathfrak{krv}_2^{\mathrm{sym}} \subset \mathfrak{krv}_2$ and the invariant subgroup by $\mathrm{KRV}_2^{\mathrm{sym}} \subset \mathrm{KRV}_2$.

PROPOSITION 8.9. *The group* $\mathrm{KRV}_2^{\mathrm{sym}}$ *acts on the set* SolKV^τ *by multiplications on the right. This action is free and transitive.*

Proof. Let $g \in \mathrm{KRV}_2^{\mathrm{sym}}$ and $F \in \mathrm{SolKV}^\tau$. By Theorem 5.7, $Fg \in \mathrm{SolKV}$. 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, $Fg \in \mathrm{SolKV}^\tau$.

Consider two elements $F_1, F_2 \in \mathrm{SolKV}^\tau$. We denote $g = F_1^{-1}F_2$ and compute

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

as required. $\square$

Remark 8.10. Note that the element $t = (y, x)$ as well as the image of the injection $\nu : \mathfrak{grt}_1 \to \mathfrak{krv}_2$ is contained in $\mathfrak{krv}_2^{\mathrm{sym}}$. In fact, it is not known whether any nonsymmetric elements of $\mathfrak{krv}_2$ exist. If the conjecture stated in the end of Section 4 is correct, it implies $\mathfrak{krv}_2 = \mathfrak{krv}_2^{\mathrm{sym}}$.

PROPOSITION 8.11. *Let* $F \in \mathrm{SolKV}^\tau$, *and let* $\Phi \in \mathrm{KRV}^0{}_3$ *be the corresponding solution of the pentagon equation. Then,*

$$\Phi^{1,2,3}\Phi^{3,2,1} = e, \tag{29}$$

$$e^{(t^{1,3}+t^{2,3})/2} = \Phi^{2,1,3}e^{t^{1,3}/2}(\Phi^{2,3,1})^{-1}e^{t^{2,3}/2}\Phi^{3,2,1}, \tag{30}$$

and

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

Proof. Equation (29) follows by Proposition 8.5. In order to prove equation (30) recall that $R^{12,3} = R^{1,3}R^{2,3} = (\exp(-\operatorname{ad}_z), \exp(-\operatorname{ad}_z), 1) \in \mathrm{TAut}_3$. 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

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

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 (30). Equation (31) follows by applying the (13)-permutation to equation (30) and by using the inversion formula (29). □

Remark 8.12. Equations (30) and (31) are called as *hexagon equations*. They were first introduced in [8] (see equations (2.14a) and (2.14b)).

9. **Associators**

In this section we consider joint solutions of pentagon and hexagon equations called KV-*associators* (with values in the group $\mathrm{KRV^0}_3$). We show that Drinfeld's associators defined in [8] 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 $\Phi \in \mathrm{KRV^0}_3$ is called a KV-associator if it satisfies the pentagon equation (25), hexagon equations (30) and (31), and the inversion property (29).

PROPOSITION 9.2. *Let* $\Phi = \exp(\phi) = \exp\left(\sum_{k=2}^\infty \phi_k\right) \in \mathrm{KRV^0}_3$ *be a* KV-*associator. Then,* $\pi(\phi_2) = 1/8$.

Proof. The degree two component of the hexagon equation (30) 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 9.3. *Let* $\Phi = \exp(\phi) = \exp\left(\sum_{k=2}^\infty \phi_k\right) \in \mathrm{KRV^0}_3$ *be a solution of equations* (25) *and* (29) *with* $\pi(\phi_2) = 1/8$. *Then, each* $F \in \mathrm{SolKV}$ *which verifies equation* (26) *is a symmetric solution of the KV problem,* $F \in \mathrm{SolKV}^\tau$.

Proof. Theorem 7.5 implies that equation (26) admits solutions $F = \exp\left(\sum_{k=1}^\infty f_k\right) \in \mathrm{SolKV}$. 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 3.11, Lie algebras $\mathfrak{t}_n$ inject into $\mathfrak{krv}^0{}_n$. In particular, $\mathfrak{t}_3$ injects into $\mathfrak{krv}^0{}_3$, and the corresponding group T_3 is a subgroup of $\mathrm{KRV}^0{}_3$.

Definition 9.4. A KV-associator $\Phi \in \mathrm{KRV}^0{}_3$ 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 $\mathfrak{krv}^0{}_n$ since coface maps restrict to Lie subalgebras $\mathfrak{t}_n$ in a natural way. In [7], Drinfeld proved the following fundamental theorem.

THEOREM 9.5. *The set of Drinfeld's associators is nonempty.*

This implies the following result.

THEOREM 9.6. *The set of symmetric solutions of the* KV *problem* SolKV^τ *is nonempty.*

Proof. Each Drinfeld's associator $\Phi = \exp(\phi) = \exp\left(\sum_{k=2}^\infty \phi_k\right)$ is a KV-associator with $\pi(\phi_2) = 1/8$. Then, by Theorem 7.5, there is an element $F = \exp\left(\sum_{k=1}^\infty f_k\right) \in \mathrm{TAut}_2$ with $f_1 = r/2$ which solves equation (26). By Proposition 7.4, this automorphism is a solution of the KV problem, and by Proposition 9.3 this solution is symmetric. $\square$

Remark 9.7. In the case of Drinfeld associators, there is a constructive proof of Theorem 7.5 (see [2]). It gives an explicit formula for F solving the twist equation (26) in terms of the Drinfeld associator Φ.

Remark 9.8. The KV problem has been settled in [3]. The solution is based on the Kontsevich deformation quantization scheme [17] and on the earlier work of the second author [24]. Theorem 9.6 gives a new proof of the KV conjecture by reducing it to the existence theorem for Drinfeld's associators.

PROPOSITION 9.9. *Let* $\Phi = \exp(\phi) \in T_3$ *be a Drinfeld's associator, and let* $F \in \mathrm{SolKV}$ *be a solution of the* KV *problem which satisfies equation* (26). *Write* $\phi = h(\mathrm{ad}_{t^{2,3}})t^{1,2} + \dots$, *where* $h \in x\mathbb{K}[[x]]$ *and* $\dots$ *stand for terms whose degree with respect to* $t^{1,2}$ *is greater than one. Then, the Duflo function* $f(x)$ *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 $B(x, 0, z)_{x-\mathrm{lin}} = h(\mathrm{ad}_z)x$. Then, by Proposition 7.7, we obtain $f'(x) = h(x)$, as required. $\square$

Example 9.10. Consider the Knizhnik-Zamolodchikov associator (with values in T_3) constructed by Drinfeld. Equation (2.15) of [8] yields the function $h(x)$:

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

Note that associators defined in this paper are obtained by taking an inverse of associators in the 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. The formula for $f(x)$ matches (up to a sign change) the expression $\ln(F_{\text{nice}}(x))$ in [16].

9.2. *Actions of the group* GRT_1. 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_1 as a subset of Lie_2 defined by a number of relations (see [8, §5]) and equipped with the new multiplication

$$(h_1 *_{\mathrm{GRT}_1} h_2)(x, y) = h_1(x, h_2(x, y) y h_2^{-1}(x, y)) h_2(x, y).$$

Remark 9.11. Note that we have chosen to act on the second argument y of the function h rather than on x (the first argument) as in [8].

Let $\psi \in \mathfrak{grt}_1$ and consider a one parameter subgroup of GRT_1 defined by ψ, $h_s = \exp_{\mathrm{GRT}_1}(s\psi)$. Write $h_t = h_{t-s} *_{\mathrm{GRT}_1} h_s$ 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 $\exp_{\mathrm{GRT}_1}$ in a unique way.

PROPOSITION 9.12. *Let* $\psi \in \mathfrak{grt}_1$, $h = \exp_{\mathrm{GRT}_1}(\psi) \in \mathrm{GRT}_1$, *and* $g = \exp(\nu(\psi)) \in \mathrm{KRV}_2$. *Then,*

$$\hat{g} = (g^{12,3})^{-1} (g^{1,2})^{-1} g^{2,3} g^{1,23} = h(t^{1,2}, t^{2,3}) \in {\mathrm{KRV}^0}_3.$$

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 $\hat{g}_s = (g_s^l)^{-1} g_s^r$:

$$\begin{aligned} \frac{d\hat{g}_s}{ds} &= (g_s^l)^{-1} \left(\frac{dg_s^r}{ds} (g_s^r)^{-1} - \frac{dg_s^l}{ds} (g_s^l)^{-1} \right) g_s^r \\ &= (g_s^l)^{-1} (\mathrm{d}\nu(\psi)) g_s^r \end{aligned}$$

$$
\begin{aligned}
&= (g^l_s)^{-1}\psi(t^{1,2},t^{2,3})g^r_s \\
&= \psi(t^{1,2},(g^l_s)^{-1}t^{2,3}g^l_s)(g^l_s)^{-1}g^r_s \\
&= \psi(t^{1,2},(g^l_s)^{-1}g^r_s t^{2,3}(g^r_s)^{-1}g^l_s)\hat{g}_s \\
&= \psi(t^{1,2},\hat{g}_s t^{2,3}(\hat{g}_s)^{-1})\hat{g}_s.
\end{aligned}
$$

To establish the second equality, we make use of $(dg^l_s/ds)(g^l_s)^{-1} = \nu(\psi)^{1,2} + \nu(\psi)^{12,3}$ and $(dg^r_s/ds)(g^r_s)^{-1} = \nu(\psi)^{2,3} + \nu(\psi)^{1,23}$. The third equality follows from Proposition 4.7. For the fourth and fifth equalities, we are using that t is central in $\mathfrak{sder}_2$.

Observe that $\hat{g}_0 = e \in \mathrm{KRV}^0{}_3$. Then, $h(t^{1,2},t^{2,3})$ 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 $\nu : \mathfrak{grt}_1 \to \mathfrak{krv}_2$ gives rise to a subgroup of KRV_2 isomorphic to GRT_1. The group KRV_2 acts on the set of solutions of the KV problem and on the set of associators with values in $\mathrm{KRV}^0{}_3$ (see equation (27)). In [8] (see §5) Drinfeld defines a free and transitive action of the group GRT_1 on the set of associators with values in T_3. This action is given by the following formula:

$$
g : \Phi(t^{1,2},t^{2,3}) \mapsto \Phi(t^{1,2}, g t^{2,3} g^{-1}) g, \tag{32}
$$

where $g = \exp_{\mathrm{GRT}_1}(\psi) \in \mathrm{GRT}_1$ 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 9.13. *When restricted to the set of Drinfeld's associators, the action of the group* GRT_1 *on KV-associators coincides with the canonical action* (32).

Proof. Let $g \in \mathrm{KRV}_2$ and rewrite the action (27) 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 $\psi \in \mathfrak{grt}_1$ and $g = \exp(\nu(\psi))$. Then, by Proposition 9.12 we have $\hat{g} = (\exp_{\mathrm{GRT}_1}(\psi))(t^{1,2},t^{2,3})$, and the action (27) coincides with the canonical action (32). □

Remark 9.14. If the conjecture of Section 4 is correct, we have $\mathrm{KRV}_2 \cong \mathbb{K}t \times \nu(\mathrm{GRT}_1)$, where the additive group $\mathbb{K}t$ injects into KRV_2 via the exponential map, $\lambda t \mapsto \exp(\lambda t)$. In particular, this implies $\mathrm{KRV}_2 = \mathrm{KRV}_2^{\mathrm{sym}}$ since both $\mathbb{K}t$ and $\nu(\mathrm{GRT}_1)$ are contained in $\mathrm{KRV}_2^{\mathrm{sym}}$. Note that the action of $\mathbb{K}t$ on KV-associators is trivial and the action of GRT_1 on the set of Drinfeld's associators is transitive. The action of $\mathrm{KRV}_2^{\mathrm{sym}}$ on KV-associators is also transitive, and we conclude that all KV-associators are Drinfeld's associators.

Remark 9.15. For Drinfeld's associators, Furusho [12] showed that the hexagon equations (30), (31), and the inversion property (29) follow from the pentagon equation, and the normalization condition $\pi(\phi_2) = 1/8$. In the case of KV-associators, Proposition 8.11 shows that the hexagon equations (30) and (31) follow from the pentagon equation, the inversion property, and the normalization condition $\pi(\phi_2) = 1/8$. If we assumed $\mathrm{KRV}_2 = \mathrm{KRV}_2^{\mathrm{sym}}$, the inversion property would be automatic and we would get the analogue of Furusho's result for KV-associators. If the conjecture of Section 4 holds true, we recover the Furusho's result.

Appendix A. Cohomology computations

In this appendix, we collect the cohomology computations needed in the paper. We give a detailed account for cohomology in low degrees. A more enlightened approach can be found in [22] and [27].

Proof of Theorem 2.8. 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 2.7.

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

$$f(y,z) - f(x+y,z) + f(x,y+z) - f(x,y) = 0. \tag{33}$$

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

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

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

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

Combining these two equations gives an identity

$$\begin{aligned} &f((1+s)x,z) + f(x,(1+s)z) \\ &\qquad = 2f(x,z) + f(sx,x+z) + f(x+z,sz) - f(sx,x) - f(z,sz) \end{aligned}$$

and differentiating both sides in s at $s=0$ yields

$$\begin{aligned} nf(x,z) &= \frac{d}{ds}\left(f((1+s)x,z) + f(x,(1+s)z)\right)|_{s=0} \\ &= \frac{d}{ds}\left(f(sx,x+z) + f(x+z,sz) - f(sx,x) - f(z,sz)\right)|_{s=0}. \end{aligned} \tag{34}$$

First, we solve equation (34) for $f \in \mathfrak{lie}_2$. In this case, $f(sx,x) = f(z,sz) = 0$ 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 (33).

For $n \geq 3$, consider equation (33) and first put $y = -z$ to get $f(x, -z) = -f(x - z, z)$ which implies $f(x, z) = -f(x + z, -z)$. Then, put $y = -x$ to obtain $f(-x, z) = -f(x, z - x)$ which implies $f(x, z) = -f(-x, x + z)$. Hence,

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

This implies $\alpha - \beta = 0$ and $f(x, z) = 0$ since $\mathrm{ad}_z^{n-1} x \neq -\mathrm{ad}_x^{n-1} z$ (in $\mathfrak{lie}_2$) unless $n = 2$. 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 (34) 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

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

Introduce a basis of monomial cyclic words in $\mathfrak{tr}_3$ (e.g., $\mathrm{tr}(y^n)$, $\mathrm{tr}(y^{n-1}x) = \mathrm{tr}(xy^{n-1})$, $\mathrm{tr}(y^{n-2}xz)$, etc.). With respect to this basis, the coefficient of the cyclic monomial $\mathrm{tr}(y^{n-2}xz)$ in the decomposition of δf is equal to $(\beta - \alpha)(n - 2)$. 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.

Remark. In the proof of Theorem 2.8 we have shown that $\ker(\delta : \mathfrak{lie}_2 \to \mathfrak{lie}_3) = \mathbb{K}[x, y]$. That is, the only solution of equation (33) is $f(x, y) = \alpha[x, y]$. Equation (33) has been previously considered in the proof of Proposition 5.7 in [8]. There it is stated that equation (33) has no nontrivial symmetric (that is, $f(x, y) = f(y, x)$) solutions in $\mathfrak{lie}_2$.

Proof of Proposition 2.10. 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 $H^1(\mathfrak{tr}, \tilde{\delta})$, 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 "…" stand for the terms of degree greater than k).

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

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 $f \in \mathfrak{tr}_2$, the 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 $g = \tilde{\delta}h$.

Proof of Theorem 3.17. 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 $\mathrm{d}u = u^{2,3} - u^{12,3} + u^{1,23} - u^{1,2}$. The 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 $b(x, y) = b(x + y, 0) - b(y, 0) = \beta x$. 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 $\mathrm{d}u = u^{2,3,4} - u^{12,3,4} + u^{1,23,4} - u^{1,2,34} + u^{1,2,3}$. The equation $\mathrm{d}u = 0$ yields

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

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 fourth equation for $\tilde{c}$ yields $l(x + y, z + w) = l(y, z + w)$ which implies $l = 0$. Hence, $\tilde{u} = (0, \tilde{b}, 0)$. Denote $h(x, y) =$

$\tilde{b}(x,0,y)$. First put $y=0$ in the second equation for $\tilde{b}$ to get $\tilde{b}(x,z,w) = h(x,z+w)-h(x,z)$, then put $z=0$ in the third equation for $\tilde{b}$ 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 2.8, $h(x,y)=\gamma[x,y]$ 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 $\gamma \neq 0$.

Appendix B. Proof of Proposition 4.7

In this appendix we give a proof of Proposition 4.7. It is inspired by the proof of Proposition 5.7 in [8].

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

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

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 $\mathfrak{t}_4$:

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

Here, in passing from the first to the second equation, 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 equation 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 third to the fourth equation we used a (3214) permutation of the equation (13). 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:

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

Here we used the (1324) and (3124) permutations of equation (13) as well as equation (12), 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:

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

where we used the equation (13) (no permutation needed). We conclude that

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

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

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