About Approximations of Exponentials *

P.-V. Koseleff **

Équipe "Analyse Algébrique", Institut de Mathématiques,
Université Pierre & Marie Curie, Case 247
4 place Jussieu, F-75252 Paris cedex 05

e-mail: koseleff@mathp6.jussieu.fr

Abstract. We look for the approximation of $\exp(A_1 + A_2)$ by a product in form $\exp(x_1A_1)\exp(y_1A_2)\cdots\exp(x_nA_1)\exp(y_nA_2)$. We specially are interested in minimal approximations, with respect to the number of terms. After having shown some isomorphisms between specific free Lie subalgebras, we will prove the equivalence of the search of such approximations and approximations of $\exp(A_1 + \cdots + A_n)$. The main result is based on the fact that the Lie subalgebra spanned by the homogeneous components of the Hausdorff series is free.

1 Introduction

Let $A_1 + A_2$ be an hamiltonian vector fields. We want to approximate the flow $\exp(t(A_1 + A_2))$ and suppose that it is much easier to evaluate $\exp(tA_1)$ so as $\exp(tA_2)$. Thus we try to approximate $\exp(A_1 + A_2)$ by a product of exponentials $\exp(x_1A_1)\exp(x_2A_2)\cdots\exp(x_nA_1)\exp(y_nA_2)$. The transformation obtained is the time-evolution of an hamiltonian system close to the original one. In particular, some quantities are invariant trough the transformation.

Many methods are known and are used to calculate the so-called symplectic integrators at any order. We are interested here in minimal approximations, that is to say in which a minimum number of exponentials are involved. We will see such identities as universal Lie algebraic identities. We will work in a free Lie algebra and we will study the conditions that must satisfy such approximants.

In this paper, we will prove an assertion that has been proposed by R. MacLachlan ([5]). It shows that the getting of approximations for $\exp(A_1 + A_2)$ gives approximants for any $\exp(\sum A_i)$, as product of first-order approximants. The main step is the fact that the Lie subalgebra generated by the homogeneous components of the Hausdorff series of A_1 and A_2 is free. We then prove algebraic isomorphisms between the several sets of solutions we are looking at.

All these minimal integrators have been computed up to order 6 and we remark that they are all products of second-order approximants. An interesting question would be to know if that fact is preserved at any order.

* Proceedings of AAECC'11 Conference, Paris, juillet 1995, LNCS **948**, 12 p.

** Research supported by the CNRS GDR 1026 (MEDICIS) and the Computer Algebra Lab. (GAGE) at the École Polytechnique

2 Notations and presentation of the main results

R is a commutative ring which contains the rational numbers. X is a weighted alphabet, that is to say an ordered set in which each letter has a positive integer weight. Without any indication, we will suppose that any letter has a weight 1.

2.1 Free Lie algebras

X^* is the free monoid on X. X^* is an ordered set with the lexicographic order. $M(X)$ denotes the free magma on X. $\mathcal{A}(X)$ is the free associative R-algebra on X. $L(X)$ is the free Lie R-algebra whose Lie bracket is denoted by $[,]$.

We will denote by $\mathrm{ad}x$ the map $y \mapsto [x,y]$.

On $L(X)$ so as on $\mathcal{A}(X)$, we consider the following gradations:

The length $x \mapsto |x|$ is the unique morphism on X^* that extends the function $x \mapsto 1$ on X. $L_n(X)$ (resp. $\mathcal{A}_n(X)$) is the free module generated by monomials of length n.

One defines on X^* (resp. $M(X)$) the weight $x \mapsto ||x||$ as the unique morphism that extends the weight on X. $\tilde{L}_n(X)$ (resp. $\tilde{\mathcal{A}}_n(X)$) is the free module generated by monomials of weight n.

2.2 Formal Lie series

Let us define the formal Lie series and the series of words as

$$\tilde{L}(X) = \prod_{n\geq 0} \tilde{L}_n(X) \quad \text{and} \quad \tilde{\mathcal{A}}(X) = \prod_{n\geq 0} \tilde{\mathcal{A}}_n(X). \tag{1}$$

We will write $x = \sum_{n\geq 0} x_n \in \tilde{L}(X)$. If $x, y \in \tilde{L}(X)$, we define classically

$$([x,y])_n = \sum_{p+q=n} [x_p, y_q] \tag{2}$$

that furnishes a Lie algebra structure to $\tilde{L}(X)$. Let $\tilde{L}(X)^+$ (resp. $\tilde{\mathcal{A}}(X)^+$), be the ideal of $\tilde{L}(X)$ (resp. $\tilde{\mathcal{A}}(X)$) generated by elements of strictly positive weight. Exponential is defined by

$$\begin{array}{rcl} \exp : \tilde{\mathcal{A}}(X)^+ & \rightarrow & 1 + \tilde{\mathcal{A}}(X)^+ \\ x & \mapsto & \sum_{n\geq 0} \dfrac{x^n}{n!}. \end{array}$$

Let us remind the Campbell-Hausdorff theorem:

Lemma 1. *If $x, y \in \tilde{L}(X)^+$, then $\exp(x)\exp(y) = \exp(H(x,y))$ where $H(x,y) \in \tilde{L}(X)^+$. Furthermore, we have $H_1(x,y) = x_1 + y_1$.*

2.3 Main result

The original problem we are looking at is the following.

Problem 1. *Considering the alphabet $A = \{A_1, A_2\}$, an order $k \in \mathbb{N}$ and an integer n, find a sequence $(x_1, \ldots, x_n)$ of length n, such that*

$$\begin{cases} \exp(x_1 A_1) \cdots \exp(x_n A_n) = \exp(A_1 + A_2 + R_k), \\ R_k \in \prod_{n>k} L_n(A). \end{cases} \tag{3}$$

Here $A_i = A_{i (\mathrm{mod}\, 2)+1}$

⋆⋆⋆

Considering the transformations

$$S^+(x) = \exp(xA_1)\exp(xA_2), \ S^-(x) = \exp(xA_2)\exp(xA_1), \tag{4}$$

MacLachlan ([5]) shows that any sequence $(y_1, \ldots, y_{n-1})$ which satisfies the

Problem 2.

$$\begin{cases} S^+(y_1)S^-(y_2)\cdots S^{\pm}(y_{n-1}) = \exp(A_1 + A_2 + R_k), \\ R_k \in \prod_{n>k} L_n(A). \end{cases} \tag{5}$$

gives a solution for the problem 1. Here $S^{\pm}(y_{n-1})$ is equal to $S^+(y_{n-1})$ if n is even, $S^-(y_{n-1})$ otherwise.

⋆⋆⋆

Considering that $S^+(x) = \exp(\sum_{n\geq 1} x^n H_n)$, where H_n is the homogeneous components of weight n of the Hausdorff series $H(A_1, A_2)$ in lemma 1, we have

$$S^-(x) = {S^+}^{-1}(-x) = \exp(-\textstyle\sum_{n\geq 1}(-x)^n H_n). \tag{6}$$

Considering an infinite alphabet $X = \{X_i, ||X_i|| = i, \ i \geq 1\}$, and

$$\phi^+(x) = \exp(\textstyle\sum_{n\geq 1} x^n X_n), \ \phi^-(x) = \exp(-\sum_{n\geq 1}(-x)^n X_n), \tag{7}$$

problem 2 may be generalized to

Problem 3. *Find a sequence $(y_1, \ldots, y_{n-1})$, such that*

$$\begin{cases} \phi^+(y_1)\phi^-(y_2)\cdots\phi^{\pm}(y_{n-1}) = \exp(X_1 + R_k), \\ R_k \in \prod_{n>k} \tilde{L}_n(X). \end{cases} \tag{8}$$

⋆⋆⋆

We will prove in this paper the assertion proposed by R. MacLachlan ([5]): *The solutions of problems 3 and 2 are equals and there is a one-to-one correspondance between these solutions and the solutions of the problem 1.*

More precisely we will prove the following results.

Proposition 2. *The set of solutions of problems 1, 2 and 3 are algebraic varieties. The first one is isomorphic to the others that are equals.*

Let us give now the successive steps of the proof.

- We will prove that the subalgebra of $L(A_1, A_2)$ generated by the homogeneous components of the Hausdorff series $H(A_1, A_2)$ is free. What is more is that the sum of this subalgebra and the line generated by A_2 is equal to $L(A_1, A_2)$, so their submodules spanned by elements of same weight are equals. This results makes use the Lazard elimination theorem and some combinatoric properties related to the Witt's formula.
- We will show that the solutions of the 3 problems we are considering are the solutions of a finite set of polynomial equations, that will prove that they are algebraic varieties.
- The two first steps will prove that the solutions of problems 2 and 3 are equals.
- The isomorphism between these varieties, will be shown by considering transformations in some commutative polynomial rings.

3 Some free Lie algebra isomorphisms

Let us first remind the

Theorem 3 (Elimination theorem of M. Lazard). *Let X be an alphabet, $S \subset X$ and $T = \{(s_1, \ldots, s_n, x),\ n \geq 0,\ s_1, \ldots, s_n \in S, x \in X - S\}$.*

- *$L(X)$ is the direct sum of $L(X - S)$ and of the ideal $\mathcal{S}$ spanned by S.*
- *$L(T)$ and $\mathcal{S}$ are isomorphic through $(s_1, \ldots, s_n, x) \mapsto \mathrm{ad}s_1 \cdots \mathrm{ad}s_n x$.*

Corollary 4. *By taking $A = \{A_1, A_2\}$ and $S = \{A_2\}$, we then deduce that*

$$\begin{aligned} L(\{A_1, A_2\}) &= L(\{A_2\}) + L(\{(\mathrm{ad}A_2)^n A_1,\ n \geq 0\}) \\ &= R.A_2 + L(\{(\mathrm{ad}A_2)^n A_1,\ n \geq 0\}). \end{aligned} \tag{9}$$

3.1 Dimensions of the homogeneous submodules

Let Y be any weighted alphabet. For a given $\alpha \in \mathbb{N}^{(Y)}$, let us consider $L^\alpha(Y)$ the submodule of $L(Y)$ generated by elements of multi-degree α. Let $l(\alpha)$ be the dimension of $L^\alpha(Y)$. From the Poincaré-Birkhoff-Witt theorem ([1]), we get the formal identity

$$1 - \sum_{y \in Y} T_y = \prod_{\alpha \in \mathbb{N}^{(Y)} - \{0\}} (1 - T^\alpha)^{l(\alpha)}\,. \tag{10}$$

Let $Y = A$ and consider $l_n = \sum_{|\alpha| = n} l(\alpha)$, the dimension of $L_n(A)$. In (10), let us substitute the same unknown U to T_{A_1} and T_{A_2}, we get

$$1 - 2U = \prod_{\alpha \in \mathbb{N}^{(A)} - \{0\}} (1 - U^{|\alpha|})^{l(\alpha)} = \prod_{n > 0} (1 - U^n)^{l_n}. \tag{11}$$

Let $X = Y$ and consider $\tilde{l}_n = \sum_{||\alpha||=n} l(\alpha)$ the dimension of $\tilde{L}_n(X)$. In formula (10), let us substitute U^i to T_{X_i}, we then obtain

$$1 - \sum_{i \geq 1} U^i = \frac{1-2U}{1-U} = \prod_{r>0} \prod_{||\alpha||=r} (1 - U^{||\alpha||})^{p_\alpha} = \prod_{r>0} (1-U^r)^{\tilde{l}_r}. \qquad (12)$$

We therefore deduce the following results using formulas (11) and (12):

Isomorphism 1. *Let $X = \{X_i, ||X_i|| = i,\ i \geq 1\}$. For each $n \geq 2$, $L_n(\{A_1, A_2\})$ and $\tilde{L}_n(X)$ are isomorphic. Furthermore*

$$\dim L_1(A) = 2,\ \dim \tilde{L}_1(X) = 1,\ \dim L_n(A) = \dim \tilde{L}_n(X),\ n \geq 2. \qquad (13)$$

We thus deduce, using corollary 4 and isomorphism 1 that

Corollary 5. *For any $d \geq 2$, $L_d(\{A_1, A_2\}) = \tilde{L}_d(\{(\mathrm{ad}A_2)^n A_1,\ n \geq 0\})$.*

4 Hausdorff series

Let us show the following result:

Isomorphism 2. *Let $A = \{A_1, A_2\}$ and $H(A_1, A_2) = \sum_{n \geq 1} H_n$. $\{H_n,\ n \geq 1\}$ freely generates the free Lie algebra $L(\{(\mathrm{ad}A_2)^n A_1,\ n \geq 0\})$.*

Sketch of proof. — We first show that

$$\tilde{L}_d(\{H_n(A_1 + A_2, -A_2),\ n \geq 1\}) \simeq \tilde{L}_d(\{H_n(A_1, A_2),\ n \geq 1\}), \qquad (14)$$

by using the Lie algebra morphism

$$\begin{aligned} \Phi_{x,y} : \tilde{L}(\{H_n(x,y),\ n \geq 1\}) &\to \tilde{L}(\{H_n(x+y,-y),\ n \geq 1\}) \\ H_n(x,y) &\mapsto H_n(x+y,-y). \end{aligned} \qquad (15)$$

Exhibing $\Phi_{x+y,-y} : \tilde{L}(\{H_n(x+y,-y),\ n \geq 1\}) \to \tilde{L}(\{H_n(x,y),\ n \geq 1\})$, shows that $\Phi_{x,y}$ is an isomorphism. Using corollary 5 and the following (cf. [1])

Lemma 6. *Let $K_{r,s}$ be the (r,s)-component in (A_1, A_2) of $H(A_1 + A_2, -A_2)$. We have*

$$K_{1,n} = \frac{1}{(n+1)!} (\mathrm{ad}A_2)^n A_1,\ n \geq 0. \qquad (16)$$

We conclude by showing that for any $d \geq 2$, we have

Lemma 7.

$$\begin{aligned} \tilde{L}_d(\{(\mathrm{ad}A_2)^n A_1,\ n \geq 0\}) &\subset \tilde{L}_d(\{H_n(A_1 + A_2, -A_2),\ n \geq 1\}) \\ &\subset \tilde{L}_d(\{A_1, A_2\}) \\ &= \tilde{L}_d(\{(\mathrm{ad}A_2)^n A_1,\ n \geq 0\}). \quad \square \end{aligned} \qquad (17)$$

Remark. — A direct proof is given in ([4]) by considering the transformations $Tw : \mathcal{A}(X)^+ \to 1 + \mathcal{A}^+(X)$, defined by

$$(Tw)_0 = 1, (Tw)_n = \textstyle\sum_{p=1}^{n} \frac{p}{n} w_p (Tw)_{n-p}. \quad (18)$$

We have $T(A_1) = \exp(A_1)$, $T(A_2) = \exp(A_2)$ and $T(A_1)T(A_2) = T(C)$, where $C = A_1 + \sum_{n\geq 0} \frac{1}{n+1!}(\mathrm{ad}A_2)^n A_1$. We would have concluded by pointing out that $H_n - C_n \in \tilde{L}_n(C_1, \ldots, C_{n-1})$.

5 Approximations of the exponential

Before starting the proof of the proposition 2, let us introduce some notations. For given n and k, let us denote by

- $\mathcal{P}_{n,k} = \{\mathbf{x} = (x_1, \ldots, x_n)\}$ the set of solutions of

$$\begin{cases} \exp(x_1 A_1) \cdots \exp(x_n A_n) = \exp(A_1 + A_2 + R_k) \\ R_k \in \prod_{n>k} \tilde{L}_n(A_1, A_2). \end{cases} \quad (19)$$

- $\mathcal{R}_{n,k} = \{\mathbf{z} = (z_1, \ldots, z_n)\}$ the set of solutions of

$$\begin{cases} S^+(z_1) S^-(z_2) \cdots S^{\pm}(z_n) = \exp(A_1 + A_2 + R_k) \\ R_k \in \prod_{n>k} \tilde{L}_n(A_1, A_2). \end{cases} \quad (20)$$

Here S^+ and S^- are defined in (4).

- $\mathcal{Q}_{n,k} = \{\mathbf{z} = (z_1, \ldots, z_n)\}$ the set of solutions of

$$\begin{cases} \phi^+(z_1) \phi^-(z_2) \cdots \phi^{\pm}(z_n) = \exp(X_1 + R_k), \\ R_k \in \prod_{n>k} \tilde{L}_n(Y). \end{cases} \quad (21)$$

Here $X = \{X_i, i \geq 1\}$, and ϕ^+, ϕ^- are defined in problem 3.

- $\mathbf{R}$ is the polynomial ring $\mathbb{Q}[Z_1, \ldots, Z_n]$.

⋆⋆⋆

Proposition 8. *For each $n, k \in \mathbb{N}$, $\mathcal{P}_{n,k}$, $\mathcal{Q}_{n,k}$ and $\mathcal{R}_{n,k}$ are algebraic varieties. Therefore $\mathcal{Q}_{n,k} = \mathcal{R}_{n,k}$.*

Proof. — Let $A = \{A_1, A_2\}$ and $(A_{d,i})_{i=1,\ldots,l_d}$ be a basis (the Lyndon basis) of $L_d(A)$. We have for example $A_{1,1} = A_1,\ A_{1,2} = A_2,\ A_{2,1} = [A_1, A_2]$. Let $\mathbf{x} = (x_1, \ldots, x_n)$. Using the Campbell-Hausdorff theorem, one can write

$$\exp(x_1 A_1) \cdots \exp(x_n A_n) = \exp(\textstyle\sum_{d\geq 1} \sum_{i=1}^{l_d} P_{d,i}^{(n)}(\mathbf{x}) A_{d,i}). \quad (22)$$

where $P_{d,i}^{(n)} \in \mathbf{R}$. Condition (19) is now equivalent to

$$\{P_{1,1}^{(n)}(\mathbf{x}) - 1 = P_{1,2}^{(n)}(\mathbf{x}) - 1 = 0,\ P_{d,i}^{(n)}(\mathbf{x}) = 0,\ 2 \leq d \leq k, 1 \leq i \leq l_d\}. \quad (23)$$

We thus deduce that $\mathcal{P}_{n,k} = Z(\mathcal{I}_{n,k})$ where

$$\mathcal{I}_{n,k} = (P_{1,1} - 1, P_{1,2} - 1) + (P_{d,i}^{(n)},\ 2 \le d \le k, 1 \le i \le l_d). \tag{24}$$

Let $(X_{d,i})_{1 \le i \le \tilde{l}_d}$ be a basis (the Lyndon basis) of $\tilde{L}_d(X)$. For $\mathbf{z} = (z_1, \ldots, z_n)$, we get

$$\phi^+(z_1)\phi^-(z_2)\cdots\phi^\pm(z_n) = \exp(\textstyle\sum_{d\ge1}\sum_{i=1}^{l_d} Q_{d,i}^{(n)}(\mathbf{z})X_{d,i}) \tag{25}$$

where $Q_{d,i}^{(n)} \in R$. We thus deduce that $\mathcal{Q}_{n,k} = Z(\mathcal{J}_{n,k})$ where

$$\mathcal{J}_{n,k} = (Q_{1,1}^{(n)} - 1) + (Q_{d,i}^{(n)},\ 2 \le d \le k, 1 \le i \le l_d). \tag{26}$$

Let $\psi : \tilde{L}(X) \to \tilde{L}(\{H_n,\ n \ge 1\})$ the Lie algebra isomorphism defined by $\psi(X_i) = H_i$. $H_{d,j} = \psi(X_{d,j})$ is a basis of $\tilde{L}(\{H_n,\ n \ge 1\})$ and we get

$$S^+(z_1)S^-(z_2)\cdots S^\pm(z_n) = \exp(\psi(\textstyle\sum_{d\ge1}\sum_{i=1}^{l_d} Q_{d,i}^{(n)}(\mathbf{z})X_{d,i})) \tag{27}$$

$$= \exp(\textstyle\sum_{d\ge1}\sum_{i=1}^{l_d} Q_{d,i}^{(n)}(\mathbf{z})H_{d,i}). \tag{28}$$

We thus deduce that $\mathcal{Q}_{n,k} = Z(\mathcal{J}_{n,k})$ and therefore $\mathcal{Q}_{n,k} = \mathcal{R}_{n,k}$. ∎

Remark. — Using lemma 1, we have

$$P_{1,1}^{(n)} = \textstyle\sum_{p=1}^{\left[\frac{n+1}{2}\right]} Z_{2p-1}, P_{1,2}^{(n)} = \sum_{p=1}^{\left[\frac{n}{2}\right]} Z_{2p}, \tag{29}$$

$$Q_{1,1}^{(n)} = \textstyle\sum_{p=1}^{n} Z_p = P_{1,1}^{(n)} + P_{1,2}^{(n)}. \tag{30}$$

⋆⋆⋆

We then show the following lemma proposed by R. MacLachlan ([5])

Lemma 9. *For each $n \ge 2$, let $\mathbf{u} = (u_1, \ldots, u_n)$ and $\mathbf{v} = (v_1, \ldots, v_n)$ given by*

$$u_1 = v_1,\ v_i = \sum_{p=1}^{i} (-1)^{p+i} u_i,\ u_i = v_i + v_{i-1},\ 2 \le i \le n. \tag{31}$$

Then we have

$$\exp(u_1A_1)\cdots\exp(u_nA_n) = S^+(v_1)S^-(v_2)\cdots S^\pm(v_{n-1})\exp(v_nA_n). \tag{32}$$

Proof. — If $n = 2$, we have $v_1 = u_1, v_2 = u_2 - u_1$ and

$$\exp(u_1A_1)\exp(u_2A_2) = S^+(u_1)\exp((u_2 - u_1)A_2). \tag{33}$$

Suppose now that the result yields for n. Let us consider

$$\mathbf{u} = (u_1, \ldots, u_{n+1}),\ \mathbf{v} = (v_1, \ldots, v_{n+1}). \tag{34}$$

We get (by posing $S^\varepsilon(v_{n-1}) = S^+(v_{n-1})$ if n is even)

$$\begin{aligned}
\exp(u_1A_1)\cdots\exp(u_{n+1}A_2) &= \exp(u_1A_1)\cdots\exp(u_nA_1)\cdot\exp(u_{n+1}A_2)\\
&= S^+(v_1)\cdots S^\varepsilon(v_{n-1})\exp(v_nA_n)\cdot\exp(u_{n+1}A_{n+1})\\
&= S^+(v_1)\cdots S^\varepsilon(v_{n-1})\cdot\exp(v_nA_n)\exp(v_nA_{n+1})\cdot\\
&\qquad \exp((u_{n+1}-v_n)A_{n+1})\\
&= S^+(v_1)\cdots S^\varepsilon(v_{n-1})S^{-\varepsilon}(v_n)\cdot\exp(v_{n+1}A_{n+1}).
\end{aligned} \tag{35}$$

and the result is again valid for $n+1$. ∎

⋆⋆⋆

Lemma 10. *The change of variables*

$$\psi_n : Z_i \mapsto \textstyle\sum_{p=1}^{i}(-1)^{p+i}Z_p,\ \ i=1,\ldots,n \tag{36}$$

induces a ring isomorphism

$$\psi_n^* : \mathbb{Q}[Z_1,\ldots,Z_n] \to \mathbb{Q}[Z_1,\ldots,Z_n]. \tag{37}$$

Using this lemma and formula (30), we get

$$\psi_n^* Z_n = \sum_{p=1}^{n}(-1)^{n+p}Z_p = (-1)^n(P_{1,2}^{(n)} - P_{1,1}^{(n)}). \tag{38}$$

Let us consider the following commutative diagram

$$\begin{array}{ccc}
\mathbb{Q}[Z_1,\ldots,Z_n] & \xrightarrow{\ \psi_n^*\ } & \mathbb{Q}[Z_1,\ldots,Z_n]\\
\downarrow{\scriptstyle \pi_{\mathcal{R}}} & & \downarrow{\scriptstyle \pi_{\mathcal{P}}}\\
\mathbb{Q}[Z_1,\ldots,Z_n]/(Z_n) & \xrightarrow[\ \psi_n'^*\ ]{} & \mathbb{Q}[Z_1,\ldots,Z_n]/(P_{1,2}^{(n)} - P_{1,1}^{(n)})
\end{array}$$

Let us work now in $\mathbf{R} = \mathbb{Q}[Z_1,\ldots,Z_n]$. Formula (32) becomes

$$\exp(Z_1A_1)\cdots\exp(Z_nA_n) = S^+(\psi_n^*(Z_1))\cdots S^\pm(\psi_n^*(Z_{n-1}))\exp(\psi_n^*(Z_n)A_n) \tag{39}$$

In $\mathbb{Q}[Z_1,\ldots,Z_n]/(\psi_n^* Z_n)$, equation (39) becomes

$$\exp(\pi_{\mathcal{P}}(Z_1)A_1)\cdots\exp(\pi_{\mathcal{P}}(Z_n)A_n) = S^+(\psi_n'^*(Z_1))\cdots S^\pm(\psi_n'^*(Z_{n-1})) \tag{40}$$

We thus have

$$\sum_{d=1}^{n}\sum_{i=1}^{l_d}\pi_{\mathcal{P}}(P_{d,i}^{(n)})A_{d,i} = \sum_{d=1}^{n}\sum_{i=1}^{\tilde{l}_d}\psi_n'^*(Q_{d,i}^{(n)})H_{d,i}. \tag{41}$$

•For $d = 1$, equation (41) becomes

$$\pi_{\mathcal{P}} P_{1,1}^{(n)} A_{1,1} + \pi_{\mathcal{P}} P_{1,2}^{(n)} A_{1,2} = \psi_n'^* Q_{1,1}^{(n)} H_{1,1} \tag{42}$$

and $\pi_{\mathcal{P}}(P_{1,1}^{(n)}) = \pi_{\mathcal{P}}(P_{1,2}^{(n)})$. From $H_{1,1} = A_{1,1} + A_{1,2} = A_1 + A_2$, we thus deduce that

$$\pi_{\mathcal{P}}(P_{1,1}^{(n)}) = \psi_n'^*(Q_{1,1}^{(n)}), \tag{43}$$

so

$$(P_{1,1}^{(n)} - 1) + (P_{1,2}^{(n)} - P_{1,1}^{(n)}) = (\psi_n^* Z_n) + (\psi_n^* Q_{1,1}^{(n)} - 1). \tag{44}$$

•For $d \geq 2$, let us consider the linear isomorphism

$$\begin{aligned} \xi_d : \tilde{L}_d(A) &\to \tilde{L}_d(\{H_n,\ n \geq 1\}) \\ A_{d,i} &\mapsto H_{d,i},\ i = 1, \ldots, l_d = \tilde{l}_d. \end{aligned} \tag{45}$$

Equation (41) becomes for each d

$$\begin{aligned} \sum_{i=1}^{l_d} \pi_{\mathcal{P}}(P_{d,i}^{(n)}) A_{d,i} &= \sum_{i=1}^{l_d} \psi_n'^*(Q_{d,i}^{(n)}) H_{d,i} \\ &= \sum_{i=1}^{l_d} \psi_n'^*(Q_{d,i}^{(n)}) \xi_d A_{d,i}. \end{aligned} \tag{46}$$

Using the dual map ξ_d^*, we thus get

$$\pi_{\mathcal{P}}(P_{d,i}^{(n)}) = \xi_d^* \circ \psi_n'^*(Q_{d,i}^{(n)}),\ 1 \leq i \leq l_d \tag{47}$$

and by considering the generated ideals, we obtain

$$(\pi_{\mathcal{P}}(P_{d,i}^{(n)}),\ 1 \leq i \leq l_d) = (\psi_n'^*(Q_{d,i}^{(n)}),\ 1 \leq i \leq l_d) \tag{48}$$

and therefore

$$(P_{1,1}^{(n)} - P_{1,2}^{(n)}) + (P_{d,i}^{(n)},\ 1 \leq i \leq l_d) = (\psi_n^*(Z_n)) + (\psi_n^*(Q_{d,i}^{(n)}),\ 1 \leq i \leq l_d) \tag{49}$$

•Combining equations (44) and (49), we get

$$\mathcal{I}_{n,k} = \psi_n^* \left[(\mathcal{J}_{n,k}) + (Z_n) \right] \qquad \square \tag{50}$$

⋆⋆⋆

From

$$S^+(z_1) \cdots S^{\varepsilon}(z_{n-1}) = S^+(z_1) \cdots S^{\varepsilon}(z_{n-1}) S^{-\varepsilon}(0) \tag{51}$$

we deduce a one-to-one correspondance between $\mathcal{R}_{n-1,k}$ and $\mathcal{R}_{n,k} \cap \{z_n = 0\}$.

⋆⋆⋆

We then obtain the announced result, that is to say

$$\mathcal{I}_{n,k} \simeq \psi_n^*(\mathcal{J}_{n-1,k}) \simeq \mathcal{J}_{n-1,k}, \tag{52}$$

or equivalently

$$\mathcal{P}_{n,k} \simeq \mathcal{R}_{n-1,k}. \qquad \square \tag{53}$$

6 Examples

All the following results have been obtained with algorithms on Lie series and have been implemented t in Axiom ([2]). We then obtain the polynomials that define the variety we look at. For low orders, these can be described ([3]).

- The solution for $k = 1$ is given by $c_1 = d_1 = 1$ and

$$S_1(x) = S^{(2)}(x) = \exp(xA_1)\exp(xA_2) = S^+(x). \tag{54}$$

- The solution for $k = 2$ is given by

$$S_2(x) = S^{(3)}(x) = \exp(\tfrac{x}{2}A_1)\exp(xA_2)\exp(\tfrac{x}{2}A_1) = S^+(\tfrac{x}{2})S^-(\tfrac{x}{2}) \tag{55}$$

  This approximant is reversible, that is to say satisfies $S_2^- = S_2$.
- Solutions for $k = 3$ are

$$\begin{aligned} S_3(x) &= \exp(cxA_1)\exp(2cxA_2)\exp(cxA_1)\exp(\bar{c}xA_1)\exp(2\bar{c}xA_2)\exp(\bar{c}xA_1) \\ &= S_2(2cx)S_2(2\bar{c}x) \end{aligned} \tag{56}$$

  where $c^2 - \frac{1}{2}\,c + \frac{1}{12} = 0$.
- When $k = 4$, we find two sets of solutions and 5 solutions. If $c^3 - c^2 + \frac{1}{4}c = \frac{1}{48}$, we get

$$S_4(x) = S_2(2cx)S_2((1-4c)x)S_2(2cx) \tag{57}$$

  These solutions are known and have been given also by Yoshida ([9]).
  If c is a root of $c^2 - \frac{1}{4}c + \frac{1}{24} = 0$, we get two other solutions

$$S_4(x) = S_2(2cx)S_2((2c+2\bar{c})x)S_2(2\bar{c}x). \tag{58}$$

- For $k = 5$, one gets exactly 46 solutions as product of approximants S_2.
- For $k = 6$, an exhaustive list is still unknown. If we add the condition of being reversible, we get exactly 39 solutions and they are all products of approximants S_2.

7 Conclusion

If we look at $\mathcal{Q}_{n,k}$, one sees that the solutions lie in $\{z_{2i-1} = z_{2i},\ 1 \leq i \leq [\frac{n}{2}]\}$ and correspond to products of S_2 approximants (up to order 6).

Let us look at $\mathcal{R}_{n,k}$, we get

$$\begin{aligned} S^+(x)S^-(y) &= \exp(xA_1)\exp((x+y)A_2)\exp(yA_1) \\ &= \exp(\tfrac{(x-y)}{2}A_1)S_2(\tfrac{x+y}{2})\exp(-\tfrac{(x-y)}{2}A_1) \end{aligned} \tag{59}$$

which is conjugate to S_2. Approximants are therefore products of conjugates of S_2. We have shown that up to order 6, these conjugates were all trivial.

Let us remind that we know how to built approximant at any order. Suzuki ([6]) did show that when S_{2k} is a $2k$-order approximant, then

$$S_{2k+2} = S_{2k}(x_k)S_{2k}(1-2x_k)S_{2k}(x_k) \tag{60}$$

is also an approximant of order $2k+2$ when

$$x_k^{2k+1} + (1-2x_k)^{2k+1} = 0. \tag{61}$$

They are not minimal approximants.

⋆⋆⋆

From approximants of $\exp(A_1 + A_2)$, we deduce approximants for each $\exp(A_1+\cdots+A_n)$, as product of ϕ^+ and ϕ^- where ϕ^+ is a first order approximant as suggested in ([5]):

$$\phi^+(x) = \exp(xA_1)\cdots\exp(xA_n). \tag{62}$$

Unfortunately, nothing proves that they are minimal.

References

1. **N. Bourbaki**, *Groupes et Algèbres de Lie*, Éléments de Mathématiques, Hermann, Paris, 1972
2. **P.-V. Koseleff**, *Calcul formel pour les méthodes de Lie en mécanique hamiltonienne*, Thèse de troisième cycle, École Polytechnique, 1993
3. **P.-V. Koseleff**, *Relations among Formal Lie Series and Construction of Symplectic Integrators*, AAECC'10 proceedings, Lecture Notes in Computer Science **673** (1993)
4. **P.-V. Koseleff**, *Relations among Formal Lie Series Transformations and isomorphisms between free Lie algebras*, accepted in SFCA'95, Marne-la-Vallée (1995)
5. **R. I. MacLachlan**, *On the numerical integration of ordinary differential equations by symmetric composition methods*, SIAM J. Sci. Comp. **16(1)** (1995), 151–168
6. **M. Suzuki**, *Fractal Decomposition of Exponential Operators with Applications to Many-Body Theories and Monte Carlo Simulations*, Physic Letters A **146** (1990), 319–323
7. **M. Suzuki**, *General nonsymetric higher-order decompositions of exponential operators and symplectic integrators*, Physic Letters A **165** (1993), 387–395
8. **H. Yoshida**, *Conserved Quantities of Symplectic Integrators for Hamiltonian Systems*, Physica D (1990)
9. **H. Yoshida**, *Construction Of Higher Order Symplectic Integrators*, Physics Letters A **150,** (1990), 262–268

This article was processed using the LaTeX macro package with LLNCS style