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► **To cite this version:**

Jean-Christophe Novelli, Thierry Paul, David Sauzin, Jean-Yves Thibon. Rayleigh-Schrödinger series and Birkhoff decomposition. *Letters in Mathematical Physics*, 2018, 108 (7), pp.1583-1600. 10.1007/s11005-017-1040-1 . hal-01351108v2

HAL Id: hal-01351108

<https://hal.science/hal-01351108v2>

Submitted on 14 Jan 2017

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RAYLEIGH-SCHRÖDINGER SERIES AND BIRKHOFF DECOMPOSITION

JEAN-CHRISTOPHE NOVELLI, THIERRY PAUL, DAVID SAUZIN, AND JEAN-YVES THIBON

ABSTRACT. We derive new expressions for the Rayleigh-Schrödinger series describing the perturbation of eigenvalues of quantum Hamiltonians. The method, somehow close to the so-called dimensional renormalization in quantum field theory, involves the Birkhoff decomposition of some Laurent series built up out of explicit fully non-resonant terms present in the usual expression of the Rayleigh-Schrödinger series. Our results provide new combinational formulae and a new way of deriving perturbation series in Quantum Mechanics. More generally we prove that such a decomposition provides solutions of general normal form problems in Lie algebras.

1. Introduction

Rayleigh-Schrödinger expansion is a powerful tool in quantum mechanics, chemistry and more generally applied sciences. It consists in expanding the spectrum of an operator (finite or infinite dimensional) which is a perturbation of a bare one, around the unperturbed spectrum. Besides, let us mention that perturbation theory has been a clue in the discovery of quantum dynamics by Heisenberg in 1925 [Bo25, He25]. Considering the huge bibliography on the subject, we only quote in the present article the two classical textbooks [Ka88, RS80], and present in this introduction an elementary formal derivation of the Rayleigh-Schrödinger expansion.

Let us consider a self-adjoint operator H_0 on a Hilbert space \mathcal{H} whose spectrum $\{E_0(n), n \in J \subseteq \mathbb{N}\}$ is supposed (for the moment) to be discrete and non-degenerate, and a perturbation V of H_0 , namely a self-adjoint bounded operator of “small size”. It is well-known that one can unitarily conjugate $H := H_0 + V$, formally at any order in the size of V , to an operator of the form $H_0 + N$ where N is diagonal on the eigenbasis of H_0 . More precisely

$$\exists C, \text{ unitary, such that } C(H_0 + V)C^{-1} \sim H_0 + N, \quad [H_0, N] = 0, \quad (1.1)$$

the symbol \sim meaning (in the good cases) that $\|C(H_0 + V)C^{-1} - (H_0 + N)\| = O(\|V\|^\infty)$, for some suitable norm $\|\cdot\|$.

An elegant way of building this pair (N, C) consists in using the so-called Lie algorithm, see e.g. [DEGH91]: let us look for C of the form $C = e^{\frac{1}{i\hbar}W}$ with W self-adjoint (which will ensure that C is unitary). Expanding $W = W_1 + W_2 + \dots$ and $N = N_1 + N_2 + \dots$ “in powers of V ”,

and using Hadamard's lemma $e^{\frac{1}{i\hbar}W} H e^{-\frac{1}{i\hbar}W} = H + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{1}{i\hbar}\right)^k \underbrace{[W, [W, \dots [W, H] \dots]]}_{k \text{ times}}$, we get

$$\begin{aligned}
\frac{1}{i\hbar}[H_0, W_1] + N_1 &= V_1, & V_1 &:= V \\
\frac{1}{i\hbar}[H_0, W_2] + N_2 &= V_2, & V_2 &:= \frac{1}{i\hbar}[W_1, V] - \frac{1}{2\hbar^2}[W_1, W_1, H_0] \\
\frac{1}{i\hbar}[H_0, W_3] + N_3 &= V_3, & V_3 &:= \frac{1}{i\hbar}[W_2, V] - \frac{1}{2\hbar^2}[W_1, W_1, V] - \frac{1}{2\hbar^2}[W_1, [W_2, H_0]] \\
&&& - \frac{1}{2\hbar^2}[W_2, [W_1, H_0]] - \frac{1}{6i\hbar^3}[W_1, [W_1, [W_1, H_0]]] \\
&&& \vdots \\
\frac{1}{i\hbar}[H_0, W_k] + N_k &= V_k, & V_k &:= \dots
\end{aligned} \tag{1.2}$$

These equations, together with the commutation relations $[H_0, N_k] = 0$, are solved recursively by

$$\begin{aligned}
(e_n, N_k e_m) &= (e_n, V_k e_m) \delta_{nm}, \\
(e_n, W_k e_m) &= \frac{i\hbar}{E_0(n) - E_0(m)} (e_n, V_k e_m) \text{ if } n \neq m,
\end{aligned}$$

where we have denoted by e_n an eigenvector of H_0 of eigenvalue $E_0(n)$, because H_0 has simple spectrum and $(e_n, \frac{1}{i\hbar}[H_0, A]e_m) = \frac{1}{i\hbar}(E_0(n) - E_0(m))(e_n, A e_m)$ for an arbitrary operator A . Note that $N_k = \text{Diag}(V_k)$ (diagonal part of V_k on the eigenbasis of H_0), but the diagonal part of W_k remains undetermined; one can check that the N_k 's are uniquely determined by (1.1).

Using the Dirac notation $\langle n | A | m \rangle := (e_n, A e_m)$ for an arbitrary operator A , we easily arrive at

$$\langle n | N_k | n \rangle = \sum_{n_1, n_2, \dots, n_{k-1}} c_{n_1, \dots, n_{k-1}, n} \langle n | V | n_1 \rangle \langle n_1 | V | n_2 \rangle \cdots \langle n_{k-1} | V | n \rangle \tag{1.3}$$

where the coefficients $c_{n_1, \dots, n_{k-1}, n}$ have to be determined recursively.

This is the standard way the Rayleigh-Schrödinger series is usually expressed: the correction to the eigenvalue $E_0(n)$ is given at order k by the r.h.s. of (1.3), that is the diagonal matrix elements of the (diagonal) normal form N_k .

Looking at the hierarchy of equations (1.2), one realises that only commutators should be involved in (1.3) for $k \geq 2$. One way of achieving this has been developed recently by two of us in [PS16a]: let

$$\mathcal{N} := \left\{ \frac{1}{i\hbar}(E_0(\ell) - E_0(k)) \mid k, \ell \in \mathbb{N} \right\}, \tag{1.4}$$

and define, for $\lambda \in \mathcal{N}$,

$$V_\lambda := \sum_{\substack{(k,\ell) \text{ such that} \\ E_0(\ell) - E_0(k) = i\hbar\lambda}} \langle k | V | \ell \rangle | \ell \rangle \langle k | \quad (1.5)$$

with the Dirac notation $| \ell \rangle \langle k | \psi := (e_\ell, \psi) e_k$ for an arbitrary vector ψ , so that

$$\frac{1}{i\hbar} [H_0, V_\lambda] = \lambda V_\lambda \quad \text{and} \quad V = \sum_{\lambda \in \mathcal{N}} V_\lambda. \quad (1.6)$$

We will suppose that V is finite-band, that is to say that the sum in (1.6) is finite. According to [PS16a], *for every $k \geq 1$ there exist coefficients $R^{\lambda_1, \dots, \lambda_k} \in \mathbb{C}$ such that*

$$N_k = \sum_{\lambda_1, \dots, \lambda_k \in \mathcal{N}} \frac{1}{k} R^{\lambda_1, \dots, \lambda_k} \frac{1}{i\hbar} [V_{\lambda_1}, \frac{1}{i\hbar} [V_{\lambda_2}, \dots \frac{1}{i\hbar} [V_{\lambda_{k-1}}, V_{\lambda_k}] \dots]]. \quad (1.7)$$

The coefficients $R^{\lambda_1, \dots, \lambda_k}$ are computable recursively together with coefficients $S^{\lambda_1, \dots, \lambda_k}$ appearing in a similar expansion for the formal unitary operator C — see (1.12).

The family of pairs $(R^{\lambda_1, \dots, \lambda_k}, S^{\lambda_1, \dots, \lambda_k})$ is obtained by solving a universal “mould equation” (independent of V and depending on H_0 only through \mathcal{N}) studied in [PS16a] and recalled in the next section. In general, this mould equation has more than one solution (the set of all solutions is described in [PS16a]), so the decomposition (1.7) is not unique, though N_k is. Using (1.5) and introducing a decomposition of the identity on the unperturbed eigenbasis in (1.7), one would certainly recover (1.3), but probably with a big combinatorial complexity in the expressions as $k \rightarrow \infty$.

One of the main goal of this note is to introduce a new (to our knowledge) way of finding a solution to the mould equation, and thus a family of coefficients $R^{\lambda_1, \dots, \lambda_k}$ satisfying (1.7). It consists in applying a method actually very similar to the so-called dimensional regularisation in quantum field theory (but much simpler): we will add a dependence in an undetermined parameter ε . This will lead us to a modified mould equation with a unique solution, for which the coefficients are given by explicit Laurent series

$$T^{\lambda_1, \dots, \lambda_k}(\varepsilon) \in K := \mathbb{C}((\varepsilon)).$$

The correct expression for $R^{\lambda_1, \dots, \lambda_k}$ will then be obtained, up to a factor k , by taking the residue of the polar part of the so-called “Birkhoff decomposition” of this family of Laurent series, relative to the decomposition

$$K = K_+ \oplus K_-, \quad K_+ := \mathbb{C}[[\varepsilon]], \quad K_- = \varepsilon^{-1} \mathbb{C}[\varepsilon^{-1}].$$

More precisely, let $\underline{\mathcal{N}}$ be the set of words on the alphabet \mathcal{N} (finite sequences of elements of \mathcal{N}) and denote by $r(\underline{\lambda})$ the length of the word $\underline{\lambda} = \lambda_1 \lambda_2 \dots \lambda_{r(\underline{\lambda})}$. We will consider the set of functions

from $\underline{\mathcal{N}}$ to K , that is

$$K^{\underline{\mathcal{N}}} := \{M : \underline{\lambda} \in \underline{\mathcal{N}} \mapsto M^{\underline{\lambda}} \in K\}. \quad (1.8)$$

On $\underline{\mathcal{N}}$, we define word concatenation by $\underline{\lambda}\underline{\lambda}' = \lambda_1 \cdots \lambda_\ell \lambda'_1 \cdots \lambda'_m$ for $\underline{\lambda} = \lambda_1 \cdots \lambda_\ell$, $\underline{\lambda}' = \lambda'_1 \cdots \lambda'_m$ and, on $K^{\underline{\mathcal{N}}}$, we define the product

$$(M \times N)^{\underline{\lambda}} := \sum_{\underline{a}\underline{b}=\underline{\lambda}} M^{\underline{a}} N^{\underline{b}} \in K \quad (1.9)$$

with unit $\mathbb{1} \in K^{\underline{\mathcal{N}}}$ defined by $\mathbb{1}^\emptyset = 1_K$ and $\mathbb{1}^{\underline{\lambda}} = 0$ for $\underline{\lambda} \neq \emptyset$.

Let $T : \underline{\mathcal{N}} \rightarrow K$, $\underline{\lambda} \mapsto T^{\underline{\lambda}}(\varepsilon)$ be given by

$$T^{\underline{\lambda}}(\varepsilon) := \frac{1}{(\lambda_1 + \varepsilon)(\lambda_1 + \lambda_2 + 2\varepsilon) \cdots (\lambda_1 + \cdots + \lambda_{r(\underline{\lambda})} + r(\underline{\lambda})\varepsilon)},$$

considered of course as a formal Laurent series in ε (note that $T^{\underline{\lambda}}(\varepsilon) \in K_+$ only for those $\underline{\lambda} \in \underline{\mathcal{N}}$ such that the partial sums $\lambda_1 + \cdots + \lambda_j$ are all nonzero). Its ‘‘Birkhoff decomposition’’ is the following: *there exists a unique pair $(U_+, U_-) \in K^{\underline{\mathcal{N}}} \times K^{\underline{\mathcal{N}}}$ such that*

$$U_-^\emptyset = U_+^\emptyset = 1_K, \quad U_- - \mathbb{1} \in K_-^{\underline{\mathcal{N}}}, \quad U_+ \in K_+^{\underline{\mathcal{N}}}, \quad U_- \times T = U_+.$$

This will be proved in the next section as Proposition 2.2 (in a more general setting), together with recurrence relations in order to compute U_- and U_+ .

Since $U_- \in \mathbb{1} + K_-^{\underline{\mathcal{N}}}$, one can evaluate $\varepsilon U_-^{\underline{\lambda}}(\varepsilon)$ at $\varepsilon = \infty$ for each word $\underline{\lambda} \neq \emptyset$. We are now in position of stating one of the main results of this article.

Theorem A. *For any $k \geq 1$, one can write*

$$N_k = \sum_{\lambda_1, \dots, \lambda_k \in \mathcal{N}} N^{\lambda_1 \cdots \lambda_k} \frac{1}{i\hbar} [V_{\lambda_1}, \frac{1}{i\hbar} [V_{\lambda_2}, \dots \frac{1}{i\hbar} [V_{\lambda_{k-1}}, V_{\lambda_k}] \dots]], \quad (1.10)$$

with

$$N^{\lambda_1 \cdots \lambda_k} := -\text{residue of } U_-^{\lambda_1 \cdots \lambda_k} = -[\varepsilon U_-^{\lambda_1 \cdots \lambda_k}(\varepsilon)]_{\varepsilon=\infty}. \quad (1.11)$$

We will prove much more in the following sections. In particular we will show that the coefficients $S^{\underline{\lambda}} := U_+^{\underline{\lambda}}(\varepsilon)|_{\varepsilon=0}$ give rise to a formal unitary operator

$$C = \sum_{k=0}^{\infty} \sum_{\lambda_1, \dots, \lambda_k \in \mathcal{N}} \left(\frac{1}{i\hbar}\right)^k S^{\lambda_1 \cdots \lambda_k} V_{\lambda_1} V_{\lambda_2} \cdots V_{\lambda_k} \quad (1.12)$$

which satisfies the conjugacy equation (1.1). We will also remove the simplicity condition on the spectrum of H_0 .

This paper is organized as follows. In Section 2 we briefly recall elements of Ecalle’s mould calculus (i.e. the manipulation of families of coefficients indexed by words) and, in the more general setting of a normalization problem in a complete filtered Lie algebra \mathcal{L} , the mould equation

implying (1.1); then we prove the underlying Birkhoff decomposition and the main results of this article, Theorems B and C. In Section 3 we prove the general “quantum” result, Theorem D, implying Theorem A. In Section 4 we present different situations where Theorem C applies, including perturbations of Hamiltonian vector fields in classical dynamics. For the sake of completeness, we have included the derivation of the mould equation in appendix.

The techniques used here have been introduced in various papers dealing with normal forms of dynamical systems [EV95, Me09, Me13, PS16a, PS16b], quantum mechanics [PS16a, PS16b] and renormalization in QFT [CK00]. Some of them use the language of Ecalle’s mould calculus, while others rely only on the formalism of Hopf algebras. The idea of using Birkhoff decomposition for normal form problems appears in the pioneering work of F. Menous¹ [Me09, Me13]. The article [Me13] notably deals with an abstract Lie-algebraic context, however it considers completed graded Lie algebras with finite-dimensional components and does not express the results in terms of mould expansions, whereas, for our most general result and its application to the Rayleigh-Schrödinger expansion, we need complete filtered Lie algebras without dimensional restriction, and we aim at emphasizing the explicit character of the coefficients which are involved in the solution of the normalization problem (correspondingly, we apply the Birkhoff decomposition to an element of the mould algebra, rather than to an element of the enveloping algebra of \mathcal{L}). The algebraic expansion that we obtain for the left-hand side of (1.10) in Theorem A (or (3.2) in Theorem D) is, to our knowledge, new. We point out that no prerequisite on mould calculus or Hopf algebras is needed to read this article.

2. Mould calculus and Birkhoff decomposition

In full generality, we are interested in the following situation: given $X_0 \in \mathcal{L}$ and $B \in \mathcal{L}_{\geq 1}$, where

$$\mathcal{L} = \mathcal{L}_{\geq 0} \supset \mathcal{L}_{\geq 1} \supset \mathcal{L}_{\geq 2} \supset \dots$$

is a complete filtered Lie algebra² over a field \mathbf{k} of characteristic zero, we look for a Lie algebra automorphism Ψ which maps $X_0 + B$ to an element $X_0 + N$ of \mathcal{L} which commutes with X_0 :

$$\Psi(X_0 + B) = X_0 + N, \quad [X_0, N] = 0, \quad \Psi \in \text{Aut}(\mathcal{L}). \quad (2.1)$$

¹Since the first version of this paper has been posted, we have learnt that F. Menous [Me16] had announced results in the same line of research.

²This means that $[\mathcal{L}_{\geq m}, \mathcal{L}_{\geq n}] \subset \mathcal{L}_{\geq m+n}$ for all $m, n \in \mathbb{N}$, $\bigcap \mathcal{L}_{\geq m} = \{0\}$ and \mathcal{L} is a complete metric space for the distance $d(X, Y) := 2^{-\text{ord}(Y-X)}$, where we denote by $\text{ord}: \mathcal{L} \rightarrow \mathbb{N} \cup \{\infty\}$ the order function associated with the filtration (function characterized by $\text{ord}(X) \geq m \Leftrightarrow X \in \mathcal{L}_{\geq m}$).

Then Ψ is called a “normalizing automorphism” and $X_0 + N$ a “normal form” of $X_0 + B$. Our key assumption will be that B can be decomposed into a formally convergent series $B = \sum_{n \in \mathcal{N}} B_n$ of eigenvectors of the inner derivation $\text{ad}_{X_0}: Y \mapsto [X_0, Y]$, namely

$$[X_0, B_n] = \varphi(n)B_n, \quad B_n \in \mathcal{L}_{\geq 1} \text{ for each } n \in \mathcal{N}, \quad (2.2)$$

for some function $\varphi: \mathcal{N} \rightarrow \mathbf{k}$.

In [PS16a], solutions (N, Ψ) are constructed by means of the ansatz

$$\begin{cases} N &= \sum_{r \geq 1} \sum_{n_1, n_2, \dots, n_r \in \mathcal{N}} \frac{1}{r} R^{n_1 \dots n_r} [B_{n_1}, [\dots [B_{n_{r-1}}, B_r] \dots]] \\ \Psi &= \sum_{r \geq 0} \sum_{n_1, n_2, \dots, n_r \in \mathcal{N}} S^{n_1 \dots n_r} \text{ad}_{B_{n_1}} \dots \text{ad}_{B_{n_r}} \end{cases} \quad (2.3)$$

where $(R^{n_1 \dots n_r})$ and $(S^{n_1 \dots n_r})$ are suitable families of coefficients. A family of coefficients indexed by all the words $n_1 \dots n_r$ is called a “mould”. It is shown in [PS16a] that (2.3) yields a solution as soon as the moulds $(R^{n_1 \dots n_r})$ and $(S^{n_1 \dots n_r})$ satisfy a certain “mould equation”, equation (2.10) below. We give in Section 2.1 the basics of mould calculus and state the mould equation; we then show in Sections 2.2–2.3 a new method to solve the mould equation.

2.1. Moulds. Mould calculus has been introduced and developed by Jean Écalle ([Ec81], [Ec93]) in the 80-90’s, initially in relation with the free Lie algebra of alien operators in resurgence theory, providing also powerful tools for handling problems in local dynamics, typically the normalization of vector fields or diffeomorphisms at a fixed point [EV95].

Let \mathcal{N} be a nonempty set and \mathbf{k} a commutative ring. Similarly to (1.8), we consider the set $\mathbf{k}^{\underline{\mathcal{N}}}$ of all families of coefficients $M^{\underline{\lambda}}$ indexed by words $\underline{\lambda} \in \underline{\mathcal{N}}$. A “ \mathbf{k} -valued mould” is an element of $\mathbf{k}^{\underline{\mathcal{N}}}$. Mould multiplication is defined by (1.9) and makes $\mathbf{k}^{\underline{\mathcal{N}}}$ a \mathbf{k} -algebra. A mould can be identified with a linear form on $\mathbf{k}\underline{\mathcal{N}}$, the linear span of the words; the mould product can then be identified with the convolution product of linear forms corresponding to the comultiplication $\underline{n} \mapsto \sum_{\underline{n}=\underline{a}\underline{b}} \underline{a} \otimes \underline{b}$.

The “shuffle algebra” is $\mathbf{k}\underline{\mathcal{N}}$ viewed as a Hopf algebra, with the previous comultiplication (with counit $\emptyset \mapsto 1_{\mathbf{k}}$ and $\underline{n} \mapsto 0$ for a nonempty word \underline{n}), the antipode map $n_1 \dots n_r \mapsto (-1)^r n_r \dots n_1$, and the “shuffle product” Δ , which can be recursively defined by the formula

$$\lambda \underline{a} \Delta \mu \underline{b} = \lambda(\underline{a} \Delta \mu \underline{b}) + \mu(\lambda \underline{a} \Delta \underline{b}) \text{ where } \lambda, \mu \text{ are letters and } \underline{a}, \underline{b} \text{ are words} \quad (2.4)$$

(the unit being \emptyset), giving rise to structure coefficients $\text{sh}(\frac{\underline{a}, \underline{b}}{\underline{n}})$ known as “shuffling coefficients”:

$$\underline{a} \Delta \underline{b} = \sum_{\underline{n} \in \underline{\mathcal{N}}} \text{sh}(\frac{\underline{a}, \underline{b}}{\underline{n}}) \underline{n} \quad (2.5)$$

(see e.g. Section 2.2 of [PS16a] for their definition in terms of permutations of $r(\underline{n})$ elements: $\text{sh}(\frac{\underline{a}, \underline{b}}{\underline{n}})$ is the number of ways \underline{n} can be obtained by interdigitating the letters of \underline{a} and \underline{b} while preserving their internal order in \underline{a} or \underline{b}).

By duality, this leads to Écalle's definition of symmetrality, which is fundamental. A mould M is said to be “symmetral” if the corresponding linear form is a character of the shuffle algebra [Me09], i.e. $M^\varnothing = 1_{\mathbf{k}}$ and

$$M^{\underline{a}\Delta\underline{b}} = M^{\underline{a}}M^{\underline{b}} \quad \text{for all } \underline{a}, \underline{b} \in \underline{\mathcal{N}}, \quad (2.6)$$

which boils down to the condition $\sum_{\underline{n} \in \underline{\mathcal{N}}} \text{sh}(\frac{\underline{a}, \underline{b}}{\underline{n}})M^{\underline{n}} = M^{\underline{a}}M^{\underline{b}}$ for any nonempty words $\underline{a}, \underline{b}$ [Ec81].

Its multiplicative inverse M^{-1} then coincides with the mould \tilde{M} defined by

$$\tilde{M}^{n_1 \cdots n_r} := (-1)^r M^{n_r \cdots n_1} \quad (2.7)$$

(this is a manifestation of the antipode of the shuffle algebra; see e.g. Proposition 5.2 of [Sa09]).

For us, symmetrality is useful because whenever a mould S is symmetral, the operator Ψ to which it gives rise by mould expansion as in the second part of (2.3) is a Lie algebra automorphism, and its inverse Ψ^{-1} is given by the mould expansion associated with $S^{-1} = \tilde{S}$. This is because the $\text{ad}_{B_{n_i}}$'s are derivations of the Lie algebra \mathcal{L} , hence the composite operators $\mathcal{B}_{\underline{n}} := \text{ad}_{B_{n_1}} \cdots \text{ad}_{B_{n_r}}$ satisfy the generalized Leibniz rule

$$\mathcal{B}_{\underline{n}}[X, Y] = \sum_{\underline{a}, \underline{b} \in \underline{\mathcal{N}}} \text{sh}(\frac{\underline{a}, \underline{b}}{\underline{n}}) [\mathcal{B}_{\underline{a}}X, \mathcal{B}_{\underline{b}}Y]. \quad (2.8)$$

Let us define the mould $I_{\mathbf{k}} \in \mathbf{k}^{\underline{\mathcal{N}}}$ by $I_{\mathbf{k}}^{\underline{n}} = \delta_{r(\underline{n}), 1} 1_{\mathbf{k}}$ and the operator $M \mapsto \nabla_{\varphi} M$ of $\mathbf{k}^{\underline{\mathcal{N}}}$ by

$$\nabla_{\varphi} M^{\underline{n}} := (\varphi(n_1) + \cdots + \varphi(n_{r(\underline{n})})) M^{\underline{n}} := \varphi(\underline{n}) M^{\underline{n}}, \quad (2.9)$$

with the eigenvalue function $\varphi: \mathcal{N} \rightarrow \mathbf{k}$ of (2.2) thus extended to a monoid morphism $\varphi: \underline{\mathcal{N}} \rightarrow \mathbf{k}$. These are the ingredients of a “mould equation”, whose solutions (R, S) yield solutions (Ψ, N) of the normalization problem (2.1), as proved in Section 3.4 of [PS16a]:

Proposition 2.1 ([PS16a]). *When \mathbf{k} is a field of characteristic 0, equation (2.1) is solved by the ansatz (2.3) if the pair of moulds (R, S) satisfies the “mould equation”*

$$\begin{cases} \nabla_{\varphi} S = S \times I_{\mathbf{k}} - R \times S \\ \nabla_{\varphi} R = 0 \\ S \text{ symmetral.} \end{cases} \quad (2.10)$$

For the sake of completeness and clarity, we give the proof in appendix.

All the solutions of the mould equation (2.10) are constructed in [PS16a] (this is the generalization of some of the statements of the preprint [EV95], which introduced the mould equation in the context of local holomorphic vector fields and diffeomorphisms).

We now show an alternative method to obtain a particular solution (R, S) . From now on, we suppose that \mathbf{k} is a field of characteristic 0.

2.2. Birkhoff decomposition. We call “resonant” any word \underline{n} such that $\varphi(\underline{n}) = 0$. In the case when the function $\varphi: \mathcal{N} \rightarrow \mathbf{k}$ is such that \emptyset is the only resonant word, it is easy to check that there is a unique solution to (2.10), given by $R = 0$ and $S^{n_1 \cdots n_r} = \frac{1}{\varphi(n_1)\varphi(n_1 n_2) \cdots \varphi(n_1 \cdots n_r)}$, but in general the latter expression is ill-defined. We will extend the field \mathbf{k} to the field \mathbf{K} of formal Laurent series with coefficients in \mathbf{k} and replace φ by a \mathbf{K} -valued function for which there is no resonant word except the empty one. The new mould equation (2.10) will therefore be easily solvable by an expression similar to the one just mentioned. The original situation will be recovered by taking some kind of residue of the Birkhoff decomposition of this explicit solution.

The Birkhoff decomposition has been originally introduced by G. D. Birkhoff for matrices of Laurent series. It has been extended by Connes and Kreimer [CK00] to Hopf algebras of Feynman diagrams, and abstract versions for general Hopf algebras appear in several papers [EFGM06, Ma03].

Let $\mathbf{K} := \mathbf{k}((\varepsilon))$ and $\mathbf{K}_+ := \mathbf{k}[[\varepsilon]]$, so that $\mathbf{K} = \mathbf{K}_+ \oplus \mathbf{K}_-$ with $\mathbf{K}_- = \varepsilon^{-1}\mathbf{k}[\varepsilon^{-1}]$. Note that $\mathbf{k} \subset \mathbf{K}$, by identifying elements of \mathbf{k} with constant formal series, so $\mathbf{k}^{\mathcal{N}} \subset \mathbf{K}^{\mathcal{N}}$. Let us consider the function $\Phi: n \in \mathcal{N} \mapsto \varphi(n) + \varepsilon 1_{\mathbf{k}} \in \mathbf{K}$ and, correspondingly, the operator $M \mapsto \nabla_{\Phi} M$ of $\mathbf{K}^{\mathcal{N}}$ defined by

$$\nabla_{\Phi} M^{\underline{n}}(\varepsilon) = (\varphi(\underline{n}) + r(\underline{n})\varepsilon)M^{\underline{n}}(\varepsilon).$$

Since \mathbf{K} is a field and $\varphi(\underline{n}) + r(\underline{n})\varepsilon \neq 0$ for $\underline{n} \neq \emptyset$ (even if $\varphi(\underline{n}) = 0!$), the mould equation associated with (Φ, \mathbf{K}) (in place of (φ, \mathbf{k})) has a unique solution, given by $R = 0$ and

$$T^{n_1 \cdots n_r}(\varepsilon) = \frac{1}{(\varphi(n_1) + \varepsilon)(\varphi(n_1 n_2) + 2\varepsilon) \cdots (\varphi(n_1 \cdots n_r) + r\varepsilon)}. \quad (2.11)$$

The symmetrality of T is easily checked e.g. by induction on the sum of the lengths of \underline{a} and \underline{b} in (2.6). Of course $T^{n_1 \cdots n_r}(\varepsilon)$, considered as a rational function, is singular at $\varepsilon = 0$ when some words $n_1 \cdots n_{\ell}$, $\ell \leq r$, are φ -resonant.

Any \mathbf{K} -valued symmetrality mould can be interpreted as a character of the shuffle algebra $\mathbf{K}\mathcal{N}$ and, therefore, admits a Birkhoff decomposition with respect to the decomposition $\mathbf{K} = \mathbf{K}_+ \oplus \mathbf{K}_-$ (see e.g. [Ma03]). For the sake of completeness, we state this as a proposition which we will prove from scratch in the context of moulds.

Proposition 2.2. *Suppose T is an arbitrary \mathbf{K} -valued symmetrality mould. Then there exists a unique pair (U_+, U_-) of \mathbf{K} -valued moulds such that*

$$U_-^{\emptyset} = U_+^{\emptyset} = 1_{\mathbf{k}}, \quad U_- - \mathbb{1} \in \mathbf{K}_-^{\mathcal{N}}, \quad U_+ \in \mathbf{K}_+^{\mathcal{N}}, \quad U_- \times T = U_+. \quad (2.12)$$

Their values on an arbitrary word \underline{n} are determined by induction on $r(\underline{n})$ by the formulae $U_-^\varnothing = U_+^\varnothing = 1_{\mathbf{k}}$ and

$$\underline{n} \neq \varnothing \quad \Rightarrow \quad U_-^{\underline{n}} = -\pi_-(D^{\underline{n}}), \quad U_+^{\underline{n}} = \pi_+(D^{\underline{n}}) \quad \text{with} \quad D^{\underline{n}} = \sum_{\underline{n}=\underline{a}\underline{b}, \underline{b} \neq \varnothing} U_-^{\underline{a}} T^{\underline{b}}, \quad (2.13)$$

where $\pi_{\pm}: \mathbf{K} \rightarrow \mathbf{K}_{\pm}$ are the projectors associated with the decomposition $\mathbf{K} = \mathbf{K}_+ \oplus \mathbf{K}_-$.

Moreover, U_+ and U_- are symmetrical.

Proof.

- Uniqueness: Suppose (U_-, U_+) and $(\tilde{U}_-, \tilde{U}_+)$ satisfy (2.12). We have $U_-^{-1} \times U_+ = \tilde{U}_-^{-1} \times \tilde{U}_+$ so that $\mathbb{1} + \mathbf{K}_-^{\mathcal{N}} \ni \tilde{U}_- \times U_-^{-1} = \tilde{U}_+ \times U_+^{-1} \in \mathbf{K}_+^{\mathcal{N}}$. Therefore $\tilde{U}_- \times U_-^{-1} = \tilde{U}_+ \times U_+^{-1} = \mathbb{1}$, since $\mathbf{K}_- \cap \mathbf{K}_+ = \{0\}$.

- Existence: Let us define U_- and U_+ by $U_-^\varnothing = U_+^\varnothing = 1_{\mathbf{k}}$ and (2.13). Setting $D := U_- \times (T - 1)$, we get $U_- = \mathbb{1} - \pi_- D$ and $U_+ = \mathbb{1} + \pi_+ D$, whence $U_+ - U_- = D$, i.e. $U_+ = U_- \times T$.

- Symmetry: Define the *dimoulds* as the functions $\underline{\mathcal{N}} \times \underline{\mathcal{N}} \rightarrow \mathbf{K}$, and their multiplication as

$$(M \times N)^{(\underline{a}, \underline{b})} := \sum_{(\underline{a}, \underline{b}) = (\underline{a}^1, \underline{b}^1)(\underline{a}^2, \underline{b}^2)} M^{(\underline{a}^1, \underline{b}^1)} N^{(\underline{a}^2, \underline{b}^2)},$$

where the concatenation in $\underline{\mathcal{N}} \times \underline{\mathcal{N}}$ is defined by $(\underline{a}^1, \underline{b}^1)(\underline{a}^2, \underline{b}^2) = (\underline{a}^1 \underline{a}^2, \underline{b}^1 \underline{b}^2)$. A dimould is therefore the same as a linear form on the tensor square of the shuffle algebra $\mathbf{K}\underline{\mathcal{N}}$. Dualizing (2.5), we define a map $\Delta: \mathbf{K}\underline{\mathcal{N}} \rightarrow \mathbf{K}\underline{\mathcal{N}} \times \underline{\mathcal{N}}$ by $(\Delta M)^{\underline{a}, \underline{b}} := \sum_{\underline{n} \in \underline{\mathcal{N}}} \text{sh}\left(\frac{\underline{a}, \underline{b}}{\underline{n}}\right) M^{\underline{n}}$ for any $(\underline{a}, \underline{b}) \in \underline{\mathcal{N}} \times \underline{\mathcal{N}}$. According to [Sa09], Δ is a morphism of associative algebras (thanks to the compatibility between the comultiplication and the shuffle product of $\mathbf{K}\underline{\mathcal{N}}$) and, given $M \in \mathbf{K}\underline{\mathcal{N}}$,

$$M \text{ is symmetrical if and only if } M^\varnothing = 1 \text{ and } \Delta(M) = M \otimes M, \quad (2.14)$$

with the notation $(M \otimes N)^{\underline{a}, \underline{b}} = M^{\underline{a}} N^{\underline{b}}$ for any $M, N \in \mathbf{K}\underline{\mathcal{N}}$.

Let us define $A := \Delta U_-$ and $B := \Delta U_+$. Since $U_+ = U_- \times T$, A and B satisfy

$$B = A \times \Delta T, \quad A \in \mathbb{1} + \mathbf{K}_-^{\underline{\mathcal{N}} \times \underline{\mathcal{N}}}, \quad B \in \mathbf{K}_+^{\underline{\mathcal{N}} \times \underline{\mathcal{N}}}. \quad (2.15)$$

It is immediate to see that equation (2.15) has a unique (pair of dimoulds) solution, by the same argument as in the proof of the uniqueness part of Proposition 2.2. Moreover the symmetry of T implies that $\Delta T = T \otimes T$, and one checks easily that this implies that $(U_- \otimes U_-, U_+ \otimes U_+)$ solves (2.15) too. Therefore $\Delta U_- = U_- \otimes U_-$ and $\Delta U_+ = U_+ \otimes U_+$, hence U_- and U_+ are symmetrical by (2.14). \square

2.3. Main results.

Theorem B. Let $T \in \mathbf{K}^{\mathcal{N}}$ be defined by (2.11), and let (U_-, U_+) be its Birkhoff decomposition as stated in Proposition 2.2. Define the moulds $R, S \in \mathbf{k}^{\mathcal{N}}$ by

$$R^{\underline{n}} = -r(\underline{n})(\text{residue of } U_-^{\underline{n}}(\varepsilon)), \quad S^{\underline{n}} = \text{constant term of } U_+^{\underline{n}}(\varepsilon). \quad (2.16)$$

Then (R, S) solves (2.10).

By ‘‘constant term’’ and ‘‘residue’’ of a Laurent series $\sum_{n \in \mathbb{Z}} c_n \varepsilon^n$ we mean respectively c_0 and c_{-1} . In view of Proposition 2.1, Theorem B entails

Theorem C. Define $U_-^{\emptyset}(\varepsilon) = U_+^{\emptyset}(\varepsilon) = 1_{\mathbf{k}}$ and, for nonempty \underline{n} , define $U_-^{\underline{n}}(\varepsilon) \in \varepsilon^{-1} \mathbf{k}[\varepsilon^{-1}]$ and $U_+^{\underline{n}}(\varepsilon) \in \mathbf{k}[[\varepsilon]]$ by (2.11) and (2.13), and then $R^{\underline{n}}, S^{\underline{n}} \in \mathbf{k}$ by (2.16). Then the mould expansions (2.3) provide a solution (Ψ, N) to the normalization problem (2.1).

The proof of Theorem B will rely on

Lemma 2.3. Let S be as in (2.16) and $\tilde{R} := S \times I_{\mathbf{k}} \times S^{-1} - \nabla_{\varphi} S \times S^{-1} \in \mathbf{k}^{\mathcal{N}} \subset \mathbf{K}^{\mathcal{N}}$. Then

- (i) $\nabla_{\Phi} U_- = -\tilde{R} \times U_-$
- (ii) $\nabla_{\Phi} U_+ = U_+ \times I_{\mathbf{k}} - \tilde{R} \times U_+$
- (iii) $\tilde{R}^{\underline{n}} = -(\varepsilon \nabla_{1_{\mathbf{k}}} U_-^{\underline{n}}(\varepsilon))|_{\varepsilon=\infty}$

where $\nabla_{1_{\mathbf{k}}}$ is the operator of $\mathbf{K}^{\mathcal{N}}$ defined by $M^{\underline{n}}(\varepsilon) := r(\underline{n})M^{\underline{n}}(\varepsilon)$.

Proof of Lemma 2.3. Observe that $\nabla_{\Phi} = \nabla_{\varphi} + \varepsilon \nabla_{1_{\mathbf{k}}}$ and that $\nabla_{1_{\mathbf{k}}}$, ∇_{φ} and ∇_{Φ} are derivations of the associative algebra $\mathbf{K}^{\mathcal{N}}$. Since $U_- \times T = U_+$ and $\nabla_{\Phi} T = T \times I_{\mathbf{k}}$, we get

$$\nabla_{\Phi} U_+ = U_- \times T \times I_{\mathbf{k}} + \nabla_{\Phi} U_- \times T = U_+ \times I_{\mathbf{k}} - \mathcal{R} \times U_+$$

with $\mathcal{R} := -\nabla_{\Phi} U_- \times U_-^{-1}$. So

$$\mathcal{R} = U_+ \times I_{\mathbf{k}} \times U_+^{-1} - \nabla_{\Phi} U_+ \times U_+^{-1} \in \mathbf{K}_+^{\mathcal{N}} \quad (2.17)$$

since $\mathbf{K}_+^{\mathcal{N}}$ is invariant by ∇_{Φ} . On the other hand,

$$\mathcal{R} = -\nabla_{\varphi} U_- \times U_-^{-1} - \varepsilon \nabla_{1_{\mathbf{k}}} U_- \times U_-^{-1} = P + \varepsilon Q, \quad P, Q \in \mathbf{K}_-^{\mathcal{N}}. \quad (2.18)$$

Since $\mathbf{K}_+ \cap \mathbf{K}_- = \{0\}$, we deduce from (2.17–2.18) that $\mathcal{R} = (\varepsilon Q)|_{\varepsilon=\infty}$, i.e.

$$\mathcal{R} = -(\varepsilon \nabla_{1_{\mathbf{k}}} U_- \times U_-^{-1})|_{\varepsilon=\infty} = -(\varepsilon \nabla_{1_{\mathbf{k}}} U_-)|_{\varepsilon=\infty}$$

since $U_-^{-1} \in \mathbb{1} + \mathbf{K}_-^{\mathcal{N}}$ so that $U_-^{-1}|_{\varepsilon=\infty} = \mathbb{1}$.

Returning to (2.17), since \mathcal{R} is constant in ε , we get

$$\mathcal{R} = (U_+ \times I_{\mathbf{k}} \times U_+^{-1} - \nabla_{\Phi} U_+ \times U_+^{-1})|_{\varepsilon=0} = S \times I_{\mathbf{k}} \times S^{-1} - \nabla_{\varphi} S \times S^{-1} = \tilde{R}.$$

The three assertions (i)–(iii) are proven. \square

Proof of Theorem B. Lemma 2.3(iii) says that \tilde{R} coincides with the mould R defined by (2.16), hence $\nabla_\varphi S = S \times I_{\mathbf{k}} - R \times S$. The symmetry of S follows from that of U_+ . Therefore it is enough to prove that $\nabla_\varphi R = 0$.

We will show by induction on the length of \underline{n} that $[\varphi(\underline{n}) \neq 0 \Rightarrow U_{\underline{n}}^{\underline{n}}(\varepsilon) = 0 \text{ and } R^{\underline{n}} = 0]$. By definition $\varphi(\emptyset) = 0$, nothing to prove. Suppose $\varphi(\underline{n}) \neq 0$. By Lemma 2.3(i), we have

$$-(\varphi(\underline{n}) + \varepsilon r(\underline{n}))U_{\underline{n}}^{\underline{n}}(\varepsilon) = R^{\underline{n}} + \sum^* R^{\underline{a}}U_{\underline{b}}^{\underline{b}}(\varepsilon) \quad (2.19)$$

with \sum^* representing summation over all non-trivial decompositions $\underline{n} = \underline{a}\underline{b}$, because $U_{\emptyset}^{\emptyset} = 1_{\mathbf{k}}$ and $R^{\emptyset} = 0$. Since $0 \neq \varphi(\underline{n}) = \varphi(\underline{a}) + \varphi(\underline{b})$, at least one of these two terms is different from 0, therefore the induction hypothesis implies that $R^{\underline{a}}U_{\underline{b}}^{\underline{b}}(\varepsilon) = 0$, so the sum in (2.19) vanishes. Moreover, since $\varphi(\underline{n}) \neq 0$, $\varphi(\underline{n}) + \varepsilon r(\underline{n})$ is invertible in \mathbf{K}_+ , hence $\mathbf{K}_- \ni U_{\underline{n}}^{\underline{n}}(\varepsilon) = -\frac{R^{\underline{n}}}{\varphi(\underline{n}) + \varepsilon r(\underline{n})} \in \mathbf{K}_+$ and therefore $U_{\underline{n}}^{\underline{n}}(\varepsilon) = 0$ and $R^{\underline{n}} = 0$. \square

Remark 2.4. Theorem B could appear as a particular case of Theorem 5 of [Me13] were it not for the fact that the latter reference deals with completed graded Lie algebras with finite-dimensional components and their enveloping algebras, a situation to which $\mathbf{K}^{\mathcal{N}}$ is not readily amenable.

3. Proof of Theorem A and more

Given a self-adjoint operator H_0 on a separable Hilbert space \mathcal{H} which is diagonal in an orthonormal basis $\mathbf{e} = (e_k)_{k \in J \subseteq \mathbb{N}}$ with eigenvalues $E_0(k)$, one considers in [PS16a] the space $\mathcal{L}^{\mathbb{R}} := \mathcal{L}_{\mathbf{e}}^{\mathbb{R}}[[\mu]]$ where $\mathcal{L}_{\mathbf{e}}^{\mathbb{R}}$ consists of all symmetric operators whose domain is the dense subspace $\text{Span}_{\mathbb{C}}(\mathbf{e})$ and which preserve $\text{Span}_{\mathbb{C}}(\mathbf{e})$. Since $\mathcal{L}_{\mathbf{e}}^{\mathbb{R}}$ is a Lie algebra over \mathbb{R} for the Lie bracket $[\cdot, \cdot]_{\text{qu}} := \frac{1}{i\hbar} \times \text{commutator}$, $\mathcal{L}^{\mathbb{R}}$ is a complete filtered Lie algebra over \mathbb{R} , filtered by order in μ . In what follows, we denote commutators by $[\cdot, \cdot]$.

To decompose an arbitrary perturbation as a sum of eigenvectors of $\text{ad}_{H_0} := \frac{1}{i\hbar}[H_0, \cdot]$, we notice that, for $B \in \mathcal{L}^{\mathbb{R}}$ with matrix $(\beta_{k,\ell}(\mu))_{k,\ell \in J}$ on the basis \mathbf{e} (with $\beta_{k,\ell}(\mu) \in \mathbb{C}[[\mu]]$), we can write $B = \sum_{(k,\ell) \in J \times J} \beta_{k,\ell}(\mu)|\ell\rangle\langle k|$. The sum might be infinite, but it is well-defined because the action of B in $\text{Span}_{\mathbb{C}}(\mathbf{e})$ is finitary. For the sake of simplicity, we suppose that B is finite-band, which means that there exists $D \in \mathbb{N}$ such that $\beta_{k,\ell} = 0$ when $|k - \ell| > D$.

Since $\frac{1}{i\hbar}[H_0, |\ell\rangle\langle k|] = \frac{E_0(\ell) - E_0(k)}{i\hbar}|\ell\rangle\langle k|$, we set

$$\mathcal{N} := \left\{ \frac{1}{i\hbar}(E_0(\ell) - E_0(k)) \mid (k, \ell) \in J \times J \right\} \quad \text{and} \quad B_\lambda := \sum_{\substack{(k,\ell) \text{ such that} \\ E_0(\ell) - E_0(k) = i\hbar\lambda}} \beta_{k,\ell}(\mu)|\ell\rangle\langle k|, \quad (3.1)$$

so that we have $B = \sum_{\lambda \in \mathcal{N}} B_\lambda$ and $\frac{1}{i\hbar}[H_0, B_\lambda] = \lambda B_\lambda$ in the complex Lie algebra $\mathcal{L}^{\mathbb{C}} := \mathcal{L}_{\mathbf{e}}^{\mathbb{C}}[[\mu]]$, where $\mathcal{L}_{\mathbf{e}}^{\mathbb{C}}$ is defined like $\mathcal{L}_{\mathbf{e}}^{\mathbb{R}}$ but without the symmetry requirement. With these notations, we have the following result, more general than Theorem A:

Theorem D. *Define, for $\underline{\lambda} \in \underline{\mathcal{N}}$,*

$$N^{\underline{\lambda}} := -\text{residue of } U_{-}^{\underline{\lambda}}(\varepsilon), \quad S^{\underline{\lambda}} := \text{constant term of } U_{+}^{\underline{\lambda}}(\varepsilon),$$

where (U_{-}, U_{+}) is the Birkhoff decomposition of the $\mathbb{C}((\varepsilon))$ -valued mould

$$T^{\underline{\lambda}}(\varepsilon) := \frac{1}{(\lambda_1 + \varepsilon)(\lambda_1 + \lambda_2 + 2\varepsilon) \cdots (\lambda_1 + \cdots + \lambda_{r(\underline{\lambda})} + r(\underline{\lambda})\varepsilon)}$$

inductively determined by (2.13) with $K_{-} = \varepsilon^{-1}\mathbb{C}[\varepsilon^{-1}]$ and $K_{+} = \mathbb{C}[[\varepsilon]]$. Then the formulae

$$N := \sum_{\underline{\lambda} \in \underline{\mathcal{N}}} N^{\underline{\lambda}} \frac{1}{i\hbar}[B_{\lambda_1}, \frac{1}{i\hbar}[B_{\lambda_2}, \dots \frac{1}{i\hbar}[B_{\lambda_{r(\underline{\lambda})-1}}, B_{\lambda_{r(\underline{\lambda})}}] \dots]] \quad (3.2)$$

$$\Psi(\cdot) := \sum_{\underline{\lambda} \in \underline{\mathcal{N}}} S^{\underline{\lambda}} \frac{1}{i\hbar}[B_{\lambda_1}, \frac{1}{i\hbar}[B_{\lambda_2}, \dots \frac{1}{i\hbar}[B_{\lambda_{r(\underline{\lambda})}}, \cdot] \dots]] \quad (3.3)$$

define respectively an element of $\mathcal{L}^{\mathbb{R}}$ and a unitary conjugation satisfying

$$\Psi(H_0 + B) = H_0 + N \quad \text{and} \quad [H_0, N] = 0.$$

Moreover, $\Psi(A) = CAC^{-1}$ with a unitary C given by the mould expansion

$$C := \sum_{\underline{\lambda} \in \underline{\mathcal{N}}} \left(\frac{1}{i\hbar}\right)^{r(\underline{\lambda})} S^{\underline{\lambda}} B_{\lambda_1} B_{\lambda_2} \cdots B_{\lambda_{r(\underline{\lambda})}} \quad (3.4)$$

(using the natural underlying structure of complete filtered associative algebra of $\mathcal{L}^{\mathbb{C}}$).

The proof of Theorem D requires two lemmas.

Lemma 3.1. *For any symmetral $S \in \mathbb{C}^{\underline{\mathcal{N}}}$, the formula (3.3) defines a Lie algebra automorphism Ψ of $\mathcal{L}^{\mathbb{C}}$ which is of the form $\Psi(A) = CAC^{-1}$ with $C \in \mathcal{L}^{\mathbb{C}}$ given by the mould expansion (3.4).*

Proof. For arbitrary $D \in \mathcal{L}^{\mathbb{C}}$, we use the notations $\mathcal{L}_D: A \mapsto DA$ and $\mathcal{R}_D: A \mapsto AD$ for the left and right multiplication operators in the associative algebra $\mathcal{L}^{\mathbb{C}}$. Then we can rewrite (3.3) as

$$\Psi = \sum_{\underline{\lambda} \in \underline{\mathcal{N}}} \left(\frac{1}{i\hbar}\right)^{r(\underline{\lambda})} S^{\underline{\lambda}} (\mathcal{L}_{B_{\lambda_1}} - \mathcal{R}_{B_{\lambda_1}}) \cdots (\mathcal{L}_{B_{\lambda_{r(\underline{\lambda})}}} - \mathcal{R}_{B_{\lambda_{r(\underline{\lambda})}}}).$$

For each $\underline{\lambda} \in \underline{\mathcal{N}}$, since left and right multiplications commute, we can expand

$$(\mathcal{L}_{B_{\lambda_1}} - \mathcal{R}_{B_{\lambda_1}}) \cdots (\mathcal{L}_{B_{\lambda_{r(\underline{\lambda})}}} - \mathcal{R}_{B_{\lambda_{r(\underline{\lambda})}}}) = \sum_{\underline{a}, \underline{b}} \text{sh}\left(\frac{\underline{a}, \underline{b}}{\underline{\lambda}}\right) (-1)^{r(\underline{b})} \mathcal{L}_{B_{a_1}} \cdots \mathcal{L}_{B_{a_{r(\underline{a})}}} \mathcal{R}_{B_{b_1}} \cdots \mathcal{R}_{B_{b_{r(\underline{b})}}}$$

with the same shuffling coefficients as in (2.5). We thus get

$$\Psi = \sum_{a,b,\lambda} (-1)^{r(\underline{b})} \left(\frac{1}{i\hbar}\right)^{r(\underline{\lambda})} \operatorname{sh}\left(\frac{a,\underline{b}}{\underline{\lambda}}\right) S^\lambda \mathcal{L}_{B_{\underline{a}}} \mathcal{R}_{B_{\underline{b}}},$$

where $\underline{b} \mapsto \tilde{\underline{b}}$ denotes word reversing. Symmetry then yields

$$\Psi = \sum_{a,b} (-1)^{r(\underline{b})} \left(\frac{1}{i\hbar}\right)^{r(a)+r(\underline{b})} S^a S^{\underline{b}} \mathcal{L}_{B_{\underline{a}}} \mathcal{R}_{B_{\underline{b}}} = \left(\sum_a \left(\frac{1}{i\hbar}\right)^{r(a)} S^a \mathcal{L}_{B_{\underline{a}}} \right) \left(\sum_{\underline{b}} (-1)^{r(\underline{b})} \left(\frac{1}{i\hbar}\right)^{r(\underline{b})} S^{\tilde{\underline{b}}} \mathcal{R}_{B_{\underline{b}}} \right).$$

We end up with $\Psi = \mathcal{L}_C \mathcal{R}_{\tilde{C}}$, with C defined by the mould expansion (3.4), and \tilde{C} defined by the analogous mould expansion associated to \tilde{S} defined by (2.7). But $S \times \tilde{S} = \tilde{S} \times S = \mathbf{1}$, by symmetry of S , and this clearly entails $C\tilde{C} = \tilde{C}C = \operatorname{Id}_{\mathcal{H}}$. \square

Lemma 3.2. *For any $N \in \mathbb{C}^{\mathcal{N}}$ such that the complex conjugate of $N^{\lambda_1, \dots, \lambda_r}$ is $N^{-\lambda_1, \dots, -\lambda_r}$, the mould expansion $N \in \mathcal{L}^{\mathbb{C}}$ defined by (3.2) is in $\mathcal{L}^{\mathbb{R}}$.*

For any symmetrized $S \in \mathbb{C}^{\mathcal{N}}$ such that the complex conjugate of $S^{\lambda_1, \dots, \lambda_r}$ is $S^{-\lambda_1, \dots, -\lambda_r}$, the mould expansion $C \in \mathcal{L}^{\mathbb{C}}$ defined by (3.4) is unitary.

Proof. Observe that the adjoint of the operator B_λ is $B_{-\lambda}$ for every $\lambda \in \mathcal{N}$. Since taking the adjoint is a real Lie algebra automorphism of $\mathcal{L}^{\mathbb{C}}$, this yields that the mould expansion N is a symmetric operator.

In the case of C , we find that the adjoint is given by the mould expansion associated to \tilde{S} defined by (2.7), which is C^{-1} as already mentioned. \square

Proof of Theorem D. Apply Theorem C to the normalization problem in $\mathcal{L}^{\mathbb{C}} = \mathcal{L}_e^{\mathbb{C}}[[\mu]]$ viewed as Lie algebra over $\mathbf{k} = \mathbb{C}$ with Lie bracket $[\cdot, \cdot]_{\text{qu}}$, filtered by order in μ , and with $\varphi(\lambda) \equiv \lambda$ in (2.11). Observe that, since $\mathcal{N} \subset i\mathbb{R}$, the complex conjugate of $T^{\lambda_1, \dots, \lambda_r}$ is $T^{-\lambda_1, \dots, -\lambda_r}$; it is easy to see that this property is inherited by U_- and U_+ , and hence by the constant moulds N and S . \square

Remark 3.3. Using the \mathbb{C} -valued mould $G = \log S$ defined in appendix, we see that $C = e^{\frac{1}{i\hbar}W}$ with $W = \sum_{\underline{\lambda} \in \underline{\mathcal{N}} \setminus \{\emptyset\}} \frac{1}{r(\underline{\lambda})} G^\lambda \frac{1}{i\hbar} [B_{\lambda_1}, \frac{1}{i\hbar} [B_{\lambda_2}, \dots, \frac{1}{i\hbar} [B_{\lambda_{r(\underline{\lambda})-1}}, B_{\lambda_{r(\underline{\lambda})}}] \dots]] \in \mathcal{L}^{\mathbb{R}}$.

Proof of Theorem A. Take V in Section 1 as $\mu B \in \mathcal{L}^{\mathbb{R}} = \mathcal{L}_e^{\mathbb{R}}[[\mu]]$, and identify the homogeneous terms in μ and in V (see the Addendum of Theorem A in [PS16a] for a more precise statement). \square

4. Extensions

In [PS16a], four other examples of complete filtered algebras are considered, corresponding to four dynamical situations: Poincaré-Dulac normal forms, Birkhoff normal forms, multiphase averaging and the semiclassical approximation of the situation of the present article. In all these

examples, as in Section 3, the results are derived exclusively out of a mould equation of the form (2.10). Therefore statements similar to theorem D can be established.

More quantitative results are proven in [PS16b] in the situation of an equation of the form (2.1) stated on Banach scales of Lie algebras: precise estimates (in convenient norms) are given when mould expansions are truncated. They also rely exclusively on mould equations and so can be rephrased using Birkhoff decompositions.

Precise formulations for all these cases are left to the interested reader.

Appendix A.

A.1. Mould exponential and alternality. Let \mathbf{k} be a ring and \mathcal{N} a nonempty set, and consider the set of moulds $\mathbf{k}^{\mathcal{N}}$ as in Section 2.1. We define a decreasing filtration by declaring that, for $m \geq 0$, a mould M is of order $\geq m$ if $M^{\underline{n}} = 0$ whenever $r(\underline{n}) < m$; this is easily seen to be compatible with mould multiplication, and in fact $\mathbf{k}^{\mathcal{N}}$ is a complete filtered associative algebra. We can thus define the mutually inverse exponential and logarithm maps by the usual series

$$M^{\emptyset} = 0 \quad \Rightarrow \quad e^M := \mathbf{1} + \sum_{k \geq 1} \frac{1}{k!} (M)^{\times k}, \quad \log(\mathbf{1} + M) := \sum_{k \geq 1} \frac{(-1)^{k-1}}{k} (M)^{\times k},$$

which are formally summable (only finitely many terms contribute to the evaluation of e^M or $\log(\mathbf{1} + M)$ on a given word).

A mould M is said to be “alternal” if $M^{\emptyset} = 0$ and $\sum_{\underline{n} \in \mathcal{N}} \text{sh}\left(\frac{\underline{a}, \underline{b}}{\underline{n}}\right) M^{\underline{n}} = 0$ for any nonempty words \underline{a} and \underline{b} . Equivalently, using the map Δ mentioned in the paragraph containing (2.14), M is alternal if and only if $\Delta M = M \otimes \mathbf{1} + \mathbf{1} \otimes M$. Since Δ is a morphism of associative algebras, alternal moulds form a Lie subalgebra of $\text{Lie}(\mathbf{k}^{\mathcal{N}})$ (the space $\mathbf{k}^{\mathcal{N}}$ viewed as a Lie algebra for which bracketing is defined by commutators).

The exponential map $M \mapsto e^M$ induces a bijection between alternal moulds and symmetrised moulds (use Δ and (2.14)).

Notice that, when identifying moulds with linear forms on the shuffle algebra, alternal moulds are identified with infinitesimal characters:

$$M^{\underline{a}\Delta\underline{b}} = \eta(\underline{a})M^{\underline{b}} + \eta(\underline{b})M^{\underline{a}} \quad \text{for all } \underline{a}, \underline{b} \in \mathcal{N}, \quad (\text{A.1})$$

where we denote by η the counit.

A.2. Proof of Proposition 2.1. Suppose that, in the situation described at the beginning of Section 2, we have a solution (R, S) to the mould equation (2.10). We must prove that the mould expansions (2.3) define a solution (N, Ψ) to (2.1).

Let us introduce the notations $B_{[\underline{n}]} := [B_{n_1}, [\dots [B_{n_{r-1}}, B_{n_r}] \dots]]$ and $\mathcal{B}_{\underline{n}} := \text{ad}_{B_{n_1}} \cdots \text{ad}_{B_{n_r}}$ for an arbitrary word $\underline{n} = n_1 \cdots n_r$, with the conventions $B_{[\emptyset]} = 0$ and $\mathcal{B}_{\emptyset} = \text{Id}$. Because \mathcal{L} is a complete filtered Lie algebra and each $B_{n_i} \in \mathcal{L}_{\geq 1}$, it is easily checked that one can define two linear maps $\mathcal{L}: \mathbf{k}^{\mathcal{N}} \rightarrow \mathcal{L}$ and $\mathcal{E}: \mathbf{k}^{\mathcal{N}} \rightarrow \text{End}_{\mathbf{k}}(\mathcal{L})$ (\mathbf{k} -linear operators) by the formulae

$$\mathcal{L}(M) := \sum_{\underline{n} \in \mathcal{N} \setminus \{\emptyset\}} \frac{1}{r(\underline{n})} M^{\underline{n}} B_{[\underline{n}]}, \quad \mathcal{E}(M) := \sum_{\underline{n} \in \mathcal{N}} M^{\underline{n}} \mathcal{B}_{\underline{n}}. \quad (\text{A.2})$$

In particular, $N = \mathcal{L}(R)$ and $\Psi = \mathcal{E}(S)$ are well-defined.

As already mentioned in the paragraph containing (2.8), Ψ is a Lie algebra automorphism because S is symmetral. By induction on $r(\underline{n})$, we deduce from (2.2) that $[X_0, B_{[\underline{n}]}] = \varphi(\underline{n}) B_{[\underline{n}]}$, whence

$$[X_0, \mathcal{L}(M)] = \mathcal{L}(\nabla_{\varphi} M) \text{ for any mould } M. \quad (\text{A.3})$$

In particular, $\nabla_{\varphi} R = 0$ entails $[X_0, N] = 0$, and we are just left with the verification of the first relation in (2.1). This will be obtained by means of the two identities

$$\Psi(B) = \mathcal{L}(S \times I_{\mathbf{k}} \times S^{-1}), \quad (\text{A.4})$$

$$\Psi(X_0) - X_0 = -\mathcal{L}(\nabla_{\varphi} S \times S^{-1}), \quad (\text{A.5})$$

the sum of which will yield the desired result, namely $\Psi(X_0 + B) - X_0 = N$, in view of the relation $S \times I_{\mathbf{k}} \times S^{-1} - \nabla_{\varphi} S \times S^{-1} = R$ granted by the mould equation.

Before proving (A.4) and (A.5), we show that $\Psi = e^{\text{ad}_W}$ with W in the range of \mathcal{L} . Let $G := \log S$. As explained in Section A.1, this is an alternal mould. Since $\mathcal{B}_{\underline{a}\underline{b}} = \mathcal{B}_{\underline{a}} \mathcal{B}_{\underline{b}}$, the map \mathcal{E} is clearly a morphism of filtered associative algebras, hence $\Psi = \mathcal{E}(e^G) = e^{\mathcal{E}(G)}$. Let $\mathcal{B}_{[\underline{n}]} := [\text{ad}_{B_{n_1}}, [\dots [\text{ad}_{B_{n_{r-1}}}, \text{ad}_{B_{n_r}}] \dots]]$ for an arbitrary word $\underline{n} = n_1 \cdots n_r$. The alternality of G entails

$$\mathcal{E}(G) = \sum_{\underline{n} \in \mathcal{N}} G^{\underline{n}} \mathcal{B}_{\underline{n}} = \sum_{\underline{n} \in \mathcal{N} \setminus \{\emptyset\}} \frac{1}{r(\underline{n})} G^{\underline{n}} \mathcal{B}_{[\underline{n}]} = \text{ad}_{\mathcal{L}(G)}. \quad (\text{A.6})$$

Indeed, the middle equality in (A.6) is obtained for any alternal mould from the identity

$$\mathcal{B}_{[\underline{n}]} = \sum_{(\underline{a}, \underline{b}) \in \mathcal{N} \times \mathcal{N}} (-1)^{r(\underline{b})} r(\underline{a}) \text{sh}\left(\frac{\underline{a}, \underline{b}}{\underline{n}}\right) \mathcal{B}_{\underline{a}\underline{b}} \quad \text{for all } \underline{n} \in \mathcal{N}$$

(where we denote by $\underline{b} \mapsto \tilde{\underline{b}}$ order reversal), which results from a classical computation (related to the Dynkin-Specht-Wever idempotent — see [vW66] or [PS16a]), and the last equality in (A.6) follows from the obvious relation $\mathcal{B}_{[\underline{n}]} = \text{ad}_{B_{[\underline{n}]}}$. Therefore, $\Psi = e^{\text{ad}_W}$ with $W = \mathcal{L}(G)$.

Proof of (A.4). An identity similar to the middle equality in (A.6), but at the level of \mathcal{L} and its universal enveloping algebra, implies that *the restriction of \mathcal{L} to alternal moulds is a morphism*

of Lie algebras. It follows that $\text{ad}_W(\mathcal{L}(M)) = \mathcal{L}(\text{ad}_G M)$ for any alternal M (denoting by ad the adjoint representations of \mathcal{L} and $\text{Lie}(\mathbf{k}^{\mathcal{N}})$), hence

$$e^{\text{ad}_W} \mathcal{L}(M) = \mathcal{L}(e^{\text{ad}_G} M) = \mathcal{L}(S \times M \times S^{-1})$$

(we have used Hadamard's lemma in $\mathbf{k}^{\mathcal{N}}$ for the last equality: $e^{\text{ad}_G} M = e^G \times M \times e^{-G}$). Since $I_{\mathbf{k}}$ is an alternal mould satisfying $\mathcal{L}(I_{\mathbf{k}}) = B$, we get as a particular case $\Psi(B) = e^{\text{ad}_W} \mathcal{L}(I_{\mathbf{k}}) = \mathcal{L}(S \times I_{\mathbf{k}} \times S^{-1})$. \square

Proof of (A.5). By (A.3), $\text{ad}_W X_0 = -\mathcal{L}(\nabla_{\varphi} G)$. Using again the morphism of Lie algebras induced by \mathcal{L} , we derive $\text{ad}_W^k X_0 = -\text{ad}_W^{k-1} \mathcal{L}(\nabla_{\varphi} G) = -\mathcal{L}(\text{ad}_G^{k-1} \nabla_{\varphi} G)$ for all $k \geq 1$, whence

$$\Psi(X_0) - X_0 = -\mathcal{L}(M), \quad M := \sum_{k \geq 1} \frac{1}{k!} \text{ad}_G^{k-1} \nabla_{\varphi} G.$$

A classical computation³ yields $M = \nabla_{\varphi}(e^G) \times e^{-G}$, whence $\Psi(X_0) - X_0 = -\mathcal{L}(\nabla_{\varphi} S \times S^{-1})$, as desired. \square

Remark A.1. There is another proof of Proposition 2.1, which consists in defining on the universal enveloping algebra $U(\mathcal{L})$ of \mathcal{L} a decreasing filtration of associative algebra which is separated and complete, so as to be able to define a morphism of filtered associative algebras $\mathcal{U} : \mathbf{k}^{\mathcal{N}} \rightarrow U(\mathcal{L})$ analogous to \mathcal{E} (this extra work can be dispensed with in the case of the Lie algebra $\mathcal{L}^{\mathbb{C}}$ of Section 3, since it has a natural structure of complete filtered associative algebra). One then checks that the restrictions of \mathcal{U} and \mathcal{L} to alternal moulds coincide, and that the normalization problem is solved by $N := \mathcal{U}(R)$ and the conjugation automorphism $\Psi : A \mapsto CAC^{-1}$ where $C := \mathcal{U}(S)$ (because $\mathcal{U}(\nabla_{\varphi} S) = [X_0, C]$, $\mathcal{U}(S \times I_{\mathbf{k}}) = CB$ and $\mathcal{U}(R \times S) = NC$).

Acknowledgments: This work has been partially carried out thanks to the support of the A*MIDEX project (n° ANR-11-IDEX-0001-02) funded by the ‘‘Investissements d’Avenir’’ French Government program, managed by the French National Research Agency (ANR). T.P. thanks also the Dipartimento di Matematica, Sapienza Università di Roma, for its kind hospitality during the elaboration of this work. D.S. thanks Fibonacci Laboratory (CNRS UMI 3483), the Centro Di Ricerca Matematica Ennio De Giorgi and the Scuola Normale Superiore di Pisa for their kind hospitality. This work has received funding from the French National Research Agency under the reference ANR-12-BS01-0017.

³Check that $\sum \frac{1}{k!} (U - V)^{k-1} = \sum \frac{1}{(p+q+1)!} U^p V^q e^{-V}$ in $\mathbb{Q}[[U, V]]$ e.g. by multiplying both sides by $(U - V)e^V$, substitute for U and V the operators of left and right multiplication by G in $\mathbf{k}^{\mathcal{N}}$ which commute, apply the resulting operator to $\nabla_{\varphi} G$, and remember that ∇_{φ} is a derivation.

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UNIVERSITÉ PARIS-EST MARNE-LA-VALLÉE, LABORATOIRE D'INFORMATIQUE GASPARD-MONGE (CNRS - UMR 8049), 77454
MARNE-LA-VALLÉE CEDEX 2, FRANCE (NOVELLI AND THIBON)

E-mail address: `novelli@univmlv.fr`, `jyt@univmlv.fr`

CMLS, ECOLE POLYTECHNIQUE, CNRS, UNIVERSITÉ PARIS-SACLAY, 91128 PALAISEAU CEDEX, FRANCE

E-mail address: `thierry.paul@polytechnique.edu`

CNRS UMR 8028 – IMCCE, OBSERVATOIRE DE PARIS, 77 AV. DENFERT-ROCHEREAU, 75014 PARIS, FRANCE

E-mail address: `david.sauzin@obspm.fr`