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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. More generally we prove that such a decomposition provides solutions of a universal “mould equation” introduced in [P16], which solves 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 [B25, H25].

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

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

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

An elegant way of building this pair (N, C) consists in using the so-called Lie algorithm, see, e.g. [D91]: let us look at C of the form $C = e^{i\frac{W}{\hbar}}$, W being self-adjoint (which ensure automatically that U is unitary). Expanding $W = W_1 + W_2 + \dots$, $N = N_1 + N_2 + \dots$ in “powers of V ”, we

get, since $e^{-i\frac{W}{\hbar}} H e^{i\frac{W}{\hbar}} = H + \sum_{k=1}^{\infty} \frac{1}{k!} (\frac{-i}{\hbar})^k [W, [W, \dots H] \dots]$, that

$$\begin{aligned}
-\frac{i}{\hbar}[W_1, H_0] &= \text{Diag}(V) - V \\
-\frac{i}{\hbar}[W_2, H_0] &= \text{Diag}(V_2) - V_2, \quad V_2 = -\frac{i}{\hbar}[W_1, V] - \frac{1}{2\hbar^2}[W_1, W_1, H_0] \\
-\frac{i}{\hbar}[W_3, H_0] &= \text{Diag}(V_3) - V_3, \quad V_3 = -\frac{i}{\hbar}[W_2, V] - \frac{1}{2\hbar^2}[W_1, W_1, V] - \frac{1}{2\hbar^2}[W_1, [W_2, H_0]] \\
&\quad - \frac{1}{2\hbar^2}[W_2, [W_1, H_0]] + \frac{i}{6\hbar^3}[W_1, [W_1, [W_1, H_0]]] \\
&\quad \cdot \\
-\frac{i}{\hbar}[W_k, H_0] &= \text{Diag}(V_k) - V_k
\end{aligned} \tag{1.2}$$

where $\text{Diag}(V)$ is the diagonal part of V on the eigenbasis of H_0 and the V_k s are computed recursively. Since the kernel of the derivation $W \mapsto -\frac{i}{\hbar}[W, H_0]$ is precisely the set of diagonal operators (H_0 has simple spectrum), one can solve the preceding hierarchy of equations by

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

(here we have denoted by e_n the eigenvector of H_0 of eigenvalue $E_0(n)$), the diagonal part of W_k remaining undetermined by the equation.

Using the Dirac notation $\langle n | V | m \rangle := (e_n, V e_m)$, $|n\rangle\langle m| \psi = (e_m, \psi) e_n$, and the hierarchy, we easily arrive to

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

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 (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 [P16]: 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 $\lambda \in \mathcal{N}$,

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

so that

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

We will suppose that V is finite-band, that is to say that the sum in (1.6) is finite.

Proposition 1.1 ([P16]). *For any $k \geq 1$, there exist coefficients $R^{\lambda_1, \dots, \lambda_k}$ 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 the coefficients $S^{\lambda_1, \dots, \lambda_k}$ appearing in a similar expansion for the operator of conjugation by C (see (2.2) with $\Psi(\cdot) = C^{-1} \cdot C$). The family of pairs $(R^{\lambda_1, \dots, \lambda_k}, S^{\lambda_1, \dots, \lambda_k})$ satisfies a universal ‘‘mould equation’’ (independent of V and depending on H_0 only through \mathcal{N}) studied in [P16] and recalled in the next section. Using (1.5) and introducing decomposition of the identity on the unperturbed eigenbasis in (1.7), one certainly recover (1.3), but probably with a big combinatorial complexity in the expressions as $k \rightarrow \infty$. Note that the decomposition (1.7) is NOT unique, though N_k is.

One of the main goal of this note is to introduce a new (to our knowledge) way of computing the coefficients $R^{\lambda_1, \dots, \lambda_k}$. It consist 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 an explicit expression for the solution of the modified ‘‘mould equation’’ coefficients as Laurent series in ε . The correct expression for $R^{\lambda_1, \dots, \lambda_k}$ will then be obtained by taking the residue of the polar part of the so-called Birkhoff decomposition of these Laurent series.

More precisely:

- (1) let $K_+ := \mathbb{C}[[\varepsilon]]$ and let $K := \mathbb{C}((\varepsilon))$ the field of the fractions of K_+ , so that $K = K_+ \oplus K_-$ with $K_- = \varepsilon^{-1} \mathbb{C}[[\varepsilon^{-1}]]$.
- (2) let $\underline{\mathcal{N}}$ be the set of words on the alphabet \mathcal{N} (ordered sequences of elements of \mathcal{N}). We will consider the set of functions from $\underline{\mathcal{N}}$ to K , that is $K^{\underline{\mathcal{N}}} = \{f, \underline{\lambda} \mapsto f^{\underline{\lambda}}\}$. We denote by $r(\underline{\lambda})$ the length of the word $\underline{\lambda} = \lambda_1 \lambda_2 \dots \lambda_{r(\underline{\lambda})}$.
- (3) for $\underline{\lambda} = \lambda_1 \dots \lambda_l$, $\underline{\lambda}' = \lambda'_1 \dots \lambda'_m$ we define $\underline{\lambda \lambda'} = \lambda_1 \dots \lambda_l \lambda'_1 \dots \lambda'_m$ and on $K^{\underline{\mathcal{N}}}$ we define the product

$$(f \times g)^{\underline{\lambda}} := \sum_{\underline{ab} = \underline{\lambda}} f^{\underline{a}} g^{\underline{b}} \in K.$$

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

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

considered of course as a formal Laurent series in ε . Note that $T^\lambda(\varepsilon)$ always exists as Laurent series in ε , even when $\lambda_1 + \dots + \lambda_{r(\underline{\lambda})} = 0$.

The ‘‘Birkhoff decomposition’’ (proven in the next section) states the following result.

Proposition 1.2 (Theorem B below). *Let $J \in K^{\mathcal{N}}$ be defined by $J^\varnothing = 1_K$, $J^\lambda = 0$ otherwise.*

There exist a unique pair $U_+, U_- \in K^{\mathcal{N}}$ such that $U_-^\varnothing = U_+^\varnothing = 1_K$, $U_- \in J + K + K_-^{\mathcal{N}}$, $U_+ \in K_+^{\mathcal{N}}$ and

$$U_- \times T = U_+.$$

The proof will be given in the next Section (in a more general setting), together with recurrence relations in order to compute U_- and U_+ .

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

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

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

for

$$N^{\lambda_1, \dots, \lambda_k} = -\text{Residue of } U_-^{\lambda_1, \dots, \lambda_k} = -[\varepsilon U_-^{\lambda_1, \dots, \lambda_k}(\varepsilon)]_{\varepsilon=\infty}.$$

We will prove much more in the following sections. In particular we will show that conjugation by C as in (1.1) has an expansion:

$$C^{-1}HC \sim H + \sum_{k=1}^{\infty} \sum_{\lambda_1, \dots, \lambda_k \in \mathcal{N}} G^{\lambda_1, \dots, \lambda_k} \frac{1}{i\hbar} [V_{\lambda_1}, \frac{1}{i\hbar} [V_{\lambda_2}, \dots \frac{1}{i\hbar} [V_{\lambda_k}, H] \dots]]$$

where $G^\lambda = U_+^\lambda(\varepsilon)|_{\varepsilon=0}$, and we will also remove the simplicity condition on the spectrum of H_0 .

F. Menous considers in [M09] the Birkhoff decomposition of moulds in order to solve normalization problems necessitating (possibly) logarithmically ramified conjugating maps. Let us note that the problems studied in [M09], and the methods used to solve them, concern local dynamics (vector fields) in a situation where there is no need of normal form (absence of resonances): the vector field is normalized to its ‘‘linear (unperturbed) part’’. For these reasons, the results and methods of [M09] cannot apply to our situation.

This paper is organized as follows. In Section 2 we briefly recall elements of mould theory and the mould equation implying (1.1), prove the underlying Birkhoff decomposition and prove the main result of this article, Theorem C. In Section 3 we prove the general ‘‘quantum’’ result implying Theorem A. In Section 4 we present different situations where Theorem C applies, including perturbations of Hamiltonian vector fields in classical dynamics.

2. Mould theory and Birkhoff decomposition

In full generality, we are interested in the following situation: given $X_0, B \in \mathcal{L}$, where \mathcal{L} is a Lie algebra over a field \mathbf{k} of characteristic zero, we look for a Lie algebra automorphism Ψ which maps $X_0 + B$ to an element of \mathcal{L} which commutes with X_0 . We call such a Ψ a “normalizing automorphism” and $X_0 + B$ satisfying

$$\Psi(X_0 + B) := X_0 + N, [X_0, N] = 0, \quad (2.1)$$

is then called a “normal form” of $X_0 + B$. Our key assumption will be that B can be decomposed into a sum $B = \sum_{n \in \mathcal{N}} B_n$ of eigenvectors of the inner derivation $\text{ad}_{X_0}: Y \mapsto [X_0, Y]$, namely $[X_0, B_n] = \varphi(n)B_n$ for some function $\varphi: \mathcal{N} \rightarrow \mathbf{k}$.

It was proven in [P16] that such a pair (Ψ, N) exists when \mathcal{L} is a complete filtered algebra¹ and that (Ψ, N) can be expressed by mould expansions, that is

$$\begin{cases} N &= \sum_{r \geq 1} \sum_{n_1, n_2, \dots, n_r \in \mathcal{N}} \frac{1}{r} R^{n_1 \dots n_r} [B_{n_1}, [\dots [B_{n_{r-1}}, B_r] \dots]] \\ \Psi(\cdot) &= \sum_{r \geq 1} \sum_{n_1, n_2, \dots, n_r \in \mathcal{N}} S^{n_1 \dots n_r} [B_{n_1}, [\dots [B_{n_r}, \cdot] \dots]] \end{cases} \quad (2.2)$$

where the functions $n_1 \dots n_r \mapsto R^{n_1 \dots n_r}, S^{n_1 \dots n_r}$ are moulds satisfying the mould equation (2.3) below.

Note that normal forms in completed graded Lie algebras have been studied in [M13] with a more Hopf-algebraic point of view and without involving moulds theory.

2.1. Moulds. Mould calculus has been introduced and developed by Jean Écalle ([E81], [E93]) in the 80-90’s in order to give powerful tools for handling problems in local dynamics, typically the normalization of vector fields or diffeomorphisms at a fixed point.

Let \mathcal{N} be a non empty set and \mathbf{k} a ring. We will denote by $\underline{\mathcal{N}}$ the set of words on the alphabet \mathcal{N} , $r(\underline{n})$ the length of $\underline{n} \in \underline{\mathcal{N}}$, and define the set of moulds which take values in \mathbf{k} as $\mathbf{k}^{\underline{\mathcal{N}}}$: a mould is a map $M: \underline{\mathcal{N}} \rightarrow \mathbf{k}$, $\underline{n} \mapsto M^{\underline{n}}$.

¹that is a Lie algebra $(\mathcal{L}, [\cdot, \cdot])$ together with a sequence of subspaces

$$\mathcal{L} = \mathcal{L}_{\geq 0} \supset \mathcal{L}_{\geq 1} \supset \mathcal{L}_{\geq 2} \supset \dots \quad \text{with } [\mathcal{L}_{\geq m}, \mathcal{L}_{\geq n}] \subset \mathcal{L}_{\geq m+n} \text{ for all } m, n \in \mathbb{N}$$

(exhaustive decreasing filtration compatible with the Lie bracket) such that $\bigcap \mathcal{L}_{\geq m} = \{0\}$ (the filtration is separated) 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 $\text{ord}(X) \geq m \Leftrightarrow X \in \mathcal{L}_{\geq m}$).

Mould multiplication is induced by word concatenation²,

$$(M \times N)^{\underline{n}} := \sum_{\underline{n}=\underline{a}\underline{b}} M^{\underline{a}}N^{\underline{b}} \text{ with } \underline{ab} := a_1 \dots a_{r(\underline{a})}b_1 \dots b_{r(\underline{b})}.$$

Écalle's definitions of symmetrality is fundamental. It is based on word shuffling. Roughly speaking, the shuffling of two words \underline{a} and \underline{b} is the set of all words obtained by interdigitating the letters of \underline{a} and \underline{b} while preserving their internal order in \underline{a} or \underline{b} ; the number of different ways a word \underline{n} can be obtained out of \underline{a} and \underline{b} is called shuffling coefficient, denoted by $\text{sh}\left(\frac{\underline{a}, \underline{b}}{\underline{n}}\right)$: let \mathfrak{S}_r be the symmetric group of degree r , then (see [P16], Section 2.2 for precisions): $\text{sh}\left(\frac{\underline{a}, \underline{b}}{\underline{n}}\right) = \text{card}\{\tau \in \mathfrak{S}_r \mid n_{\tau(1)} \dots n_{\tau(r(\underline{n}))} = \underline{ab}, \tau(1) < \dots < \tau(r(\underline{a})), \tau(r(\underline{a})+1) < \dots < \tau(r(\underline{n}))\}$.

A mould M is “symmetral” if $M^\emptyset = 1$ and $\sum_{\underline{n} \in \mathcal{N}} \text{sh}\left(\frac{\underline{a}, \underline{b}}{\underline{n}}\right) M^{\underline{n}} = M^{\underline{a}}M^{\underline{b}}$ for any nonempty words $\underline{a}, \underline{b}$. In other words, a symmetral mould is a character of a shuffle algebra.

It is explained in [P16] that, in the case of complete filtered Lie algebras over a field \mathbf{k} of characteristic 0, the equation (2.1) is solved by the ansatz (2.2) if the two moulds R and S are solution of the mould equation:

$$\begin{cases} \nabla_\varphi S = S \times I_{\mathbf{k}} - R \times S \\ \nabla_\varphi R = 0 \\ S \text{ symmetral} \end{cases} \quad (2.3)$$

where $I_{\mathbf{k}}$ is the mould defined by $I_{\mathbf{k}}^{\underline{n}} = \delta_{r(\underline{n}), 1} 1_{\mathbf{k}}$ and $\nabla_\varphi M^{\underline{n}} = (\varphi(n_1) + \dots + \varphi(n_{r(\underline{n})}))M^{\underline{n}}$.

By a slight abuse of notation we define $\varphi(\underline{n}) = \varphi(n_1) + \dots + \varphi(n_{r(\underline{n})})$.

2.2. Birkhoff decomposition.

Note that, in the case where $[\varphi(\underline{n}) = 0 \Leftrightarrow \underline{n} = \emptyset]$ (non resonant case) the unique solution of (2.3) is $R = 0$ and $S^{n_1 \dots n_r} = \frac{1}{\varphi(n_1)\varphi(n_1 n_2) \dots \varphi(n_1 \dots n_r)}$ (the symmetrality requirement is easy to check in that case), this last expression being possibly ill-defined in the general resonant case. We will therefore extend the field \mathbf{k} to the field of formal Laurent series with coefficients in \mathbf{k} . This will allow us to change the derivation ∇_φ into a non resonant one. The new mould equation (2.3) associated to this new derivation will be therefore easily solvable by an expression similar to the

²Let us notice that $\mathbf{k}^{\mathcal{N}}$ can also be seen as a completed filtered Lie algebra with the bracketing $[M, N] = M \times N - N \times M$ and the order function $\text{ord}: \mathbf{k}^{\mathcal{N}} \rightarrow \mathbb{N} \cup \{\infty\}$ which is defined by

$$\text{ord}(M^\bullet) \geq m \Leftrightarrow M^{\underline{n}} = 0 \text{ whenever } r(\underline{n}) < m.$$

one just mentioned. The original situation will be recovered by taking some kind of residues of the Birkhoff decomposition of this explicit solution.

More precisely, let $\mathbf{K}_+ := \mathbf{k}[[\varepsilon]]$ and $\mathbf{K} = \mathbf{k}((\varepsilon))$ the field of fractions of \mathbf{K}_+ , 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 $\Phi := \varphi + \varepsilon 1_k : \mathcal{N} \rightarrow K$, so that

$$\nabla_{\Phi} M^{\underline{n}}(\varepsilon) = (\varphi(\underline{n}) + r(\underline{n})\varepsilon)M^{\underline{n}}(\varepsilon) = \Phi(\underline{n})M^{\underline{n}}(\varepsilon) \in \mathbf{K},$$

with the same abuse of notation for $\Phi(\underline{n})$ as we did before for $\varphi(\underline{n})$.

Since $r(\underline{n}) \geq 1$ for $\underline{n} \neq \emptyset$, $r(\underline{n})\varepsilon \neq 0$ in \mathbf{K} and so is $\varphi(\underline{n}) + r(\underline{n})\varepsilon$, even if $\varphi(\underline{n}) = 0$. Therefore the mould equation (2.3) associated to (Φ, \mathbf{K}) (in place of (φ, \mathbf{k})) reduces to $R = 0$ and

$$\nabla_{\Phi} T = T \times I_K \tag{2.4}$$

and the (symmetral) solution is easily shown to be given explicitly by

$$T^{n_1 \dots n_r}(\varepsilon) = \frac{1}{(\varphi(n_1) + \varepsilon)(\varphi(n_1 n_2) + 2\varepsilon) \dots (\varphi(n_1 \dots n_r) + r(\underline{n})\varepsilon)}. \tag{2.5}$$

Of course $T^{n_1 \dots n_r}(\varepsilon)$, considered as a function, is singular at $\varepsilon = 0$ when some words $n_1 \dots n_l$, $l \leq r$, are resonant. The next result will give a precise product structure to T viewed as a mould.

Theorem B (Birkhoff decomposition of T). *Let $J \in \mathbf{K}^{\mathcal{N}}$ be defined by $J^{\emptyset} = 1_{\mathbf{K}}$, $J^{\lambda} = 0$ otherwise.*

There exist a unique pair $U_+, U_- \in \mathbf{K}^{\mathcal{N}}$ such that $U_-^{\emptyset} = U_+^{\emptyset} = 1_{\mathbf{K}}$, $U_- \in J + \mathbf{K}_-^{\mathcal{N}}$, $U_+ \in \mathbf{K}_+^{\mathcal{N}}$ and

$$U_- \times T = U_+.$$

Before to prove Theorem B, let us remark that, if we define $S^{\underline{n}} = U_+^{\underline{n}}(\varepsilon)|_{\varepsilon=0}$ (by this we mean that $S^{\underline{n}}$ is the constant term of the formal series $U_+^{\underline{n}}(\varepsilon)$), and $R = S \times I_k \times S^{-1} - \nabla_{\varphi} S \times S^{-1} \in \mathbf{k}^{\mathcal{N}}$ we have tautologically that

$$\nabla_{\varphi} S = S \times I_{\mathbf{k}} - R \times S$$

that is, (S, R) solves (2.3) at the condition that S is symmetral and R is resonant.

Proof.

- Uniqueness

Let us take two decompositions (U_-, U_+) and $(\widetilde{U}_-, \widetilde{U}_+)$. We have $U_-^{-1} \times U_+ = \widetilde{U}_-^{-1} \times \widetilde{U}_+$ so that $J + \mathbf{K}_-^{\mathcal{N}} \ni \widetilde{U}_- \times U_-^{-1} = \widetilde{U}_+ \times U_+^{-1} \in \mathbf{K}_+^{\mathcal{N}}$. Therefore $U_- \times U_-^{-1} = \widetilde{U}_+ \times U_+^{-1} = 1_{\mathbf{K}}$ since $\mathbf{K}_- \cap \mathbf{K}_+ = \{0\}$.

- Existence

Let π_{\pm} be the projectors $\mathbf{K} \rightarrow \mathbf{K}_{\pm}$. Since $U_{-}^{\emptyset}(\varepsilon) = U_{+}^{\emptyset}(\varepsilon) = \mathbf{1}_{\mathbf{K}}$, the formulae

$$\begin{cases} U_{-} &= \mathbf{1}_{\mathbf{K}} - \pi_{-}(U_{-} \times (T - \mathbf{1}_{\mathbf{K}})) \\ U_{+} &= \mathbf{1}_{\mathbf{K}} + \pi_{+}(U_{-} \times (T - \mathbf{1}_{\mathbf{K}})) \end{cases}$$

determine the values of $U_{-}^{\underline{n}}(\varepsilon)$ and $U_{+}^{\underline{n}}(\varepsilon)$ by induction on the length of \underline{n} . Moreover $U_{+} - U_{-} = U_{-} \times (T - \mathbf{1}_{\mathbf{K}})$, i.e. $U_{+} = U_{-} \times T$. \square

2.3. Main result.

Theorem C. *Let T the mould of $\mathbf{K}^{\mathcal{N}}$ defined by (2.5) and (U_{-}, U_{+}) its Birkhoff decomposition as stated in Theorem B. Define the moulds S, R of $\mathbf{k}^{\mathcal{N}}$ by*

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

Then (S, R) solves (2.3), and therefore (Ψ, N) , defined by (2.2), solves (2.1).

By *constant term* and *residue* of a Laurent series $\sum_{n \in \mathbb{Z}} c_n \varepsilon^n$ we mean respectively the coefficient c_0 and c_{-1} .

Proof.

Lemma 2.1. *Let S be as in Theorem C and $R' = S \times I_{\mathbf{K}} \times S^{-1} - \nabla_{\varphi} S \times S^{-1} \in \mathbf{k}^{\mathcal{N}} \subset \mathbf{K}^{\mathcal{N}}$. Then*

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

where $\nabla_{\mathbf{1}_{\mathbf{K}}} M^{\underline{n}}(\varepsilon) = r(\underline{n})M^{\underline{n}}(\varepsilon)$.

Note that, by (iii), we have that $\nabla_{\varphi} S = S \times I_{\mathbf{K}} - R \times S$. Therefore it is enough in order to prove the Theorem to prove that S is symmetral and R resonant.

- U_{-} and U_{+} are symmetral.

The symmetrality of U_{-} and U_{+} is derived easily³ from the one of T (T is symmetral since it is the unique solution of an equation of type (2.3)) by using the machinery of dimoulds introduced in [S09] and applied to our purpose in [P16].

A *dimould* is any map $M : \underline{\mathcal{N}} \times \underline{\mathcal{N}} \rightarrow \mathbf{K}$, $(\underline{a}, \underline{b}) \mapsto M^{\underline{a}, \underline{b}}$. Multiplication of dimoulds follows multiplication of moulds:

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

where the concatenation in $\underline{\mathcal{N}} \times \underline{\mathcal{N}}$ is defined by $(\underline{a}^1, \underline{b}^1)(\underline{a}^2, \underline{b}^2) = (\underline{a}^1 \underline{a}^2, \underline{b}^1 \underline{b}^2)$.

³It is immediate from the Birkhoff decomposition theorem, [C00], as stated for example in [Mn]. It is well known that expressions like $T(\varepsilon)$ define characters of shuffle algebras, so that their Birkhoff factors are both characters.

Decomposable dimoulds are dimoulds of the form $P = M \otimes N$, where it is meant that M and N are (ordinary) moulds and $P^{\underline{a}, \underline{b}} = M^{\underline{a}} N^{\underline{b}}$. Using the shuffling coefficients defined earlier, we introduce the map $\Delta : \mathbf{K}^{\mathcal{N}} \rightarrow \mathbf{K}^{\mathcal{N} \times \mathcal{N}}$, defined by $(\Delta M)^{\underline{a}, \underline{b}} := \sum_{\underline{n} \in \mathcal{N}} \text{sh}(\frac{\underline{a}, \underline{b}}{\underline{n}}) M^{\underline{n}}$ for any $(\underline{a}, \underline{b}) \in \mathcal{N} \times \mathcal{N}$, which happens to be a morphism of associative algebras. With the help of Δ , symmetrality reads now (see [S09, P16]):

$$M \text{ is symmetrical if and only if } M^\varnothing = 1 \text{ and } \Delta(M) = M \otimes M. \quad (2.6)$$

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

$$B = A \times \Delta T, \quad A \in J + \mathbf{K}_-^{\mathcal{N} \times \mathcal{N}} \text{ and } B \in \mathbf{K}_+^{\mathcal{N} \times \mathcal{N}}. \quad (\star)$$

It is immediate to see that the equation (\star) has a unique (pair of dimoulds) solution, by the same argument as in the proof of the uniqueness part of Theorem B. Moreover the symmetrality of T implies that $\Delta T = T \otimes T$, and one checks easily that this implies that $(U_- \otimes U_-, U_+ \otimes U_+)$ solves (\star) too. Therefore $\Delta U_- = U_- \otimes U_-$ and $\Delta U_+ = U_+ \otimes U_+$, and U_-, U_+ are symmetrical by (2.6).

- R is resonant.

We will show by induction on the length of \underline{n} that $[\varphi(\underline{n}) \neq 0 \Rightarrow R^{\underline{n}} = U_-^{\underline{n}}(\varepsilon) = 0]$. By definition \varnothing is a resonant word, nothing to prove. By (i) we have, since $U_-^\varnothing = 1_{\mathbf{K}}$ and, by (iii), $R^\varnothing = 0$, that

$$-(\varphi(\underline{n}) + \varepsilon r(\underline{n})) U_-^{\underline{n}}(\varepsilon) = R^{\underline{n}} + \sum_{\substack{\underline{a}\underline{b}=\underline{n} \\ \underline{a} \neq \varnothing \neq \underline{b}}} R^{\underline{a}} U_-^{\underline{b}}(\varepsilon) \quad (2.7)$$

Since $0 \neq \varphi(\underline{n}) = \varphi(\underline{a}) + \varphi(\underline{b})$, one of them must be different from 0. Therefore the induction hypothesis implies that $R^{\underline{a}} U_-^{\underline{b}}(\varepsilon) = 0$ when $\underline{a}\underline{b} = \underline{n}$, $\underline{a} \neq \varnothing \neq \underline{b}$, so the sum in (2.7) vanishes. Moreover, since $\varphi(\underline{n}) \neq 0$, $\varphi(\underline{n}) + \varepsilon r(\underline{n})$ is invertible in \mathbf{K}_+ . So $\mathbf{K}_- \ni -U_-^{\underline{n}}(\varepsilon) = \frac{R^{\underline{n}}}{\varphi(\underline{n}) + \varepsilon r(\underline{n})} \in \mathbf{K}_+$ and therefore $R^{\underline{n}} = U_-^{\underline{n}}(\varepsilon) = 0$. Theorem C is proven. \square

Proof of Lemma 2.1. Since $U_- \times T = U_+$, $\nabla_\Phi T = T \times I_{\mathbf{K}}$ and ∇_Φ is a derivation, we get that

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

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

$$U_+ \times I_{\mathbf{K}} \times U_+^{-1} - \nabla_\Phi U_+ \times U_+^{-1} = \mathcal{R} \in \mathbf{K}_+^{\mathcal{N}} \quad (2.8)$$

since $\mathbf{K}_+^{\mathcal{N}}$ is invariant by ∇_Φ and, on the other side,

$$\nabla_\Phi U_- \times U_-^{-1} + \varepsilon \nabla_1 U_- \times U_-^{-1} = -\mathcal{R} = P + \varepsilon Q, \quad P, Q \in \mathbf{K}_+^{\mathcal{N}}. \quad (2.9)$$

Since $\mathbf{K}_+ \cap \mathbf{K}_- = \{0\}$, we get, by (2.8 - 2.9),

$$\mathcal{R} = -(\varepsilon \nabla_1 U_- \times U_-^{-1})|_{\varepsilon=\infty} = -(\varepsilon \nabla_1 U_-)|_{\varepsilon=\infty}$$

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

Returning to (2.8), we have that $\mathcal{R} = U_+ \times I_{\mathbf{K}} \times U_+^{-1} - \nabla_{\Phi} U_+ \times U_+^{-1}$ is constant in ε and therefore

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

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

3. Proof of Theorem A and more

Given an 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 [P16] the algebra $\mathcal{L}^{\mathbb{R}} := \mathcal{L}_{\mathbf{e}}^{\mathbb{R}}[[\mu]]$ 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 $\text{Span}_{\mathbb{C}}(\mathbf{e})$. This is a complete filtered Lie algebra over \mathbb{R} , filtered by order in μ .

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 $B = \sum_{(k,\ell) \in J \times J} \beta_{k,\ell}(\mu) |e_{\ell}\rangle \langle e_k|$. 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 $|k - \ell| > D$.

By $\frac{1}{i\hbar}[H_0, |e_{\ell}\rangle \langle e_k|] = \frac{E_0(\ell) - E_0(k)}{i\hbar} |e_{\ell}\rangle \langle e_k|$, we immediately get that $B = \sum_{\lambda \in \mathcal{N}} B_{\lambda}$ with

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

Then applying Theorem A and formulae (1.9) and (1.10) in [P16] to our main result Theorem C, with φ equal to the identity in (2.3), we get the following one, more general than Theorem A,

Theorem D. *Let*

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

where (U_-, U_+) is the Birkhoff decomposition of the mould

$$T^{\Delta}(\varepsilon) = \frac{1}{(\lambda_1 + \varepsilon)(\lambda_1 + \lambda_2 + 2\varepsilon) \dots (\lambda_1 + \dots + \lambda_{r(\Delta)} + r(\Delta)\varepsilon)}.$$

Then the formulae

$$\begin{aligned}
N &= \sum_{\lambda \in \mathcal{N}} N^\lambda \frac{1}{i\hbar} [B_{\lambda_1}, \frac{1}{i\hbar} [B_{\lambda_2}, \dots \frac{1}{i\hbar} [B_{\lambda_{r(\Delta)-1}}, B_{\lambda_{r(\Delta)}}] \dots]] \\
\Psi(\cdot) &= \sum_{\lambda \in \mathcal{N}} S^\lambda \frac{1}{i\hbar} [B_{\lambda_1}, \frac{1}{i\hbar} [B_{\lambda_2}, \dots \frac{1}{i\hbar} [B_{\lambda_{r(\Delta)}}, \cdot] \dots]]
\end{aligned}$$

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

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

Taking now V in Section 1 as $\mu B \in \mathcal{L}^{\mathbb{R}}[[\mu]]$ and using the Addendum of Theorem A in [P16], we get Theorem A of the present paper by identifying the homogeneous terms in μ and in V .

4. Extensions

One considers in [P16] four more examples of complete filtered algebras corresponding to four dynamical situation: 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 the mould equation of the form (2.3). Therefore statements similar to theorem D can be established.

More quantitative results are proven in [P16] 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 expansion 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.

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