Hyperoctahedral Chen calculus for effective Hamiltonians

Christian Brouder
Institut de Minéralogie et de Physique des Milieux Condensés,
CNRS UMR7590, Universités Paris 6 et 7, IPGP,
140 rue de Lourmel, 75015 Paris, France.

Frédéric Patras
Laboratoire J.-A. Dieudonné, CNRS UMR 6621,
Université de Nice,
Parc Valrose, 06108 Nice Cedex 02, France.

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Abstract

We tackle the problem of unraveling the algebraic structure of computations of effective Hamiltonians. This is an important subject in view of applications to chemistry, solid state physics or quantum field theory. We show, among other things, that the correct framework for these computations is provided by the hyperoctahedral group algebras. We define several structures on these algebras and give various applications. For example, we show that the adiabatic evolution operator (in the time-dependent interaction representation of an effective Hamiltonian) can be written naturally as a Picard-type series and has a natural exponential expansion.

Introduction

We start with a short overview of the classical theory of Chen calculus, that is, iterated integral computations. The subject is classical but is rarely presented from the suitable theoretical perspective -that is, emphasizing the role of the convolution product on the direct sum of the symmetric groups group algebras. We give therefore a brief account of the theory that takes into account this point of view -this will be useful later in the article. Then, we recall the construction of effective Hamiltonians in the time-dependent interaction representation.

The third section is devoted to the investigation of the structure of the hyperoctahedral group algebras. Although we are really interested in the applications of these objects to the study of effective Hamiltonians, and although the definitions we introduce are motivated by the behavior of the iterated integrals showing up in this setting, we postpone the description of the way the two theories interact to a later stage of the article. Roughly stated, we show that the descent algebra approach to Lie calculus, as emphasized in Reutenauer's [25] can be lifted to the hyperoctahedral setting. This extends previous works [14, 1, 5, 2, 19] on the subject and shows that these results (focussing largely on Solomon's algebras of hyperoctahedral groups and other wreath product group algebras) are naturally connected to the study of physical systems through the properties of their Hamiltonians and of the corresponding differential equations, very much as the classical theory of free Lie algebras relates naturally to the study of differential equations and topological groups. Notice however that the statistics we introduce here on hyperoctahedral groups seems to be new –and is different from the statistics naturally associated to the noncommutative representation theoretic approach to hyperoctahedral groups, as it appears in these works.

The fourth section studies the effective adiabatic evolution operator and shows that it can be expanded

as a generalized Picard series by means of the statistics introduced on hyperoctahedral groups[1]. As a corollary, we derive in the last section an exponential expansion for the evolution operator. Such expansions are particularly useful in view of numerical computations, since they usually lead to approximating series converging much faster than the ones obtained from the Picard series.

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1 The algebra of iterated integrals

Let us recall the basis of Chen's iterated integrals calculus, starting with a first order linear differential equation (with, say, operator or matrix coefficients):

$$A'(t) = H(t)A(t),\ A(0) = 1$$

The solution can be expanded as the Picard series:

$$A(t) = 1 + \int_0^t H(x)dx + \int_0^t \int_0^{t_1} H(t_1)H(t_2)dt_1dt_2 + ... + \int_{\Delta_n^t} H(t_1)...H(t_n) + ...$$

where $\Delta_n^t := \{0 \leq t_n \leq ... \leq t_1 \leq t\}$ and where the measure $dt_1 \dots dt_n$ is implicit. Notice, for further use, that when we allow for a general initial condition $A(x) = 1$, with possibly $x = -\infty$, the integration simplex Δ_n^t should be replaced by $\Delta_n^{[x,t]} := \{x \leq t_n \leq ... \leq t_1 \leq t\}$.

Solving for $A(t) = \exp(\Omega(t))$ (see [3, 16]), and more generally any computation with $A(t)$, requires the computation of products of iterated integrals of the form:

$$< \sigma >:= \int_{\Delta_n^t} H(t_{\sigma(1)})...H(t_{\sigma(n)}),\ \sigma = (\sigma(1), ..., \sigma(n)) \in S_n,$$

where S_n stands for the symmetric group of order n. Notice that we represent an element σ in S_n by the sequence $(\sigma(1), ..., \sigma(n))$.

In general, for any $\mu = \sum_n \sum_{\sigma \in S_n} \mu_\sigma \cdot \sigma \in \mathbf{S} := \bigoplus_n \mathbb{Q}[S_n]$, the direct sum of the group algebras of the symmetric groups S_n over the rationals, we will write $< \mu >$ for $\sum_n \sum_{\sigma \in S_n} \mu_\sigma \cdot < \sigma >$. This allows, for example, to write $A(t)$ as $< I >$, where $I := \sum_n (1, ..., n)$ is the formal sum of the identity elements in the symmetric group algebras.

The formula for the product of $< \sigma >$ with $< \beta >$ is a variant of Chen's formula for the product of two iterated integrals of functions or of differential forms (a proof of the formula will be given in Section 3 in a more general framework; the formula also holds for arbitrary integration bounds, that is when Δ_n^t is replaced by $\Delta_n^{[x,t]}$):

$$< \sigma > \cdot < \beta > = < \sigma * \beta >,$$

where $\sigma * \beta$ is the convolution product[2] of the two permutations, that is, for $\sigma \in S_n,\ \beta \in S_m$: $\sigma * \beta$ is the sum of the $\binom{n+m}{n}$ permutations $\gamma \in S_{n+m}$ with $st(\gamma(1), ..., \gamma(n)) = (\sigma(1), ..., \sigma(n))$ and $st(\gamma(n+1), ..., \gamma(n+m)) = (\beta(1), ..., \beta(m))$. Here, st stands for the standardization map, the action of which on sequences is obtained by replacing $(i_1, ..., i_n), i_j \in \mathbb{N}^*$ by the (necessarily unique) permutation $\sigma \in S_n$, such that $\sigma(p) < \sigma(q)$ for $p < q$ if and only if $i_p \leq i_q$. In words, each number i_j is replaced by the position

[1] Picard series are often referred to as Dyson or Dyson-Chen series in the literature, especially in contemporary physics, but we prefer to stick to the most classical terminology

[2] This is one possible definition of the convolution product, there are several equivalent ones that can be obtained using the various natural set automorphisms of the symmetric groups (such as inversion or conjugacy by the element of maximal length). They result into various (but essentially equivalent) associative algebra structures on the direct sum of the symmetric groups group algebras, see e.g. [13]

of i_j in the increasing ordering of $i_1, \ldots, i_n$. If we take the example of $(5,8,2)$, the position of 5, 8 and 2 in the ordering $2<5<8$ is 2, 3 and 1. Thus, $st(5,8,2)=(2,3,1)$. For instance,

$$\begin{aligned}(2,3,1)*(1) &= (2,3,1,4)+(2,4,1,3)+(3,4,1,2)+(3,4,2,1),\\ (1,2)*(2,1) &= (1,2,4,3)+(1,3,4,2)+(1,4,3,2)+(2,3,4,1)+(2,4,3,1)+(3,4,2,1).\end{aligned}$$

The convolution product relates to the shuffle product ш [25] as it appears in Chen's work [7] and in the parametrization of the product of iterated integrals of functions or differential forms. Indeed, for σ, β as above:

$$\sigma^{-1}*\beta^{-1}=(\sigma ш \beta[n])^{-1}$$

where $\beta[n]$ stands for the sequence $(\beta(1)+n, ..., \beta(m)+n)$. Recall, for completeness sake, that the shuffle product $A ш B$ of two words (or sequences) $A=aA'=aa_2...a_k$, $B=bB'=bb_2...b_l$ is defined recursively by

$$A ш B = a(A' ш B)+b(A ш B')$$

we refer to [27] and [25] for details. Associativity of $*$ follows immediately from the definition, the unit is $1\in \mathbf{S}_0=\mathbb{Q}$, and the graduation on $\mathbf{S}=\bigoplus_n \mathbb{Q}[S_n]$ is compatible with $*$, so that:

Lemma 1.1. *The convolution product provides* $\mathbf{S}$ *with the structure of a graded connected associative (but noncommutative) unital algebra.*

For completeness, recall that connected means simply that $\mathbf{S}_0=\mathbb{Q}$. In fact, $\mathbf{S}$ carries the richer structure of a Hopf algebra, and as such is referred to as the Malvenuto-Reutenauer Hopf algebra [13]. From the point of view of the theory of noncommutative symmetric functions, the elements of $\mathbf{S}$ should be understood as free quasisymmetric functions [8]. This definition of the convolution product on $\mathbf{S}$ allows, for example, to express simply the coefficients of the continuous Baker-Campbell-Hausdorff formula (compare with the original solution [16]):

$$\Omega(t)=<\log(I)>.$$

Here $\log(I)$ identifies, in $\mathbf{S}$, with the formal sum of Solomon's (also called Eulerian or canonical) idempotents [28]. We refer to [20, 25, 21, 22, 9] for an explanation and a Hopf algebraic approach to these idempotents and, more generally, for a Hopf algebraic approach to Lie computations. We will return later with more details to Solomon's idempotent but mention only, for the time being, that one of the main purposes of the present article is to extend these ideas to the more general framework required by the study of effective Hamiltonians.

2 Iterated integrals in time-dependent perturbation theory

The ultimate aim of quantum physics is the knowledge of the eigenvalues and eigenstates of the Hamiltonian H describing a physical system. In most cases, the eigenvalue problem cannot be solved exactly, but the eigenvalues and eigenstates of a simpler and closely related Hamiltonian H_0 are known, at least numerically. Then, H can be rewritten $H=H_0+V$, where V is referred to as the perturbation term. For example, in molecular physics, H_0 is the Hamiltonian describing the interactions of N_e electrons with N_n nuclei, whereas H describes the interaction of the N_e electrons with themselves *and* with the N_n nuclei. In that case, the perturbation V describes the electron-electron interaction, this simple approach paving the way to most of the numerical methods in the field.

In other terms, perturbation theory provides a systematic way to calculate an eigenstate of H from an eigenstate of H_0. In the time-dependent perturbation theory, we first define a time-dependent Hamiltonian $H(t)=H_0+\mathrm{e}^{-\epsilon|t|}V$. When ϵ is small, this means physically that the interaction is very slowly switched on from $t=-\infty$ where $H(-\infty)=H_0$ to $t=0$ where $H(0)=H$. The basic idea is that, if ϵ is small enough, then an eigenstate of H_0 can be transformed into an eigenstate of H by the time-dependent perturbation $\mathrm{e}^{-\epsilon|t|}V$. For example, the ground state $|\Phi_0>$ (the eigenstate associated to the lowest eigenvalue E_0 of H_0) should hopefully be transformed into the ground state of H. We also assume for the time being that the ground state is non degenerate, that is that the eigenspace associated to the

highest eigenvalue E_0 is one-dimensional. We write from now on $|\Phi_i>$ for the eigenvectors of H_0 and assume that the eigenvalues E_i are ordered increasingly ($E_i \leq E_{i+1}$).

To implement this picture of perturbation theory, the time-dependent Schrödinger equation $i\partial|\Psi_S(t)\rangle/\partial t = H(t)|\Psi_S(t)\rangle$ should be solved. However, the solutions $|\Psi_S(t)\rangle$ of this equation vary like $\mathrm{e}^{-iE_0t}|\Phi_0\rangle$ for large negative t (where $|\Phi_0\rangle$ satisfies $H_0|\Phi_0\rangle = E_0|\Phi_0\rangle$) and have no limit for $t \to -\infty$. To compensate for this time variation, one looks instead for $|\Psi(t)\rangle = \mathrm{e}^{iH_0t}|\Psi_S(t)\rangle$ that satisfies $i\partial|\Psi(t)\rangle/\partial t = H_{\mathrm{I}\epsilon}(t)|\Psi(t)\rangle$, with $H_{\mathrm{I}\epsilon} = \mathrm{e}^{iH_0t}V\mathrm{e}^{-iH_0t}\mathrm{e}^{-\epsilon|t|}$. Now $H_{\mathrm{I}\epsilon}(-\infty) = 0$, and $|\Psi(-\infty)\rangle$ makes sense. Using $H_{\mathrm{I}\epsilon}$, we can start consistently from the ground state $|\Phi_0\rangle$ of H_0 and solve the time-dependent Schrödinger equation with the boundary condition $|\Psi(-\infty)\rangle = |\Phi_0\rangle$. When no eigenvalue crossing takes place, $|\Phi_0\rangle$ should be transformed into the ground state $|\Psi(0)\rangle$ of H.

At first sight, solving the time-dependent Schrödinger equation for $|\Psi(t)\rangle$ does not look simpler than solving the time-independent Schrödinger equation with the Hamiltonian H. However, if V is small enough, fairly accurate approximations of the true eigenstates can be obtained from the first terms of the perturbative expansion of $|\Psi(t)\rangle$. In general, instead of calculating directly $|\Psi(t)\rangle$, it is convenient to define the unitary operator $U_\epsilon(t)$ as the solution of $i\partial U_\epsilon(t)/\partial t = H_{\mathrm{I}\epsilon}(t)U_\epsilon(t)$, with the boundary condition $U_\epsilon(-\infty) = 1$. Thus, $|\Psi(t)\rangle = U_\epsilon(t)|\Phi_0\rangle$. The connection with iterated integrals appears when solving iteratively the equation for $U_\epsilon(t)$:

$$U_\epsilon(t) \quad = \quad 1 + (-i)\int_{-\infty}^{t} \mathrm{d}t_1 H_{\mathrm{I}\epsilon}(t_1) + (-i)^2 \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 H_{\mathrm{I}\epsilon}(t_1)H_{\mathrm{I}\epsilon}(t_2) + \dots$$

A straightforward calculation [11] gives us

$$U_\epsilon(0)|\Phi_0\rangle \quad = \quad |\Phi_0\rangle + \sum_{n=1}^{\infty} \sum_{i_1 \dots i_n} \frac{|\Phi_{i_n}\rangle\langle\Phi_{i_n}|V|\Phi_{i_{n-1}}\rangle \dots \langle\Phi_{i_2}|V|\Phi_{i_1}\rangle\langle\Phi_{i_1}|V|\Phi_0\rangle}{(E_0 - E_{i_n} + ni\epsilon)\dots(E_0 - E_{i_2} + 2i\epsilon)(E_0 - E_{i_1} + i\epsilon)}, \tag{1}$$

where we use the completeness relation $1 = \sum_i |\Phi_i\rangle\langle\Phi_i|$. However, it immediately appears that this expression has no limit for $\epsilon \to 0$ because the sum over all i_p contains the terms $i_p = 0$, for which the denominator has a factor $pi\epsilon$. In 1951, Gell-Mann and Low [10] conjectured that

$$|\Psi_{\mathrm{GL}}\rangle \quad = \quad \lim_{\epsilon \to 0} \frac{U_\epsilon(0)|\Phi_0\rangle}{\langle\Phi_0|U_\epsilon(0)|\Phi_0\rangle}$$

exists and is an eigenstate of H. The fact that the Gell-Mann and Low formula indeed removes all the divergences of equation (1) was proved much later by Nenciu and Rasche [18].

The above scheme works nicely when the ground state of H_0 is non degenerate. When it is degenerate, that is when the eigenspace E_0 associated to the lowest eigenvalue of H_0 has dimension > 1, the problem is more subtle, see [17, 6, 15]. To understand the algebraic phenomena underlying time-dependent perturbation theory for degenerate systems is actually the purpose of the present article.

Let us write P for the projection on this eigenspace. The natural extension of the Gell-Mann and Low formula then reads as a definition of a "Gell-Mann and Low" operator acting on the degenerate eigenspace E_0:

$$U_{GL} \quad := \quad \lim_{\epsilon \to 0} U_\epsilon(0)P(PU_\epsilon(0)P)^{-1}, \tag{2}$$

or, $U_{GL} = \lim_{\epsilon \to 0} U_{GL}(\epsilon)$, $U_{GL}(\epsilon) := U_\epsilon(0)P(PU_\epsilon(0)P)^{-1}$. It can be shown that the operator $PU_\epsilon(0)P$ is invertible within the image of P if no vector in the image of $U_\epsilon(0)P$ is annihilated by P [4]. We will assume that this property is satisfied by the systems we consider. The operator U_{GL} was first proposed by Morita in 1963 [17]. It shows up e.g. in the time-dependent interaction representation of the effective Hamiltonian $H_{\mathrm{eff}} := \lim_{\epsilon \to 0} PHU_\epsilon(0)P[PU_\epsilon(0)P]^{-1}$ classically used to solve the eigenvalue problem.

This operator U_{GL} is the one we will be interested in here, postponing to further work the analysis of concrete applications to the study of degenerate systems. In other terms, we will investigate and unravel the fine algebraic structure of the iterative expansions of $U_\epsilon(t)$ and $U_{GL}(\epsilon)$.

3 Wreath product convolution algebras

Let us explain further our motivation. In the previous section, we observed that the study of effective Hamiltonians leads to the study of Picard-type expansions involving the operators $H_{\mathrm{I}\epsilon}(t)$ and $PH_{\mathrm{I}\epsilon}(t)$ or, equivalently, $A(t) := -i(1-P)H_{\mathrm{I}\epsilon}(t)$ and $B(t) := iPH_{\mathrm{I}\epsilon}(t)$. Expanding these expressions will lead to the study of iterated integrals involving the two operators $A(t)$ and $B(t)$ such as, say: $\int_{\Delta_3^t} A(t_2)B(t_3)A(t_1)$. The idea underlying the forthcoming algebraic constructions is to encode such an expression by a signed permutation and to lift computations with iterated integrals to an abstract algebraic setting: in the previous example, the signed permutation would be $(2, \bar{3}, 1)$ (see below for precise definitions).

In more abstract (but equivalent) terms, iterated integrals on two operators are conveniently encoded by elements of the hyperoctahedral groups, whereas iterated integrals on k operators would be conveniently encoded by more general colored permutations or elements of the wreath product of S_n with the cyclic group of order k. Recall the definition of the hyperoctahedral group B_n of order n. The hyperoctahedral group is the group defined either as the wreath product of the symmetric group of order n with the cyclic group of order 2, or, in a more concrete way, as the group of "signed permutations" the elements of which are written as sequences of integers $i \in \mathbb{N}^*$ and of integers with an upper bar $\bar{i}, i \in \mathbb{N}^*$, so that, when the bars are erased, one recovers the expression of a permutation. The composition rule is the usual one for permutations, together with the sign rule for bars: for example, if $\bar{\sigma} \in B_3 = (2, \bar{3}, 1)$ and $\bar{\beta} = (\bar{3}, 1, \bar{2})$, then:

$$\bar{\beta} \circ \bar{\sigma}(2) = \bar{\beta}(\bar{3}) = \bar{\bar{2}} = 2,$$
$$\bar{\beta} \circ \bar{\sigma}(3) = \bar{\beta}(1) = \bar{3}.$$

By analogy with $\mathbf{S}$, we equip $\mathbf{B} := \bigoplus_n B_n$ with the structure of a graded connected (associative but noncommutative) algebra with a unit. This algebra structure agrees with the ones introduced in [1, 19, 2] (possibly up to an isomorphism: for example, the relationship between the product we consider and the shifted shuffle product of [19] reflects the relationship between the convolution and (shifted) shuffle product on $\mathbf{S}$ that we recalled in the first section of the present article).

The standardization *st* of a signed sequence $\bar{w}$ (i.e. a sequence of integers and of integers marked with an upper bar) is defined analogously to the classical standardization, except for the fact that upper bars are left unchanged (or, equivalently, have to be reintroduced at their initial positions after the standardization of the sequence w has been performed, where we write w for $\bar{w}$ where the upper bars have been erased). For example, $st(\bar{2}, 7, \bar{1}, 2) = (\bar{2}, 4, \bar{1}, 3)$.

Definition 3.1. *Let $\bar{\sigma}, \bar{\beta}$ belong to B_n, resp. B_m. Their convolution product is defined by:*

$$\bar{\sigma} * \bar{\beta} := \sum_{\bar{\tau}} \bar{\tau}$$

where $\bar{\tau}$ runs over the $\binom{n+m}{n}$ elements of B_{n+m} with $st(\bar{\tau}(1), ..., \bar{\tau}(n)) = \bar{\sigma}$, $st(\bar{\tau}(n+1), ..., \bar{\tau}(n+m)) = \bar{\beta}$.

For instance,

$$\begin{aligned}(\bar{2}, 3, 1) * (\bar{1}) &= (\bar{2}, 3, 1, \bar{4}) + (\bar{2}, 4, 1, \bar{3}) + (\bar{3}, 4, 1, \bar{2}) + (\bar{3}, 4, 2, \bar{1}),\\ (1, \bar{2}) * (2, \bar{1}) &= (1, \bar{2}, 4, \bar{3}) + (1, \bar{3}, 4, \bar{2}) + (1, \bar{4}, 3, \bar{2}) + (2, \bar{3}, 4, \bar{1}) + (2, \bar{4}, 3, \bar{1}) + (3, \bar{4}, 2, \bar{1}).\end{aligned}$$

Notice that this definition is dictated, for us, by iterated integrals computations, similarly to the classical one-Hamiltonian case dealt with in the first section. Indeed, let $A(t), B(t)$ be two time-dependent operators. For $\bar{\sigma} \in B_n$, let us write $< \bar{\sigma} >$ for the iterated integrals obtained by the usual process, with the extra prescription that upper indices (empty set or bar) in $\bar{\sigma}$ indicate that the operator used at the corresponding level of the integral is A or B, so that e.g., $\bar{\sigma} = (\bar{3}, 1, \bar{2})$ is associated to: $\int_{\Delta_3^t} B(t_3)A(t_1)B(t_2)$. For an arbitrary $\bar{\gamma} = \sum_n \sum_{\bar{\sigma} \in B_n} a_{\bar{\sigma}} \cdot \bar{\sigma} \in \mathbf{B}$, we write $< \bar{\gamma} >$ for $\sum_n \sum_{\bar{\sigma} \in B_n} a_{\bar{\sigma}} \cdot < \bar{\sigma} >$.

Proposition 3.2. *The product of two iterated integrals $< \bar{\sigma} > \times < \bar{\beta} >$ is given by:*

$$< \bar{\sigma} > \times < \bar{\beta} > = < \bar{\sigma} * \bar{\beta} >$$

This formula is a noncommutative variant of the classical Chen formulas for the product of iterated integrals of differential forms [7]. It includes as a particular case the formula for the product of two iterated integrals depending on a single time-dependent Hamiltonian given in the first section of the article. We detail the proof for the sake of completeness, and since the formula is crucial for our purposes.

For a permutation $\bar{\sigma}$ we denote by σ the same permutation without bars (e.g. if $\bar{\sigma} = (\bar{2}, 3, \bar{1})$, then $\sigma = (2, 3, 1)$) and we define $X(t_{\sigma(i)}) = A(t_{\sigma(i)})$ if $\bar{\sigma}(i)$ has no bar and $X(t_{\sigma(i)}) = B(t_{\sigma(i)})$ if $\bar{\sigma}(i)$ has a bar. Therefore,

$$< \bar{\sigma} > \times < \bar{\beta} > \;=\; \int_0^t dt_1 \ldots \int_0^{t_{n-1}} dt_n X(t_{\sigma(1)}) \ldots X(t_{\sigma(n)}) \int_0^t dt_{n+1} \ldots \int_0^{t_{n+m-1}} dt_{n+m} X(t_{n+\beta(1)}) \ldots X(t_{n+\beta(m)}).$$

By Fubini's theorem, this can be rewritten as the integral of $X(t_{\sigma(1)}) \ldots X(t_{n+\beta(m)})$ over the domain $\Delta_n^t \times \Delta_m^t$. The idea is now to rewrite this domain as a sum of $\binom{n+m}{n}$ domains isomorphic to Δ_{n+m}^t. For instance, the product of the domain $0 \leq t_n \leq \cdots \leq t_1 \leq t$ with the domain $0 \leq t_{n+1} \leq t$ is the sum of the $n+1$ domains obtained by inserting t_{n+1} between 0 and t_1, then between t_1 and t_2, up to between t_n and t. More generally the product of Δ_n^t by Δ_m^t is the sum of all the domains obtained by "mixing" the two conditions $0 \leq t_n \leq \cdots \leq t_1 \leq t$ and $0 \leq t_{n+m} \leq \cdots \leq t_{n+1} \leq t$, i.e. by ordering the $n+m$ variables t_i so that these conditions are satisfied. If $\rho(i)$ is the position of variable t_i in one of these orderings (where the variables are ordered from the largest to the smallest), the conditions imply that $\rho(1) < \cdots < \rho(n)$ and $\rho(n+1) < \cdots < \rho(n+m)$. For example, if $0 \leq t_2 \leq t_1 \leq t$ and $0 \leq t_4 \leq t_3 \leq t$, for the domain $0 \leq t_4 \leq t_2 \leq t_1 \leq t_3 \leq t$, t_3 is in the first place (i.e. largest), t_1 in the second, t_2 in the third and t_4 in the fourth (smallest), and the permutation is $\rho = (2, 3, 1, 4)$. In general, we get:

$$\Delta_n^t \times \Delta_m^t = \bigcup_\tau \{(t_{\tau(1)}, ..., t_{\tau(n+m)}) | 0 \leq t_{n+m} \leq ... \leq t_1 \leq t\},$$

where τ runs over the permutations in S_{n+m} such that $\tau(1) < \cdots < \tau(n)$ and $\tau(n+1) < \cdots < \tau(n+m)$. Equivalently, τ runs over the permutations such that: $st(\tau(1), \ldots, \tau(n)) = (1, \ldots, n)$ and $st(\tau(n+1), \ldots, \tau(n+m)) = (1, \ldots, m)$. Now,

$$\int_{\{(x_1 = t_{\tau(1)}, \ldots, x_{n+m} = t_{\tau(n+m)}) | 0 \leq t_{n+m} \leq \ldots \leq t_1 \leq t\}} X(x_{\sigma(1)}) ... X(x_{\sigma(n)}) X(x_{n+\beta(1)}) \ldots X(x_{n+\beta(m)})$$

$$= \int_{\{0 \leq t_{n+m} \leq \ldots \leq t_1 \leq t\}} X(t_{\tau(\sigma(1))}) ... X(t_{\tau(\sigma(n))}) X(t_{\tau(n+\beta(1))}) ... X(t_{\tau(n+\beta(m))})$$

so that finally, taking into account the bars of the permutations (that is the fact that X is A or B, depending only on its position in the sequence $X(t_{\tau(\sigma(1))}) ... X(t_{\tau(\sigma(n))}) X(t_{\tau(n+\beta(1))}) ... X(t_{\tau(n+\beta(m))})$), we obtain $< \bar{\sigma} > \times < \bar{\beta} > = \sum_{\bar{\gamma}} < \bar{\gamma} >$, with $st(\bar{\gamma}(1) \ldots \bar{\gamma}(n)) = (\bar{\sigma}(1), \ldots, \bar{\sigma}(n))$ and $st(\bar{\gamma}(n+1) \ldots \bar{\gamma}(n+m)) = (\bar{\beta}(1), \ldots, \bar{\beta}(n))$. This concludes the proof.

Remark 3.3. *The same proof leads to a general noncommutative Chen formula. Let $A_1, \ldots, A_n$ and $B_1, \ldots, B_m$ be noncommutative (e.g. matrix-valued) functions and let*

$$\begin{aligned} A_\alpha &= \int_0^t dt_1 \ldots \int_0^{t_{n-1}} dt_n A_1(t_{\alpha(1)}) \ldots A_n(t_{\alpha(n)}), \\ B_\beta &= \int_0^t dt_1 \ldots \int_0^{t_{m-1}} dt_m B_1(t_{\beta(1)}) \ldots B_m(t_{\beta(m)}), \\ (AB)_\sigma &= \int_0^t dt_1 \ldots \int_0^{t_{n+m-1}} dt_{n+m} A_1(t_{\sigma(1)}) \ldots A_n(t_{\sigma(n)}) B_1(t_{\sigma(n+1)}) \ldots B_m(t_{\sigma(n+m)}), \end{aligned}$$

then $A_\alpha \times B_\beta = (AB)_{\alpha * \beta}$.

Proposition 3.4. *The convolution product provides* **B** *with the structure of an associative (but noncommutative) algebra with a unit.*

The Proposition can be checked directly from the combinatorial definition of the convolution product, we refer to the original proofs [1, 19]. In our setting, it also follows from the associativity of the product of iterated integrals. Notice that the general noncommutative Chen formula would relate similarly to the algebraic structures on colored permutations and wreath product group algebras introduced in [19].

4 Progressions and regressions

Modern noncommutative representation theory originates largely in the work of Solomon [29]. From this point of view, it is natural to partition hyperoctahedral groups into "descent classes", similarly to the partition of symmetric groups into descent classes (such a partition is often referred to as a statistics on S_n).

Recall that a permutation $\sigma \in S_n$ has a descent in position $i < n$ if and only if $\sigma(i) > \sigma(i+1)$. The descent set $Desc(\sigma)$ of σ is the set of all $i < n$ such that σ has a descent in position i. The partition into descent classes read: $S_n = \bigcup_{I \subset [n-1]} \{\sigma, Desc(\sigma) = I\}$. The *descent algebra* $\mathcal{D}$ is the linear span of Solomon's elements $D_S^n := \sum_{\sigma \in S_n, Desc(\sigma) \subseteq S} \sigma$, where $S \subseteq [n-1]$ and $n \in \mathbb{N}^*$ (with the convention $D_\emptyset^0 = 1$). It is provided with a free associative algebra structure by the convolution product $*$ on $\mathbf{S} \supset \mathcal{D}$, see [25, Chap.9]. This algebra has various natural generating families as a free associative algebra -for instance, the family of the $D_\emptyset^n$. It is therefore also isomorphic to the algebra of noncommutative symmetric functions **Sym**, from which it follows that the structure theorems for these functions can be carried back to the descent algebra -a point of view introduced and developed in [9] and a subsequent series of articles starting with [12].

The corresponding descent statistics on B_n is obtained by considering the total order $\bar{n} < \overline{n-1} < ... < \bar{1} < 1 < ... < n$. A signed permutation $\bar{\sigma} \in B_n$ has a descent in position $i < n$ if and only if $\bar{\sigma}(i) > \bar{\sigma}(i+1)$ [14, Def. 3.2]. Descent classes are defined accordingly. The problem with this noncommutative representation theoretical statistics and with the corresponding algebraic structures is that they do not fit the needs of iterated integral computations for effective Hamiltonians, as we shall see in the forthcoming sections. Neither do the generalized descent algebras of [19, Sect 5]. Notice that this is not the case when symmetric groups are considered: the statistics of descent classes fits the needs of noncommutative representation theory *as well as* the needs of Lie theoretical computations, as emphasized in [25, 9].

For this reason, we introduce another statistics on B_n. It seems to be new, and has surprisingly nice properties, in that it allows to generalize very naturally many algebraic properties of symmetric groups descent classes.

We say that an element $\bar{\alpha} = (\alpha(1), ..., \alpha(n)) \in B_n$ has a progression in position i if either:

1. $|\alpha(i)| < |\alpha(i+1)|$ and $\alpha(i+1) \in \mathbf{N}^*$
2. $|\alpha(i)| > |\alpha(i+1)|$ and $\alpha(i+1) \in \bar{\mathbf{N}}^*$

Else, we say that α has a regression in position i. Here, the operation $|\ |$ is the operation of forgetting the bars, so that e.g. $|\bar{6}| = 6$. The terminology is motivated by the quantum physical idea that particles (associated to unmarked integers) propagate forward in time, whereas holes (associated to marked integers in our framework) propagate backward. We refer the reader to Goldstone diagrams expansions [11] of the Gell-Mann Low eigenstate $|\Psi_{GL}>$ for further insights into the physical motivations. Further details on these topics are contained in the following sections of this article, but we do not develop here fully the physical implications of our approach, the focus being on their mathematical background.

We write $Reg(\alpha)$ for the set of regressions of α. For example: $Reg(4, \bar{3}, \bar{5}, 6, \bar{2}, 1) = \{2, 5\}$ since the sequence $(4, \bar{3}, \bar{5}, 6, \bar{2}, 1)$ has only two regressions, in positions 2 and 5. For an arbitrary subset S of $[n-1]$, we mimic now the descent statistics and write $R_S^n := \sum_{\sigma \in B_n, Reg(\sigma) = S} \sigma$. It is also convenient to introduce the elements $T_S^n := \sum_{\sigma \in B_n, Reg(\sigma) \subseteq S} \sigma = \sum_{U \subseteq S} R_U^n$.

Lemma 4.1. *The elements R_S^n (resp. T_S^n), $S \subseteq [n-1]$, form a family of linearly independent elements in the group algebra $\mathbb{Q}[B_n]$.*

The first assertion follows from the very definition of the R_S^n, since it is easily checked that $\{\bar{\sigma} \in B_n, Reg(\bar{\sigma}) = S\} \neq \emptyset$ for any $S \subseteq [n-1]$. The second case follows from the Möbius inversion formula:

$$R_S^n = \sum_{U \subseteq S} (-1)^{|S|-|U|} T_S^n,$$

where $|S|$ stands for the number of elements in S.

Lemma 4.2. *We have, for $S \subseteq [n-1],\ U \subseteq [m-1]$:*

$$T_S^n * T_U^m = T_{S \cup \{n\} \cup (U+n)},$$

where $U + n = \{u + n, u \in U\}$.

Indeed, by definition, for $\bar{\sigma} \in B_n,\ \bar{\beta} \in B_m$, with $Reg(\bar{\sigma}) = X \subseteq S,\ Reg(\bar{\beta}) = Y \subseteq U$, $\bar{\sigma} * \bar{\beta} = \sum_{\bar{\tau}} \bar{\tau}$, where $\bar{\tau}$ runs over the elements of B_{n+m} with $st(\bar{\tau}(1), ..., \bar{\tau}(n)) = \bar{\sigma}$ and $st(\bar{\tau}(n+1), ..., \bar{\tau}(n+m)) = \bar{\beta}$. In particular, for any such $\bar{\tau}$ and by definition of the standardization process:

$$Reg(\bar{\tau}) \subseteq X \cup \{n\} \cup (Y + n).$$

Conversely, any $\bar{\tau} \in B_{n+m}$ appears in the expansion of $st(\bar{\tau}(1), ..., \bar{\tau}(n)) * st(\bar{\tau}(n+1), ..., \bar{\tau}(n+m))$ by the very definition of $*$ and does not appear in the expansion of any other product $\bar{\sigma} * \bar{\beta}$ with $Reg(\bar{\sigma}) = Reg(st(\bar{\tau}(1), ..., \bar{\tau}(n)))$, $Reg(\bar{\beta}) = Reg(st(\bar{\tau}(n+1), ..., \bar{\tau}(n+m))$, from which the lemma follows.

Corollary 4.3. *For S, U as above, with the notation of the previous sections:*

$$< T_S^n > \times < T_U^m > = < T_{S \cup \{n\} \cup (U+n)}^{n+m} >$$

so that:

$$< T_\emptyset^{n_1} > \times ... \times < T_\emptyset^{n_k} > = < T_{\{n_1, ..., n_1 + ... + n_{k-1}\}}^{n_1 + ... + n_k} > .$$

Theorem 4.1. *The linear span $\mathcal{R}$ of the elements T_S^n (equivalently, of the R_S^n), $n \in \mathbb{N},\ S \subseteq [n-1]$, is closed under the convolution product in* **B**. *This algebra, referred to from now on as the (hyperoctahedral) Regression algebra, is isomorphic to the descent algebra $\mathcal{D}$ and to the algebra of noncommutative symmetric functions* **Sym**.

The second part of the Theorem follows from the product rule in $\mathcal{D}$, that reads:

$$D_S^n * D_U^m = D_{S \cup \{n\} \cup (U+n)}^{n+m}.$$

The proof for this last identity can be obtained similarly to the one in Lemma 4.2 -see also [25].

Now we study in more detail the elements $R_\emptyset^n$ that will play an important role in the following. The lowest order $R_\emptyset^n$ are

$$\begin{aligned}
R_\emptyset^1 &= (1) + (\bar{1}), \\
R_\emptyset^2 &= (1,2) + (\bar{1},2) + (2,\bar{1}) + (\bar{2},\bar{1}), \\
R_\emptyset^3 &= (1,2,3) + (\bar{1},2,3) + (1,3,\bar{2}) + (\bar{1},3,\bar{2}) + (2,\bar{1},3) + (\bar{2},\bar{1},3) + (2,3,\bar{1}) + (\bar{2},3,\bar{1}) \\
&\quad + (3,\bar{1},2) + (\bar{3},\bar{1},2) + (3,\bar{2},\bar{1}) + (\bar{3},\bar{2},\bar{1}).
\end{aligned}$$

We first observe that, if $\bar{\sigma} \in B_n$ is a term of $R_\emptyset^n$ (and therefore has no regression), then the barred integers of $\bar{\sigma}$ are entirely determined by the permutation $\sigma = (|\bar{\sigma}(1)|, \ldots, |\bar{\sigma}(n)|)$, except for $\bar{\sigma}(1)$. Indeed, by definition of a progression, $\bar{\sigma}(i+1) \in \mathbf{N}^*$ if $\sigma(i) < \sigma(i+1)$ and $\bar{\sigma}(i+1) \in \bar{\mathbf{N}}^*$ if $\sigma(i) > \sigma(i+1)$. In other words, $\bar{\sigma}(i+1) \in \bar{\mathbf{N}}^*$ iff σ has a descent at i. The integer $\bar{\sigma}(1)$ is not determined by σ and can be barred or not. Therefore, the number of terms of $R_\emptyset^n$ is $2 \cdot n!$.

5 A Picard-type hyperoctahedral expansion

When it comes to expand Ψ_{GL} or U_{GL}, as introduced in Section 2, the classical strategy introduced by Goldstone (at least for nondegenerate states, that is for Ψ_{GL} [11]) consists in appealing to the hole/particle duality of quantum physics. Goldstone's theory was generalized to degenerate states by Michels and Suttorp [15], but this part of the theory has remained largely in infancy and relies on shaky mathematical grounds. The purpose of this section is to show that hyperoctahedral groups provide a convenient way to derive and study such expansions, so as to build the foundations of a group-theoretic approach to the perturbative computation of the ground states of physical systems, with a particular view toward the degenerate case.

To sum up, we want to compute $U_{GL}(\epsilon) = U_\epsilon(0)P(PU_\epsilon(0)P)^{-1}$. Let us write H_i for $-iH_{\mathrm{I}\epsilon}$ and $A(t) := (1-P)H_i(t)$, $B(t) := -PH_i(t)$ (notice the -1 sign in the definition of B). From the Picard expansion, we have:

$$U_\epsilon(0) = 1 + \int_{-\infty}^{0} H_i(x)dx + \int_{-\infty}^{0}\int_{-\infty}^{t_1} H_i(t_1)H_i(t_2)dt_1dt_2 + ... + \int_{\Delta_n^{[-\infty,0]}} H_i(t_1)...H_i(t_n) + ...$$

In this section (following a suggestion by the referee whose remarks helped us to simplify notably the presentation of the following computations -we take the opportunity to thank him or her warmly), we introduce a new encoding of iterated integrals involving A, B and H_i.

The notation is best explained through an example:

$$\int_{-\infty}^{0}\int_{-\infty}^{t_1}\int_{-\infty}^{t_2}\int_{-\infty}^{t_3}\int_{-\infty}^{t_4} A(t_3)H_i(t_1)B(t_2)B(t_5)H_i(t_4)dt_1dt_2dt_3dt_4dt_5 =: [\hat{2},\bar{3},1,\hat{5},\bar{4}].$$

Concretely, in an arbitrary iterated integral involving A, B and H_i, we look recursively at the positions $i_1, ..., i_n$ of t_1,...,t_n in the integrand and decorate i_j with a bar (resp. a hat, resp. no decoration) if the corresponding operator is B (resp. H_i, resp. A). In our example, t_1 (resp. t_2...) is in position 2 (resp. 3...) in the product $A(t_3)H_i(t_1)B(t_2)B(t_5)H_i(t_4)$ and appears as a parameter for H_i (resp. B), so that we map 1 to $\hat{2}$, 2 to $\bar{3}$, and so on. The so-obtained sequence of decorated integers is written inside brackets to avoid confusion with our previous notation. Notice that, if $\bar{\sigma} \in B_n$, $< \bar{\sigma} >= [\bar{\sigma}^{-1}(1), ..., \bar{\sigma}^{-1}(n)]$ (where we use the definition of Section 3 for $< \bar{\sigma} >$). We will also use some self-explaining multilinear extensions of this notation, so that, for example: $[3, (\bar{1}, \hat{2}) + (2, \hat{1})] = [3, \bar{1}, \hat{2}] + [3, 2, \hat{1}]$, and so on. Notice in particular that the identity $H_i = A - B$ translates formally into $\hat{k} = k - \bar{k}$ so that, for example, $[\hat{1}, \bar{2}] = [1, \bar{2}] - [\bar{1}, \bar{2}]$.

Theorem 5.1. *The effective adiabatic evolution operator U_{GL} has the hyperoctahedral Picard-type expansion:*

$$U_{GL} = \lim_{\epsilon \to 0} P + (1-P)(\sum_{n \in \mathbf{N}^*} < R_\emptyset^n >)P$$

Indeed, let us expand $[\hat{1}, ..., \hat{n}] = \int_{\Delta_n^{[-\infty,0]}} H_i(t_1)...H_i(t_n)$ with the A and B operators. In order to do so, we introduce still another notation: for $\bar{\sigma} \in B_k$, $k < n$, we set:

$$< \bar{\sigma}; n-k >= \int_{\Delta_k^{[-\infty,0]} \times \Delta_{n-k}^{[-\infty, t_{\sigma(k)}]}} X(t_{\sigma(1)})...X(t_{\sigma(k)})H_i(t_{k+1})...H_i(t_n)$$

where $\Delta_k^{[-\infty,0]} \times \Delta_{n-k}^{[-\infty,t_{\sigma(k)}]}$ is a shortcut for:

$$\{(t_1, ..., t_n) | -\infty \leq t_k \leq ... \leq t_1 \leq 0,\ -\infty \leq t_n \leq ... \leq t_{k+1} \leq t_{\sigma(k)}\};$$

where σ stands, as usual, for the image of $\bar{\sigma}$ in S_k (obtained by forgetting the decorations), and where $X(t_{\sigma(i)}) = A(t_{\sigma(i)})$ if $\sigma(i) = \bar{\sigma}(i)$ and $B(t_{\sigma(i)})$ else. For example,

$$< (2\bar{1}3); 2 >= \int_{\Delta_3^{[-\infty,0]} \times \Delta_2^{[-\infty,t_3]}} A(t_2)B(t_1)A(t_3)H_i(t_4)H_i(t_5),$$

$$< (2\bar{3}1); 2 >= \int\limits_{-\infty \le t_3 \le t_2 \le t_1 \le 0,\ -\infty \le t_5 \le t_4 \le t_1} A(t_2)B(t_3)A(t_1)H_i(t_4)H_i(t_5).$$

The more general symbols $< X; n-k >$ are defined, as usual, by extending linearly these conventions to arbitrary elements $X \in \mathbb{Q}[B_k]$, $k < n$.

Lemma 5.1. *The symbol $< \bar{\sigma}; n-k >$ can be expanded as:*

$$< \bar{\sigma}; n-k >= [\bar{\sigma}^{-1}(1), ..., \bar{\sigma}^{-1}(i), (\bar{\sigma}^{-1}(i+1), ..., \bar{\sigma}^{-1}(k))\sqcup\!\sqcup(\widehat{k+1}, ..., \hat{n})],$$

where $\bar{\sigma} \in B_k$ and $i := \sigma(k)$.

Indeed:

$$\{(t_1, ..., t_n)| -\infty \le t_k \le ... \le t_1 \le 0,\ -\infty \le t_n \le ... \le t_{k+1} \le t_{\sigma(k)}\} =$$
$$\{(t_1, ..., t_n)| -\infty \le t_k \le ... \le t_{\sigma(k)},\ -\infty \le t_n \le ... \le t_{k+1} \le t_{\sigma(k)}, t_{\sigma(k)} \le ... \le t_1 \le 0\}$$
$$= \{(t_1, t_2, ..., t_n)| -\infty \le t_{\sigma(k)} \le ... \le t_1 \le 0, (t_{\sigma(k)+1}, ..., t_n) \in$$
$$\{(u_1, ..., u_{k-\sigma(k)})| -\infty \le u_{\sigma(k)} \le ... \le u_1 \le t_{\sigma(k)}\} \times \{(v_1, ..., v_{n-k})| -\infty \le v_{n-k} \le ... \le v_1 \le t_{\sigma(k)}\}\},$$

where $\times$ stands for the cartesian product. Since the Cartesian product of simplices is reflected in the shuffle product (see e.g. the proof of Prop. 3.2), the Lemma follows.

We then have:

$$\begin{aligned}
[\hat{1}, ...\hat{n}] &= [1, \hat{2}, ...\hat{n}] - [\bar{1}, \hat{2}, ..., \hat{n}] = -[\bar{1}, \hat{2}, ..., \hat{n}] + [1, 2, \hat{3}, ...\hat{n}] - [1, \bar{2}, \hat{3}, ..., \hat{n}] \\
&= P[\hat{1}, ...\hat{n}] + [1, 2, \hat{3}, ...\hat{n}] - [1, \bar{2}, \hat{3}, ..., \hat{n}] \\
&= P[\hat{1}, ...\hat{n}] + [1, 2, \hat{3}, ...\hat{n}] - [1, \bar{2}, \hat{3}, ..., \hat{n}] + (-[\bar{2}, (1)\sqcup\!\sqcup(\hat{3}, ..., \hat{n})] + [\bar{2}, (1)\sqcup\!\sqcup(\hat{3}, ..., \hat{n})]).
\end{aligned}$$

Now, from the recursive definition of the shuffle product:

$$[1, \bar{2}, \hat{3}, ..., \hat{n}] + [\bar{2}, (1)\sqcup\!\sqcup(\hat{3}, ..., \hat{n})] = [(1)\sqcup\!\sqcup(\bar{2}, \hat{3}, ..., \hat{n})]$$

$$= [\int\limits_{-\infty}^{0} A(t)dt] \int\limits_{\Delta_{n-1}^{[-\infty,0]}} B(t_1)H_i(t_2)...H_i(t_{n-1})$$

$$= -(1-P) < R_\emptyset^1 > P[\hat{1}, ..., \widehat{n-1}].$$

Here, we have used that P is a projection, so that $(1-P)B(t) = -(1-P)PH_i(t) = 0$, to rewrite

$$[\int\limits_{-\infty}^{0} A(t)dt] = (1-P)[\int\limits_{-\infty}^{0} (A(t)+B(t))dt] = (1-P) < R_\emptyset^1 > .$$

We get finally, since $< (1,2); n-2 >= [1, 2, \hat{3}, ..., \hat{n}]$ and (according to the Lemma 5.1) $< (2, \bar{1}); n-2 >= [\bar{2}, (1)\sqcup\!\sqcup(\hat{3}, ..., \hat{n})]$:

$$[\hat{1}, ..., \hat{n}] = P[\hat{1}, ..., \hat{n}] + (1-P) < R_\emptyset^1 > P[\hat{1}, ..., \widehat{n-1}] + (1-P) < R_\emptyset^2; n-2 >,$$

where the last identity follows, once again, from $(1-P)B(t) = 0$ (we won't comment any more on this rewriting trick from now on).

The proof of the Theorem can be obtained along these principles by recursion. Let us indeed assume for a while that:

$$< R_\emptyset^k; n-k >=< R_\emptyset^k > P[\hat{1}, ..., \widehat{n-k}] + < R_\emptyset^{k+1}; n-k-1 > .$$

Then we get, by induction:

$$[\hat{1}, ..., \hat{n}] = P[\hat{1}, ..., \hat{n}] + (1-P) < R_\emptyset^1 > P[\hat{1}, ..., \widehat{n-1}] +$$

$$(1-P) < R_\emptyset^2 > P[\hat{1},...,\widehat{n-2}] + ... + (1-P) < R_\emptyset^{n-1} > P[\hat{1}] + (1-P) < R_\emptyset^n > .$$

Since $U_\epsilon(0) = \sum_n [\hat{1},...,\hat{n}]$, this implies

$$U_\epsilon(0) \quad = \quad PU_\epsilon(0) + (1-P)\sum_{n=1}^{\infty} < R_\emptyset^n > (P(U_\epsilon(0)-1)+1),$$

or, since $P^2 = P$:

$$U_\epsilon(0)P \quad = \quad \Big(P + (1-P)\sum_{n=1}^{\infty} < R_\emptyset^n > P\Big)PU_\epsilon(0)P,$$

and the Theorem follows.

So, let us check that the formula for $< R_\emptyset^k; n-k >$ holds. Let us consider an arbitrary element $\bar{\sigma} \in B_k$ with $Reg(\bar{\sigma}) = \emptyset$. Then, with the notation of Lemma 5.1:

$$< \bar{\sigma}; n-k >= [\bar{\sigma}^{-1}(1),...,\bar{\sigma}^{-1}(i),(\bar{\sigma}^{-1}(i+1),...,\bar{\sigma}^{-1}(k)) \sqcup\!\sqcup (k+1,\widehat{k+2},...,\hat{n})]$$

$$-[\bar{\sigma}^{-1}(1),...,\bar{\sigma}^{-1}(i),(\bar{\sigma}^{-1}(i+1),...,\bar{\sigma}^{-1}(k)) \sqcup\!\sqcup (\overline{k+1},\widehat{k+2},...,\hat{n})]$$

Let us denote the first term by T_1 and the second by T_2, so that $< \bar{\sigma}; n-k >= T_1 - T_2$. To calculate T_1, let us use another (equivalent, the equivalence follows from the recursive definition of the shuffle product and is left to the reader) recursive definition of the shuffle product, namely:

$$a_1a_2...a_k \sqcup\!\sqcup bb_2...b_l = \sum_{i=0}^{k} a_1...a_i b(a_{i+1}...a_k \sqcup\!\sqcup b_2...b_l).$$

We get:

$$T_1 = \sum_{j=i}^{k} [\bar{\sigma}^{-1}(1),...,\bar{\sigma}^{-1}(j),k+1,(\bar{\sigma}^{-1}(j+1),...,\bar{\sigma}^{-1}(k)) \sqcup\!\sqcup (\widehat{k+2},...,\hat{n})]$$

$$= \sum_{j=i}^{k} < \bar{\beta}_j; n-k-1 >$$

where $\bar{\beta}_j := (\bar{\sigma}^{-1}(1),...,\bar{\sigma}^{-1}(j),k+1,\bar{\sigma}^{-1}(j+1),...,\bar{\sigma}^{-1}(k))^{-1}$. We notice then that, for $l < k$,

$$\beta_j(l) < \beta_j(l+1) \Longleftrightarrow \sigma(l) < \sigma(l+1).$$

In particular, $\bar{\beta}_j$ has no regression in position less than k. Now, $\beta_j(k+1) = \bar{\beta}_j(k+1) = j \geq \beta_j(k) = i$, which implies that $\bar{\beta}_j$ has no regression in position k. Finally, $\bar{\beta}_j$ has no regression.

Let us enumerate the number of (necessarily distinct) signed permutations $\bar{\beta}_j$ obtained in that way. There are $2(k-1)!$ elements $\bar{\sigma}$ of $R_\emptyset^k$ with a given value j of $\sigma(k)$, where j runs from 1 to k. For a given $\bar{\sigma}$ with $\sigma(k) = j$, T_1 provides $k-j+1$ elements of $R_\emptyset^{k+1}$. Thus, the expansion of T_1 provides $(k+1)!$ different elements of $R_\emptyset^{k+1}$ when $\bar{\sigma}$ runs over $R_\emptyset^k$.

The term T_2 can be computed similarly. Using the same recursive formula for the shuffle product as above, we get:

$$T_2 = \sum_{j=i}^{k} [\bar{\sigma}^{-1}(1),...,\bar{\sigma}^{-1}(j),\overline{k+1},(\bar{\sigma}^{-1}(j+1),...,\bar{\sigma}^{-1}(k)) \sqcup\!\sqcup (\widehat{k+2},...,\hat{n})]$$

$$= [(\bar{\sigma}^{-1}(1),...,\bar{\sigma}^{-1}(k)) \sqcup\!\sqcup (\overline{k+1},...,\bar{n})]$$

$$- \sum_{j<i} [(\bar{\sigma}^{-1}(1),...,\bar{\sigma}^{-1}(j),\overline{k+1},(\bar{\sigma}^{-1}(j+1),...,\bar{\sigma}^{-1}(k)) \sqcup\!\sqcup (\widehat{k+2},...,\hat{n})]$$

In the first term in this expansion of T_2, we recognize $- < \bar{\sigma} > P[\hat{1}, ..., \widehat{n-k}]$, so that these terms sum up to $- < R_\emptyset^k > P[\hat{1}, ..., \widehat{n-k}]$ when $\bar{\sigma}$ runs over elements in B_k without regressions. In the second term (the sum over $j < i$), the same reasoning as for T_1 shows that each term of the expansion is of the form $< \bar{\beta}_j; n-k-1 >$, where $\bar{\beta}_j$ has no regression. Again, when $\bar{\sigma}$ runs over elements in B_k without regressions, this provides $(k+1)!$ such elements in the expansion. These terms are pairwise distinct and pairwise distinct from the elements showing up in the expansion of T_1, from which we conclude:

$$T_1 - T_2 =< R_\emptyset^k > P[\hat{1}, ..., \widehat{n-k}] + < R_\emptyset^{k+1}; n-k+1 > .$$

The Theorem follows.

6 A Magnus expansion for the evolution operator

In the classical case, that is when the solution $X(t)$ of a first order linear differential equation is obtained from its Picard series expansion, the resulting approximating series converges relatively slowly to the solution. This problem –let us call it the Magnus problem– is solved by reorganizing the series expansion, often by looking for an exponential expansion $X(t) = \exp \Omega(t)$ of the solution, known as its Magnus expansion. Many numerical techniques have been developed along this idea that go much beyond the formal-algebraic problem of deriving a formal expression for $\Omega(t)$. However, deriving such an expression is a decisive step towards the understanding of the behavior of $\Omega(t)$. This problem was solved, in the classical case, by Bialynicki-Birula, Mielnik and Plebański [3, 16] who obtained a formula for $\Omega(t)$ in terms of Solomon's elements D_S^n.

The purpose of the present section is to solve the Magnus problem for the analysis of solutions in time-dependent perturbation theory. This provides the general term of time-dependent coupled-cluster theory [26]. Our previous results pave the way toward the solution of the problem. Namely, as it appears from Thm 5.1, the natural object to look at is not so much the effective Hamiltonian

$$\mathcal{H} = \lim_{\epsilon \to 0} P_0 H U_{GL}(\epsilon)$$

or the effective adiabatic evolution operator U_{GL}, than the Picard-type series

$$Pic := \sum_{n \in \mathbb{N}} < R_\emptyset^n > .$$

Notice that we define Pic as the sum of the $< R_\emptyset^n >$ over all the integers (and not over $\mathbb{N}^*$) in order to have the identity operator $1 = H_{R_\emptyset^0}$ as the first term of the series. Of course, we have:

$$U_{GL}(\epsilon) = P + (1-P)(\sum_{n \in \mathbb{N}^*} < R_\emptyset^n >)P = P + (1-P)(\sum_{n \in \mathbb{N}} < R_\emptyset^n >)P = P + (1-P)\ Pic\ P$$

In other terms, we are interested in the expansion:

$$U_{GL}(\epsilon) = P + (1-P)\exp(\Omega_\epsilon)P,$$

where

$$\Omega_\epsilon = \log(\sum_{n \in \mathbb{N}} < R_\emptyset^n >) =< \log(\sum_{n \in \mathbb{N}} R_\emptyset^n) > .$$

Since $R_\emptyset^{n_1} * ... * R_\emptyset^{n_k} = R^{n_1+...+n_k}_{\{n_1, ..., n_1+...+n_{k-1}\}}$, a first expression of $\Omega_R = \log \sum_{n \in \mathbb{N}} R_\emptyset^n$ follows:

$$\Omega_R = \sum_{n \in \mathbb{N}^*} \sum_{S \subseteq [n-1]} \frac{(-1)^{|S|}}{|S|+1} R_S^n,$$

where one can recognize the hyperoctahedral analogue of Solomon's Eulerian idempotent [25, Chap.3, Lem.3.14]:

$$sol_n = \sum_{S \subseteq [n-1]} \frac{(-1)^{|S|}}{|S|+1} D_S^n.$$

The analogy is not merely formal and follows from the isomorphism of Thm 4.1 together with the existence of a logarithmic expansion of sol_n, which is actually best understood from an Hopf algebraic point of view, see [20, 25, 21, 22]:

$$\sum_{n\in\mathbb{N}^*} sol^n = \log(\sum_{n\in\mathbb{N}} D^n_\emptyset).$$

As a corollary of Thm 4.1, we also get the expansion of Ω_R in the canonical basis of $\bigoplus_{n\in\mathbb{N}^*} \mathbb{Q}[B_n]$:

Proposition 6.1. *We have:*

$$\Omega_R = \sum_{n\in\mathbb{N}^*} \sum_{S\subseteq[n-1]} \frac{(-1)^{|S|}}{n} \binom{n-1}{|S|}^{-1} T^n_S$$

$$= \sum_{n\in\mathbb{N}^*} \sum_{S\subseteq[n-1]} \sum_{\bar\sigma\in B_n, Reg(\sigma)=S} \frac{(-1)^{|S|}}{n} \binom{n-1}{|S|}^{-1} \bar\sigma$$

The Proposition follows from the analogous expansion for sol_n [25], together with the algebra isomorphism Thm 4.1:

$$sol_n = \sum_{n\in\mathbb{N}^*} \sum_{S\subseteq[n-1]} \sum_{\sigma\in S_n, Desc(\sigma)=S} \frac{(-1)^{|S|}}{n} \binom{n-1}{|S|}^{-1} \sigma.$$

Corollary 6.2. *The hyperoctahedral Magnus expansion of the effective Hamiltonian $\mathcal{H}$ reads, when truncated at the third order:*

$$\mathcal{H} = \lim_{\epsilon\to 0} PH_I(P+(1-P)\exp(H_{(1)}+H_{(\bar1)}+\frac{1}{2}[H_{(12)}+H_{(\bar12)}+H_{(2\bar1)}+H_{(\bar2\bar1)}-H_{(1\bar2)}-H_{(\bar1\bar2)}-H_{(21)}-H_{(\bar21)}]+$$

$$\frac{1}{3}[H_{(123)}+H_{(\bar123)}+H_{(13\bar2)}+H_{(\bar13\bar2)}+H_{(2\bar13)}+H_{(\bar2\bar13)}+H_{(23\bar1)}+H_{(\bar23\bar1)}+H_{(3\bar2\bar1)}+H_{(\bar3\bar2\bar1)}+H_{(3\bar12)}+H_{(\bar3\bar12)}$$

$$+H_{(321)}+H_{(\bar321)}+H_{(2\bar31)}+H_{(\bar2\bar31)}+H_{(1\bar2\bar3)}+H_{(\bar1\bar2\bar3)}+H_{(1\bar32)}+H_{(\bar1\bar32)}+H_{(21\bar3)}+H_{(\bar21\bar3)}+H_{(31\bar2)}+H_{(\bar31\bar2)}]$$

$$-\frac{1}{6}[H_{(132)}+H_{(\bar132)}+H_{(231)}+H_{(\bar231)}+H_{(213)}+H_{(\bar213)}+H_{(312)}+H_{(\bar312)}+H_{(1\bar32)}+H_{(\bar1\bar32)}+H_{(1\bar23)}+H_{(\bar1\bar23)}+H_{(2\bar13)}$$

$$+H_{(\bar2\bar13)}+H_{(3\bar12)}+H_{(\bar3\bar12)}+H_{(2\bar31)}+H_{(\bar2\bar31)}+H_{(3\bar21)}+H_{(\bar3\bar21)}+H_{(12\bar3)}+H_{(\bar12\bar3)}+H_{(32\bar1)}+H_{(\bar32\bar1)}])P).$$

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