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Hyeroctahedral 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

The algebraic structure of iterated integrals has been encoded by Chen. It is mostly incorporated in the modern theory of free Lie algebras. Here, 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 shuffle 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, but postpone their detailed study.

The third section is devoted to the investigation of the structure of the hyperoctahedral group algebras. Although we are really interested into 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 once again 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 [21] can be lifted to the hyperoctahedral setting. This extends previous work by Mantaci-Reutenauer [11], Aguiar-Mahajan and Bonnafé-Hohlweg [2] on Solomon's algebras of hyperoctahedral groups. However, the statistics we introduce here 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 groups¹. As a

¹Picard 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

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.

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):

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

The solution can be expanded as the Picard series:

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

where $\Delta_n^t := \{0 \leq t_n \leq \dots \leq t_1 \leq t\}$. Solving for $A(t) = \exp(\Omega(t))$ (see [1, 13]), and more generally any computation with $A(t)$, requires the computation of products of iterated integrals of the form:

$$H_\sigma := \int_{\Delta_n^t} H(t_{\sigma(1)})\dots H(t_{\sigma(n)}), \quad \sigma = (\sigma(1), \dots, \sigma(n)) \in S_n,$$

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

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 H_μ for $\sum_n \sum_{\sigma \in S_n} \mu_\sigma \cdot H_\sigma$. This allows, for example, to write $A(t)$ as H_I , where $I := \sum_n (1, \dots, n)$ is the formal sum of the identity elements in the symmetric group algebras. When allowing for a general initial condition $A(x) = 1$, with possibly $x = -\infty$, and/or when we want to emphasize the t -dependency, we will indicate explicitly this dependency. For example, $H_\sigma(-\infty, t)$ means that the integrations take place between $-\infty$ and t , so that $H_1(-\infty, t) = \int_{-\infty}^t H(x)dx$,

and so on. Similarly, we write $\Delta_n^{[a,b]} := \{a \leq t_n \leq \dots \leq t_1 \leq b\}$.

The formula for the product of H_σ with H_β 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):

$$H_\sigma \cdot H_\beta = H_{\sigma*\beta},$$

where $\sigma*\beta$ is the shuffle product² 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 $st(\gamma(1), \dots, \gamma(n)) = (\sigma(1), \dots, \sigma(n))$ and $st(\gamma(n+1), \dots, \gamma(n+m)) = (\beta(1), \dots, \beta(m))$. Here, st stands for the standardization map, the action of which on sequences is obtained by replacing $(i_1, \dots, i_n), i_j \in \mathbb{N}^*$ 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 of i_j in the increasing ordering of i_1, \dots, 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,

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

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:

²This is one possible definition of the shuffle 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. [10]

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

For completeness, recall that connected means simply that $\mathbf{S}_0 = \mathbb{Q}$. From the point of view of the theory of noncommutative symmetric functions, the elements of \mathbf{S} can be understood as free quasymmetric functions [5]. This definition of the shuffle product on \mathbf{S} allows, for example, to express simply the coefficients of the continuous Baker-Campbell-Hausdorff formula (compare with the original solution [13]):

$$\Omega(t) = H_{\log(I)}.$$

Here $\log(I)$ identifies, in \mathbf{S} , with the formal sum of Solomon's Eulerian idempotents [23]. We refer to [16, 21, 17, 18, 6] 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 problem we are ultimately interested in is the eigenvalue problem for a time-independent Hamiltonian $H = H_0 + V$, with V a perturbation term, and where the eigenstates of H_0 are known but not those of H .

Recall first the basic idea of the time-dependent approach for the computation of the ground state of a physical system (the eigenstate of the Hamiltonian with the lowest eigenvalue). We first define a time-dependent Hamiltonian $H(t) = H_0 + e^{-\epsilon|t|}V$. 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 $H(0) = H$. It is hoped that, if ϵ is small enough, then an eigenstate of H_0 is transformed into an eigenstate of H .

To implement this picture, the time-dependent Schrödinger equation $i\partial|\Psi_S(t)\rangle/\partial t = H(t)|\Psi_S(t)\rangle$ should be solved. However, looking for a solution $|\Psi_S(t)\rangle$ is not convenient because, due to H_0 , it tends to oscillate according to $e^{iH_0 t}$ when $t \rightarrow -\infty$. Therefore, one looks instead at $|\Psi(t)\rangle = e^{iH_0 t}|\Psi_S(t)\rangle$ that satisfies $i\partial|\Psi(t)\rangle/\partial t = H_{\text{int}}(t)|\Psi(t)\rangle$, with $H_{\text{int}} = e^{iH_0 t}V e^{-iH_0 t}e^{-\epsilon|t|}$. Now $H_{\text{int}}(-\infty) = 0$, and $|\Psi(-\infty)\rangle$ makes sense. Using H_{int} , we can start 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 .

Now, instead of calculating directly $|\Psi(t)\rangle$ it is convenient to define the unitary operator $U(t)$ as the solution of $i\partial U(t)/\partial t = H_{\text{int}}(t)U(t)$, with the boundary condition $U(-\infty) = 1$. Thus, $|\Psi(t)\rangle = U(t)|\Phi_0\rangle$. Note that $U(t)$ depends on ϵ , as $H_{\text{int}}(t)$. But is $\lim_{\epsilon \rightarrow 0} U(0)|\Phi_0\rangle$ an eigenstate of H ? It would if the limit existed, but it does not. However, Gell-Mann and Low [7] discovered in 1951 that

$$|\Psi_{\text{GL}}\rangle = \lim_{\epsilon \rightarrow 0} \frac{U(0)|\Phi_0\rangle}{\langle \Phi_0|U(0)|\Phi_0\rangle}$$

exists and is an eigenstate of H . A mathematical proof of this fact for reasonable Hamiltonians came much later [15].

The above scheme works 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 [14, 3, 12]. 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 :

$$U_{\text{GL}} := \lim_{\epsilon \rightarrow 0} U_\epsilon, \quad U_\epsilon := U(0)P(PU(0)P)^{-1}$$

This operator shows up e.g. in the time-dependent interaction representation of the effective Hamiltonian $H_{\text{eff}} := \lim_{\epsilon \rightarrow 0} PHU(0)P[PU(0)P]^{-1} = \lim_{\epsilon \rightarrow 0} PHU_\epsilon$ classically used to solve the eigenvalue problem. This is the operator we will be interested in, postponing to further work the analysis of concrete applications to the study of degenerate systems.

The Picard expansion allows to write $U(0)$ and U_ϵ formally in terms of iterated integrals:

$$U(0) = (-iH_{\text{int}})_I, \quad U_\epsilon = (-iH_{\text{int}})_I P [P(-iH_{\text{int}})_I P]^{-1},$$

with initial condition $U(-\infty) = 1$. We will be interested in unraveling the fine algebraic structure of this expression for U_ϵ similarly to the analysis of $U(0)$ in terms of symmetric group actions performed in the first section of the present article.

3 Wreath product shuffle 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 $H_{\text{int}}(t)$ and $PH_{\text{int}}(t)$ or, equivalently, $A(t) := -i(1-P)H_{\text{int}}(t)$ and $B(t) := iPH_{\text{int}}(t)$. Expanding these expressions will lead to the study of iterated integrals involving the two operators $A(t)$ and $B(t)$ such as, say: $\int_{\Delta_3^i} A(t_2)B(t_3)A(t_1)$.

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. 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:

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

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. 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, $st(\bar{2}, 7, \bar{1}, 2) = (\bar{2}, 4, \bar{1}, 3)$. Similarly, the map $\bar{\sigma} \mapsto \bar{\sigma}|_I$ for $\bar{\sigma} \in B_n$ and $I \subset [n] := \{1, \dots, n\}$ is defined by extracting from the sequence $\bar{\sigma}$ the subsequences of elements in I with their upper indices: $(\bar{2}, 4, \bar{1}, 3)|_{\{1,4\}} = (4, \bar{1})$.

Definition 3.1. Let $\bar{\sigma}, \bar{\beta}$ belong to B_n , resp. B_m . Their shuffle 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 $st(\bar{\tau}(1), \dots, \bar{\tau}(n)) = \bar{\sigma}$, $st(\bar{\tau}(n+1), \dots, \bar{\tau}(n+m)) = \bar{\beta}$.

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 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 $H_{\bar{\sigma}}$ 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: $\int_{\Delta_3^i} B(t_3)A(t_1)B(t_2)$). For an

arbitrary $\bar{\gamma} = \sum_n \sum_{\bar{\sigma} \in B_n} a_{\bar{\sigma}} \cdot \bar{\sigma} \in \mathbf{B}$, we write $H_{\bar{\gamma}}$ for $\sum_n \sum_{\bar{\sigma} \in B_n} a_{\bar{\sigma}} \cdot H_{\bar{\sigma}}$.

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

$$H_{\bar{\sigma}} \times H_{\bar{\beta}} = H_{\bar{\sigma} * \bar{\beta}}$$

Proof. As already alluded to, this kind of formula is essentially a (natural, noncommutative) variant of the classical Chen formulas for the product of iterated integrals of differential forms [4]. 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,

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

By Fubini's theorem, this can be rewritten as the integral of $X(t_{\sigma(1)}) \dots X(t_{n+\beta(m)})$ 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 $0 \leq t_n \leq \dots \leq t_1 \leq t$ 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 $0 \leq t_n \leq \dots \leq t_1 \leq t$ and $0 \leq t_{n+m} \leq \dots \leq t_{n+1} \leq t$, 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 $\rho(1) < \dots < \rho(n)$ and $\rho(n+1) < \dots < \rho(n+m)$. 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:

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

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

$$\begin{aligned} & \int_{\{(x_1=t_{\tau(1)}, \dots, x_{n+m}=t_{\tau(n+m)}) | 0 \leq t_{n+m} \leq \dots \leq t_1 \leq t\}} X(x_{\sigma(1)}) \dots X(x_{\sigma(n)}) X(x_{n+\beta(1)}) \dots X(x_{n+\beta(m)}) \\ &= \int_{\{0 \leq t_{n+m} \leq \dots \leq t_1 \leq t\}} X(t_{\tau(\sigma(1))}) \dots X(t_{\tau(\sigma(n))}) X(t_{\tau(n+\beta(1))}) \dots X(t_{\tau(n+\beta(m))}) \end{aligned}$$

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 $X(t_{\tau(\sigma(1))}) \dots X(t_{\tau(\sigma(n))}) X(t_{\tau(n+\beta(1))}) \dots X(t_{\tau(n+\beta(m))})$), we obtain $H_{\bar{\sigma}} \times H_{\bar{\beta}} = \sum_{\bar{\gamma}} H_{\bar{\gamma}}$, with $st(\bar{\gamma}(1) \dots \bar{\gamma}(n)) = (\bar{\sigma}(1), \dots, \bar{\sigma}(n))$ and $st(\bar{\gamma}(n+1) \dots \bar{\gamma}(n+m)) = (\bar{\beta}(1), \dots, \bar{\beta}(n))$. This concludes the proof. \square

Proposition 3.3. *The shuffle product provides \mathbf{B} with the structure of an associative (but noncommutative) algebra with a unit.*

This is a consequence of the associativity of the product of iterated integrals. The Proposition can also be checked directly from the combinatorial definition of the shuffle product.

We refer to the work of Mantaci-Reutenauer [11] and Bonnafé-Hohlweg [2] for further insights into the algebraic structure of the group algebras of hyperoctahedral groups, together with their applications to noncommutative representation theory. From this later point of view that originates in the work of Solomon [24], it is natural to partition hyperoctahedral groups into "descent classes", similarly to the partition of symmetric groups into descent classes (such a partition is also 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: $S_n = \bigcup_{I \subseteq [n-1]} \{\sigma, Desc(\sigma) = I\}$. 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 shuffle product $*$ on $\mathbf{S} \supset \mathcal{D}$, see [21, 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 [6] and a subsequent series of articles starting with [9].

The corresponding descent statistics on B_n is obtained by considering the total order $\bar{n} < \overline{n-1} < \dots < \bar{1} < 1 < \dots < n$. A signed permutation $\bar{\sigma} \in B_n$ has a descent in position $i < n$ if and only if $\bar{\sigma}(i) > \bar{\sigma}(i+1)$ [11, 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. 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 [21, 6].

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 $\bar{\alpha} = (\alpha(1), \dots, \alpha(n)) \in B_n$ 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 [8] of the Gell-Mann Low eigenstate $|\Psi_{GL}\rangle$ 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 3.4. *The elements R_S^n (resp. T_S^n), $S \subseteq [n-1]$, form a family of linearly independent elements in the group algebra $\mathbb{Q}[S_n]$.*

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:

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

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

Lemma 3.5. *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 $st(\bar{\tau}(1), \dots, \bar{\tau}(n)) = \bar{\sigma}$ and $st(\bar{\tau}(n+1), \dots, \bar{\tau}(n+m)) = \bar{\beta}$. 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 $st(\bar{\tau}(1), \dots, \bar{\tau}(n)) * st(\bar{\tau}(n+1), \dots, \bar{\tau}(n+m))$ by the very definition of $*$ and does not appear in the expansion of any other product $\bar{\sigma} * \bar{\beta}$ with $Reg(\bar{\sigma}) = Reg(st(\bar{\tau}(1), \dots, \bar{\tau}(n)))$, $Reg(\bar{\beta}) = Reg(st(\bar{\tau}(n+1), \dots, \bar{\tau}(n+m)))$, from which the lemma follows.

Corollary 3.6. *For S, U as above:*

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

so that:

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

Theorem 3.1. *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 shuffle product in \mathbf{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 \mathbf{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 3.5 -see also [21].

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 , then the barred integers of $\bar{\sigma}$ are entirely determined by permutation $\sigma = (|\bar{\sigma}(1)|, \dots, |\bar{\sigma}(n)|)$, 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 $2n!$.

4 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} [8]) consists in appealing to the hole/particle duality of quantum physics. Goldstone's theory was generalized to degenerate states by Michels and Suttorp [12], 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 $U_\epsilon = U(0)P(PU(0)P)^{-1}$. Let us write H_i for $-iH_{int}$ 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:

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

We encode iterated integrals in A and B as previously. For example,

$$\int_{-\infty}^0 \int_{-\infty}^{t_1} \int_{-\infty}^{t_2} A(t_2)B(t_1)A(t_3)dt_1dt_2dt_3 =: H_{(2,\bar{1},3)}.$$

For an arbitrary element $X = \sum_{\bar{\sigma} \in B_n} \mu_{\bar{\sigma}} \cdot \bar{\sigma}$ in the group algebra $\mathbb{Q}[B_n]$, we write H_X for $\sum_{\bar{\sigma} \in B_n} \mu_{\bar{\sigma}} \cdot H_{\bar{\sigma}}$.

Theorem 4.1. *The effective adiabatic evolution operator U_{GL} has the hyperoctahedral Picard-type expansion:*

$$U_{GL} = \lim_{\epsilon \rightarrow 0} P + (1 - P) \left(\sum_{n \in \mathbb{N}} H_{R_n^0} \right) P$$

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

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

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

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

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,

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

$$V_{(2\bar{3}1); 2} = \int_{-\infty \leq t_3 \leq t_2 \leq t_1 \leq 0, -\infty \leq t_5 \leq t_4 \leq t_1} A(t_2)B(t_3)A(t_1)H_i(t_4)H_i(t_5).$$

The integrals $V_{X, n-k}$ are defined, as usual, by extending these conventions to arbitrary elements $X \in \mathbb{Q}[B_k]$, $k < n$.

We then have:

$$\begin{aligned} V_n &= \int_{\Delta_n^{[-\infty, 0]}} (P + (1 - P)) H_i(t_1) \dots H_i(t_n) = PV_n + \int_{\Delta_n^{[-\infty, 0]}} A(t_1) H_i(t_2) \dots H_i(t_n) \\ &= PV_n + V_{(1); n-1} = PV_n + \int_{\Delta_n^{[-\infty, 0]}} A(t_1) (A - B)(t_2) H_i(t_3) \dots H_i(t_n) \\ &= PV_n + V_{(12); n-2} - V_{(1\bar{2}); n-2} \\ &= PV_n + V_{(12); n-2} - V_{(1\bar{2}); n-2} + (-V_{(2\bar{1}); n-2} + V_{(2\bar{1}); n-2}). \end{aligned}$$

By interchanging the integration variables t_1 and t_2 , $V_{(2\bar{1}); n-2}$ can be rewritten

$$\int_{-\infty}^0 \int_{t_1}^0 \int_{\Delta_{n-2}^{[-\infty, t_2]}} A(t_1) B(t_2) H_i(t_3) \dots H_i(t_n)$$

so that:

$$V_{(1\bar{2}); n-2} + V_{(2\bar{1}); n-2} = \left[\int_{-\infty}^0 A(t) dt \right] \int_{\Delta_{n-1}^{[-\infty, 0]}} B(t_1) H_i(t_2) \dots H_i(t_{n-1})$$

$$= -(1-P)H_{R_0^1}PV_{n-1},$$

where we have used that $(1-P)B(t) = 0$ to rewrite

$$\left[\int_{-\infty}^0 A(t)dt \right] = (1-P) \left[\int_{-\infty}^0 (A(t) + B(t))dt \right] = (1-P)H_{R_0^1}.$$

We get:

$$V_n = PV_n + (1-P)H_{R_0^1}PV_{n-1} + V_{(12);n-2} + V_{(2\bar{1});n-2} = PV_n + (1-P)H_{R_0^1}PV_{n-1} + (1-P)V_{R_0^2;n-2},$$

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:

$$(1-P)V_{R_0^k;n-k} = (1-P)H_{R_0^k}PV_{n-k} + (1-P)V_{R_0^{k+1};n-k-1}.$$

Then we get, by induction:

$$V_n = PV_n + (1-P)H_{R_0^1}PV_{n-1} + (1-P)H_{R_0^2}PV_{n-2} + \dots + (1-P)H_{R_0^n}PV_0.$$

Since $U_0 = \sum_n V_n$, this implies

$$U_0 = PU_0 + (1-P) \sum_{n=1}^{\infty} H_{R_0^n}PU_0,$$

or

$$U_0P = \left(P + (1-P) \sum_{n=1}^{\infty} H_{R_0^n}P \right) PU_0P,$$

and the Theorem follows.

So, let us check that the formula for $(1-P)V_{R_0^k;n-k}$ holds. This property is crucial and we give a detailed proof of it. Let us consider an arbitrary element $\bar{\sigma} \in B_k$ with $Reg(\bar{\sigma}) = \emptyset$. Then,

$$\begin{aligned} V_{\bar{\sigma};n-k} &= \int_{\Delta_k^{[-\infty,0]} \times \Delta_{n-k}^{[-\infty,t_{\sigma(k)}}} X(t_{\sigma(1)}) \dots X(t_{\sigma(k)}) H_i(t_{k+1}) \dots H_i(t_n) \\ &= \int_{\Delta_k^{[-\infty,0]} \times \Delta_{n-k}^{[-\infty,t_{\sigma(k)}}} X(t_{\sigma(1)}) \dots X(t_{\sigma(k)}) (A-B)(t_{k+1}) \dots H_i(t_n) \\ &= \int_{\Delta_k^{[-\infty,0]} \times \Delta_{n-k}^{[-\infty,t_{\sigma(k)}}} X(t_{\sigma(1)}) \dots X(t_{\sigma(k)}) A(t_{k+1}) \dots H_i(t_n) \\ &\quad - \int_{\Delta_k^{[-\infty,0]} \times \Delta_{n-k}^{[-\infty,t_{\sigma(k)}}} X(t_{\sigma(1)}) \dots X(t_{\sigma(k)}) B(t_{k+1}) \dots H_i(t_n). \end{aligned}$$

Let us denote the first term by T_1 and the second by T_2 , so that $V_{\bar{\sigma};n-k} = T_1 + T_2$. To calculate T_1 , we define $V_n(t) := \int_{\Delta_n^{[-\infty,t]}} H_i(t_1) \dots H_i(t_n)$. This gives us

$$T_1 = \int_{\Delta_k^{[-\infty,0]}} X(t_{\sigma(1)}) \dots X(t_{\sigma(k)}) \int_{-\infty}^{t_{\sigma(k)}} A(t_{k+1}) V_{n-k-1}(t_{k+1}).$$

The domain $\Delta_k^{[-\infty, 0]}$ of the first integral is defined by the inequalities $-\infty \leq t_k \leq \dots \leq t_1 \leq 0$. The domain of the second integral is $-\infty \leq t_{k+1} \leq t_{\sigma(k)}$, where we recall that $\sigma(i) = |\bar{\sigma}(i)|$. To decompose this product of domains into a sum of domains isomorphic to $\Delta_{k+1}^{[-\infty, 0]}$, we proceed as in the proof of proposition 3.2. We see that t_{k+1} can be between $-\infty$ and t_k , between t_k and t_{k-1} , up to between $t_{\sigma(k)+1}$ and $t_{\sigma(k)}$. Thus, if we denote by $\rho(i)$ the position of t_i in the ordering of the time variables t_1, \dots, t_k and t_{k+1} (starting from the largest), we have $\sigma(k)+1 \leq \rho(k+1) \leq k+1$, $\rho(i) = i$ for $i < \rho(k+1)$ and $\rho(i) = i+1$ for $k \geq i \geq \rho(k+1)$. If we take the example of $\bar{\sigma} = (2, \bar{1})$, we have $k = 2$, $\sigma(k) = 1$, and two possibilities for $\rho(k+1)$: (i) $\rho(k+1) = 2$, with $-\infty \leq t_2 \leq t_3 \leq t_1 \leq 0$ and $\rho = (1, 3, 2)$ and (ii) $\rho(k+1) = 3$, with $-\infty \leq t_3 \leq t_2 \leq t_1 \leq 0$ and $\rho = (1, 2, 3)$. To put the variables in increasing order, we change variables to $s_i = t_i$ for $i < \rho(k+1)$, $s_{\rho(k+1)} = t_{k+1}$ and $s_i = t_{i-1}$ for $i > \rho(k+1)$. Therefore, the product $X(t_{\sigma(1)}) \dots X(t_{\sigma(k)}) A(t_{k+1})$ becomes $X(s_{\tau(1)}) \dots X(s_{\tau(k)}) A(s_{\tau(k+1)})$ (where we assume that X takes the same value A or B as in the previous expressions), with $\tau(i) = \sigma(i)$ for $\sigma(i) < \rho(k+1)$, $\tau(i) = \sigma(i) + 1$ for $\sigma(i) \geq \rho(k+1)$ and $\tau(k+1) = \rho(k+1)$. Therefore, the descents of $(\tau(1), \dots, \tau(k))$ and σ are at the same positions. Moreover, $\sigma(k) < \rho(k+1)$ implies $\tau(k) = \sigma(k) < \rho(k+1) = \tau(k+1)$ and τ has no descent at k . If we define now $\bar{\tau}$ by $|\bar{\tau}(i)| = \tau(i)$ and the sign of $\bar{\tau}(i)$ is the same as the sign of $\bar{\sigma}(i)$ for $1 \leq i \leq k$ and $\bar{\sigma}(k+1) = \rho(k+1)$, then $\bar{\tau}$ has no regression and $X(t_{\sigma(1)}) \dots X(t_{\sigma(k)}) A(t_{k+1}) = X(s_{\tau(1)}) \dots X(s_{\tau(k)}) X(s_{\tau(k+1)})$. We note that all terms of T_1 contribute to $V_{R_0^{k+1}; n-k-1}$. Finally, we enumerate the signed permutations $\bar{\tau}$ that are obtained in T_1 . There are $2(k-1)!$ elements $\bar{\sigma}$ of R_0^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_0^{k+1} . Thus, T_1 provides $(k+1)!$ different elements of R_0^{k+1} when $\bar{\sigma}$ runs over R_0^k .

The term T_2 is slightly more difficult to take into account. We have

$$\begin{aligned} T_2 &= - \int_{\Delta_k^{[-\infty, 0]}} X(t_{\sigma(1)}) \dots X(t_{\sigma(k)}) \int_{-\infty}^{t_{\sigma(k)}} B(t_{k+1}) V_{n-k-1}(t_{k+1}) dt_{k+1} \\ &= - \int_{\Delta_k^{[-\infty, 0]}} X(t_{\sigma(1)}) \dots X(t_{\sigma(k)}) \int_{-\infty}^0 B(t_{k+1}) V_{n-k-1}(t_{k+1}) dt_{k+1} \\ &\quad + \int_{\Delta_k^{[-\infty, 0]}} X(t_{\sigma(1)}) \dots X(t_{\sigma(k)}) \int_{t_{\sigma(k)}}^0 B(t_{k+1}) V_{n-k-1}(t_{k+1}) dt_{k+1}. \end{aligned}$$

In the first term of this last expansion, when summing up over $\bar{\sigma} \in B_k$ with $Reg(\bar{\sigma}) = \emptyset$, we recognize $H_{R_0^k} P V_{n-k}$.

For the second term, we proceed as for the calculation of T_1 . We expand the product of the domain $-\infty \leq t_k \leq \dots \leq t_1 \leq 0$ with the domain $t_{\sigma(k)} \leq t_{k+1} \leq 0$ into domains isomorphic to $\Delta_{k+1}^{[-\infty, 0]}$. The position $\rho(k+1)$ of t_{k+1} in such a domain satisfies now $1 \leq \rho(k+1) \leq \sigma(k)$. As for T_1 , we find that each $\bar{\sigma}$ generates $\sigma(k)$ signed permutations $\bar{\tau} \in B_{k+1}$ and the relation between $\bar{\sigma}$ and $\bar{\tau}$ is the same as for T_1 except for $\bar{\tau}(k+1)$. We still have $\tau(k+1) = \rho(k+1)$ but now $\sigma(k) \geq \rho(k+1)$ implies $\tau(k) = \sigma(k) + 1 > \rho(k+1) = \tau(k+1)$ and τ has a descent at k . However, we have now $X(s_{\tau(k+1)}) = B(s_{\tau(k+1)})$ so that $\bar{\tau}(k+1) \in \bar{\mathbf{N}}^*$, and the permutation $\bar{\tau}$ has no regression. Again, this process generates $(k+1)!$ elements of R_0^{k+1} , that are all different from the elements generated by the calculation of T_1 (because $\bar{\tau}(k+1)$ is now in $\bar{\mathbf{N}}^*$). The sum of these terms and of those coming from T_1 gives us $V_{R_0^{k+1}; n-k-1}$. Therefore

$$V_{R_0^k; n-k} = H_{R_0^k} P V_{n-k} + V_{R_0^{k+1}; n-k-1}.$$

The theorem is obtained by multiplying this equation by $(1 - P)$.

5 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 Białynicki-Birula, Mielnik and Plebański [1, 13] 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 [22]. Our previous results pave the way toward the solution of the problem. Namely, as it appears from Thm 4.1, the natural object to look at is not so much the effective Hamiltonian

$$\mathcal{H} = \lim_{\epsilon \rightarrow 0} P_0 H U_\epsilon$$

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

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

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

$$U_\epsilon = P + (1 - P) \left(\sum_{n \in \mathbb{N}^*} H_{R_\emptyset^n} \right) P = P + (1 - P) \left(\sum_{n \in \mathbb{N}} H_{R_\emptyset^n} \right) P = P + (1 - P) Pic P$$

In other terms, we are interested in the expansion:

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

where

$$\Omega_\epsilon = \log \left(\sum_{n \in \mathbb{N}} H_{R_\emptyset^n} \right) = H_{\log \left(\sum_{n \in \mathbb{N}} R_\emptyset^n \right)}.$$

Since $R_\emptyset^{n_1} * \dots * R_\emptyset^{n_k} = R_{\{n_1, \dots, n_1 + \dots + n_{k-1}\}}^{n_1 + \dots + n_k}$, 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 [21, 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 3.1 together with the existence of a logarithmic expansion of sol_n , which is actually best understood from an Hopf algebraic point of view, see [16, 21, 17, 18]:

$$\sum_{n \in \mathbb{N}^*} sol^n = \log \left(\sum_{n \in \mathbb{N}} D_\emptyset^n \right).$$

As a corollary of Thm 3.1, we also get the expansion of Ω_R in the canonical basis of $\bigoplus_{n \in \mathbb{N}^*} \mathbb{Q}[B_n]$:

Proposition 5.1. *We have:*

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

The Proposition follows from the analogous expansion for sol_n [21], together with the algebra isomorphism Thm 3.1:

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

Corollary 5.2. *The hyperoctahedral Magnus expansion of the effective Hamiltonian \mathcal{H} reads, when truncated at the third order:*

$$\begin{aligned} \mathcal{H} = & \lim_{\epsilon \rightarrow 0} PH_I(P + (1-P) \exp(H_{(1)} + H_{(\bar{1})} + \frac{1}{2}[H_{(12)} + H_{(\bar{1}\bar{2})} + H_{(2\bar{1})} + H_{(\bar{2}\bar{1})} - H_{(1\bar{2})} - H_{(\bar{1}\bar{2})} - H_{(21)} - H_{(\bar{2}1)}] + \\ & \frac{1}{3}[H_{(123)} + H_{(\bar{1}\bar{2}\bar{3})} + H_{(13\bar{2})} + H_{(\bar{1}\bar{3}\bar{2})} + H_{(2\bar{1}\bar{3})} + H_{(\bar{2}\bar{1}\bar{3})} + H_{(23\bar{1})} + H_{(\bar{2}\bar{3}\bar{1})} + H_{(3\bar{2}\bar{1})} + H_{(\bar{3}\bar{2}\bar{1})} + H_{(31\bar{2})} + H_{(\bar{3}\bar{1}\bar{2})} \\ & + H_{(321)} + H_{(\bar{3}\bar{2}\bar{1})} + H_{(2\bar{3}\bar{1})} + H_{(\bar{2}\bar{3}\bar{1})} + H_{(1\bar{2}\bar{3})} + H_{(\bar{1}\bar{2}\bar{3})} + H_{(1\bar{3}\bar{2})} + H_{(\bar{1}\bar{3}\bar{2})} + H_{(21\bar{3})} + H_{(\bar{2}\bar{1}\bar{3})} + H_{(31\bar{2})} + H_{(\bar{3}\bar{1}\bar{2})}] \\ & - \frac{1}{6}[H_{(132)} + H_{(\bar{1}\bar{3}\bar{2})} + H_{(231)} + H_{(\bar{2}\bar{3}\bar{1})} + H_{(213)} + H_{(\bar{2}\bar{1}\bar{3})} + H_{(312)} + H_{(\bar{3}\bar{1}\bar{2})} + H_{(1\bar{3}\bar{2})} + H_{(\bar{1}\bar{3}\bar{2})} + H_{(1\bar{2}\bar{3})} + H_{(\bar{1}\bar{2}\bar{3})} + H_{(21\bar{3})} \\ & + H_{(\bar{2}\bar{1}\bar{3})} + H_{(31\bar{2})} + H_{(\bar{3}\bar{1}\bar{2})} + H_{(2\bar{3}\bar{1})} + H_{(\bar{2}\bar{3}\bar{1})} + H_{(3\bar{2}\bar{1})} + H_{(\bar{3}\bar{2}\bar{1})} + H_{(1\bar{2}\bar{3})} + H_{(\bar{1}\bar{2}\bar{3})} + H_{(3\bar{2}\bar{1})} + H_{(\bar{3}\bar{2}\bar{1})}])P). \end{aligned}$$

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