Tree expansion in time-dependent perturbation theory

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The computational complexity of time-dependent perturbation theory is well-known to be largely combinatorial whatever the chosen expansion method and family of parameters (combinatorial sequences, Goldstone and other Feynman-type diagrams...). We show that a very efficient perturbative expansion, both for theoretical and numerical purposes, can be obtained through an original parametrization by trees and generalized iterated integrals. We emphasize above all the simplicity and naturality of the new approach that links perturbation theory with classical and recent results in enumerative and algebraic combinatorics. These tools are applied to the adiabatic approximation and the effective Hamiltonian. We prove perturbatively and non-perturbatively the convergence of Morita's generalization of the Gell-Mann and Low wavefunction. We show that summing all the terms associated to the same tree leads to an utter simplification where the sum is simpler than any of its terms. Finally, we recover the time-independent equation for the wave operator and we give an explicit non-recursive expression for the term corresponding to an arbitrary tree.

I. INTRODUCTION

Effective Hamiltonians provide a way to determine the low-energy eigenvalues of a (possibly infinite dimensional) Hamiltonian by diagonalizing a matrix defined in a subspace of small dimension, called the *model space* and hereafter denoted by M. Because of this appealing feature, effective Hamiltonians are used in nuclear, atomic, molecular, chemical and solid-state physics[1].

These theories are plagued with a tremendous combinatorial complexity because of the presence of folded diagrams (to avoid singularities of the adiabatic limit), partial resummations, subtle "linkedness" properties and the exponential growth of the number of graphs with the order of perturbation. This complexity has two consequences: on the one hand, few results are proved in the mathematical sense of the word, on the other hand, it is difficult to see what is the underlying structure of the perturbative expansion that could lead to useful resummations and non-perturbative approximations.

To avoid these pitfalls, we take a bird's-eye view of the problem and consider a general time-dependent Hamiltonian $H(t)$. This way, we disentangle the problem from the various particular forms that can be given to the Hamiltonian and which have lead in the past to various perturbative expansions. To be precise, take the example of fermions in molecular systems. The Coulomb interaction between the electrons (say V) can be viewed as a perturbation of a "free Hamiltonian" modeling the interaction with the nuclei (in the Born-Oppenheimer approximation). One can take advantage of the particular form of V (which is a linear combination of products of two creation and two annihilation operators in the second quantization picture) to represent the perturbative expansions using a given family of Goldstone diagrams (see e.g. ref. 2 for such a family). However, the general results on perturbative expansions (such as the convergence of the time-dependent wave operator) do not depend on such a particular choice.

Thus, we consider an Hamiltonian $H(t)$ and we build its evolution operator $U(t,t_0)$, which is the solution of the Schrödinger equation (in units $\hbar = 1$)

$$\imath \frac{\partial U(t,t_0)}{\partial t} \;=\; H(t)U(t,t_0), \tag{1}$$

with the boundary condition $U(t_0,t_0) = 1$. In perturbation theory, $H(t) := \mathrm{e}^{-\epsilon|t|}\mathrm{e}^{\imath H_0 t} V \mathrm{e}^{-\imath H_0 t}$ is the adiabatically switched interaction Hamiltonian in the interaction picture (here H_0 and V stand respectively for the "free" and interaction terms of the initial Hamiltonian) and singularities show up in the adiabatic limit ($t_0 \to -\infty$ and $\epsilon \to 0$). Morita discovered[2] that, in this setting, the *time-dependent wave operator*

$$\Omega(t,t_0) \;:=\; U(t,t_0)P\big(PU(t,t_0)P\big)^{-1},$$

where P is the projection onto the model space M, has no singularity in the adiabatic limit. Moreover, the wave

operator determines the effective Hamiltonian because

$$H_{\text{eff}} := \lim_{\epsilon \to 0} PH\Omega(0, -\infty). \tag{2}$$

However, as we have already alluded to, the effective computation of these operators raises several combinatorial and analytical problems that have been addressed in a long series of articles (several of which will be referred to in the present article).

In the first sections of the paper, we consider a general time-dependent Hamiltonian $H(t)$ (not necessarily in the interaction picture). In this broader setting, Jolicard[3] found that the time-dependent wave operator provides also a powerful description of the evolution of quantum systems (see ref. 4 for applications). Then, we derive three (rigorously proven) series expansions of the wave operator. The first one is classical and can be physically interpreted as the replacement of causality (i.e. the Heaviside step function $\theta(t-t')$) by a "propagator" $\theta_P(t-t') := \theta(t-t')Q - \theta(t'-t)P$, where $Q = 1 - P$. This "propagator" is causal out of the model space ($\theta_P(t-t') = 0$ for $t < t'$ on the image of Q) and anticausal on it, like the Feynman propagator of quantum field theory[5]. However, this sum of causal and anticausal orderings is cumbersome to use in practice. A second series expansion is obtained by writing the wave operator as a sum of integrals over all possible time orderings of the Hamiltonians $H(t_i)$ (see Sect. II B). This expansion, parametrized by all the permutations (or equivalent families), is used in many-body theory and gives rise to a large number of complicated terms. The third expansion is obtained by noticing that some time orderings can be added to give simpler expressions. This series is naturally indexed by trees and is the main new tool developed in the present paper. Among others, we derive a very simple recurrence relation for the terms of the series. We also show that the very structure of the corresponding generalized iterated integrals showing up in the expansion is interesting on its own. These integrals carry naturally a rich algebraic structure that is connected to several recent results in the field of combinatorial Hopf algebras and noncommutative symmetric functions. The corresponding algebraic results that point out in the direction of the existence of a specific Lie theory for effective Hamiltonians (generalizing the usual Lie theory) are gathered in an Appendix.

In the last sections of the paper, we restrict $H(t)$ to the interaction picture and we consider the adiabatic limit. We first prove that the adiabatic limit exists non perturbatively. We show that the effective Hamiltonian defined by eq. (2) has the expected properties. Then, we expand the series and we give a rigorous (but lengthy) proof that the term corresponding to each time ordering has an adiabatic limit. Then, we consider the series indexed by trees and we give a short and easy proof of the existence of that limit. Finally, we provide a direct rule to calculate the term corresponding to a given tree and establish the connection between the time-dependent approach and the time-independent equations discovered by Lindgren[6] and Kvasnička[7].

The existence of this series indexed by trees can be useful in many ways: (i) It describes a sort of superstructure that is common to all many-body theories without knowing the exact form of the interaction Hamiltonian; (ii) It considerably simplifies the manipulation of the general term of the series by providing a powerful recurrence relation; (iii) It provides simple algorithms to calculate the terms of the series; (iv) The number of trees of order n, $\frac{1}{n+1}\binom{2n}{n} \approx \frac{4^n}{n^{\frac{3}{2}}\sqrt{\pi}}$ being subexponential, it improves the convergence of the series[8,9]; (v) It can deal with problems where the Hamiltonian H_0 is not quadratic. Indeed, many-body theories most often require the Hamiltonian H_0 to be free, i.e. to be a quadratic function of the fields[10]. As noticed by Bulaevskii[11], this is not the good point of view for some applications. For example, in the microscopic theory of the interaction of radiation with matter, it is natural to take for H_0 the Hamiltonian describing electrons and nuclei in Coulomb interaction[12], the perturbation being the interaction with the transverse electric field. In that case, quadratic free Hamiltonians many-body theories break down whereas our approach is still valid. Actually, it is precisely for that reason that we originally developed the tree series approach; (vi) Last, but not least, the tree-theoretical approach connects many-body theories with a large field of knowledge that originates in the "birth of modern bijective combinatorics" in the seventies with in particular the seminal works of Foata, Schützenberger and Viennot[13,14]. See e.g. ref. 15 for a survey of the modern combinatorial theory of tree-like structures.

From the physical point of view, the tree expansion is particularly interesting in the adiabatic limit. Indeed, the denominator of each of its terms is a product of $E_i^Q - E_j^P$ factors, where E_j^P is the energy of a state in the model space M and E_j^Q the energy of a state not belonging to M. In the usual many-body expansions, the denominators are products of $\sum_i E_i^Q - \sum_j E_j^P$ factors, where the sums contain various numbers of elements (corresponding therefore to multiple transitions between low-energy and excitated levels). In that sense, the tree expansion is the simplest possible because each term is a product of single transitions between two states.

We now list the main new results of this paper: (i) A recursion formula that generates the simplified terms of the time-dependent perturbation series (theorem 5); (ii) when the interaction is adiabatically switched on, a non-perturbative proof of the convergence of the wave operator and a characterization of the states of the model space that are transformed into eigenstates of H by the wave operator (theorem 6); (iii) a proof of the existence of the

adiabatic limit for the terms of the series expansion of the wave operator (theorem 9); (iv) a recursive formula (lemma 13) and an explicit form (theorem 14) for the general term of the time-independent perturbation series.

II. TIME-DEPENDENT HAMILTONIAN AND COMBINATORICS

We consider a time-dependent Hamiltonian $H(t)$, which is a self-adjoint operator on a Hilbert space $\mathcal{H}$, and its evolution operator $U(t,t_0)$ defined in eq. (1). Since we are interested in the combinatorial aspects of the problem, we consider the simple case where $H(t)$ is a strongly continuous map from $\mathbb{R}$ into the bounded self-adjoint operators on $\mathcal{H}$[16]. In that case, the Picard-Dyson series

$$1+\sum_{n=1}^{\infty}(-\imath)^n\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\ldots\int_{t_0}^{t_{n-1}}\mathrm{d}t_n H(t_1)\ldots H(t_n),$$

converges in the uniform operator topology to $U(t,t_0)$ and $U(t,t_0)$ is a jointly strongly continuous two-parameter family of unitaries on $\mathcal{H}$ (see section X.12 of ref. 17).

Following Morita[2], Jolicard[3] established a connection between the evolution operator and the effective Hamiltonian approach by defining

$$\Omega(t,t_0) \;:=\; U(t,t_0)P\big(PU(t,t_0)P\big)^{-1},$$

where P is a projection operator onto M and $\big(PU(t,t_0)P\big)^{-1}$ is the inverse of $PU(t,t_0)P$ as a map from $M=P\mathcal{H}$ to itself. This map is invertible if and only if there is no state $|\phi\rangle$ in M such that $\langle\phi|U(t,t_0)P=0$. This condition is similar to the one of time-independent perturbation theory[18]. We assume from now on that the condition is satisfied and we define three expansions for $\Omega(t,t_0)$.

A. First expression for Ω

We start by proving an elegant expression for Ω, that was stated by Michels and Suttorp[19] and Dmitriev and Solnyshkina[20].

Theorem 1

$$\Omega(t,t_0) \;=\; P+Q\sum_{n=1}^{\infty}(-\imath)^n\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t}\mathrm{d}t_2\ldots\int_{t_0}^{t}\mathrm{d}t_n H(t_1)\theta_P(t_1-t_2)H(t_2)\ldots\theta_P(t_{n-1}-t_n)H(t_n)P, \tag{3}$$

where $Q=1-P$ and $\theta_P(t)=\theta(t)Q-\theta(-t)P$, with θ the Heaviside step function.

Proof. We first rewrite the Picard-Dyson series as $U(t,t_0)=1+\sum_n U_n(t,t_0)$ with $U_1(t,t_0):=-\imath\int_{t_0}^{t}\mathrm{d}t_1 H(t_1)$ and, for $n>1$,

$$U_n(t,t_0) \;:=\; (-\imath)^n\int_{t_0}^{t}\mathrm{d}t_1\ldots\int_{t_0}^{t}\mathrm{d}t_n H(t_1)\theta(t_1-t_2)\ldots\theta(t_{n-1}-t_n)H(t_n).$$

Then, by using $\theta(t)+\theta(-t)=1$, we notice that

$$\theta(t) \;=\; P+\theta(t)-\theta(t)P-\theta(-t)P=P+\theta_P(t).$$

Now, we replace $\theta(t)$ by the sum of operators $P+\theta_P(t)$ in the expression for $U_n(t,t_0)$. This gives us 2^{n-1} terms with various numbers of P and θ_P. Denote by $C_n(t,t_0)$ the term with no P (with the particular case $C_1(t,t_0)=U_1(t,t_0)$). Take then any other term. There is an index i such that the first P from the left occurs after $H(t_i)$. Therefore, the integrand of this term is

$$H(t_1)\theta_P(t_1-t_2)\ldots\theta_P(t_{i-1}-t_i)H(t_i)PH(t_{i+1})\ldots$$

Observe that the integral over $t_1,\ldots,t_i$ is independent from the integral over $t_{i+1},\ldots,t_n$. The first integral gives $C_i(t,t_0)$, the second integral is a term of the Picard-Dyson series for $U_{n-i}(t,t_0)$. Thus, the sum of the 2^{n-1} terms yields

$$U_n(t,t_0) \;=\; C_n(t,t_0)+\sum_{i=1}^{n-1}C_i(t,t_0)PU_{n-i}(t,t_0).$$

If we denote by $K(t,t_0)$ the sum of all the $C_n(t,t_0)$ with $n>0$, we obtain $U=1+K+KP(U-1)$, so that

$$UP \;=\; P+KPUP. \tag{4}$$

The operator K is called the *reduced evolution operator* by Lindgren and collaborators[21]. If we define $\omega := P+QKP$, eq. (4) becomes

$$UP \;=\; P+(\omega-P+PKP)PUP = P+\omega PUP-PUP+PKPUP.$$

This equation can be simplified by using eq. (4) again

$$UP \;=\; P+\omega PUP-PP = \omega PUP.$$

Thus, $\omega=\Omega$ and eq. (3) is satisfied. □

Despite its elegance, eq. (3) is not immediately usable. To illustrate this point, consider the third-order term

$$\Omega_3 \;=\; \imath Q\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t}\mathrm{d}t_2\int_{t_0}^{t}\mathrm{d}t_3 H(t_1)\theta_P(t_1-t_2)H(t_2)\theta_P(t_2-t_3)H(t_3)P.$$

If we expand $\theta_P(t)=\theta(t)Q-\theta(-t)P$, we obtain four terms

$$\begin{aligned}
&\imath QH(t_1)QH(t_2)QH(t_3)P && \text{for } t_1\geq t_2 \text{ and } t_2\geq t_3,\\
-&\imath QH(t_1)QH(t_2)PH(t_3)P && \text{for } t_1\geq t_2 \text{ and } t_2\leq t_3,\\
-&\imath QH(t_1)PH(t_2)QH(t_3)P && \text{for } t_1\leq t_2 \text{ and } t_2\geq t_3,\\
&\imath QH(t_1)PH(t_2)PH(t_3)P && \text{for } t_1\leq t_2 \text{ and } t_2\leq t_3.
\end{aligned}$$

The first and last terms have integration range $t_1\geq t_2\geq t_3$ and $t_3\geq t_2\geq t_1$, respectively and give rise to iterated integrals. The integration range of the second term is $t_1\geq t_2$ and $t_2\leq t_3$. Such an integration range is not convenient because the relative position of t_1 and t_3 is not specified. The integration range has to be split into the two subranges $t_1\geq t_3\geq t_2$ and $t_3\geq t_1\geq t_2$. Each subrange defines now an iterated integral. For example $t_1\geq t_3\geq t_2$ gives

$$-\imath\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_3\int_{t_0}^{t_3}\mathrm{d}t_2 QH(t_1)QH(t_2)PH(t_3)P.$$

Similarly, the integration range of the third term ($t_1\leq t_2$ and $t_2\geq t_3$) is the union of $t_2\geq t_1\geq t_3$ and $t_2\geq t_3\geq t_1$. We see that Ω_3 is sum of six iterated integrals corresponding to the six possible orderings of t_1, t_2 and t_3.

B. Ω in terms of permutations

We consider again the previous example, and we change variables to have a fixed integration range $s_1\geq s_2\geq s_3$. If we sum over all time orderings, we obtain

$$\begin{aligned}
\Omega_3 \;=\; \imath\int_{t_0}^{t}\mathrm{d}s_1\int_{t_0}^{s_1}\mathrm{d}s_2\int_{t_0}^{s_2}\mathrm{d}s_3\Big(&QH(s_1)QH(s_2)QH(s_3)P-QH(s_1)QH(s_3)PH(s_2)P-QH(s_2)QH(s_3)PH(s_1)P\\
&-QH(s_2)PH(s_1)QH(s_3)P-QH(s_3)PH(s_1)QH(s_2)P+QH(s_3)PH(s_2)PH(s_1)P\Big).
\end{aligned} \tag{5}$$

In ref. 22, we showed that this result can be generalized to all orders and that Ω_n is a sum of $n!$ iterated integrals corresponding to all the orderings of $t_1,\ldots,t_n$. More precisely, we obtained the series expansion for Ω

$$\Omega(t,t_0) \;=\; P+\sum_{n=1}^{\infty}\sum_{\sigma\in\mathcal{S}_n}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\ldots\int_{t_0}^{t_{n-1}}\mathrm{d}t_n X(t_{\sigma(1)})\ldots X(t_{\sigma(n)}), \tag{6}$$

where $\mathcal{S}_n$ is the group of permutations of n elements. The operators X are defined, for $n=1$, by $X(t):=-\imath QH(t)P$ and, for $n>1$ and any $\sigma\in\mathcal{S}_n$, by $X(t_{\sigma(1)}):=-\imath QH(t_{\sigma(1)})$ and

$$\begin{aligned}
X(t_{\sigma(p)}) \;&:=\; -\imath QH(t_{\sigma(p)}) \text{ if } 1<p<n \text{ and } \sigma(p)>\sigma(p-1),\\
X(t_{\sigma(p)}) \;&:=\; \imath PH(t_{\sigma(p)}) \text{ if } 1<p<n \text{ and } \sigma(p)<\sigma(p-1),\\
X(t_{\sigma(n)}) \;&:=\; -\imath QH(t_{\sigma(n)})P \text{ if } \sigma(n)>\sigma(n-1),\\
X(t_{\sigma(n)}) \;&:=\; \imath PH(t_{\sigma(n)})P \text{ if } \sigma(n)<\sigma(n-1).
\end{aligned}$$

Each term of eq. (6) is now written as an iterated integral. However, the expansion (6) is still not optimal because some of its terms can be summed to get a simpler expression. As an example, consider the fourth and fifth terms of eq. (5), where we replace s_i by t_i.

$$Z \;:=\; -\imath \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \int_{t_0}^{t_2} \mathrm{d}t_3 \Big(QH(t_2)PH(t_1)QH(t_3)P + QH(t_3)PH(t_1)QH(t_2)P \Big).$$

The first and second terms of the right hand side of this equation are denoted by Z_1 and Z_2, respectively. We transform Z_2 by exchanging variables t_2 and t_3.

$$Z_2 \;=\; -\imath \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_3 \int_{t_0}^{t_3} \mathrm{d}t_2 QH(t_2)PH(t_1)QH(t_3)P = -\imath \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \int_{t_2}^{t_1} \mathrm{d}t_3 QH(t_2)PH(t_1)QH(t_3)P,$$

where we also exchanged the order of the integrations over t_3 and t_2. This can be added to Z_1 and we obtain the simpler expression

$$Z \;=\; -\imath \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \int_{t_0}^{t_1} \mathrm{d}t_3 QH(t_2)PH(t_1)QH(t_3)P.$$

Such a simplification is not possible for the other terms of Ω_3. In the next section, we determine how this simplification can be extended to the general term of Ω.

Before closing this section, we need to specify more precisely the relation between the permutations σ and the sequence of P and Q in the expansion of eq. (3). When we expand all the $\theta_P(t_i - t_{i+1})$ in eq. (3), we obtain an integrand of the form $(-\imath)^n QH(t_1)R_1H(t_2)\dots R_{n-1}H(t_n)P$, multiplied by a product of Heaviside functions, where R_i takes the value $-P$ or Q. We aim to determine the relation between the sequence $R_1 \dots R_{n-1}$ and the permutations σ in eq. (6). From the definition of $X(t_{\sigma(i)})$, it appears that $R_i = -P$ if $\sigma(i) > \sigma(i+1)$ and $R_i = Q$ if $\sigma(i) < \sigma(i+1)$. The set of indices i such that $\sigma(i) > \sigma(i+1)$ is called the *descent set* of σ, denoted by D_σ. It is also called the *shape* of the permutation[23]. For instance, the descent set of the permutations (213) and (312) is $\{1\}$, corresponding to $(R_1, R_2) = (-P, Q)$.

C. Permutations and trees

In many-body physics, the expansion in Goldstone diagrams corresponds (among other things) to the expansion of Ω into all time orderings Ω_σ. In that context, several authors noticed that some diagrams corresponding to different orderings can be added to give a simple sum[1,19,24–27], as we saw in the previous section. These are special cases of the simplification that we shall present which, as far as we know, was never stated in full generality. The first difficulty is to find the proper combinatorial object to represent the sets of permutations that lead to simplified sums. We shall find it after a short algebraic detour meant to recall the notion of tree and its relation to permutations[13,23]. The trees we consider have received various names in the literature: binary trees in ref. 23, but also (to quote only a few occurrences) plane rooted complete binary tree[28], extended binary trees[29] or planar binary trees[30]. Since these objects are rarely used in physics, we first link them with the trees commonly found in graph theory. This lengthy definition will then be replaced by a much easier one.

A *common tree* is a connected graph without loops. In other words, a common tree is a set of vertices linked by edges such that there is a unique way to go from any vertex to any another one by travelling along edges. An example of a common tree is given in fig. 1(a). A *rooted tree* is a common tree where one vertex was selected. This particular vertex is called the *root*. The *level* of a vertex in a rooted tree is the number of edges that separates this vertex from the root. The root has level 0. It is natural to draw a rooted tree by putting the root at the bottom and drawing a vertex above another one if its level is larger. The rooted tree of fig. 1(b) was obtained by selecting as the root the lowest left vertex of fig. 1(a). The root is indicated by a white dot and a dangling line. In a rooted tree, the *children* of a vertex v are the vertices v' that are linked to v by an edge and such that the level of v' is larger than the level of v. A *plane rooted binary tree* is a rooted tree where each vertex has zero, one or two children, and each edge is oriented either to the left or to the right. If a vertex has two children, then one of the edges is oriented to the left and the other one to the right. Fig. 1(c) shows one of the plane rooted trees that can be obtained from the rooted tree of fig. 1(b). The adjective "plane" means that an edge going to the right cannot be identified with, or deformed into an edge going to the left. A *plane rooted complete binary tree* is a plane rooted binary tree where each vertex is "completed" by drawing *leaves* as follows: if a vertex has no child, draw a leaf (i.e. a line) to the left and one to the right, if a vertex has one child, then draw a leaf to the right if the child is to the left and draw it to the left if the child is to the right. Fig. 1(d) shows the plane rooted complete binary tree that is obtained from the plane rooted

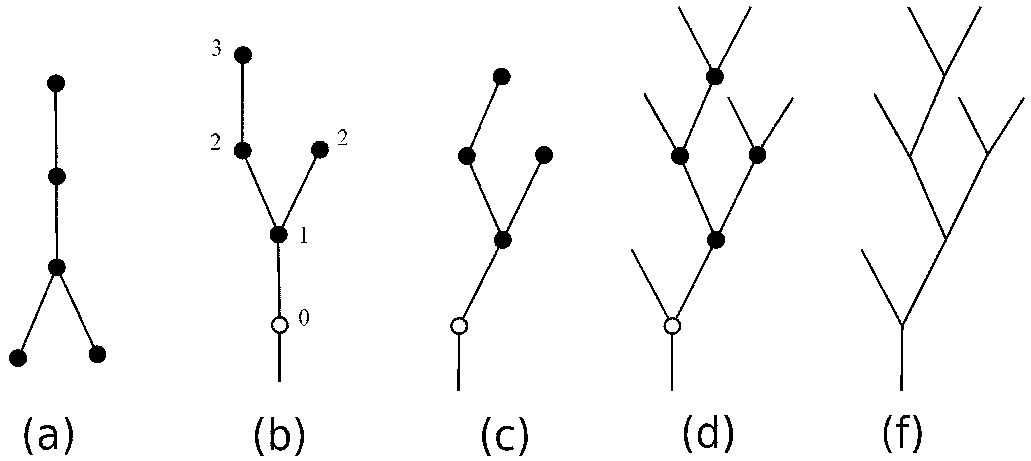

FIG. 1: Construction of plane rooted complete binary tree. (a) a common tree; (b) a rooted tree with its vertex levels; (c) a plane rooted binary tree; (d) a plane rooted complete binary tree; (f) a simplified plane rooted complete binary tree.

binary tree of fig. 1(c). In practice, the vertices are no longer necessary and they are not drawn, as in fig. 1(f). If Y_n denotes the set of plane rooted complete binary trees with n vertices, we see that $Y_1 = \{ \curlyvee \}$, $Y_2 = \{ \curlyvee\!\curlyvee , \curlyvee\!\curlyvee \}$, $Y_3 = \{ \curlyvee\!\curlyvee\!\curlyvee , \curlyvee\!\curlyvee\!\curlyvee , \curlyvee\!\curlyvee\!\curlyvee , \curlyvee\!\curlyvee\!\curlyvee , \curlyvee\!\curlyvee\!\curlyvee \}$. They are much more numerous than the common trees (there is only one common tree with one, two or three vertices). For notational convenience, plane rooted complete binary trees will be simply called "trees" in the rest of the paper.

Fortunately, there exists a much simpler definition of the trees, that use a sort of building rule. We first denote the *empty tree*, i.e. the tree with no vertex, by $|$, which is a dangling line without root (a dangling line with a root and no other vertex belongs to the tree $\curlyvee$). Then, for any integer n, Y_n, is defined recursively by $Y_0 := \{ | \}$ and, for $n > 0$, $Y_n := \{T_1 \vee T_2 \,:\, T_1 \in Y_k, T_2 \in Y_{n-k-1},\, k = 0, \ldots, n-1\}$, where $T_1 \vee T_2$ is the grafting of the two trees T_1 and T_2, by which the dangling lines of T_1 and T_2 are brought together and a new root (with its own dangling line) is grown at their juncture. For example, $| \vee | = \curlyvee$, $| \vee \curlyvee = \curlyvee\!\curlyvee$, $\curlyvee \vee \curlyvee = \curlyvee\!\curlyvee\!\curlyvee$. Note that each tree of Y_n has n vertices (including a root) and $n+1$ leaves. The order $|T|$ of a tree T is the number of its vertices.

If C_n denotes the number of elements of Y_n, the recursive definition of Y_n implies that $C_0 = 1$ and $C_n = \sum_{k=0}^{n-1} C_k C_{n-k-1}$, so that $C_n = \frac{1}{n+1}\binom{2n}{n}$ are the famous Catalan numbers. For n=0 to 10, C_n=1, 1, 2, 5, 14, 42, 132, 429, 1430, 4862, 16796. The Catalan numbers enumerate a large number of (sometimes quite different) combinatorial objects[31]. The main practical interest of trees with respect to other combinatorial interpretations is that their recursive definition is very easy to implement.

We noticed in the previous section that, at order three, the terms Ω_σ corresponding to two specific permutations σ can be added to give a simple result. At the general order, we shall see that the sum of Ω_σ is simple if it is carried out over permutations σ associated with the same tree. But for this, we need to associate a tree to each permutation. The relevant map from permutations to trees belongs to "the ABC's of classical enumeration"[32] and is historically one of the founding tools of modern bijective and algebraic combinatorics[13,23,33]. We describe it in the next section.

1. From permutations to trees

We first map any n-tuple $I = (i_1, \ldots, i_n)$ of distinct integers to a tree $T \in Y_n$. The mapping ϕ is defined recursively as follows: if $I = (i)$ contains a single integer, then $\phi(I) := \curlyvee$; otherwise, pick up the smallest element i_k of I, then

$$\begin{aligned}
\phi(I) &:= | \vee \phi\big((i_2, \ldots, i_n)\big), \text{ if } k = 1,\\
\phi(I) &:= \phi\big((i_1, \ldots, i_{n-1})\big) \vee | \,, \text{ if } k = n,\\
\phi(I) &:= \phi\big((i_1, \ldots, i_{k-1})\big) \vee \phi\big((i_{k+1}, \ldots, i_n)\big), \text{ otherwise.}
\end{aligned}$$

In the following, we frequently abuse notation by writing $\phi(i_1,\dots,i_n)$ or even $\phi(i_1\dots i_n)$ instead of $\phi\big((i_1,\dots,i_n)\big)$. For a permutation $\sigma\in\mathcal{S}_n$, the corresponding tree is $\phi(\sigma)=\phi\big(\sigma(1),\dots,\sigma(n)\big)$. For example

$$\begin{aligned}
\phi(1) &= \curlyvee\,,\\
\phi(12) &= \curlyvee\,, \quad \phi(21) = \curlyvee\,,\\
\phi(123) &= \curlyvee\,, \quad \phi(132) = \curlyvee\,, \quad \phi(213) = \curlyvee\,,\\
\phi(231) &= \curlyvee\,, \quad \phi(312) = \curlyvee\,, \quad \phi(321) = \curlyvee\,.
\end{aligned}$$

Note that the two permutations (213) and (312) correspond to the same tree, and they are also the two permutations that add up to a simple sum in the calculation of Z at the end of section II B. This is not a coincidence.

To simplify the proofs, we embrace the three cases of the definition of ϕ into a single one as follows. We first define the *concatenation product* of two tuples $I=(i_1,\dots,i_n)$ and $J=(j_1,\dots,j_m)$ as $I\cdot J=(i_1,\dots,i_n,j_1,\dots,j_m)$. We extend this definition to the case of the zero-tuple $I_0=\emptyset$ by $I_0\cdot I=I\cdot I_0=I$. Then, for any n-tuple I of distinct integers, we define $\phi(I)$ by $\phi(I)=|$ if $n=0$ and $\phi(I)=\phi(I_1)\vee\phi(I_2)$ otherwise, where I_1 and I_2 are determined by $I=I_1\cdot(\min I)\cdot I_2$. Note that I_1 or I_2 can be the zero-tuple.

We first prove an easy lemma.

Lemma 2 *If the elements of the two n-tuples $I=(i_1,\dots,i_n)$ and $J=(j_1,\dots,j_n)$ of distinct integers have the same ordering (i.e. if $i_k<i_l$ if and only if $j_k<j_l$ for all k and l in $\{1,\dots,n\}$), then $\phi(I)=\phi(J)$.*

Proof. The proof is by induction. If $n=0$, then $I=J=\emptyset$ and $\phi(I)=\phi(J)=|$. Assume that the property is true for k-tuples of distinct integers up to $k=n-1$ and take two n-tuples I and J having the same ordering. Then, the minimum element of both is at the same position k (i.e. $\min I=i_k$ and $\min J=j_k$) and $I=I_1\cdot(i_k)\cdot I_2$, $J=J_1\cdot(j_k)\cdot J_2$, where I_1 and J_1 (I_2 and J_2, respectively) are two $(k-1)$-tuples ($(n-k)$-tuples, respectively) of distinct integers have the same ordering. By the recursion hypothesis, we have $\phi(I_1)=\phi(J_1)$ and $\phi(I_2)=\phi(J_2)$ and the definition of ϕ gives us $\phi(I)=\phi(I_1)\vee\phi(I_2)=\phi(J_1)\vee\phi(J_2)=\phi(J)$. □

As a useful particular case, we consider the situation where J describes the ordering of the elements of I: we order the elements of $I=(i_1,\dots,i_n)$ increasingly as $i_{k_1}<\dots<i_{k_n}$. Then j_l is the position of i_l in this ordering. More formally, $J:=(\tau^{-1}(1),\dots,\tau^{-1}(n))$, where τ is the permutation $(k_1,\dots,k_n)$. The n-tuple J is called the *standardization* of I and it is denoted by $st(I)$. If we take the example of $I=(5,8,2)$, the position of 5, 8 and 2 in the ordering $2<5<8$ is 2, 3 and 1, respectively. Thus, $st(5,8,2)=(2,3,1)$. By construction, I and $st(I)$ have the same ordering and $\phi(I)=\phi(st(I))$. We extend the standardization to the case of $I=\emptyset$ by $st(\emptyset)=\emptyset$.

2. From trees to permutations

Conversely, we shall need to know the permutations corresponding to a given tree: $S_T:=\{\sigma\in\mathcal{S}_{|T|}\,:\,\phi(\sigma)=T\}$ (we extend this definition to the case of $T=|$ by defining the zero-element permutation group $\mathcal{S}_0:=\{\emptyset\}$). The solution of this problem is given by

Lemma 3 *If $T=T_1\vee T_2$, where $|T_1|=n$ and $|T_2|=m$ (n or m can be zero), all the permutations of S_T have the form $I=I_1\cdot(1)\cdot I_2$, where I_1 is a subset of n elements of $\{2,\dots,n+m+1\}$ ordered according to a permutation α of S_{T_1} (i.e. $st(I_1)=\alpha$) and I_2 is the complement of I_1 in $\{2,\dots,n+m+1\}$, ordered according to a permutation β of S_{T_2} (i.e. $st(I_2)=\beta$).*

Proof. The proof is given in refs. 29 and 30, but we can sketch it here for completeness. The simplest examples are $S_T=\{\emptyset\}$ for $T=|$ and $S_T=\{(1)\}$ for $T=\curlyvee$. Now take $T=T_1\vee T_2$ as in the lemma. By the definition of ϕ, the minimum of the tuple $I=(\sigma(1),\dots,\sigma(n+m+1))$ is $\sigma(n+1)=1$ and $I=I_1\cdot(1)\cdot I_2$, where $\phi(I_1)=T_1$ and $\phi(I_2)=T_2$. We saw in the previous section that $\phi(I_1)=\phi(st(I_1))$. By definition $st(I_1)$ is a permutation of $\mathcal{S}_n$. Therefore, $st(I_1)$ belongs to S_{T_1} and, similarly, $st(I_2)$ belongs to S_{T_2}. It is now enough to check that each element of S_T is obtained exactly once by running the construction over all orderings and all permutations of T_1 and T_2. □

This lemma allows us to recursively determine the number of elements of S_T, denoted by $|S_T|$, by $|S_T|=1$ for $T=|$ and $T=\curlyvee$ and, for $T=T_1\vee T_2$,

$$|S_T| \;=\; \binom{|T|-1}{|T_1|}|S_{T_1}|\,|S_{T_2}|. \tag{7}$$

See ref. 29 for an alternative approach.

Example: Consider the tree $T = T_1 \vee T_2$, with $T_1 =$  and $T_2 =$  , so that $n = 1$ and $m = 3$. S_{T_1} contains the single permutation $\alpha = (1)$ and, according to the examples given in the previous section, the two permutations of S_{T_2} are $\beta_1 = (213)$ and $\beta_2 = (312)$. We choose the permutations α and β_1, we pick up $n = 1$ element (for example 3) in the set $J = \{2, 3, 4, 5\}$, so that $I_1 = (3)$ and we order the remaining elements $\{2, 4, 5\}$ according to β_1, so that $I_2 = (4, 2, 5)$. This gives us $\sigma = (31425)$. If we pick up the other elements of J to build I_1 we obtain $(21435), (41325)$ and (51324). We add the elements obtained by choosing β_2 and we obtain eight permutations:

$$S_T = \{(21435), (21534), (31425), (31524), (41325), (41523), (51324), (51423)\}.$$

We can check that eq. (7) holds and that $|S_T| = 8$.

D. Recursion formula

The permutations corresponding to a tree can be used to make a partial summation of the terms of the Picard-Dyson expansion.

Definition 4 *For any tree T, we define $\Omega_T(t, t_0)$ by $\Omega_T(t, t_0) = P$ if $T =$* *and*

$$\Omega_T(t, t_0) \;:=\; \sum_{\sigma \in S_T} \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \ldots \int_{t_0}^{t_{n-1}} \mathrm{d}t_n X(t_{\sigma(1)}) \ldots X(t_{\sigma(n)}),$$

otherwise, where $n = |T|$.

With this notation we have obviously $\Omega(t, t_0) = \sum_T \Omega_T(t, t_0) = \sum_\sigma \Omega_\sigma(t, t_0)$, with the notation $\Omega_\sigma(t, t_0) := \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \ldots \int_{t_0}^{t_{n-1}} \mathrm{d}t_n X(t_{\sigma(1)}) \ldots X(t_{\sigma(n)})$ and where σ runs over all permutations (of all orders). The term of order 0 of this series is $\Omega_{|} = P$ and the term of order one is

$$\Omega_T(t, t_0) \;=\; -\imath \int_{t_0}^{t} \mathrm{d}s Q H(s) P,$$

for $T =$  . The other terms enjoy a remarkably simple recurrence relation:

Theorem 5 *If $|T| > 1$, then $\Omega_T(t, t_0)$ can be expressed recursively by*

$$\begin{aligned}
\Omega_T(t, t_0) \;&=\; -\imath \int_{t_0}^{t} \mathrm{d}s Q H(s) \Omega_{T_2}(s, t_0), \;\text{ if } T = \,| \,\vee T_2, \\
\Omega_T(t, t_0) \;&=\; \imath \int_{t_0}^{t} \mathrm{d}s \Omega_{T_1}(s, t_0) H(s) P, \;\text{ if } T = T_1 \vee \,| \,, \\
\Omega_T(t, t_0) \;&=\; \imath \int_{t_0}^{t} \mathrm{d}s \Omega_{T_1}(s, t_0) H(s) \Omega_{T_2}(s, t_0), \;\text{ if } T = T_1 \vee T_2,
\end{aligned}$$

where $T_1 \neq$ *and $T_2 \neq$* .

Note that a similar recursive expression was conjectured by Olszewski for the nondegenerate Rayleigh-Schrödinger expansion[27].

Proof. Let us prove the theorem recursively. Consider an arbitrary $T = T_1 \vee T_2$, $|T| > 1$, and assume the formulas to hold for all the trees T' with $|T'| < |T|$. Consider for example the case where $T_1 \neq$ and $T_2 \neq$ (the other cases are even simpler). We define:

$$A_T := \imath \int_{t_0}^{t} \mathrm{d}s \Omega_{T_1}(s, t_0) H(s) \Omega_{T_2}(s, t_0) = \sum_{\alpha \in S_{T_1}, \beta \in S_{T_2}} \imath \int_{t_0}^{t} \mathrm{d}s \Omega_\alpha(s, t_0) H(s) \Omega_\beta(s, t_0).$$

This first important point is that, for a given tree T, all the permutations $\sigma \in S_T$ have the same descent set. This is a well-known fact[23,30] that can be deduced from the characterization of S_T at the end of section II C. As a consequence,

the sequence of operators P, Q and H is the same for all α and β in A_T, and only the order of the arguments t_i varies. Therefore, the conditions of lemma 16 (see appendix A) are satisfied and we get:

$$A_T = \sum_\gamma \Omega_\gamma(t, t_0),$$

where γ runs over the permutations such that $\gamma(|T_1|+1) = 1$, $st(\gamma(1), ..., \gamma(|T_1|)) \in S_{T_1}$, $st(\gamma(|T_1|+2), ..., \gamma(|T_1| + |T_2|+1)) \in S_{T_2}$. The set of permutations γ satisfying these equations is precisely S_T, so that, finally: $A_T = \Omega_T(t, t_0)$. This concludes the proof of the theorem. □

E. Remarks

1. Nonlinear integral equation

If we denote $\chi(t, t_0) = \Omega(t, t_0) - P$, then the recurrence relations add up to

$$\imath\chi(t,t_0) \;=\; \int_{t_0}^{t} \mathrm{d}s QH(s)P + \int_{t_0}^{t} \mathrm{d}s QH(s)\chi(s,t_0) - \int_{t_0}^{t} \mathrm{d}s \chi(s,t_0)H(s)P - \int_{t_0}^{t} \mathrm{d}s \chi(s,t_0)H(s)\chi(s,t_0). \tag{8}$$

The derivative of this equation with respect to t was obtained in a different way by Jolicard[3].

2. Permutations, trees and descents

We saw that, for a given tree T, all permutations of S_T have the same descent set. We can now give more details[30,34]. The relation between the trees and the sequences of operators P and Q in eq. (3) is very simple. Consider the sequence of leaves from left to right. Each leaf pointing to the right corresponds to a P, each leaf pointing to the left correspond to a Q. For example, the tree  corresponds to the sequence $QQPP$. From the combinatorial point of view, this description emphasizes the existence of a relationship between trees and descent sets (or, equivalently, hypercubes), see e.g. refs. 23,34–37 and our Appendix.

III. ADIABATIC SWITCHING

Morita's formula is most often applied to an interaction Hamiltonian $H^\epsilon(t) := \mathrm{e}^{-\epsilon|t|}\mathrm{e}^{\imath H_0 t} V \mathrm{e}^{-\imath H_0 t}$. We write $E_0, ..., E_n, ...$ and $\Phi_0, ..., \Phi_n, ...$ for the eigenvalues of H_0 and for an orthogonal basis of corresponding eigenstates. We assume that the spectrum is discrete and that the eigenvalues are ordered by (weakly) increasing order. The ground state may be degenerate ($E_0 = E_1 = ... = E_k$ for a given k). The model space M (see the Introduction) is the vector space generated by the lowest N eigenstates of H_0 (with $N \geq k$). We assume that the energies of the eigenstates of M are separated by a finite gap from the energies of the eigenstates that do not belong to M. The projector P is the projector onto the model space M. Following the notation of the Introduction, the energies of the eigenstates that belong (resp. do not belong) to M are denoted by E_i^P (resp. E_i^Q).

In this section, we prove the convergence of each term of the perturbation expansion of the wave operator when $\epsilon \to 0$. For notational convenience, we assume that $t \leq 0$. We first give a nonperturbative proof of this convergence. Then, we expand in series and we consider the different cases of the previous sections.

A. Nonperturbative proof

The nonperturbative proof is important in this context because its range of validity is wider than the series expansion (no convergence criterion for the series is required). Moreover, the proof that the wave operator indeed leads to an effective Hamiltonian is much easier to give in the nonperturbative setting.

The first condition required in the nonperturbative setting is that the perturbation V must be relatively bounded with respect to H_0 with a bound strictly smaller than 1. This condition is satisfied for the Hamiltonian describing nuclei and electrons interacting through a Coulomb potential[38]. Before stating the second condition, we define the time independent Hamiltonian $h(\lambda) = H_0 + \lambda V$, its eigenvalues $E_j(\lambda)$ and its eigenprojectors $P_j(\lambda)$, such that

$h(\lambda)P_j(\lambda) = E_j(\lambda)P_j(\lambda)$. The second condition is that the eigenvalues $E_j(\lambda)$ coming from the eigenstates of the model space (i.e. such that $P_j(0)P = P_j(0)$) are separated by a finite gap from the rest of the spectrum. According to Kato[38], the eigenvalues and eigenprojectors can be chosen analytic in λ. Then, a recent version of the adiabatic theorem[39,40] shows that there exists a unitary operator A, independent of ϵ, such that

$$\lim_{\epsilon\to 0} ||U_\epsilon(0,-\infty)P_j(0) - \mathrm{e}^{\imath\theta_j/\epsilon}AP_j(0)|| \;=\; 0,$$

where $U_\epsilon(t,t_0)$ is the evolution operator for the Hamiltonian $H^\epsilon(t) = \mathrm{e}^{-\epsilon|t|}\mathrm{e}^{\imath H_0 t}V\mathrm{e}^{-\imath H_0 t}$ and

$$\theta_j \;=\; \int_0^1 \frac{E_j(0) - E_j(\lambda)}{\lambda}\mathrm{d}\lambda.$$

In other words, the singularity of $U_\epsilon(0,-\infty)P_j(0)$ is entirely described by the factor $\mathrm{e}^{\imath\theta_j/\epsilon}$. The operator A satisfies the intertwining property $AP_j(0) = P_j(1)A$. To connect this result with the case that we are considering in this paper, we have to choose a model space M that satisfies the following condition: there is a set I of indices j such that $P = \sum_{j\in I} P_j(0)$, where P is the projector onto M.

This enables us to give a more precise condition for the invertibility of $PU_\epsilon(0,-\infty)P$. The adiabatic theorem shows that, for small enough ϵ, $PU_\epsilon(0,-\infty)P$ is invertible if and only if PAP is invertible. If we rewrite $PAP = \sum_j PAP_j(0) = \sum_j PP_j(1)A$, the unitarity of A implies that PAP is invertible iff the kernel of $\sum_j PP_j(1)$ is trivial. We recover the well-known invertibility condition[18] that no state of the model space should be orthogonal to the vector space spanned by all the eigenstates of H with energy $E_j(1)$, where j runs over I. Note that, when the condition of invertibility is not satisfied, it can be recovered by adding the perturbation step by step[39].

Then, we have

Theorem 6 *With the given conditions, the wave operator*

$$\overline{\Omega} \;:=\; \lim_{\epsilon\to 0} U_\epsilon(0,-\infty)P(PU_\epsilon(0,-\infty)P)^{-1}$$

is well defined. Moreover, there are states $|\tilde\varphi_j\rangle$ in the model space such that $\overline{\Omega}|\tilde\varphi_j\rangle$ is an eigenstate of H with eigenvalue $E_j(1)$ and the effective Hamiltonian $H_{\mathrm{eff}} := PH\overline{\Omega}$ satisfies $H_{\mathrm{eff}}|\tilde\varphi_j\rangle = E_j(1)|\tilde\varphi_j\rangle$.

Proof. We first define $A_{jk} = P_j(0)AP_k(0)$, for j and k in I. Then an inverse B of PAP is defined by $\sum_{k\in I} A_{jk}B_{kl} = \delta_{jl}P_j(0)$ where $B_{jk} = P_j(0)BP_k(0)$. Then, $(PU_\epsilon(0,-\infty)P)^{-1} \simeq \sum_{jk} \mathrm{e}^{-\imath\theta_j/\epsilon}B_{jk}$ and

$$\Omega_\epsilon(0,-\infty) \;:=\; U_\epsilon(0,-\infty)P(PU_\epsilon(0,-\infty)P)^{-1} \simeq \sum_{jk} AP_j(0)B_{jk}.$$

Since the right hand side does not depend on ϵ, then $\Omega_\epsilon(0,-\infty)$ has no singularity at $\epsilon = 0$ and

$$\overline{\Omega} \;=\; \lim_{\epsilon\to 0}\Omega_\epsilon(0,-\infty) = \sum_{jk} AP_j(0)B_{jk}.$$

This proves the existence of the wave operator. To prove the existence of the states $|\tilde\varphi_j\rangle$ of the theorem, define $|\tilde\varphi_j\rangle = PA|\varphi_j\rangle$, where $|\varphi_j\rangle$ is an eigenstate of $P_j(0)$: $P_j(0)|\varphi_j\rangle = |\varphi_j\rangle$. Indeed, we have

$$\overline{\Omega}|\tilde\varphi_j\rangle \;=\; \overline{\Omega}PAP_j(0)|\varphi_j\rangle = \sum_{km} AP_k(0)B_{km}A_{mj}|\varphi_j\rangle = AP_j(0)|\varphi_j\rangle = P_j(1)A|\varphi_j\rangle,$$

where we used the intertwining property in the last equation. We can now check that $\overline{\Omega}|\tilde\varphi_j\rangle$ is an eigenstate of H with eigenvalue $E_j(1)$.

$$H\overline{\Omega}|\tilde\varphi_j\rangle \;=\; h(1)P_j(1)A|\phi_j\rangle = E_j(1)P_j(1)A|\phi_j\rangle = E_j(1)\overline{\Omega}|\tilde\varphi_j\rangle. \tag{9}$$

Finally, by multiplying eq. (9) by P from the left, we obtain

$$H_{\mathrm{eff}}|\tilde\varphi_j\rangle \;=\; E_j(1)P\overline{\Omega}|\tilde\varphi_j\rangle = E_j(1)|\tilde\varphi_j\rangle,$$

because $P\overline{\Omega} = P$ and $P|\tilde\varphi_j\rangle = |\tilde\varphi_j\rangle$. □

Thus, the eigenvalues of H_{eff} are eigenvalues of the full Hamiltonian H. This is exactly what is expected from an effective Hamiltonian. In practice, the operator A is not known and the states $|\tilde\varphi_j\rangle$ are obtained by diagonalizing H_{eff}.

B. Series expansion

We consider again the series expansion in terms of permutations. A straightforward calculation[41,42] of the Picard-Dyson series gives us

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

where we used the completeness relation $1=\sum_i|\Phi_i\rangle\langle\Phi_i|$. This expression clearly shows that the terms of the expansion (and the evolution operator) are divergent as $\epsilon\to 0$ when any E_{i_k} is equal to E_0.

For $\sigma\in\mathcal{S}_n$, we set $\Omega_\sigma(t):=\Omega_\sigma(t,-\infty)$. We then have

$$\begin{aligned}\Omega_\sigma(t) \;=\; (-\imath)^n\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\dots\int_{-\infty}^{t_{n-1}}\mathrm{d}t_n Q\mathrm{e}^{(\epsilon+\imath H_0)t_{\sigma(1)}}V\mathrm{e}^{-\imath H_0 t_{\sigma(1)}}R^1_\sigma\\ \mathrm{e}^{(\epsilon+\imath H_0)t_{\sigma(2)}}V\mathrm{e}^{-\imath H_0 t_{\sigma(2)}}R^2_\sigma\dots R^{n-1}_\sigma\mathrm{e}^{(\epsilon+\imath H_0)t_{\sigma(n)}}V\mathrm{e}^{-\imath H_0 t_{\sigma(n)}}P,\end{aligned}$$

where $R^k_\sigma:=Q$ if $\sigma(k+1)>\sigma(k)$ and $R^k_\sigma:=-P$ if $\sigma(k+1)<\sigma(k)$. We replace R^k_σ by $\pm\sum_{\alpha_{k+1}}|\alpha_{k+1}\rangle\langle\alpha_{k+1}|$ where, if $R^k_\sigma=Q$, then $\pm=+$ and the sum is over the image of Q, and if $R^k_\sigma=-P$, then $\pm=-$ and the sum is over the image of P. Thus

$$\begin{aligned}\Omega_\sigma(t) \;=\; (-\imath)^n(-1)^d\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\dots\int_{-\infty}^{t_{n-1}}\mathrm{d}t_n\mathrm{e}^{(\epsilon+\imath F_1-\imath F_2)t_{\sigma(1)}}\mathrm{e}^{(\epsilon+\imath F_2-\imath F_3)t_{\sigma(2)}}\dots\mathrm{e}^{(\epsilon+\imath F_n-\imath F_{n+1})t_{\sigma(n)}}\\ \sum_{\alpha_1\dots\alpha_{n+1}}|\alpha_1\rangle\langle\alpha_1|V|\alpha_2\rangle\dots\langle\alpha_n|V|\alpha_{n+1}\rangle\langle\alpha_{n+1}|,\end{aligned}\tag{10}$$

where d is the number of elements of the descent set of σ, F_i is the energy of α_i and where the sum over α_1 is over the image of Q, the sum over α_{n+1} is over the image of P and the sum over α_k for $1<k<n+1$ is over the image of Q if $\sigma(k)>\sigma(k-1)$ and over the image of P otherwise. Consider now the time integral

$$\begin{aligned}f_\sigma(t) \;&:=\; \int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\dots\int_{-\infty}^{t_{n-1}}\mathrm{d}t_n\mathrm{e}^{(\epsilon+\imath F_1-\imath F_2)t_{\sigma(1)}}\mathrm{e}^{(\epsilon+\imath F_2-\imath F_3)t_{\sigma(2)}}\dots\mathrm{e}^{(\epsilon+\imath F_n-\imath F_{n+1})t_{\sigma(n)}}\\ &=\; \int_{-\infty}^{t}\mathrm{d}s_{\tau(1)}\int_{-\infty}^{s_{\tau(1)}}\mathrm{d}s_{\tau(2)}\dots\int_{-\infty}^{s_{\tau(n-1)}}\mathrm{d}s_{\tau(n)}\mathrm{e}^{(\epsilon+\imath F_1-\imath F_2)s_1}\mathrm{e}^{(\epsilon+\imath F_2-\imath F_3)s_2}\dots\mathrm{e}^{(\epsilon+\imath F_n-\imath F_{n+1})s_n},\end{aligned}$$

where $\tau=\sigma^{-1}$. The integral over $s_{\tau(n)}$ is

$$\int_{-\infty}^{s_{\tau(n-1)}}\mathrm{d}s_{\tau(n)}\mathrm{e}^{(\epsilon+\imath F_{\tau(n)}-\imath F_{\tau(n)+1})s_{\tau(n)}} \;=\; \frac{\mathrm{e}^{(\epsilon+\imath F_{\tau(n)}-\imath F_{\tau(n)+1})s_{\tau(n-1)}}}{(\epsilon+\imath F_{\tau(n)}-\imath F_{\tau(n)+1})}.$$

The integrand of the integral over $s_{\tau(n-1)}$ becomes

$$\frac{\mathrm{e}^{(2\epsilon+\imath(F_{\tau(n)}+F_{\tau(n-1)}-F_{\tau(n)+1}-F_{\tau(n-1)+1})s_{\tau(n-1)}}}{(\epsilon+\imath F_{\tau(n)}-\imath F_{\tau(n)+1})}.$$

A straightforward recursive argument shows that

$$f_\sigma(t) \;=\; \frac{\mathrm{e}^{X_\sigma(n)t}}{X_\sigma(1)\dots X_\sigma(n)},$$

where

$$X_\sigma(k) \;:=\; k\epsilon+\imath(F_{\sigma^{-1}(n)}+\dots+F_{\sigma^{-1}(n-k+1)}-F_{\sigma^{-1}(n)+1}-\dots-F_{\sigma^{-1}(n-k+1)+1}).\tag{11}$$

Therefore,

$$\Omega_\sigma(t) \;=\; \sum_{\alpha_1\dots\alpha_{n+1}}\frac{(-\imath)^n(-1)^d\mathrm{e}^{X_\sigma(n)t}}{X_\sigma(1)\dots X_\sigma(n)}|\alpha_1\rangle\langle\alpha_1|V|\alpha_2\rangle\dots\langle\alpha_n|V|\alpha_{n+1}\rangle\langle\alpha_{n+1}|.\tag{12}$$

C. Examples

A few examples of $\Omega_\sigma(0)$ are

$$\begin{aligned}
\Omega_{(1)}(0) &= (-\imath)\sum_{\Phi_i\Phi_j}\frac{|\Phi_i\rangle\langle\Phi_i|V|\Phi_j\rangle\langle\Phi_j|}{\epsilon+\imath(E_i^Q-E_j^P)},\\
\Omega_{(12)}(0) &= (-\imath)^2\sum_{\Phi_i\Phi_j\Phi_k}\frac{|\Phi_i\rangle\langle\Phi_i|V|\Phi_j\rangle\langle\Phi_j|V|\Phi_k\rangle\langle\Phi_k|}{\big(\epsilon+\imath(E_j^Q-E_k^P)\big)\big(2\epsilon+\imath(E_i^Q-E_k^P)\big)},\\
\Omega_{(21)}(0) &= -(-\imath)^2\sum_{\Phi_i\Phi_j\Phi_k}\frac{|\Phi_i\rangle\langle\Phi_i|V|\Phi_j\rangle\langle\Phi_j|V|\Phi_k\rangle\langle\Phi_k|}{\big(\epsilon+\imath(E_i^Q-E_j^P)\big)\big(2\epsilon+\imath(E_i^Q-E_k^P)\big)}.
\end{aligned}$$

Finally we consider two examples that will prove useful:

$$\begin{aligned}
\Omega_{(213)}(0) &= -(-\imath)^3\sum_{\Phi_i\Phi_j\Phi_k\Phi_l}\frac{|\Phi_i\rangle\langle\Phi_i|V|\Phi_j\rangle\langle\Phi_j|V|\Phi_k\rangle\langle\Phi_k|V|\Phi_l\rangle\langle\Phi_l|}{\big(\epsilon+\imath(E_k^Q-E_l^P)\big)\big(2\epsilon+\imath(E_k^Q+E_i^Q-E_l^P-E_j^P)\big)\big(3\epsilon+\imath(E_i^Q-E_l^P)\big)},\\
\Omega_{(312)}(0) &= -(-\imath)^3\sum_{\Phi_i\Phi_j\Phi_k\Phi_l}\frac{|\Phi_i\rangle\langle\Phi_i|V|\Phi_j\rangle\langle\Phi_j|V|\Phi_k\rangle\langle\Phi_k|V|\Phi_l\rangle\langle\Phi_l|}{\big(\epsilon+\imath(E_i^Q-E_j^P)\big)\big(2\epsilon+\imath(E_k^Q+E_i^Q-E_l^P-E_j^P)\big)\big(3\epsilon+\imath(E_i^Q-E_l^P)\big)}.
\end{aligned}$$

By adding these two terms, we obtain a denominator involving only the difference of two energies.

$$\Omega_{(213)}(0)+\Omega_{(312)}(0) = -(-\imath)^3\sum_{\Phi_i\Phi_j\Phi_k\Phi_l}\frac{|\Phi_i\rangle\langle\Phi_i|V|\Phi_j\rangle\langle\Phi_j|V|\Phi_k\rangle\langle\Phi_k|V|\Phi_l\rangle\langle\Phi_l|}{\big(\epsilon+\imath(E_i^Q-E_j^P)\big)\big(\epsilon+\imath(E_k^Q-E_l^P)\big)\big(3\epsilon+\imath(E_i^Q-E_l^P)\big)}.$$

Note that the sum is simpler than either $\Omega_{(213)}(0)$ or $\Omega_{(312)}(0)$. This is a general statement and the simplification becomes spectacular at higher orders. For the example of $n=7$, there is a single tree T which is the sum of 80 permutations, and the denominator of Ω_T is simpler than the denominator of Ω_σ for any of the 80 permutations σ of S_T. This will be proved in section IV. Note also that, if we assume that the states in the image of P (i.e. the model space) are separated from the states in the image of Q by a finite gap δ, so that $E_i^Q-E_j^P\geq\delta$, then the denominators of all the examples are non-zero when $\epsilon\to 0$. In other words, the limit $\lim_{\epsilon\to 0}\Omega_\sigma(0)$ exists for all the examples. In the next section, we show that this result is true for all permutations σ.

D. Convergence of $\Omega_\sigma(t)$

Definition (11) is convenient for a computer implementation but it does not make it clear that $X_\sigma(k)$ is nonzero if $\epsilon=0$. For that purpose, we need an alternative expression for $X_\sigma(k)$, which is essentially a corrected version of the graphical rule given by Michels and Suttorp[19]. We first extend any permutation $\sigma\in\mathcal{S}_n$ to the sequence of $n+2$ integers $\bar\sigma=(\bar\sigma(1),\ldots,\bar\sigma(n+2))=(0,\sigma(1),\ldots,\sigma(n),0)$. Then, for $k\in\{1,\ldots,n\}$, we define the two sets

$$\begin{aligned}
S_\sigma^<(k) &:= \{i\,|\,1\leq i\leq n+1 \text{ and } \bar\sigma(i)<k\leq\bar\sigma(i+1)\},\\
S_\sigma^>(k) &:= \{i\,|\,1\leq i\leq n+1 \text{ and } \bar\sigma(i)\geq k>\bar\sigma(i+1)\}.
\end{aligned}$$

For example, if $\sigma=(41325)$, then $S_\sigma^<(1)=\{1\}, S_\sigma^<(2)=\{1,3\}, S_\sigma^<(3)=\{1,3,5\}, S_\sigma^<(4)=\{1,5\}, S_\sigma^<(5)=\{5\}$ and $S_\sigma^>(1)=\{6\}, S_\sigma^>(2)=\{2,6\}, S_\sigma^>(3)=\{2,4,6\}, S_\sigma^>(4)=\{2,6\}, S_\sigma^>(5)=\{6\}$. The graphical meaning of these sets is illustrated in Figure 2. Notice that the vertical axis is oriented downwards in order to reflect the time-ordering in the integrals $S_\sigma(t)$.

Lemma 7 *(i) $S_\sigma^<(k)$ cannot be empty and (ii) $S_\sigma^<(k)$ and $S_\sigma^>(k)$ have the same number of elements.*

The lemma follows from the graphical interpretation of the construction of $S_\sigma^>(k)$ and $S_\sigma^<(k)$. The graph of σ (constructed as in Figure 1) is a sequence of edges connecting the points $(i,\bar\sigma(i))$. Since the graph starts from $(0,0)$ and since there exists one point with ordinate n, any horizontal line with non integer ordinate y, $0<y<n$, will be crossed from above by a segment (remember the vertical axis is oriented downwards). A similar elementary topological argument shows that such a horizontal line is always crossed successively from above and below by segments, the series of crossings starting from above and ending from below, which implies $|S_\sigma^<(k)|=|S_\sigma^>(k)|$.

The key step in the proof of convergence is

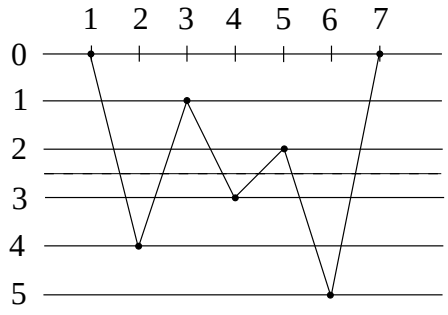

FIG. 2: Construction of $S^<_\sigma(3)$ for $\sigma = (41325)$. We build $\bar\sigma = (0, 4, 1, 3, 2, 5, 0)$, we draw a continuous line L starting from $(1, \bar\sigma(1)) = (1, 0)$ to $(2, \bar\sigma(2)) = (2, 4)$, to $(3, \bar\sigma(3)) = (3, 1)$, ..., up to $(7, \bar\sigma(7)) = (7, 0)$. To determine $S^<_\sigma(3)$, we draw a horizontal dashed line just above 3 and we gather the segments of L crossing the dashed line from above. In our case the segments are $\big((1, 0), (2, 4)\big)$, $\big((3, 1), (4, 3)\big)$ and $\big((5, 2), (6, 5)\big)$. $S^<_\sigma(3)$ is the set of abscissae of the first point of each segment: $S^<_\sigma(3) = \{1, 3, 5\}$. Similarly, $S^>_\sigma(3)$ is obtained from the segments that cross the dashed line from below: $S^>_\sigma(3) = \{2, 4, 6\}$.

Lemma 8 *For $\sigma \in \mathcal{S}_n$ and a given sequence $\alpha_1, \ldots, \alpha_{n+1}$, compatible with σ (see eq. (10)), we have*

$$X_\sigma(k) \;=\; k\epsilon + \sum_{j \in S^<_\sigma(n-k+1)} \imath F^Q_j - \sum_{j \in S^>_\sigma(n-k+1)} \imath F^P_j, \tag{13}$$

where we write $F^Q_i = F_i$ (resp. $F^P_i = F_i$) when α_i belongs to the image of Q (resp. of P).

Proof. We first show that it is true for $k = 1$. Indeed, $X_\sigma(1) = \epsilon + \imath(F_{\sigma^{-1}(n)} - F_{\sigma^{-1}(n)+1})$. Let $j = \sigma^{-1}(n)$, we have $\sigma(j) = n$. Then, either $j = 1$ and $|\alpha_1\rangle$ is in the image of Q, or $j > 1$ and $\sigma \in \mathcal{S}_n$ implies $\sigma(j) = n > \sigma(j-1)$, so that $|\alpha_j\rangle$ is in the image of Q. Thus, in all cases, $F_{\sigma^{-1}(n)} = F^Q_{\sigma^{-1}(n)}$. Consider now F_{j+1}. Either $j = n$ and $|\alpha_{j+1}\rangle = |\alpha_{n+1}\rangle$ is in the image of P, or $j < n$ and $\sigma(j+1) < \sigma(j) = n$, so that $|\alpha_{j+1}\rangle$ is in the image of P. Thus, in all cases, $F_{\sigma^{-1}(n)+1} = F^P_{\sigma^{-1}(n)+1}$. Therefore, $X_\sigma(1) = \epsilon + \imath(F^Q_{\sigma^{-1}(n)} - F^P_{\sigma^{-1}(n)+1})$. On the other hand, $S^<_\sigma(n) = \{\sigma^{-1}(n)\}$ and $S^>_\sigma(n) = \{\sigma^{-1}(n) + 1\}$ since (j, n) is the only point of the graph with ordinate n. Thus, the two members of eq. (13) are equal for $k = 1$.

Assume now that eq. (13) holds for all the $X_\sigma(i)$ with $i = 1, \ldots, k$, $k < n$, and consider the equation (which is true by definition of the $X_\sigma(i)$s):

$$X_\sigma(k+1) \;=\; X_\sigma(k) + \epsilon + \imath(F_j - F_{j+1}), \tag{14}$$

where $j = \sigma^{-1}(n-k)$. We first treat the case $1 < j < n$. Four possible situations can arise: (i) $\sigma(j-1) > \sigma(j) > \sigma(j+1)$, (ii) $\sigma(j-1) < \sigma(j) > \sigma(j+1)$, (iii) $\sigma(j-1) > \sigma(j) < \sigma(j+1)$ and (iv) $\sigma(j-1) < \sigma(j) < \sigma(j+1)$. In case (i), we have $F_j = F^P_j$ and $F_{j+1} = F^P_{j+1}$. On the other hand, condition (i) implies $\bar\sigma(j) > \bar\sigma(j+1) > \bar\sigma(j+2)$, so that $S^>_\sigma(n-k) = S^>_\sigma(n-k+1)$ and $S^<_\sigma(n-k)$ is obtained from $S^<_\sigma(n-k+1)$ by removing $\{j\}$ and adding $\{j+1\}$. eq. (14) together with the hypothesis that eq. (13) holds for $X_\sigma(k)$ imply that eq. (13) holds for $X_\sigma(k+1)$. Case (ii) implies $F_j = F^Q_j$ and $F_{j+1} = F^P_{j+1}$, case (iii) implies $F_j = F^P_j$ and $F_{j+1} = F^Q_{j+1}$, case (iv) implies $F_j = F^Q_j$ and $F_{j+1} = F^Q_{j+1}$. In all cases, these identities imply that the two expressions (14) and (13) for $X_\sigma(k+1)$ do agree.

It remains to treat the boundary cases. If $j = 1$, then $F_j = F^Q_1$ and we have either (i) $\sigma(1) < \sigma(2)$ and $F_2 = F^Q_2$ or (ii) $\sigma(1) > \sigma(2)$ and $F_2 = F^P_2$. We know that $\bar\sigma(1) = 0$, thus, case (i) corresponds to $\bar\sigma(1) < \bar\sigma(2) < \bar\sigma(3)$, so that according to eq. (13),

$$X_\sigma(k+1) - X_\sigma(k) = \imath(F^Q_1 - F^Q_2),$$

in agreement with eq. (14). In case (ii) we have $\bar\sigma(1) < \bar\sigma(2) > \bar\sigma(3)$, which amounts to add $\imath F^Q_1$ and remove $\imath F^P_2$. Again, eq. (13) holds for $k+1$. Finally, if $j = n$, then $F_{j+1} = F^P_{n+1}$ and we have (i) $\sigma(n-1) < \sigma(n)$ and $F_n = F^Q_n$ or (ii) $\sigma(n-1) > \sigma(n)$ and $F_n = F^P_n$. Case (i) corresponds to $\bar\sigma(n) < \bar\sigma(n+1) > \bar\sigma(n+2)$, case (ii) corresponds to $\bar\sigma(n) > \bar\sigma(n+1) > \bar\sigma(n+2)$. In all cases, the relation given by eq. (13) is satisfied for $k+1$ and the induction proof is complete. □

We can now ready to prove

Theorem 9 *The limit*

$$\overline{\Omega}_\sigma \;=\; \lim_{\epsilon\to 0}\Omega_\sigma(0), \tag{15}$$

is well-defined.

Proof. To prove the term-wise convergence of $\Omega_\sigma(t)$ as $\epsilon\to 0$, consider eq. (13). The sets $S^<_\sigma(n-k+1)$ and $S^>_\sigma(n-k+1)$ have the same number of elements, say n_k and, by the gap hypothesis, we have $F^Q_j - F^P_i \geq \delta$ for any i and j. Therefore, $|X_\sigma(k)|^2 \geq k^2\epsilon^2 + n_k^2\delta^2 \geq \delta^2$, since $n_k \geq 1$. Thus, the denominator remains away from zero by a finite amount for any $\epsilon \geq 0$ and the limit of $1/X_\sigma(k)$ for $\epsilon\to 0$ is well-defined. □

IV. TREES

We showed that, for each permutation σ, the wave operator $\Omega_\sigma(t,-\infty)$ has a well-defined limit as $\epsilon\to 0$. The detailed proof was rather lengthy and the final expression for $X_\sigma(k)$ suggests physically the simultaneous occurrence of transitions from states of the model space to states out of it. The convergence is actually much easier to show in terms of trees, and the expressions showing up in the expansion are simpler, mathematically and physically, each factor of the denominator corresponding to a single difference between an energy in the model space and an energy out of it.

In this section, if N is the dimension of the model space, we write $i\in Q$ for $i>N$ and $j\in P$ for $1\leq j\leq N$, both for notational simplicity, and to emphasize the meaning of the indices, that correspond respectively to eigenstates in the image of Q and in the image of P (i.e. the model space).

Proposition 10 *If $T = T_1 \vee T_2$, then, for $t\leq 0$,*

$$\Omega_T(t) := \Omega_T(t,-\infty) \;=\; \sum_{i\in Q, j\in P} \mathrm{e}^{(\imath E^Q_i - \imath E^P_j + |T|\epsilon)t}\Omega^{ij}_T\,|\Phi_i\rangle\langle\Phi_j|, \tag{16}$$

where Ω^{ij}_T is obtained recursively by:

For $T = \curlyvee$, $\Omega^{ij}_{\curlyvee} := -\imath\frac{\langle\Phi_i|V|\Phi_j\rangle}{\imath E^Q_i - \imath E^P_j + \epsilon}$.

For $T_1 = |$, $T_2\neq |$: $\Omega^{ij}_T := -\imath\sum_{k\in Q}\frac{\langle\Phi_i|V|\Phi_k\rangle\Omega^{kj}_{T_2}}{\imath E^Q_i - \imath E^P_j + |T|\epsilon}$.

For $T_1\neq |$, $T_2 = |$: $\Omega^{ij}_T := \imath\sum_{k\in P}\frac{\Omega^{ik}_{T_1}\langle\Phi_k|V|\Phi_j\rangle}{\imath E^Q_i - \imath E^P_j + |T|\epsilon}$.

For $T_1\neq |$, $T_2\neq |$: $\Omega^{ij}_T := \imath\sum_{k\in P, l\in Q}\frac{\Omega^{ik}_{T_1}\langle\Phi_k|V|\Phi_l\rangle\Omega^{lj}_{T_2}}{\imath E^Q_i - \imath E^P_j + |T|\epsilon}$.

Proof. The computation of $\Omega^{ij}_{\curlyvee}$ follows from eq. (12). Let us consider for example the case $T_1 = |$, $T_2\neq |$. Then, by applying theorem 5:

$$\Omega_T(t) \;=\; -\imath\sum_{i\in Q, j\in P}\int_{-\infty}^t \mathrm{d}s Q\mathrm{e}^{\epsilon s}\mathrm{e}^{-\imath E^Q_i s}\mathrm{e}^{(\imath E^Q_i - \imath E^P_j + |T_2|\epsilon)s}\Omega^{ij}_{T_2}\mathrm{e}^{iH_0 s}V|\Phi_i\rangle\langle\Phi_j|.$$

We replace Q by $\sum_{k\in Q}|\Phi_k\rangle\langle\Phi_k|$ and obtain, by using $|T| = |T_2|+1$,

$$\begin{aligned}\Omega_T(t) \;&=\; -\imath\sum_{k,i\in Q, j\in P}\int_{-\infty}^t \mathrm{d}s\mathrm{e}^{(\imath E^Q_k - \imath E^P_j + |T|\epsilon)s}\langle\Phi_k|V|\Phi_i\rangle\Omega^{ij}_{T_2}|\Phi_k\rangle\langle\Phi_j| \\ &=\; -\imath\sum_{k,i\in Q, j\in P}\frac{\mathrm{e}^{(\imath E^Q_k - \imath E^P_j + |T|\epsilon)t}}{\imath E^Q_k - \imath E^P_j + |T|\epsilon}\langle\Phi_k|V|\Phi_i\rangle\Omega^{ij}_{T_2}|\Phi_k\rangle\langle\Phi_j|,\end{aligned}$$

The two other cases can be treated similarly. □

Since, for arbitrary i and j, $E^Q_i - E^P_j \geq \delta$, we get:

Corollary 11 *The limit $\bar{\Omega}_T(t) = \lim_{\epsilon\to 0}\Omega_T(t)$ is well defined.*

A. Relation with the Rayleigh-Schrödinger perturbation theory

Kvasnička[7] and Lindgren[6] independenty obtained an equation for the time-independent Rayleigh-Schrödinger perturbation theory of possibly degenerate systems:

$$[\overline{\omega}, H_0]P \;=\; V\overline{\omega}P - \overline{\omega}PV\overline{\omega}P, \tag{17}$$

where the time-independent wave operator $\overline{\omega}P$ transforms eigenstates $|\Phi_0\rangle$ of H_0 into eigenstates $\overline{\omega}P|\Phi_0\rangle$ of H_0+V and where $P\overline{\omega}P = P$ (see ref. 43 p. 202 for details).

Equation (17) is an important generalization of Bloch's classical results[44] because it is also valid for a quasi-degenerate model space (i.e. when the eigenstates of H_0 in the model space have different energies). The relation between time-dependent and time-independent perturbation theory is established by the following proposition:

Proposition 12 *We have* $\overline{\omega}P = \overline{\Omega} = \lim_{\epsilon\to 0}\Omega(0)$.

Proof. We take the derivative of eq. (8) with respect to time and we substitute $\chi(t,t_0) = \Omega(t,t_0) - P$. This gives us

$$\imath\frac{\mathrm{d}}{\mathrm{d}t}\Omega(t,t_0) \;=\; H(t)\Omega(t,t_0) - \Omega(t,t_0)H(t)\Omega(t,t_0).$$

If we take $t=0$ and $t_0 = -\infty$, we obtain by continuity

$$\imath\frac{\mathrm{d}}{\mathrm{d}t}\Omega(t)|_{t=0} \;=\; V\Omega(0) - \Omega(0)V\Omega(0).$$

When we compare this equation with eq. (17), we see that $\overline{\omega}P$ and $\overline{\Omega}$ satisfy the same equation if

$$\imath\lim_{\epsilon\to 0}\frac{\mathrm{d}\Omega(t)}{\mathrm{d}t}|_{t=0} \;=\; [\lim_{\epsilon\to 0}\Omega(0), H_0]. \tag{18}$$

To show this, we prove it for each term Ω_T. Indeed, eq. (16) gives us

$$\imath\frac{\mathrm{d}\Omega_T(t)}{\mathrm{d}t} \;=\; \sum_{i\in Q, j\in P}(E_j^P - E_i^Q + \imath|T|\epsilon)\mathrm{e}^{(\imath E_i^Q - \imath E_j^P + |T|\epsilon)t}\Omega_T^{ij}\,|\Phi_i\rangle\langle\Phi_j|,$$

and

$$[\Omega_T(t), H_0] \;=\; \sum_{i\in Q, j\in P}(E_j^P - E_i^Q)\mathrm{e}^{(\imath E_i^Q - \imath E_j^P + |T|\epsilon)t}\Omega_T^{ij}\,|\Phi_i\rangle\langle\Phi_j|.$$

By continuity in ϵ, these two expressions are identical for all t when $\epsilon\to 0$. If we take $t=0$ and we sum over all trees T, then we recover eq. (18). Therefore, $\overline{\omega}P$ and $\overline{\Omega}$ satisfy the same equation. It remains to show that they have the same boundary conditions: $\overline{\Omega}P = \overline{\Omega}$ and $P\overline{\Omega} = P$. By eq. (3), these two equations are true for $\Omega(t)$ with any value of t and ϵ. □

As a corollary, proposition 10 provides a recursive construction of the wave operator $\overline{\Omega}$.

B. An explicit formula for Ω_T

In this section, we show how $\Omega_T(t)$ can be obtained non-recursively from the knowledge of T. The key idea is to replace T by another combinatorial object, better suited to that particular computation. We write therefore γ_T for the smallest permutation for the lexicographical ordering in S_T (we view a permutation as a word to make sense of the lexicographical ordering: to (35421) corresponds the word 35421, so that e.g. (35421) < (54231)). Since S_T is always non empty, the map $\gamma : T \longmapsto \gamma_T$ is well-defined and an injection from the set of trees to the set of permutations. These permutations are called Catalan permutations[29], 312-avoiding permutations (i.e. permutations for which there does not exist $i<j<k$ such that $\sigma(j) < \sigma(k) < \sigma(i)$, see ref. 31 p. 224), Kempf elements[45] or stack words[46].

Various elementary manipulations can be done to understand such a map. We list briefly some obvious properties and introduce some notation that will be useful in our forthcoming developments. If $I = (a_1, ..., a_k)$ is a sequence of integers, we write $I[n]$ for the shifted sequence $(a_1+n, ..., a_k+n)$.

Then, let $T = T_1 \vee T_2$ be a tree. The permutation $\gamma(T)$ (that we identify with the corresponding word or sequence) can be constructed recursively as $\gamma(\,|\,) = \emptyset$, $\gamma(\,\curlyvee\,) = (1)$ and

$$\gamma(T) := (\gamma(T_1)[1], 1, \gamma(T_2)[|T_1|+1])).$$

The left inverse of γ, say $\mathcal{T}$, is also easily described recursively as $\mathcal{T}(\emptyset) = |$, $\mathcal{T}(1) := \curlyvee$ and

$$\mathcal{T}(\sigma) := \mathcal{T}((\sigma(1), ..., \sigma(k))[-1]) \vee \mathcal{T}((\sigma(k+2), ..., \sigma(n))[-k-1]),$$

where $\sigma \in \mathcal{S}_n$, $\sigma = (\sigma(1), ..., \sigma(k), 1, \sigma(k+2), ..., \sigma(n))$ is in the image of γ.

Permutations in the image of γ can be characterized recursively similarly: with the same notation as in the previous paragraph, σ is in the image of γ if and only if $(\sigma(1), ..., \sigma(k))[-1]$ and $(\sigma(k+2), ..., \sigma(n))[-k-1]$ are in the image of γ, where k is the integer such that $\sigma(k) = 1$,

We are now in a position to compute $\Omega_T(t)$. Let us write $\mathcal{A}_T$ for all the sequences $\boldsymbol{\alpha} = (\alpha_1, ..., \alpha_{n+1})$ associated to $\gamma(T)$ as in equation (10). We write, as usual, F_i for the eigenvalue associated to α_i. Recall that $\alpha_1 \in Q$, $\alpha_{n+1} \in P$ whereas $\alpha_i, i \neq 1, n+1$ is in Q if $\sigma(i) > \sigma(i-1)$ and in P otherwise.

These sequences are actually common to the expansions of all the $\Omega_\sigma(t), \sigma \in S_T$ (this is because they depend only on the positions of descents in the permutations $\sigma \in S_T$, as discussed in the proof of thm. 5). They appear therefore in the expansion of $\Omega_T(t) = \sum_{\sigma \in S_T} \Omega_\sigma(t)$. They actually also correspond exactly to the sequences of eigenvectors that show up in the recursive expansion of $\Omega_T(t)$ (proposition 16) (this should be clear from our previous remarks, but can be checked directly from the definition of the recursive expansion). We can refine the recursion of proposition 10 accordingly:

Lemma 13 *We have:* $\Omega_T(t) = \sum_{\boldsymbol{\alpha}} \mathrm{e}^{(\imath F_1 - \imath F_{n+1} + |T|\epsilon)t} \Omega_T^{\boldsymbol{\alpha}} |\alpha_1\rangle\langle\alpha_{n+1}|$, *where* $\Omega_T^{\boldsymbol{\alpha}}(t)$ *is defined recursively by:*

$$\Omega_{\curlyvee}^{\Phi_i, \Phi_j} = -\imath \frac{\langle \Phi_i | V | \Phi_j \rangle}{\imath E_i^Q - \imath E_j^P + \epsilon},$$

$$\Omega_T^{\boldsymbol{\alpha}} = \imath \frac{\Omega_{T_1}^{(\alpha_1, ..., \alpha_k)} \langle \alpha_k | V | \alpha_{k+1} \rangle \Omega_{T_2}^{(\alpha_{k+1}, ..., \alpha_n, \alpha_{n+1})}}{\imath F_1 - \imath F_{n+1} + |T|\epsilon},$$

where $T = T_1 \vee T_2$ *and* $k = |T_1|$. *For* $T_1 = |$, *we have* $\Omega_{T_1}^{(\alpha_1)} = -1$ *and for* $T_2 = |$, *we have* $\Omega_{T_2}^{(\alpha_{n+1})} = 1$.

Let us now consider γ_T. For $i = 1, \ldots, n$, we set: $l(i) = \inf\{j \leq i | \forall k, j \leq k \leq i, \gamma_T(k) \geq \gamma_T(i)\}$ and $r(i) = \sup\{j \geq i | \forall l, j \geq l \geq i, \gamma_T(l) \geq \gamma_T(i)\}$. In words, $l(i)$ is defined as follows: consider all the consecutive positions k on the left of position i, such that the value of the permutation $\gamma_T(k)$ is larger than $\gamma_T(i)$. Then, $l(i)$ is the leftmost of these positions k. Similarly, $r(i)$ is the rightmost position j such that, on all positions k between i and j, the permutation $\gamma_T(k)$ is larger than $\gamma_T(i)$.

Theorem 14 *We have:*

$$\Omega_T^{\boldsymbol{\alpha}} = (-\imath)^n (-1)^{d-1} \langle \alpha_1 | V | \alpha_2 \rangle ... \langle \alpha_n | V | \alpha_{n+1} \rangle \prod_{i=1}^n \frac{1}{\imath F_{l(i)} - \imath F_{r(i)+1} + (r(i) - l(i) + 1)\epsilon},$$

or, equivalently,

$$\Omega_T(t) = (-\imath)^n (-1)^{d-1} \sum_{\boldsymbol{\alpha}} |\alpha_1\rangle\langle\alpha_1 | V | \alpha_2 \rangle ... \langle \alpha_n | V | \alpha_{n+1} \rangle \langle \alpha_{n+1}| \mathrm{e}^{(\imath F_1 - \imath F_{n+1} + |T|\epsilon)t} \prod_{i=1}^n \frac{1}{\imath F_{l(i)} - \imath F_{r(i)+1} + (r(i) - l(i) + 1)\epsilon},$$

where d *is the number of leaves of* T *pointing to the right.*

For example, if $T = \curlyvee\!\curlyvee$, then $\gamma_T = (213)$, $l = (113)$, $r = (133)$ and

$$\Omega_T^{\Phi_i \Phi_j \Phi_k \Phi_l} = -\imath \sum_{\Phi_i \Phi_j \Phi_k \Phi_l} \frac{|\Phi_i\rangle\langle\Phi_i | V | \Phi_j\rangle\langle\Phi_j | V | \Phi_k\rangle\langle\Phi_k | V | \Phi_l\rangle\langle\Phi_l|}{\big(\epsilon + \imath(E_i^Q - E_j^P)\big)\big(\epsilon + \imath(E_k^Q - E_l^P)\big)\big(3\epsilon + \imath(E_i^Q - E_l^P)\big)}.$$

Proof. We show that Ω_T^α as defined in theorem 14 satisfies the recursion relation of lemma 13. Let us first consider that $T_1 \neq |$ and $T_2 \neq |$. Let i_0 denote the index such that $\gamma_T(i_0) = 1$, with $1 < i_0 < n$. The term of the numerator corresponding to i_0 is $\langle \alpha_{i_0} | V | \alpha_{i_0+1} \rangle$, which is the central term of the recursion relation. We have $l(i_0) = 1$ and $r(i_0) = n$. Thus, the denominator is $\imath F_{l(i_0)} - \imath F_{r(i_0)+1} + (r(i_0) - l(i_0) + 1)\epsilon = \imath F_1 - \imath F_{n+1} + n\epsilon$, which is the denominator of the recursion relation. Now we check that the product of terms for $i < i_0$ in theorem 14 is $\Omega_{T_1}^{(\alpha_1,\ldots,\alpha_{i_0-1})}$. The matrix elements $\langle \alpha_1 | V | \alpha_2 \rangle \ldots \langle \alpha_{i_0-1} | V | \alpha_{i_0} \rangle$ obviously agree, so we must check that the denominators agree. Thus, we verify that, for $1 \leq i < i_0$, $l_T(i) = l_{T_1}(i)$ and $r_T(i) = r_{T_1}(i)$, where l_T and r_T denote the l and r vectors for tree T. We know that $\gamma_T(i) = \gamma_{T_1}(i) + 1$ for $1 \leq i < i_0$. Thus, for $k \leq i$, $\gamma_T(k) \geq \gamma_T(i)$ if and only if $\gamma_{T_1}(k) \geq \gamma_{T_1}(i)$ and $l_T(i) = l_{T_1}(i)$. For r_T, we notice that for $l = i_0$ we have $\gamma_T(l) = 1 < \gamma_T(i)$ and the relation $\gamma_T(l) \geq \gamma_T(i)$ does not hold. Therefore, $r_T(i) < i_0$ and $r_T(i) = r_{T_1}(i)$ by the same argument as $l_T(i) = l_{T_1}(i)$. The same reasoning holds for T_2 and the recursion relation is satisfied. The cases $T_1 = |$ or $T_2 = |$ are proved similarly. □

We conclude this section with a geometrical translation of the previous theorem. Consider a tree T with $|T| = n$ and number its leaves from 1 for the leftmost leave to $n+1$ for the rightmost one. For each vertex v of T, take the subtree T_v for which v is the root. In other words, T_v is obtained by chopping the edge below v and considering the half-edge dangling from v as the dangling line of the root of T_v. For each tree T_v, build the pair (l_v, r_v) which are the indices of the leftmost and rightmost leaves of T_v. Recall that $|\alpha_i\rangle$ belongs to the image of Q (resp. P) if leaf i points to the left (resp. right): this implies in particular that $F_{l_v} = F_{l_v}^Q$ and $F_{r_v} = F_{r_v}^P$. Then, the set of pairs (l_v, r_v) where v runs over the vertices of T is the same as the set of pairs $(l(i), r(i) + 1)$ of the theorem. The formula for Ω_T^α can be rewritten accordingly and this geometrical version can be proved recursively as theorem 14. Conversely, it can be used to determine the tree corresponding to a given denominator.

V. CONCLUSION

We considered three expansions of the wave operator and we proved their adiabatic convergence. We proposed to expand the wave operator over trees, and proved that this expansion reduced the number of terms of the expansion with respect to usual (tractable) ones, simplified the denominators of the expansion into a product of the difference of two energies and lead to powerful formulas and recursive computational methods.

We then showed that this simplification is closely related to the algebraic structure of the linear span of permutations and of a certain convolution subalgebra of trees.

As far as the many-body problem is concerned, we showed that the simplification of diagrams is not due to the details of the Hamiltonian but to the general structure of the wave operator. When the eigenstates and Hamiltonian are expressed in terms of creation and annihilation operators and quantum fields, the algebra of trees mixes with the Hopf algebraic structure of fields[47,48]. It would be interesting to investigate the interplay of these algebraic structures.

The terms of the Rayleigh-Schrödinger series are usually considered to be "quite complicated" (see ref. 49, p. 8) and difficult to work with. The general term of the Rayleigh-Schrödinger series for quasi-degenerate systems is obtained as the limit for $\epsilon \to 0$ of $\Omega_T(0)$ in theorem 14. Through our recursive and non-recursive expressions for these terms, many proofs of their properties become almost trivial. The tree structure suggests various resummations of this series, that will be explored in a forthcoming publication.

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Appendix A: A crucial lemma

In this appendix we state and prove a lemma that is crucial to demonstrate theorem 5, which is one of the main results of our paper. We first need a noncommutative analogue of Chen's formulas for products of iterated integrals. This analogue, proved in refs. 50 and 22, provides a systematic link between the theory of iterated integrals, the combinatorics of descents, free Lie algebras and noncommutative symmetric functions (see ref. 22 and Appendix B of the present article for further details).

Let $L = (L_1, ..., L_n)$ be an arbitrary sequence of time-dependent operators $L_i(t)$, satisfying the same regularity conditions as $H(t)$ in section II. Let σ be a permutation in $\mathcal{S}_n$ and define:

$$\Omega^L_\sigma(t, t_0) := \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \ldots \int_{t_0}^{t_{n-1}} \mathrm{d}t_n L_1(t_{\sigma(1)}) \ldots L_n(t_{\sigma(n)}).$$

The notation is extended linearly to combinations of permutations, so that for $\mu := \sum_{\sigma \in \mathcal{S}_n} \mu_\sigma \sigma$, with $\mu_\sigma \in \mathbb{C}$. Then $\Omega^L_\mu(t, t_0)$ is defined as the linear combination $\sum_{\sigma \in \mathcal{S}_n} \mu_\sigma \Omega^L_\sigma(t, t_0)$. For $K := (K_1, ..., K_m)$ another sequence of time-dependent operators, we write $L \cdot K$ for the concatenation product $(L_1, ..., L_n, K_1, ..., K_m)$.

We also need to define the convolution product of two permutations. If $\alpha \in \mathcal{S}_n$ and $\beta \in \mathcal{S}_m$, then $\alpha * \beta$ is the sum of the $\binom{n+m}{n}$ permutations $\gamma \in \mathcal{S}_{n+m}$ such that $st(\gamma(1), ..., \gamma(n)) = (\alpha(1), ..., \alpha(n))$ and $st(\gamma(n+1), ..., \gamma(n+m)) = (\beta(1), ..., \beta(m))$. Here, st is the standardization map defined in section II C 1. For instance,

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

In words, the product of two permutations $\alpha \in \mathcal{S}_n$ and $\beta \in \mathcal{S}_m$ is the sum of all permutations σ of $\mathcal{S}_{n+m}$ such that the elements of the sequence $(\sigma(1), \ldots, \sigma(n))$ are ordered as the elements of $(\alpha(1), \ldots, \alpha(n))$, in the sense that $\alpha(i) > \alpha(j)$ if and only if $\sigma(i) > \sigma(j)$ and the elements of $(\sigma(n+1), \ldots, \sigma(n+m))$ are ordered as the elements of $(\beta(1), \ldots, \beta(m))$.

Now, we can state the noncommutative Chen formula[50] (see also remark 3.3, p. 4111 of ref. 22)

Lemma 15 *We have:*

$$\Omega^L_\alpha(t, t_0)\Omega^K_\beta(t, t_0) = \Omega^{L \cdot K}_{\alpha * \beta}(t, t_0).$$

The following lemma can be proven similarly:

Lemma 16 *We have, for L and K as above and J a time-dependent operator:*

$$\int_{t_0}^{t} \mathrm{d}s \Omega^L_\alpha(s, t_0) J(s) \Omega^K_\beta(s, t_0) = \sum_\gamma \Omega^{L \cdot (J) \cdot K}_\gamma(t, t_0),$$

where γ runs over the permutations in $\mathcal{S}_{n+m+1}$ with $\gamma(n+1) = 1$, $st(\gamma(1), ..., \gamma(n)) = \alpha$, $st(\gamma(n+2), ..., \gamma(n+m+1)) = \beta$.

Proof. We expand Ω^L_α and Ω^K_β

$$\begin{aligned}\int_{t_0}^{t} \mathrm{d}s \Omega^L_\alpha(s, t_0) J(s) \Omega^K_\beta(s, t_0) &= \int_{t_0}^{t} \mathrm{d}s \int_{t_0}^{s} \mathrm{d}u_1 \ldots \int_{t_0}^{u_{n-1}} \mathrm{d}u_n \int_{t_0}^{s} \mathrm{d}v_1 \ldots \int_{t_0}^{v_{m-1}} \mathrm{d}v_m \\ &\quad L_1(u_{\alpha(1)}) \ldots L_n(u_{\alpha(n)}) J(s) K_1(v_{\beta(1)}) \ldots K_m(v_{\beta(m)}).\end{aligned}$$

This is the same formula as for the expansion of $\Omega^L_\alpha(s, t_0)\Omega^K_\beta(s, t_0)$, up to the term $J(s)$ and the integration $\int_{t_0}^{t} \mathrm{d}s$ that however do not change the underlying combinatorics. Therefore, lemma 15 holds in the form

$$\begin{aligned}\int_{t_0}^{t} \mathrm{d}s \Omega^L_\alpha(s, t_0) J(s) \Omega^K_\beta(s, t_0) &= \sum_\sigma \int_{t_0}^{t} \mathrm{d}s \int_{t_0}^{s} \mathrm{d}s_1 \ldots \int_{t_0}^{s_{n+m-1}} \mathrm{d}s_{n+m} \\ &\quad L_1(s_{\sigma(1)}) \ldots L_n(s_{\sigma(n)}) J(s) K_1(s_{\sigma(n+1)}) \ldots K_m(s_{\sigma(n+m)}),\end{aligned}$$

where, by the definition of $\alpha * \beta$, the sum over σ is over all the permutations of $\mathcal{S}_{n+m}$ such that $st(\sigma(1), \ldots, \sigma(n)) = \alpha$ and $st(\sigma(n+1), \ldots, \sigma(n+m)) = \beta$. Now, we change variables to $t_1 = s$, $t_{i+1} = s_i$ for $i = 1, \ldots, n+m$. The permutation γ of $t_1, \ldots, t_{n+m+1}$ corresponding to the permutation σ of $s_1, \ldots, s_{n+m}$ is characterized by $\gamma(n+1) = 1$ (because $s \geq s_i$ for all i), $\gamma(i) = \sigma(i) + 1$ for $1 \leq i \leq n$ and $\gamma(i+1) = \sigma(i) + 1$ for $n+1 \leq i \leq n+m$. Therefore,

$$\begin{aligned}\int_{t_0}^{t} \mathrm{d}s \Omega^L_\alpha(s, t_0) J(s) \Omega^K_\beta(s, t_0) &= \sum_\gamma \int_{t_0}^{t} \mathrm{d}t_1 \ldots \int_{t_0}^{t_{n+m}} \mathrm{d}t_{n+m+1} \\ &\quad L_1(t_{\gamma(1)}) \ldots L_n(t_{\gamma(n)}) J(t_{\gamma(n+1)}) K_1(t_{\gamma(n+2)}) \ldots K_m(t_{\gamma(n+m+1)}),\end{aligned}$$

where γ satisfies $\gamma(n+1) = 1$, $st(\gamma(1), ..., \gamma(n)) = \alpha$, $st(\gamma(n+2), ..., \gamma(n+m+1)) = \beta$. The lemma is proved. □

Notice that the same process would allow to derive combinatorial formulas for arbitrary products of iterated integrals and for integrals with integrands involving iterated integrals, provided these products and integrands have expressions similar to the ones considered in the two lemmas.

Appendix B: The algebraic structure of tree-shaped iterated integrals

Our exposition of tree-parametrized time-dependent perturbation theory has focussed on the derivation of convergence results and explicit formulas for the time-dependent wave operator. However, the reasons why such an approach is possible and efficient are grounded into various algebraic and combinatorial properties of trees, descents and similar objects.

These properties suggest that the theory of effective Hamiltonians is grounded into a new "Lie theory" generalizing the usual Lie theory (or, more precisely, generalizing the part of the classical Lie theory that is relevant to the study of the solutions of differential equations). First indications that such a theory exists were already pointed out in our ref. 22. Indeed, we showed in this article that descent algebras of hyperoctahedral groups and generalizations thereof are relevant to the time-dependent perturbation theory. Applications included an extension of the Magnus expansion for the time-dependent wave operator. Our results below provide complementary insights on the subject and further evidence that algebraic structures underly many-body theories.

1. The algebra structure

We know from ref. 22 and Sect II B that the family of integrals $\Omega^L_\sigma(t,t_0)$ is closed under the product. This closure property is reflected into the convolution product of permutations. This result is a natural noncommutative generalization of Chen's formula for the product of iterated integrals. We show, in the present section, that the same result holds for integrals parametrized by trees. We will explain, in the next sections, why such a result -which may seem surprising from the analytical point of view- could be expected from the modern theory of combinatorial Hopf algebras.

For $L=(L_1,...,L_n)$ a family of time-dependent operators (with the usual regularity conditions), and T a tree with n internal vertices, we write

$$\Omega^L_T(t,t_0) := \sum_{\sigma\in S_T}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\ldots\int_{t_0}^{t_{n-1}}\mathrm{d}t_n L_1(t_{\sigma(1)})L_2(t_{\sigma(2)})\ldots L_n(t_{\sigma(n)}).$$

This notation is extended to linear combinations of trees, so that e.g. if $Z=T+2T'$, where T and T' are two arbitrary trees with the same number of vertices, then $\Omega^L_Z(t,t_0)=\Omega^L_T(t,t_0)+2\Omega^L_{T'}(t,t_0)$. For $i\leq n$, we write $L_{\leq i}=(L_1,...,L_i)$, $L_{\geq i}=(L_i,...,L_n)$.

Proposition 17 *For $L=(L_1,...,L_n)$ and $K=(K_1,...,K_m)$ two families of time-dependent operators and $T=T_1\vee T_2$, $U=U_1\vee U_2$ two trees, $|T|=n,|T_1|=p,|T_2|=q,|U|=m,|U_1|=l,|U_2|=k$, we have:*

$$\Omega^L_T(t,t_0)\Omega^K_U(t,t_0)=\int_{t_0}^{t}ds\Omega^L_T(s,t_0)\Omega^{K_{\leq l}}_{U_1}(s,t_0)K_{l+1}(s)\Omega^{K_{\geq l+2}}_{U_2}(s,t_0)+\int_{t_0}^{t}ds\Omega^{L_{\leq p}}_{T_1}(s,t_0)L_{p+1}(s)\Omega^{L_{\geq p+2}}_{T_2}(s,t_0)\Omega^K_U(s,t_0).$$

In the formula, one or several of the trees T_1,T_2,U_1,U_2 may be the trivial tree $|$.

Proof. Recall the integration by parts formula. For any integrable functions f and g we define $F(t):=\int_{t_0}^t\mathrm{d}sf(s)$, $G(t):=\int_{t_0}^t\mathrm{d}sg(s)$ and $H(t):=F(t)G(t)$. Then

$$H(t) \;=\; \int_{t_0}^{t}\mathrm{d}s\frac{\mathrm{d}H(s)}{\mathrm{d}s}=\int_{t_0}^{t}\mathrm{d}sf(s)G(s)+\int_{t_0}^{t}\mathrm{d}sF(s)g(s).$$

Now, we use this identity with $F(t)=\Omega^L_T(t,t_0)$. It follows from the proof of theorem 5 that $f(s)$ is given by

$$f(s)=\Omega^{L_{\leq p}}_{T_1}(s,t_0)L_{p+1}(s)\Omega^{L_{\geq p+2}}_{T_2}(s,t_0),$$

with a similar identity for $G(t)=\Omega^K_U(t,t_0)$. The proposition follows. □

In particular, it is a consequence of the proposition and a straightforward recursion argument that the linear span of the integrals $\Omega^L_T(t,t_0)$ is closed under products.

2. Hopf algebras and Lie theory

This result may be formalized algebraically. Let us write $\mathcal{T}$ for the set of formal power series with complex coefficients over the set of trees. Proposition 17 enables us to define a product on trees, denoted by $*$, such that $\Omega_T^L(t,t_0)\Omega_U^K(t,t_0) = \Omega_{T*U}^{L\cdot K}(t,t_0)$. This product is defined recursively by the equation[30]

$$T * U := (T * U_1) \vee U_2 + T_1 \vee (T_2 * U).$$

Proof. The empty tree $|$ is the unit for the product $*$. Assume that $T*U$ is defined and satisfies the recursive relation for all trees such that $|T| + |U| < n$, and consider two trees T and U with $|T| + |U| = n$. The first term on the right hand side of proposition 17 is $\int_{t_0}^t ds\Omega_T^L(s,t_0)\Omega_{U_1}^{K_{\leq l}}(s,t_0)K_{l+1}(s)\Omega_{U_2}^{K_{\geq l+2}}(s,t_0)$. By the recursive relation, we have

$$\Omega_T^L(s,t_0)\Omega_{U_1}^{K_{\leq l}}(s,t_0) \;=\; \Omega_{T*U_1}^{L\cdot K_{\leq l}}.$$

Thus, the whole term can be written

$$\int_{t_0}^t ds\Omega_T^L(s,t_0)\Omega_{U_1}^{K_{\leq l}}(s,t_0)K_{l+1}(s)\Omega_{U_2}^{K_{\geq l+2}}(s,t_0) \;=\; \Omega_{(T*U_1)\vee U_2}^{L\cdot K}.$$

The second term of proposition 17 is treated similarly and we obtain

$$\Omega_T^L(t,t_0)\Omega_U^K(t,t_0) \;=\; \Omega_{(T*U_1)\vee U_2}^{L\cdot K} + \Omega_{(T_1\vee(T_2*U)}^{L\cdot K}$$

Therefore, the relation $\Omega_T^L(t,t_0)\Omega_U^K(t,t_0) = \Omega_{T*U}^{L\cdot K}(t,t_0)$ gives us

$$T * U = (T * U_1) \vee U_2 + T_1 \vee (T_2 * U).$$

□

Corollary 18 *The product provides $\mathcal{T}$ with the structure of an associative algebra.*

The corollary is a by-product of the associativity of the product of operators and of proposition 17.

Of course, although the analysis of tree-shaped iterated integrals leads to a straightforward proof, the associativity property is a purely combinatorial phenomenon that originates ultimately from the associativity of the shuffle product. See ref. 22 for the connections between the noncommutative Chen formula and shuffle products, see also section 4 of ref. 51 for Schützenberger's classical (but rarely quoted) analysis of the formal properties of the shuffle product -in fact, the splitting of the convolution product of trees reflects the classical splitting of shuffle products into left and right half-shuffle products that had appeared in the study of Lie polynomials and was first encoded combinatorially in ref. 51. The associativity can also be checked directly or deduced from the associativity of the convolution product $*$ of permutations, since one may verify easily, using e.g. our description of the permutations in S_T that the convolution product as introduced above is nothing but the restriction to $\mathcal{T}$ of the convolution product on the algebra $\mathcal{S} = \prod_{n\in\mathbf{N}} \mathbf{C}[\mathcal{S}_n]$.

This fact that the linear span of trees (often written **PBT**) defines a subalgebra of $\mathcal{S}$ for the convolution product (and even a Hopf subalgebra, referred to as the Hopf algebra of planar binary trees, whereas $\mathcal{S}$ is referred to as the Malvenuto-Reutenauer or Hopf algebra of free quasi-symmetric functions in the litterature) is well-known. It was first observed in ref. 30 and further investigated in a series of papers[34,36,37,52]. There is however a slight subtelty here, since the embedding of **PBT** in $\mathcal{S}$ considered e.g. in ref. 30 is not the one we consider (another projection map from permutations to trees is used) so that **PBT** and $\mathcal{T}$, although isomorphic as algebras (the product rule in **PBT** is the same as the one in $\mathcal{T}$, see e.g. proposition 3.2 of ref. 30, where **PBT** is written $\mathbf{C}[Y_\infty]$) do not agree as subalgebras of $\mathcal{S}$.

However, a corollary of this isomorphism is that the structures existing on **PBT** carry over to the analysis of the algebraic properties of tree-shaped iterated integrals. The existence of a Hopf algebra structure seems particularly meaningful since the classical applications of the theory of free Lie algebras to the analysis of differential equations can be rewritten using the framework of Hopf algebras (see e.g. the accounts in refs. 53,54).

The same observation holds for the direct sum of the hyperoctahedral group algebras, that also carries naturally a Hopf algebra structure[55,56], and which applications to time-dependent perturbative Hamiltonians were studied in ref. 22. We leave for further research the investigation of the possible role of these Hopf algebra structures in the context of many-body theories.

3. Permutations, trees and descents

Another meaningful observation, along the same lines, is that the three expansions we derived, based respectively on sequences of P and Q (as in the first expression for $\Omega(t, t_0)$), on trees (third expression) and on permutations (second expression), reflect at the analytical level the existence of projection maps and embeddings between hypercubes (or the descent algebra), planar binary trees, and permutations. Following Viennot[23], these maps have been at the origin of modern enumerative combinatorics. We refer to refs. 30,34,36,37 for a detailed study of these maps that emphasizes the existence of underlying geometrical structures that go beyond the Hopf algebraic ones.

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