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We present the first representation of the general term of the Rayleigh-Schrödinger series for quasidegenerate systems. Each term of the series is represented by a tree and there is a straightforward relation between the tree and the analytical expression of the corresponding term. The combinatorial and graphical techniques used in the proof of the series expansion allow us to derive various resummation formulas of the series. The relation with several combinatorial objects used for special cases (degenerate or non-degenerate systems) is established.

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I. INTRODUCTION

Rayleigh-Schrödinger (RS) perturbation theory is a venerable technique to calculate the eigenvalues and eigenvectors of $H = H_0 + V$ from those of H_0. It was created in 1894 by Lord Rayleigh to describe the vibrations of a string [1] and adapted to quantum mechanics by Schrödinger in 1926 [2]. RS perturbation theory has been used in all fields of quantum physics (particle, atomic, molecular, solid-state physics) and quantum chemistry.

In most textbooks, the RS series deals with the perturbation of a single nondegenerate initial state. However, in many practical applications, the initial state is either degenerate or quasidegenerate (i.e. several states are close in energy) and the basic RS approach breaks down. Quasidegenerate perturbation theory is widely used to set up effective Hamiltonians [3], for example the spin Hamiltonians of molecular chemistry and solid state physics [4, 5], or to deal with the quantum electrodynamics of atoms [6, 7].

The terms of the RS series are notoriously complex. Even mathematical physicists of the stature of Reed and Simon admit that the terms of the RS series are "quite complicated" and that "the higher order RS coefficients are hard to compute" (see ref. 8, p. 8 and 18). Computer programs are available to build the terms of the RS series [9–13], but their results are intricate expressions that do not exhibit any obvious structure and that can hardly be used to carry out resummations of the series.

In this paper, combinatorial physics is used to provide the first representation of the general term of the Rayleigh-Schrödinger (RS) perturbation theory for quasidegenerate systems. Each term is written as a tree that faithfully reflects its algebraic structure. In particular, trees illustrate the recursive structure of RS terms, that is used to prove properties of the RS series.

The purpose of this paper is to describe the general term of the RS series and to illustrate the power of our combinatorial approach by deriving a number of possible resummations of the RS series. Our aim is to set up the tools for performing such resummations and not to discuss when some resummations are more convenient than others. As a consequence, no numerical example is given.

When the system is not quasi-degenerate (i.e. when it is either fully degenerate or non-degenerate), several graphical representations of the terms of the RS series have been proposed. We give the bijection between these representations and our trees.

II. RAYLEIGH-SCHRÖDINGER SERIES

In the most general setting, we consider a model space M spanned by N eigenstates $|i\rangle$ of H_0, with energies e_i. We assume that all e_i of the model space are separated from the rest of the spectrum of H_0 by a finite gap. The projector onto the model space M is $P = \sum_i |i\rangle\langle i|$, where i runs over the basis states of M. The wave operator Ω transforms N states $|\phi_i\rangle$ of M into eigenstates $|\Phi_i\rangle = \Omega|\phi_i\rangle$ of H: $H\Omega|\phi_i\rangle = E_i\Omega|\phi_i\rangle$. We recently described [14] the way to choose the states $|\phi_i\rangle$.

We assume that $P\Omega = P$ and $\Omega P = \Omega$. Then, the eigenvalues of the effective Hamiltonian $H_{\rm eff} = PH\Omega$ are the eigenvalues E_i of H. In other words, eigenvalues of H can be obtained by diagonalizing the $M \times M$ matrix $H_{\rm eff}$. Lindgren and Kvasnička showed [15, 16] that

$$[\Omega, H_0] \;=\; V\Omega - \Omega V\Omega. \tag{1}$$

The recursive solution of this equation gives a series expansion for Ω which is the RS series for the wavefunction. However, it is not obvious that eq. (1) has a recursive solution. Indeed, we must be able to solve the equation $[X, H_0] = C$ for X. In general, the operator Sylvester equation $AX - XB = C$, where A and B are self-adjoint, has a unique solution if and only if A and B have no common eigenvalue [17, 18]. Clearly, this is not the case if $A = B = H_0$, so we recast the equation by defining $\chi = \Omega - P$, where $\chi = Q\chi P$, with $Q = 1 - P$. Thus, eq. (1) becomes an equation for χ:

$$[\chi, H_0] \;=\; QVP + QV\chi - \chi VP - \chi V\chi. \tag{2}$$

This equation is a matrix Riccati equation, for which various solution methods have been proposed in the literature [18–21]. Solutions exist also for its time-dependent form [22, 23]. Now, $[\chi, H_0] = \chi H_0 - H_0\chi = \chi PH_0 - QH_0\chi$, because P and Q commute with H_0. We obtain a Sylvester equation with $A = QH_0$ and $B = PH_0$ and its solution is unique because we assumed that there is a finite gap between the states of the model space and the rest of the spectrum.

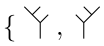
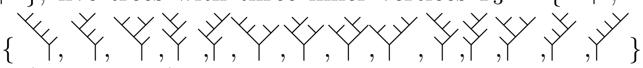
A. Combinatorial analysis

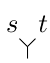
Because of its importance, the basic RS series has been dealt with in hundreds of papers. As a starting point to discover the proper combinatorial structure of the RS series, we enumerate the number of its terms: it has one term of order 0, one term of order 1, then 2, 5, 14, 42, 132, 429 terms of order 2, 3, 4, 5, 6 and 7, respectively. The number of terms of order n is the Catalan number $C_n = \frac{(2n)!}{n!(n+1)!}$. The Catalan sequence is well-know in combinatorics: "The Catalan sequence is probably the most frequently encountered sequence that is still obscure enough to cause mathematicians [...] to expend inordinate amounts of energy re-discovering formulas that were worked out long ago." [24]. An entire book is devoted to Catalan numbers [25]. They enumerate over 200 combinatorial objects [26] and in the physics literature, several of these objects were used to represent the general term of the RS series: Dyck paths [27], non-crossing partitions [28], bracketings [15, 29, 30], labelled diagrams [31] and sequences of integers [27, 32, 33]. However, these approaches could not be generalized to quasi-degenerate systems because they dealt with denominators $(e_0 - e_j)^n$ with $n > 1$, whereas more complex denominators occur in the quasi-degenerate case. Moreover, they could not be used to discover efficient resummations because they do not capture the recursive structure of the RS series.

To find out which combinatorial object is best suited to deal with the RS series, we had to use a rather elaborate algebraic analysis of the time-dependent perturbation theory [14, 34]. It turned out in the end that planar binary trees provide the most faithful representation. As we shall see, the relation beween a tree and the corresponding term of RS series is straightforward and the recursive structure of the terms is transparent. The faithfulness is demonstrated by the easiness of the proofs and by the relation between geometrical properties of the trees and analytical properties of the terms, for instance for resummation.

B. Binary trees

We first give examples of the planar binary trees that we use. We denote by Y_n the set of planar binary trees with n inner vertices. A tree is called *binary* if each vertex has either zero or two children. It is called *planar* if two trees are different when they can be deduced one from the other by moving one edge over another one. For example, the two planar trees  and  are different.

There is a single tree with zero inner vertex: $Y_0 = \{\,|\,\}$. There is one tree with one inner vertex $Y_1 = \{$  $\}$, two trees with two inner vertices $Y_2 = \{$  $\}$, five trees with three inner vertices $Y_3 = \{$  $\}$ and fourteen with four inner vertices $Y_4 = \{$  $\}$. The vertical line of a tree is called the *root*. The trees of Y_n (with $n > 0$) can be built from smaller trees by the following relation $Y_n = \{t_1 \vee t_2 \,:\, t_1 \in Y_k, t_2 \in Y_{n-k-1},\, k = 0, \ldots, n-1\}$, where $t_1 \vee t_2$ is the grafting of trees t_1 and t_2, by which the roots of t_1 and t_2 are brought together and a new root is grown from their juncture. Pictorially:

$s \vee t \;=$  .

For example, $| \vee | = \curlyvee$, $| \vee \curlyvee = \curlyvee$, $\curlyvee \vee \curlyvee = \curlyvee$. Except in figure 1, the vertices are not drawn explicitly for notational convenience. The inner vertices of a tree are the vertices to which three edges (or two edges and the root) are incident, its leaves are its vertices to which a single edge is incident. A leaf is oriented either to the left or to the right. Each tree of Y_n has n inner vertices and $n+1$ leaves. The order $|t|$ of a tree t is the number of its inner 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 is a Catalan number. The recursive definition of planar binary trees make them very easy to generate with a computer.

C. Recursive relation between trees and RS terms

In ref. 14, we showed that the wave operator can be written as the sum

$$\Omega \;=\; P + \sum_{n=1}^{\infty} \sum_{t\in Y_n} \Omega_t, \tag{3}$$

where

$$\Omega_t \;=\; \sum_{ij} |i\rangle \omega_t^{ij} \langle j|, \tag{4}$$

with $|j\rangle$ an eigenstate of H_0 in the model space and $|i\rangle$ out of it (i.e. $P|j\rangle = |j\rangle$ and $P|i\rangle = 0$). The scalars ω_t^{ij} are defined by an exceedingly simple recursive relation: for any tree t different from $|$, there are two trees t_1 and t_2 such that $t = t_1 \vee t_2$. Then,

$$\omega_t^{ij} \;=\; -\sum_{k,l} \frac{\omega_{t_1}^{ik} \langle k|V|l\rangle \omega_{t_2}^{lj}}{e_j - e_i}, \tag{5}$$

with the special cases $\omega_{t_1}^{ik} = -\delta_{i,k}$ if $t_1 = |$ and $\omega_{t_2}^{lj} = +\delta_{l,j}$ if $t_2 = |$. It is clear from the definition that Ω_t is built from a product of $|t|$ matrix elements of V. Note that, when $t_1 = |$, both i and k in $\omega_{t_1}^{ik}$ correspond to eigenstates outside the model space, while when $t_2 = |$, both i and k in $\omega_{t_1}^{ik}$ correspond to eigenstates in the model space.

We now prove that the expansion $\chi = \sum_{t\neq|} \Omega_t$ is a solution of eq. (2). First notice that taking the commutator $[\Omega_t, H_0]$ amounts to multiply ω_t^{ij} by $e_j - e_i$. Let $t = t_1 \vee t_2$. Then, $[\Omega_t, H_0]$ is equal to QVP, or $QV\Omega_{t_2}$ or $-\Omega_{t_1}VP$ or $-\Omega_{t_1}V\Omega_{t_2}$, respectively, according to whether $t_1 = t_2 = |$, or $t_1 = |$ and $t_2 \neq |$, or $t_1 \neq |$ and $t_2 = |$, or $t_1 \neq |$ and $t_2 \neq |$, respectively. The result follows by summing over all trees t_1 and t_2.

This very simple proof illustrates the fact that non trivial results can be easily obtained because trees encapsulate the recursive structure of the RS series.

A more explicit version of the recursive relation (5) will sometimes be needed. For $t = t_1 \vee t_2$, we define equivalently Ω_t by

$$\Omega_t \;=\; \sum_{ij} \frac{|i^Q\rangle\langle i^Q|V|j^P\rangle\langle j^P|}{e_j - e_i} \quad \text{if } t_1 = | \text{ and } t_2 = | \,, \tag{6}$$

$$\Omega_t \;=\; \sum_{ij} \frac{|i^Q\rangle\langle i^Q|VQ\,\Omega_{t_2}|j^P\rangle\langle j^P|}{e_j - e_i} \quad \text{if } t_1 = | \text{ and } t_2 \neq | \,, \tag{7}$$

$$\Omega_t \;=\; -\sum_{ij} \frac{|i^Q\rangle\langle i^Q|\Omega_{t_1}PV|j^P\rangle\langle j^P|}{e_j - e_i} \quad \text{if } t_1 \neq | \text{ and } t_2 = | \,, \tag{8}$$

$$\Omega_t \;=\; -\sum_{ij} \frac{|i^Q\rangle\langle i^Q|\Omega_{t_1}PVQ\,\Omega_{t_2}|j^P\rangle\langle j^P|}{e_j - e_i} \quad \text{if } t_1 \neq | \text{ and } t_2 \neq | \,, \tag{9}$$

where the exponent of $|j^P\rangle$ and $|i^Q\rangle$ means that state $|j\rangle$ is a basis state of M and $|i\rangle$ a basis state of the complementary of M.

D. Examples

As examples, we give all Ω_t for $|t|$=2 and 3, the value of Ω_t for $|t| = 1$ (i.e. $t =$ ) being given by eq. (6)).

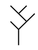
$$\Omega_t = -\sum_{i_1,i_2,i_3} \frac{|i_1^Q\rangle\langle i_1^Q|V|i_2^P\rangle\langle i_2^P|V|i_3^P\rangle\langle i_3^P|}{(e_{i_2}-e_{i_1})(e_{i_3}-e_{i_1})} \quad \text{for} \quad t =$$  ,

$$\Omega_t = \sum_{i_1,i_2,i_3} \frac{|i_1^Q\rangle\langle i_1^Q|V|i_2^Q\rangle\langle i_2^Q|V|i_3^P\rangle\langle i_3^P|}{(e_{i_3}-e_{i_2})(e_{i_3}-e_{i_1})} \quad \text{for} \quad t =$$  ,

$$\Omega_t = \sum_{i_1,i_2,i_3,i_4} \frac{|i_1^Q\rangle\langle i_1^Q|V|i_2^P\rangle\langle i_2^P|V|i_3^P\rangle\langle i_3^P|V|i_4^P\rangle\langle i_4^P|}{(e_{i_2}-e_{i_1})(e_{i_3}-e_{i_1})(e_{i_4}-e_{i_1})} \quad \text{for} \quad t =$$  ,

$$\Omega_t = -\sum_{i_1,i_2,i_3,i_4} \frac{|i_1^Q\rangle\langle i_1^Q|V|i_2^Q\rangle\langle i_2^Q|V|i_3^P\rangle\langle i_3^P|V|i_4^P\rangle\langle i_4^P|}{(e_{i_3}-e_{i_1})(e_{i_3}-e_{i_2})(e_{i_4}-e_{i_1})} \quad \text{for} \quad t =$$  ,

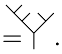
$$\Omega_t = -\sum_{i_1,i_2,i_3,i_4} \frac{|i_1^Q\rangle\langle i_1^Q|V|i_2^P\rangle\langle i_2^P|V|i_3^Q\rangle\langle i_3^Q|V|i_4^P\rangle\langle i_4^P|}{(e_{i_2}-e_{i_1})(e_{i_4}-e_{i_3})(e_{i_4}-e_{i_1})} \quad \text{for} \quad t =$$  ,

$$\Omega_t = -\sum_{i_1,i_2,i_3,i_4} \frac{|i_1^Q\rangle\langle i_1^Q|V|i_2^Q\rangle\langle i_2^Q|V|i_3^P\rangle\langle i_3^P|V|i_4^P\rangle\langle i_4^P|}{(e_{i_3}-e_{i_2})(e_{i_4}-e_{i_2})(e_{i_4}-e_{i_1})} \quad \text{for} \quad t =$$  ,

$$\Omega_t = \sum_{i_1,i_2,i_3,i_4} \frac{|i_1^Q\rangle\langle i_1^Q|V|i_2^Q\rangle\langle i_2^Q|V|i_3^Q\rangle\langle i_3^Q|V|i_4^P\rangle\langle i_4^P|}{(e_{i_4}-e_{i_3})(e_{i_4}-e_{i_2})(e_{i_4}-e_{i_1})} \quad \text{for} \quad t =$$  .

By looking at these examples, one may wonder whether some denominators could take the value zero. We show now by induction that this never happens. In other words, Ω_t is never singular. This is true for $t =$  because, in eq. (6), $|i\rangle$ belongs to M and $|j\rangle$ does not belong to M. Thus, $|e_i - e_j|$ is greater than the gap between the model space and the rest of the spectrum. Assume now that no Ω_t is singular for trees with $|t| \le n$. Take a tree t with $|t| = n+1$. Then, $t = t_1 \vee t_2$, with $|t_1| \le n$ and $|t_2| \le n$. Assume that neither t_1 nor t_2 is equal to the root $|$. Then, eq. (9) and the previous remark about $|e_i - e_j|$ shows that Ω_t is not singular. The same is true if t_1 or t_2 is equal to the root. Thus, the denominator Ω_t can never take the value 0. Again, the proof is made very simple by the recursive structure of Ω_t.

E. Direct relation between trees and RS terms

The recursive relation (5) is very useful to derive proofs, but we also need a non-recursive expression for the terms of the RS series. We now give an explicit relation between t and Ω_t [14]. This construction can be followed in figure 1 for $t =$  . Consider a tree t with $|t| = n$ and number its leaves from 1 for the leftmost leaf to $n+1$ for the rightmost one. The numerators in the expansion of Ω_t are $|i_1\rangle\langle i_1|V|i_2\rangle \dots \langle i_n|V|i_{n+1}\rangle\langle i_{n+1}|$. The state $|i_k\rangle$ belongs to M (i.e. is $|i_k^P\rangle$) if leaf k is oriented to the right and does not belong to M (i.e. is $|i_k^Q\rangle$) if leaf k is oriented to the left. In the example of fig. 1, the denominator is $|i_1^Q\rangle\langle i_1^Q|V|i_2^P\rangle\langle i_2^P|V|i_3^P\rangle\langle i_3^P|V|i_4^Q\rangle\langle i_4^Q|V|i_5^P\rangle\langle i_5^P|$

Then, for each inner vertex v of t, take the subtree t_v for which v is just above the root. In other words, t_v is obtained by chopping the edge below v and considering the edge dangling from v as the root of t_v. In the example of fig. 1, we have four inner vertices labelled a, b, c, d. For vertex a, the subtree t_a is the full tree t. For the other inner vertices the subtrees are proper (i.e. different from t) and are given in fig. 1. For each tree t_v, denote by $l(v)$ the index of its leftmost leaf and by $r(v)$ that of its rightmost leaf. Then, the denominator is the product of $e_{i_{r(v)}} - e_{i_{l(v)}}$, where v runs over the n inner vertices of the tree. In the example of fig. 1, t_a gives the denominator $(e_{i_5} - e_{i_1})$, t_b gives $(e_{i_3} - e_{i_1})$, t_c gives $(e_{i_2} - e_{i_1})$ and t_d gives $(e_{i_5} - e_{i_4})$. Finally, the whole fraction is summed over $i_1 \dots i_{n+1}$ and multiplied by $(-1)^{d-1}$, where d is the number of leaves pointing to the right. It can be easily proved that the above construction satisfies the recursive equation (5). If we take the example of the tree t of fig. 1 and consider for example the inner vertex labelled by b, we get a contribution $(e_{i_3} - e_{i_1})$ to the denominator. The total term is

$$\Omega_t = (-1)^2 \sum_{i_1 i_2 i_3 i_4 i_5} \frac{|i_1^Q\rangle\langle i_1^Q|V|i_2^P\rangle\langle i_2^P|V|i_3^P\rangle\langle i_3^P|V|i_4^Q\rangle\langle i_4^Q|V|i_5^P\rangle\langle i_5^P|}{(e_{i_5}-e_{i_1})(e_{i_2}-e_{i_1})(e_{i_3}-e_{i_1})(e_{i_5}-e_{i_4})}.$$

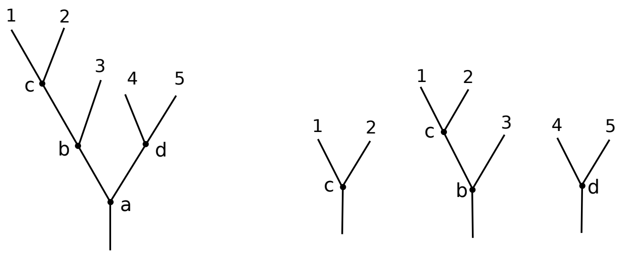


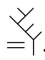
FIG. 1: A tree with its labelled leaves and its three proper subtrees. The inner vertices are labelled a, b, c and d. The couples $(l(v), r(v))$ are $(1, 5)$, $(1, 3)$, $(1, 2)$ and $(4, 5)$ for $v = a, b, c$ and d, respectively.

As far as we know, this tree representation provides the first description of the general term of the RS series for quasidegenerate systems.

III. RESUMMATIONS

The tree representation is useful, not only to prove properties of the RS series, but also to derive new resummations of it. Indeed, any way to write the set of trees as a composition of subtrees gives rise to a resummation of the RS series.

A. Summation over left combs

For any tree t, we define the sequence t_n by $t_0 = t$, $t_{n+1} = t_n \vee |$. For example, if $t =$  , we have $t_1 =$  , $t_2 =$ . For any integer n, t_n is obtained by grafting t on the leftmost leaf of a tree that has a single leaf oriented to the left and n leaves oriented to the right (such a tree is called a left comb whereas t_n, $n > 0$ is called a left comb grafting. Notice the uniqueness rewriting property: an arbitray tree u can be rewritten uniquely as t_n, where $t = |$ or $t \neq v \vee |$. The sum over graftings on left combs is made by defining

$$\Omega'_t \;=\; \Omega_t + \sum_{n=1}^{\infty} \Omega_{t_n}.$$

We can now calculate Ω'_t in terms of Ω_t. We first define

$$G^0_P(z) \;=\; P(H_0 - z)^{-1} P = \sum_j \frac{|j^P\rangle\langle j^P|}{e_j - z}.$$

Then, we use Kvasnička's trick and denote by $Q_i = |i^Q\rangle\langle i^Q|$ the projector onto the eigenspace of H_0 with eigenvalue e_i outside the model space, so that $Q = \sum_i Q_i$ and eq. (8) can be rewritten $\Omega_{t_1} = -\sum_i Q_i \Omega_t PVG^0_P(e_i)$. By repeating this argument we obtain

$$\begin{aligned}
\Omega'_t \;&=\; \sum_i Q_i \Omega_t \Big(P - PVG^0_P(e_i) + PVG^0_P(e_i) PVG^0_P(e_i) - \dots \\
&=\; \sum_i Q_i \Omega_t \Big(P + PVG^0_P(e_i) \Big)^{-1}.
\end{aligned}$$

The map $P + PVG^0_P(e_i)$ goes from the model space to itself and the inverse is taken within the model space. The dimension of the model space is generally small and the numerical calculation of the inverse is fast. We transform

$$\Big(P + PVG^0_P(e_i) \Big)^{-1} \;=\; \Big((H_0 P - e_i P + PVP) G^0_P(e_i) \Big)^{-1} = (H_0 P - e_i P)(PHP - e_i P)^{-1},$$

where $PHP = P(H_0 + V)P$ and the inverse is again from M to M. To conclude, we assume that $t = u \vee v$, where u and v are different from $|$. Then,

$$\begin{aligned}\Omega'_t &= \sum_i Q_i \Omega_u V \Omega_v G^0_P(e_i)(PH_0 - e_i P)(PHP - e_i P)^{-1} \\ &= \sum_i Q_i \Omega_u V \Omega_v (PHP - e_i P)^{-1} = \sum_{ij} \frac{|i\rangle\langle i|\Omega_u V \Omega_v|\overline{j}\rangle\langle\overline{j}|}{\overline{e}_j - e_i},\end{aligned}$$

where $|\overline{j}\rangle$ and $\overline{e}_j$ are the eigenstates and eigenvalues of PHP, so that $P = \sum_j |\overline{j}\rangle\langle\overline{j}|$. In other words, summing over all left combs amounts to replacing the eigenstates of PH_0P by the eigenstates of PHP.

B. Accelerarated summation over left combs

The formula we obtained for Ω'_t suggests to look for another expansion of the RS series involving only the eigenstates and eigenvalues of $P(H_0 + V)P$. The uniqueness rewriting property implies that $\Omega = P + \Omega' + \sum_t \Omega'_t$, where the sum is over all trees t with two or more inner vertices and such that $t \neq u \vee |$, but this resummation can still be improved.

We rewrite the Kvasnička-Lindgren equation.

$$[\chi, H_0] = \sum_i Q_i \chi H_0 - H_0 \sum_i Q_i \chi = \sum_i Q_i \chi (H_0 - e_i).$$

Thus, eq. (2) becomes $\sum_i Q_i \chi (H_0 - e_i) = QVP + QV\chi - \chi VP - \chi V \chi$ that is,

$$\sum_i Q_i \chi P(H_0 - e_i + V)P = QVP + QV\chi - \chi V \chi, \tag{10}$$

or, for all the eigenvalues e_i of H_0 outside the model space:

$$Q_i \chi P = Q_i V G_P(e_i) + Q_i V \chi G_P(e_i) - Q_i \chi V \chi G_P(e_i),$$

where

$$G_P(z) = (PH_0P + PVP - zP)^{-1} = \sum_j \frac{|\overline{j}\rangle\langle\overline{j}|}{\overline{e}_j - z}.$$

This equation is similar to the Kvasnička-Lindgren equation and can be solved graphically and recursively by the same process. Notice that the leading term of the recursive expansion of χ is now $\Omega' = \sum_i Q_i V G_P(e_i)$.

Let us call a tree t right-normalized if there is no edge in t such that the tree t' obtained by pruning the tree t at that edge can be written $t_1 \vee |$ with $t_1 \neq |$. The only left comb possibly contained in a right-normalized tree is . The number of right-normalized trees is considerably smaller than the number of trees. For n=1, 2, 3 and 4 the number of right-normalized trees is 1 ( ), 1 ( ), 2 (,) and 4 (, , ,) instead of 1, 2, 5, 14. The right-normalized trees are enumerated by the Motzkin numbers [35].

The solution of eq. (10) is then $\Omega = P + \sum_t \hat{\Omega}_t$, where t runs over right-normalized trees and $\hat{\Omega}_t$ can be defined recursively by

$$\hat{\Omega}_t = \sum_{i \notin M, j \in M} \frac{|i\rangle\langle i|V|\overline{j}\rangle\langle\overline{j}|}{\overline{e}_j - e_i} \quad \text{if } t_1 = | \text{ and } t_2 = |, \tag{11}$$

$$\hat{\Omega}_t = \sum_{i \notin M, j \in M} \frac{|i\rangle\langle i|V\hat{\Omega}_{t_2}|\overline{j}\rangle\langle\overline{j}|}{\overline{e}_j - e_i} \quad \text{if } t_1 = | \text{ and } t_2 \neq |, \tag{12}$$

$$\hat{\Omega}_t = -\sum_{i \notin M, j \in M} \frac{|i\rangle\langle i|\hat{\Omega}_{t_1} V \hat{\Omega}_{t_2}|\overline{j}\rangle\langle\overline{j}|}{\overline{e}_j - e_i} \quad \text{if } t_1 \neq | \text{ and } t_2 \neq |. \tag{13}$$

Once again, this approach reduces the number. It can be expected that this resummation considerably accelerates the convergence of the series. Indeed, when the model space is well chosen, the matrix elements of QVP are smaller than those of PVP. In this expression, all terms involving powers of PVP have been resummed.

C. Alternative accelerated tree expansion

A similar resummation, that we omit, can be obtained by summing over right combs. However, it is not so practical as the previous ones because it is usually not easy to invert $QHQ - Qz$. If this inversion is possible, then we can simultaneously sum over right and left combs, at least if we assume that a finite gap exists between the eigenvalues of QHQ and PHP. We make this assumption, proceed as before and transform the Kvasnička-Lindgren equation. We define $\overline{P}_j = |\overline{j}\rangle\langle\overline{j}|$ the projector onto the eigenspace of PHP with energy $\overline{e}_j$ and use similar notations for the projectors and energy levels of QHQ. Thus, $P = \sum_j \overline{P}_j$ and we can rewrite the lhs of eq. (10) as

$$\sum_i Q_i \chi P(H_0 - e_i + V)P \;=\; \sum_{ij} Q_i \chi P(H_0 - e_i + V)\overline{P}_j = \sum_{ij} Q_i \chi (\overline{e}_j - e_i)\overline{P}_j = \sum_j Q(\overline{e}_j - H_0)\chi \overline{P}_j.$$

Thus eq. (10) becomes $\sum_j Q(\overline{e}_j - H_0)\chi\overline{P}_j = QVP + QV\chi - \chi V \chi$, or

$$\sum_j Q(\overline{e}_j - H_0 - V)\chi\overline{P}_j \;=\; QVP - \chi V \chi.$$

For all eigenvalues $\overline{e}_j$ of PHP, this gives us

$$\chi\overline{P}_j = S(\overline{e}_j)V\overline{P}_j - S(\overline{e}_j)\chi V \chi \overline{P}_j,$$

where we set:

$$S(z) = (zQ - QHQ)^{-1}.$$

We can write directly the wave operator as a sum parametrized by trees: $\Omega = P + \sum_{t \geq |} \tilde{\Omega}_t$, where $\tilde{\Omega}_t$ is defined recursively for all trees by

$$\tilde{\Omega}_t \;=\; \sum_{i\notin M, j\in M} \frac{|\overline{i}\rangle\langle\overline{i}|V|\overline{j}\rangle\langle\overline{j}|}{\overline{e}_j - \overline{e}_i} = \sum_{j\in M} S(\overline{e}_j) QV\overline{P}_j \quad \text{if } t = | \;, \tag{14}$$

$$\tilde{\Omega}_t \;=\; -\sum_{i\notin M, j\in M} \frac{|\overline{i}\rangle\langle\overline{i}|\tilde{\Omega}_{t_1} V \tilde{\Omega}_{t_2}|\overline{j}\rangle\langle\overline{j}|}{\overline{e}_j - \overline{e}_i} = -\sum_{j\in M} S(\overline{e}_j)\tilde{\Omega}_{t_1} V \tilde{\Omega}_{t_2}\overline{P}_j \quad \text{if } t = t_1 \vee t_2. \tag{15}$$

As for the one involving a direct resummation over right combs, this resummation is not as practical as the previous one because the eigenvalues of QHQ are generally not known. However, this algorithm provides a way to express the eigenvectors of a matrix $M = \begin{pmatrix} A & C \\ C^\dagger & B \end{pmatrix}$ in terms of the eigenvalues and eigenvectors of A and B.

D. Fourth resummation

We use now another representation of trees in terms of trees. Since any tree t decomposes uniquely as $t = t_1 \vee t_2$, a recursion on the left hand side of the decomposition shows that there is a unique integer k and k unique trees v_i (with $i = 1, \ldots, k$) such that

$$t = \mathcal{L}_k(v_1, \ldots, v_k),$$

where

$$\mathcal{L}_k(v_1, \ldots, v_k) \;=\; \Big(\big(\ldots(| \;\vee v_1) \vee \ldots\big) \vee v_{k-1}\Big) \vee v_k.$$

In words, $\mathcal{L}_k(v_1, \ldots, v_k)$ is obtained by taking a left comb with k right leaves and grafting v_k on the lowest right leaf, v_{k-1} on the next one, up to v_1 on the highest right leaf.

If we sum over k and over all trees v_i we find

$$F \;=\; | \;+ \sum_{k=1}^{\infty} \mathcal{L}_k(F, \ldots, F), \tag{16}$$

where F stands for the formal sum of all trees.

We can plug the expansion of the wave operator of section III C in this equation and get for $t = \mathcal{L}_k(v_1, \ldots, v_k)$:

$$\tilde{\Omega}_t \;=\; (-1)^k \sum_{j_1 \cdots j_{k+1}} S(\overline{e}_{j_{k+1}}) \ldots S(\overline{e}_{j_1}) QV\overline{P}_{j_1} V\tilde{\Omega}_{v_1} \overline{P}_{j_2} V \ldots V\tilde{\Omega}_{v_k} \overline{P}_{j_{k+1}}.$$

Therefore, eq. (16) gives us the non-perturbative equation

$$\chi \;=\; \sum_j S(\overline{e}_j) V\overline{P}_j + \sum_{k=1}^{\infty} (-1)^k \sum_{j_1 \cdots j_{k+1}} S(\overline{e}_{j_{k+1}}) \ldots S(\overline{e}_{j_1}) QV\overline{P}_{j_1} V\chi\overline{P}_{j_2} V \ldots V\chi\overline{P}_{j_{k+1}}. \quad (17)$$

If we use instead the first expansion Eq (3) of the wave operator and plug the corresponding recursive formulas in $\mathcal{L}_k(v_1, \ldots, v_k)$, we get

$$\Omega_t = (-1)^{k-1} \sum_{j_1 \cdots j_{k+1}} S_0(e_{j_{k+1}}) ... S_0(e_{j_1}) QVP_{j_1} V\Omega_{v_1} P_{j_2} V\Omega_{v_2} ... V\Omega_{v_k} P_{j_{k+1}}$$

where $\Omega_| := P$ and $S_0(z) := (zQ - QH_0Q)^{-1}$, so that:

$$\Omega = P + \sum_{k=1}^{\infty} (-1)^{k-1} \sum_i (...((Q_i V G_p^0(e_i)) V\Omega G_p^0(e_i)) ... V\Omega G_p^0(e_i)).$$

We believe that these relations are new. Similar expansions would follow by considering the symmetric expansion of trees (using the grafting operation of a tree on the right-most leaf of another tree instead of the grafting on the left-most tree).

E. Relation with previous works

The previous works on quasidegenerate perturbation theory correspond to a summation which is symmetric to our first alternative expansion (in the sense that they focus on the operators $(e_i - QHQ)$). By following a line suggested by Kvasnička and Lindgren [15, 16], several authors transformed the Kvasnička-Lindgren equation into

$$\sum_i (e_i - QHQ)\chi P_i \;=\; QVP - \chi VP - \chi V\chi.$$

A resummation (similar, but slightly more involved than the one leading to eq. (17)) gives the equation [36, 37]

$$\chi \;=\; \sum_j S(e_j) VP_j + \sum_{k=1}^{\infty} (-1)^k \sum_{j_1 \cdots j_{k+1}} S(e_{j_{k+1}}) \ldots S(e_{j_1}) VP_{j_1} (V + V\chi) P_{j_2} (V + V\chi) \ldots (V + V\chi) P_{j_{k+1}},$$

which is a generalization of the degenerate case [38, 39]. Suzuki and Okamoto further solved this for χ but their rather complex result was not applied to concrete problems, as far as we know. Up to a left/right symmetry, their result is similar to our first alternative expansion, excepted for the fact that PVP and $PVS(e)VP$ are grouped in a single term.

The main practical difference between the result obtained by Suzuki and Okamoto and our second alternative expansion is the fact that we do not consider the term PVP as a perturbation, we treat it exactly. This is important because, when the model space is well chosen, PVP is larger than the non-diagonal terms PVQ.

IV. GREEN FUNCTION OF DEGENERATE SYSTEMS

In this section, we discuss a question related to the Green function of degenerate systems. Consider a Hamiltonian H_0 with a degenerate energy e_0. The eigenstates of H_0 with energy e_0 span a vector space M. The projector onto the model space M is denoted by P. In a series of recent papers [40–42], we proved by non-perturbative methods that there are eigenstates $|i\rangle$ of H_0, called the *parent states*, such that the usual Gell-Mann and Low wavefunction has a well-defined limit when the adiabatic parameter ϵ goes to zero:

$$|\Psi_{\mathrm{GML}}\rangle \;=\; \lim_{\epsilon \to 0} \frac{U_\epsilon(0, -\infty)|i\rangle}{\langle i|U_\epsilon(0, -\infty)|i\rangle},$$

where $U_\epsilon(t,t')$ is the evolution operator in the interaction picture. Morover, we showed that the parent states $|i\rangle$ are eigenstates of H_0 (with energy e_0) and are also eigenstates of PVP. As a consequence, $\langle i|V|j\rangle = 0$ for $i \neq j$ if $|i\rangle$ and $|j\rangle$ are parent states.

Since the parent states solve the problem in a non-perturbative approach, one might be tempted to use them in the perturbative one. In other words, we pick up a parent state, say $|0\rangle$, and we calculate the Rayleigh-Schrödinger series corresponding to the projector $|0\rangle\langle 0|$. However, as noticed by Tóth [43], a problem appears in the perturbative expansion. This problem can be illustrated by a simple example: for $t = (|\vee|)\vee|$, we have [14]

$$\Omega_t \;=\; -\sum_{i\neq 0} \frac{|i\rangle\langle i|V|0\rangle\langle 0|V|0\rangle\langle 0|}{(e_0 - e_i + i\epsilon)(e_0 - e_i + 2i\epsilon)},$$

where ϵ is the adiabatic switching operator, which tends to zero at the end of the calculation. Now, if $|i\rangle$ belongs to the model space, then $\langle i|V|0\rangle = 0$ (because $i \neq 0$) and the expression converges although $e_i = e_0$ could have brought a problem. In other words, using a basis of parent states for M has made the expression convergent. However, this trick does not always work. Indeed, for $t = |\vee(|\vee|)$, we have [14]

$$\Omega_t \;=\; \sum_{i\neq 0, j\neq 0} \frac{|i\rangle\langle i|V|j\rangle\langle j|V|0\rangle\langle 0|}{(e_0 - e_j + i\epsilon)(e_0 - e_i + 2i\epsilon)}.$$

If $|i\rangle$ belongs to the model space and $|j\rangle$ is out of it, then we have $e_i = e_0$ and the limit $\epsilon \to 0$ is not defined because nothing insures that $\langle i|V|j\rangle = 0$ or $\langle j|V|0\rangle = 0$. In other words, the convergence problem was solved at the non-perturbative level but remains at the perturbative one, so that the perturbative expansion has to be resummed in a proper way.

Now we show how to solve this problem by using a trick related to the Hamiltonian shift proposed by Silverstone [44]. We assume that $e'_i = e_i + \langle i|V|i\rangle$ are nondegenerate. Then, we rewrite $H = H_0 + V = H'_0 + V'$, where

$$\begin{aligned} H'_0 &= H_0 + \sum_{i\in M} |i\rangle\langle i|V|i\rangle\langle i|, \\ V' &= V - \sum_{i\in M} |i\rangle\langle i|V|i\rangle\langle i|. \end{aligned}$$

We build the RS series for H'_0 and V' with the one-dimensional model space M spanned by $|0\rangle$. Thus, $P' = |0\rangle\langle 0|$. This gives us $P'V'P' = 0$. As a consequence, $\Omega_t = 0$ if $t = t_1 \vee |$ with $t_1 \neq |$. We can write $Q' = Q_0 + Q$, where Q is the projector corresponding to the initial problem and $Q_0 = P - P'$ is the projector onto the basis states of M different from $|0\rangle$. Then, we have $Q_0 V' P' = 0$ and $QV' = QV$. This gives us $Q'V'P' = QV'P' = QVP'$, which simplifies the evaluation of Ω_t for $t = |\vee|$. Similarly, $P'V'Q' = P'VQ$ simplifies the evaluation of Ω_t for $t = t_1 \vee t_2$. Finally, the identity $Q_0 V' Q_0 = 0$ gives us $Q'V'Q' = Q_0 VQ + QVQ_0 + QVQ$ for the evaluation of Ω_t with $t = | \vee t_2$.

This gives us the following recursive expression for $t = t_1 \vee t_2$.

$$\begin{aligned}
\Omega_t &= \sum_i \frac{|i^Q\rangle\langle i^Q|V|0\rangle\langle 0|}{e'_0 - e_i} \quad \text{if } t_1 = | \text{ and } t_2 = |\,, \\
\Omega_t &= \sum_i \frac{|i^Q\rangle\langle i^Q|V(Q+Q_0)\,\Omega_{t_2}|0\rangle\langle 0|}{e'_0 - e_i} + \sum_i \frac{|i^{Q_0}\rangle\langle i^{Q_0}|VQ\,\Omega_{t_2}|0\rangle\langle 0|}{e'_0 - e'_i} \quad \text{if } t_1 = | \text{ and } t_2 \neq |\,, \\
\Omega_t &= 0 \quad \text{if } t_1 \neq | \text{ and } t_2 = |\,, \\
\Omega_t &= -\sum_i \frac{|i^Q\rangle\langle i^Q|\Omega_{t_1}|0\rangle\langle 0|VQ\,\Omega_{t_2}|0\rangle\langle 0|}{e'_0 - e_i} - \sum_i \frac{|i^{Q_0}\rangle\langle i^{Q_0}|\Omega_{t_1}|0\rangle\langle 0|VQ\,\Omega_{t_2}|0\rangle\langle 0|}{e'_0 - e'_i} \quad \text{if } t_1 \neq | \text{ and } t_2 \neq |\,.
\end{aligned}$$

The recursive expression shows that all terms are well defined if all $e'_i = e_i + \langle i|V|i\rangle$ are different and if e'_0 is different from the energies e^Q_j out of the model space.

V. CONTINUED FRACTIONS

We discuss here some continued-fraction resummation of the RS series. Such a (generalized) continued fraction formula was found to be very efficient for calculating nuclear properties [45]. The combinatorial structure of continued fractions was studied in detail by Flajolet [46, 47]. On the other hand, Lee and Suzuki derived a continued fraction expression for χ and the effective Hamiltonian for a degenerate system [48, 49]. Other implementations of continued fractions for pertubation theory can be found in the literature [50–54].

A. The Suzuki-Lee formula

Suzuki and Lee [49] start from the Kvasnicka-Lindgren equation

$$[\chi, H_0] \;=\; QVP + QV\chi - \chi VP - \chi V\chi.$$

For a degenerate system $PH_0 = e_0P$, so that $\chi H_0 = e_0\chi$ and $(e_0 - H_0)\chi = QVP + QV\chi - \chi VP - \chi V\chi$. This equation is then reordered into $(e_0 - QHQ + \chi VQ)\chi = QVP - \chi VP$. They consider the iterative equation (see [49], eq. (3.27) p. 2102).

$$(e_0 - QHQ + \chi_{n-1}VQ)\chi_n \;=\; QVP - \chi_{n-1}VP,$$

with the boundary condition $\chi_0 = 0$. In other words

$$\chi_n \;=\; (e_0 - QHQ + \chi_{n-1}PVQ)^{-1}(QVP - \chi_{n-1}VP).$$

B. A new continued fraction expansion

The Suzuki-Lee formula has two drawbacks: it is restricted to degenerate systems [55] and it requires the inversion of $e_0 - QHQ + \chi_{n-1}PVQ$, which is usually infinite dimensional. To solve these two problems, we start from eq. (10) and, by using $Q_iQ = Q_i$, we rewrite it $Q_i\chi P(H - e_i)P = Q_iVP + Q_iV\chi - Q_i\chi V\chi$. We transform this equation into

$$Q_i\chi\Big(P(H - e_i)P + PV\chi\Big) \;=\; Q_iVP + Q_iV\chi. \tag{18}$$

Thus, we define the system of recursive equations

$$\begin{aligned} Q_i\chi_n &= (Q_iVP + Q_iV\chi_{n-1})(PHP - e_iP + PV\chi_{n-1})^{-1}, \\ \chi_n &= \sum_i Q_i\chi_n, \end{aligned}$$

with the boundary condition $\chi_0 = 0$. This generalized continued fraction has convergence properties similar to that of Lee and Suzuki, it is well-defined for quasi-degenerate systems and the inverse is computationally easier because it is done within the model space.

VI. BIJECTIONS

Many other combinatorial objects have been used to represent the terms of the RS series in non-degenerate or degenerate cases. Each of these representations is useful for specific applications. It is therefore important to describe the relation between the most important of them (Bloch sequences, Dyck paths, braketings and non-crossing partitions) and the trees. Most of these representations are valid for degenerate systems. Thus, we start by presenting the first terms of the RS series of degenerate systems, where e_0 is the energy of the states of the model space. We also give an

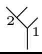
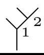
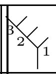
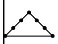
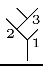
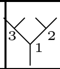
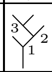
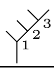
n	Tree	Bloch	Dyck	Bracketing	Partition	[28]
1		(1)		$*o\rangle$	$\|1\|$	1
2		(20)		$-*\langle o\rangle*o\rangle$	$\|12\|$	2
2		(11)		$*o*o\rangle$	$\|1\|2\|$	1
3		(300)		$*\langle o\rangle*\langle o\rangle*o\rangle$	$\|123\|$	5
3		(210)		$-*\langle o\rangle*o*o\rangle$	$\|13\|2\|$	2
3		(201)		$-*\langle o*o\rangle*o\rangle$	$\|12\|3\|$	4
3		(120)		$-*o*\langle o\rangle*o\rangle$	$\|1\|23\|$	3
3		(111)		$*o*o*o\rangle$	$\|1\|2\|3\|$	1

TABLE I: Correspondence between several representations of the RS terms for n=1,2,3: numbered tree, Bloch sequence, Dyck path, bracketing, non-crossing partition and item in Olszewski's list of examples [28].

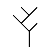
operator representation of these terms, with $R = Q(e_0 - H_0)^{-1}Q$.

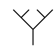
$$\Omega_t = \sum_{i_1,i_2} \frac{|i_1^Q\rangle\langle i_1^Q|V|i_2^P\rangle\langle i_2^P|}{e_0 - e_{i_1}} = RVP \quad \text{for} \quad t =$$  ,

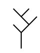
$$\Omega_t = -\sum_{i_1,i_2,i_3} \frac{|i_1^Q\rangle\langle i_1^Q|V|i_2^P\rangle\langle i_2^P|V|i_3^P\rangle\langle i_3^P|}{(e_0 - e_{i_1})(e_0 - e_{i_1})} = -R^2VPVP \quad \text{for} \quad t =$$  ,

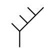
$$\Omega_t = \sum_{i_1i_2i_3} \frac{|i_1^Q\rangle\langle i_1^Q|V|i_2^Q\rangle\langle i_2^Q|V|i_3^P\rangle\langle i_3^P|}{(e_0 - e_{i_2})(e_0 - e_{i_1})} = RVRVP \quad \text{for} \quad t =$$  ,

$$\Omega_t = \sum_{i_1i_2i_3i_4} \frac{|i_1^Q\rangle\langle i_1^Q|V|i_2^P\rangle\langle i_2^P|V|i_3^P\rangle\langle i_3^P|V|i_4^P\rangle\langle i_4^P|}{(e_0 - e_{i_1})(e_0 - e_{i_1})(e_0 - e_{i_1})} = R^3VPVPVP \quad \text{for} \quad t =$$  ,

$$\Omega_t = -\sum_{i_1i_2i_3i_4} \frac{|i_1^Q\rangle\langle i_1^Q|V|i_2^Q\rangle\langle i_2^Q|V|i_3^P\rangle\langle i_3^P|V|i_4^P\rangle\langle i_4^P|}{(e_0 - e_{i_1})(e_0 - e_{i_2})(e_0 - e_{i_1})} = -R^2VRVPVP \quad \text{for} \quad t =$$  ,

$$\Omega_t = -\sum_{i_1i_2i_3i_4} \frac{|i_1^Q\rangle\langle i_1^Q|V|i_2^P\rangle\langle i_2^P|V|i_3^Q\rangle\langle i_3^Q|V|i_4^P\rangle\langle i_4^P|}{(e_0 - e_{i_1})(e_0 - e_{i_1})(e_0 - e_{i_3})} = -R^2VPVRVP \quad \text{for} \quad t =$$  ,

$$\Omega_t = -\sum_{i_1i_2i_3i_4} \frac{|i_1^Q\rangle\langle i_1^Q|V|i_2^Q\rangle\langle i_2^Q|V|i_3^P\rangle\langle i_3^P|V|i_4^P\rangle\langle i_4^P|}{(e_0 - e_{i_1})(e_0 - e_{i_2})(e_0 - e_{i_2})} = -RVR^2VPVP \quad \text{for} \quad t =$$  ,

$$\Omega_t = \sum_{i_1i_2i_3i_4} \frac{|i_1^Q\rangle\langle i_1^Q|V|i_2^Q\rangle\langle i_2^Q|V|i_3^Q\rangle\langle i_3^Q|V|i_4^P\rangle\langle i_4^P|}{(e_0 - e_{i_3})(e_0 - e_{i_2})(e_0 - e_{i_1})} = RVRVRVP \quad \text{for} \quad t =$$  .

A. Bloch sequences

Bloch [27] was the first to write the general term of Ω for degenerate systems. To describe his result, we consider the wave operator $\Omega(\lambda)$ of the Hamiltonian $H_0 + \lambda V$. We have the series expansion

$$\Omega(\lambda) = P + \sum_{n=1}^{\infty} \lambda^n \Omega_n,$$

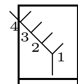
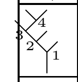
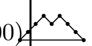
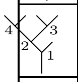
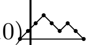
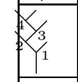
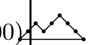
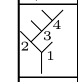
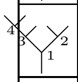
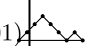
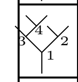
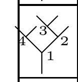
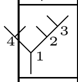
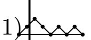
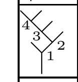
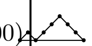
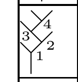
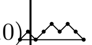
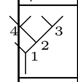
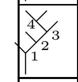
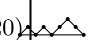
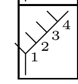
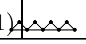
Tree	Bloch	Dyck	Bracketing	Partition	[28]
	(4000)		$-{*}\langle o\rangle{*}\langle o\rangle{*}\langle o\rangle{*}o\rangle$	$\|1234\|$	5
	(3100)		${*}\langle o\rangle{*}\langle o\rangle{*}o{*}o\rangle$	$\|134\|2\|$	6
	(3010)		${*}\langle o\rangle{*}\langle o{*}o\rangle{*}o\rangle$	$\|124\|3\|$	14
	(2200)		${*}\langle o\rangle{*}o{*}\langle o\rangle{*}o\rangle$	$\|14\|23\|$	7
	(2110)		$-{*}\langle o\rangle{*}o{*}o{*}o\rangle$	$\|14\|2\|3\|$	4
	(3001)		${*}\langle o{*}o\rangle{*}\langle o\rangle{*}o\rangle$	$\|123\|4\|$	13
	(2101)		$-{*}\langle o{*}o\rangle{*}o{*}o\rangle$	$\|13\|2\|4\|$	11
	(2020)		${*}\langle o{*}\langle o\rangle{*}o\rangle{*}o\rangle$	$\|12\|34\|$	10
	(2011)		$-{*}\langle o{*}o{*}o\rangle{*}o\rangle$	$\|12\|3\|4\|$	9
	(1300)		${*}o{*}\langle o\rangle{*}\langle o\rangle{*}o\rangle$	$\|1\|234\|$	8
	(1210)		$-{*}o{*}\langle o\rangle{*}o{*}o\rangle$	$\|1\|24\|3\|$	3
	(1201)		$-{*}o{*}\langle o{*}o\rangle{*}o\rangle$	$\|1\|23\|4\|$	12
	(1120)		$-{*}o{*}o{*}\langle o\rangle{*}o\rangle$	$\|1\|2\|34\|$	2
	(1111)		${*}o{*}o{*}o{*}o\rangle$	$\|1\|2\|3\|4\|$	1

TABLE II: Correspondence between several representations of the RS terms for n=4: numbered tree, Bloch sequence, Dyck path, bracketing, non-crossing partition and item in Olszewski's list of examples [28].

with

$$\Omega_n = \sum_{k_1,\ldots,k_n} S^{(k_1)}VS^{(k_2)}V\ldots VS^{(k_n)}VP, \tag{19}$$

where $S^0 = -P$, $S^{(k)} = R^k$ for $k > 0$, and where $k_1, \ldots, k_n$ run over the Bloch sequences. A Bloch sequence is an n-tuple $(k_1k_2\ldots k_n)$ of non-negative integers, such that $k_1+\cdots+k_m \geq m$ for $m < n$ and $k_1+\cdots+k_n = n$. The Bloch sequences for n=1, 2 and 3 are given in table I and for n=4 in table II. These combinatorial objects are enumerated by Catalan numbers (see Example 6.24 p. 180 of ref. [25] and item m^5 in Stanley's Catalan addendum). Since Bloch's publication [27], they were widely used [56–59] to represent the general term of the RS series for degenerate systems.

The bijection between trees and sequences is defined by $\phi(\curlyvee) := (1)$, $\phi(s \vee |) := K\phi(s)$, $\phi(| \vee s) := (1)\cdot\phi(s)$ and $\phi(s\vee t) := K\phi(s)\cdot\phi(t)$ where $s \neq |$, $t \neq |$, where the product on the right hand sides is the concatenation of sequences (i.e. $(k_1\ldots k_m)(k_{m+1}\ldots k_n) = (k_1\ldots k_n)$), and where the operation K acts by $K(k_1,k_2,\ldots,k_n) = (k_1+1,k_2,\ldots,k_n,0)$. Notice that ϕ is clearly one to one (injective). The fact that it is actually a bijection follows e.g. from the fact that trees and Bloch sequences are both enumerated by Catalan numbers.

We prove now its compatibility with the tree and Bloch expansions by induction. We write $t = t_1 \vee t_2$ and we consider the usual four cases. The first case is $t = \curlyvee$, $t_1 = t_2 = |$. This is the starting point of the inductive proof. We have $\Omega_t = RVP = S^1VP = \Omega_1$, where we used the fact that the only Bloch sequence for $n = 1$ is (1). Let us denote by Ω_B the contribution of Ω_n in eq. (19) corresponding to the Bloch sequence $B = (k_1\ldots k_n)$. Thus, we showed that, for $t =$ and $B = (1)$, we have $\Omega_t = \Omega_B$.

Now, assume that $\Omega_t = \Omega_{\phi(t)}$ for all trees t with $|t| \leq n$ and choose a tree t such that $|t| = n+1$. Then, $t = t_1 \vee t_2$ with $|t_1| \leq n$ and $|t_2| \leq n$. We consider the three remaining cases. If $t_1 \neq |$ and $t_2 = |$, then Ω_t is obtained from eqs. (4) and (8) $\Omega_t = -R\Omega_{t_1}PVP$. By the induction hypothesis, we have $\Omega_{t_1} = \Omega_{B_1}$ for $B_1 = \phi(t_1)$. Therefore, $\Omega_t = R\Omega_{B_1}(-P)VP$. If $B_1 = (k_1 \ldots k_n)$, then $\Omega_t = \Omega_B$ with $B = (k_1+1, k_2, \ldots, k_n, 0) = KB_1$ and the property is proved. The second case is $t_1 \neq |$ and $t_2 \neq |$. Then eqs. (4) and (9) give us $\Omega_t = R\Omega_{t_1}(-P)VQ\Omega_{t_2}$. If $\phi(t_1) = B_1 = (k_1 \ldots k_p)$ and $\phi(t_2) = B_2 = (l_1 \ldots l_q)$, then $\Omega_t = \Omega_B$ with $B = (k_1+1, k_2, \ldots, k_p, 0, l_1, \ldots, l_q) = K(B_1)B_2$. Thus, $\phi(t_1 \vee t_2) = K(B_1)B_2 = K\phi(l_1) \cdot \phi(l_2)$. The last case is $t_1 = |$ and $t_2 \neq |$. Equations (4) and (7) give us $\Omega_t = RVQ\Omega_{t_2}$. If $B_2 = \phi(t_2) = (k_1 \ldots k_n)$, then $\Omega_t = \Omega_B$ with $B = (1k_1 \ldots k_n) = (1) \cdot \phi(t_2)$.

B. Dyck paths

In ref. [27], Bloch also defined geometrical objects that are Dyck paths rotated by $\pi/4$. We prefer to use Dyck paths because they are thoroughly studied in the combinatorial literature (see, for example Item i, p. 221 of ref. [26] or Example 6.2, p. 151 of ref [25], where they are called *mountain ranges*).

The bijection between Dyck paths and Bloch sequences used in ref. [27] is well known in the combinatorial literature [25, p. 168 and 181]. To build the Dyck path corresponding to the the Bloch sequence $(k_1k_2\ldots k_n)$, start from the origin and make k_1 steps in the North-East direction, then make one step in the South-East direction, then k_2 steps in the North-East direction, then one step in the South-East direction, and so on. This bijection is illustrated in tables I and II.

C. Non-crossing partitions

The terms of the RS series of degenerate systems can also be described by non-crossing partitions. This correspondence was studied by Olszewski [28] because it leads to useful factorizations of the RS terms for non-degenerate systems.

Consider the examples at the beginning of section VI. If we just look at the denominators, we see that each of them can be deduced from the right comb by saying that some indices are equal. For the five trees with $|t| = 3$, the term corresponding to $t =$ can be obtained from that of $t =$ by stating that $e_{i_1} = e_{i_2} = e_{i_3}$. The other terms follow from $e_{i_1} = e_{i_3}$, $e_{i_1} = e_{i_2}$ and $e_{i_2} = e_{i_3}$.

More generally, for a given tree t, we say that two indices j and k are equivalent if and only if $e_{i_j} = e_{i_k}$ in the denominator of Ω_t. The sets of equivalent indices form a partition of $\{1, \ldots, n\}$. We recall that a partition $B_1|B_2|\ldots|B_k$ of $\{1, \ldots, n\}$ is a set of disjoint subsets B_i of $\{1, \ldots, n\}$ whose union is $\{1, \ldots, n\}$. Each subset B_i is called a block of the partition. The partitions corresponding to the RS terms of order 1 to 3 are given in table I and for order 4 in table II. It will be shown that these partitions are *non-crossing*. Two blocks A and B of a partition are said to be crossing if there are a, b in A and x, y in B such that $a < x < b < y$ or $x < a < y < b$. A partition is called non-crossing if no two of its blocks cross.

We build by induction a partition from a tree. Note first that for tree t of order n we deal with partitions of $\{1, \ldots, n\}$. A tree of order n has $n+1$ leaves. Thus, the index of the rightmost leaf is not used in the partition.

For a given tree $t = t_1 \vee t_2$, we call P (P_1, P_2, respectively) the partition corresponding to t (t_1, t_2, respectively). We consider the usual four cases. (i) For $t_1 = t_2 = |$ we associate the partition $P = |1|$. (ii) For $t_1 \neq |$ and $t_2 = |$, eq. (8) gives us the additional denominator $e_0 - e_1$. Therefore, an additional index is equivalent to 1. This index is that of the rightmost leaf of t_1, which was not used in P_1. Therefore, the partition P of t is obtained from P_1 by adding to the block of P_1 containing 1 the index of the rightmost leaf of t_1, which is $|t_1| + 1$. (iii) For $t_1 = |$ and $t_2 \neq |$, eq. (7) gives us the additional denominator $e_0 - e_1$. However, the leaf denoted by 1 is new and no block of P_2 should contain it. Therefore, the partition P of t is obtained from P_2 by increasing all numbers of P_2 by 1 and by adding the block $|1|$. (iv) For $t_1 \neq |$ and $t_2 \neq |$, we compose the previous cases. We build P by adding the index $|t_1| + 1$ to the block of P_1 containing the index 1 and we increase all indices of P_2 by $|t_1| + 1$. We check that, in all cases, the resulting partition is non-crossing.

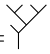
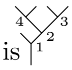
Note that Olszewski [28] does not explicitly use non-crossing partitions. He describes the general term of the RS series for non-degenerate systems by drawing a circle with n points and pinching some of these points. The relation with non-crossing partitions is straightforward: all points that are pinched together belong to the same block of the partition. However, his correspondence between partitions and terms of the RS series is not the same as ours.

D. Bracketing

Following a suggestion by Brueckner [60], Huby and Tong [29, 30] proposed, for the energy of nondegenerate systems, a solution in terms of bracketing, that is isomorphic with Stanley's problem e^5 in his "Catalan addendum".

Consider the example of $t =$ . We have $\Omega_t = R^2VPVP$. For a nondegenerate system $P = |0\rangle\langle 0|$ and $\Omega_T|0\rangle = R^2V|0\rangle\langle 0|V|0\rangle$. The rule of the game is now to insert expectation values to disjoin powers of R. Thus, $\Omega_T|0\rangle = -R\langle 0|V|0\rangle RV|0\rangle$. We use Tong's pictorial representation, where R is replaced by $*$, V by o, $\langle 0|$ by $\langle$ and $|0\rangle$ by $\rangle$, so that $\Omega_T|0\rangle = -*\langle o\rangle * o\rangle$. The bracketings for $|t|$=1,2 and 3 are given in table I and for order 4 in table II. Brueckner's bracketing is a powerful way to simplify the RS series, for instance by including the vacuum expectation value $\langle 0|V|0\rangle$ into H_0, so that all RS terms involving it cancel. More details and examples can be found in some textbooks [61] or review papers [62].

We now describe the connection between trees and bracketings. Denote by $b(t)$ the bracketing corresponding to t in Tong's representation. Assume that $b(t)$ is known for all trees t with $|t| \leq n$ and take a tree $t = t_1 \vee t_2$ of degree n. It $t_1 = \vert$ and $t_2 \neq \vert$, then $\Omega_t|0\rangle = RV\Omega_{t_2}|0\rangle$, so that $b(t) = *ob(t_2)$. It $t_1 \neq \vert$ and $t_2 = \vert$, then $\Omega_t|0\rangle = -R\Omega_{t_1}|0\rangle\langle 0|V|0\rangle = -R\langle 0|V|0\rangle\Omega_{t_1}|0\rangle$, so that $b(t) = -*\langle o\rangle b(t_1)$. It $t_1 \neq \vert$ and $t_2 \neq \vert$, then $\Omega_t|0\rangle = -R\Omega_{t_1}|0\rangle\langle 0|V\Omega_{t_2}|0\rangle = -R\langle 0|V\Omega_{t_2}|0\rangle\Omega_{t_1}|0\rangle$, so that $b(t) = -*\langle ob(t_2)b(t_1)$. Note that this bijection is different from the one used by Tong [30].

An equivalent bijection is obtained by numbering the inner vertices of the trees. The operation ν that associates to each tree t its numbered tree is defined as follows. We denote by $\nu(t)[k]$ the numbered tree obtained from $\nu(t)$ by adding k to all the vertex numbers. Then, $\nu(t)$ can be defined recursively. If $t = \vert$, then $\nu(t) = \vert$ (no number). If $t =$ , then $\nu(t)$ is obtained by assigning the number 1 to the root. If $t = t_1 \vee t_2$, then the root has number 1, the inner vertices of t_2 (if any) are numbered as $\nu(t_2)[1]$ and the inner vertices of t_1 (if any) are numbered as $\nu(t_1)[|t_2|+1]$. The numbered trees for $|t| \leq 3$ are given in table table I and for $|t| = 4$ in table II. For any tree t, we can build the sets of numbers belonging to the same line oriented to the left. For example, if $t =$ , the numbering is  and the sets are $|1|24|3|$. These sets form a non-crossing partition which is the same as that used by Olszewski [28]. To obtain $b(t)$, first number the $|t|$ stars of $b(t)$ from 1 to $|t|$ from the left to the right. Then, consider a block $B = k_1 \ldots k_p$ of the partition. If $p = 1$, do nothing, if $p > 1$, then write a $\langle$ after star number k_1, a $\rangle$ before star number k_p and replace star number k_i with $1 < i < p$ (if any) by $\rangle * \langle$.

VII. CONCLUSION

Combinatorial physics is an emerging field that uses modern tools of algebraic combinatorics to solve physical problems. It was born with the investigation of the algebraic structure of renormalization in quantum field theory [63] and showed its ability to deal with many-body problems [64].

We showed that combinatorial physics is able to solve such long-standing problems as time-independent perturbation theory. The RS series is at the heart of many applications of quantum mechanics. It is also equivalent to more sophisticated methods such as Feynman diagrams [65]. It is even related to Wilson's renormalization group [66].

Our combinatorial methods provided easy resummations of the RS series. It remains now to test their convergence properties.

Note that Arnol'd also used trees in perturbation theory [67]. However, his trees are essentially different from ours because they describe the successive degeneracy splitting due to higher order terms [68].

VIII. ACKNOWLEDGEMENT

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