Ann. Inst. H. Poincaré D
Comb. Phys. Interact. 11 (2024), 383–407
DOI 10.4171/AIHPD/173

A basis- and integral-free representation of time-dependent perturbation theory via the Omega matrix calculus

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Abstract. We obtain a basis- and integral-free representation of the n-term in time-dependent perturbation theory of the quantum time-evolution operator. The main technical tool to construct the aforementioned representation comprises the Omega matrix calculus; that is, an extension of MacMahon's partition analysis to the realm of matrix calculus. In particular, we show that if we specialize our formulation to the time-independent and finite-dimensional case, we recover Putzer (1966) original formulation to compute the matrix exponential avoiding the Jordan canonical form. Furthermore, if we use an explicit basis for the time-independent part of the generator of evolution, then our work implies a representation of the perturbation expansion similar to an approach discussed in the recent work of Kalev and Hen (2021) using divided differences. Finally, we obtain closed form expressions which generalize and unify all the perturbation calculations considered in Kalev and Hen (2021) and advance some considerations regarding degeneracy associated with the unperturbed Hamiltonian in the context of adiabatic switching.

1. Introduction

The solution of the time-dependent Schrödinger equation (in units $\hbar \equiv 1$)

$$\imath \boldsymbol{\psi}'(t) = \boldsymbol{H}(t)\boldsymbol{\psi}(t) \quad \text{and} \quad \boldsymbol{\psi}(t_0) = \boldsymbol{\psi}_0, \tag{1.1}$$

where $\imath$ is the imaginary unit, is given by

$$\boldsymbol{\psi}(t) = \boldsymbol{U}(t, t_0)\boldsymbol{\psi}_0, \tag{1.2}$$

where $\boldsymbol{U}(t, t_0)$ is the time-evolution operator

$$\boldsymbol{U}(t, t_0) = \mathcal{T} \exp\Big(-\imath \int_{t_0}^{t} \boldsymbol{H}(s)\, ds\Big)$$

2020 Mathematics Subject Classification. Primary 05A10; Secondary 05A15, 15A16, 81Q15.
Keywords. Time-dependent perturbation, Dyson series, basis-free, integral-free, Omega matrix calculus, Putzer's representation, divided differences.

with the time-ordering operator $\mathcal{T}$ [20, Chapter 1] and a time-dependent Hamiltonian operator $\boldsymbol{H}(t)$ acting on the Hilbert space $\mathcal{H}$. The determination of $\boldsymbol{U}(t, t_0)$ is of paramount importance in a variety of applications, but, unfortunately, this status is contrasted with the difficulty in determining $\boldsymbol{U}(t, t_0)$ either by non-perturbation methods or using perturbation theory [23, 31]. For example, the usual computation of time-dependent perturbation theory of the evolution operator starting with the iterated integrals involving time-ordered product of operators turns out to be rather difficult even for simple cases [31]. Therefore, new methods to compute time-dependent perturbation theory which shed light on the intricate nature of the iterated integrals are of great value. It turns out that methods based on combinatorics (discrete structures) turn out to be quite useful in computing $\boldsymbol{U}(t, t_0)$. We mention notably graph rules for functions of the time-evolution operator [14], ordered labeled rooted trees and convergence criteria for series of integrals [35], tree parametrization of iterated integrals [9, 10], the method of path-sums based on resummations on graphs [24, 25], and, recently, an integral-free method for the Dyson series based on divided differences [31]. For other time-dependent perturbation treatments including Magnus- and Fer-type expansions with applications and connections with the time-ordered product, we refer the reader to [4, 8, 32, 39].

Here we take another unexplored route to compute time-dependent perturbation theory, but this time using combinatorial analysis rooted in the partition of natural numbers. MacMahon's partition analysis (MPA) or Omega calculus is a powerful and easy to apply tool of combinatorial analysis originally devised to construct generating functions describing the solutions of Diophantine systems in the context of the partition of natural numbers [37]. MPA was mainly concerned with scalar problems until recently when an extension of MacMahon's formalism to matrix analysis, referred here as Omega matrix calculus or OMC for short, was introduced in [17]. Later on, OMC was applied to problems of continuum mechanics; that is, the computation of matrix derivatives [16]. Recently, exact formulas for the powers of matrices of general interest such as the companion, tridiagonal, and triangular matrices were obtained [19] as well as an extension of Putzer's representation [40] to general analytic functions including the Mittag-Leffler function and fractional matrix exponentials [18].

In this work, we obtain a basis- and integral-free representation of time-dependent perturbation theory by recasting the terms of the expansion in the framework of OMC. Our approach is quite simple and easy to apply since all we need is the computation of rather simple Omega generating functions and the solution of an elementary initial value problem (IVP) for ordinary differential equations (ODEs). Using our representation, we obtain an exact expression for the n-term of the time-dependent perturbation expansion of the evolution operator which gives as special cases all the examples considered in [31]. We also advance some considerations regarding degeneracy associated with the unperturbed Hamiltonian in the context of adiabatic switching [11, 12, 22, 34].

Here we consider the generator of dynamics composed of a time-independent Hamiltonian plus a time-dependent interaction term. As we will show by setting to zero the time-dependent interaction, we recover Putzer original formulation in [40, Theorem 1], and if we introduce a basis for the time-independent Hamiltonian, then we recover a result equivalent to [31]. Therefore, our work can be interpreted in at least two distinct ways: as an extension of Putzer's representation in the context of the time-dependent case and as a basis-free approach to the integral-free representation of the time-dependent perturbation theory described in [31].

This work is organized as follows. In Section 2, we establish the necessary background in order to introduce our main results in Section 3. Some examples show the usefulness of our approach in Section 4. Section 5 is devoted to the concluding remarks.

2. Basic definitions and auxiliary results

2.1. Brief review of Omega matrix calculus

We recall the basic definitions of OMC following [17]. See also [1,2,37] for the original formulation in the scalar case and for the implementation of the Omega package, a computer algebra package in MATHEMATICA suited for the Omega calculus. We write $\mathbf{0}_n = (0, \dots, 0) \in \mathbb{C}^n$ throughout this work.

Definition 2.1. Let $\boldsymbol{X}_{\boldsymbol{a}} \in \mathbb{C}^{N \times N}$ for each $\boldsymbol{a} \in \mathbb{Z}^n$ and $\boldsymbol{\lambda}^{\boldsymbol{a}} = \lambda_1^{a_1} \cdots \lambda_n^{a_n}$. We define the linear operators acting on absolutely convergent matrix valued expansions

$$\underset{=}{\overset{\boldsymbol{\lambda}}{\Omega}} \sum_{a_1=-\infty}^{\infty} \cdots \sum_{a_n=-\infty}^{\infty} \boldsymbol{X}_{\boldsymbol{a}} \boldsymbol{\lambda}^{\boldsymbol{a}} \stackrel{\text{def}}{=} \boldsymbol{X}_{\mathbf{0}_n} \tag{2.1}$$

in an open neighborhood of the complex circles $|\lambda_i| = 1$.

Remark 2.2. The convergence of the series in (2.1) guarantees that no singularities in the variable λ_i in an open neighborhood of the circle $|\lambda_i| = 1$ exists. As remarked in [1], this is an important ingredient avoiding ambiguous results and leading to unique Laurent expansions. Note also that since the Omega operators are linear operators, they commute with the derivative $\partial_{(\boldsymbol{X}_a)_{ij}}$, where we write $(\boldsymbol{X}_a)_{ij}$ for the entry in row i and column j of $\boldsymbol{X}_a$. Without further mention we use this observation whenever necessary.

Definition 2.1 encodes the essence of the Omega calculus: the elimination of the Omega variables. Note that the left-hand side of (2.1) contains the Omega variable $\boldsymbol{\lambda}$ which after applying the Omega operator is eliminated resulting in the right-hand side of (2.1). It turns out that it is not always straightforward to eliminate the Omega variables, but luckily our formalism fits in the most simple case. The Omega expressions considered here are all of the type

$$\underset{=}{\overset{\lambda}{\Omega}} \frac{\lambda^n}{P(\boldsymbol{x}/\lambda)} \tag{2.2}$$

with $n > 0$ and a factored polynomial $P(\boldsymbol{x}) \in \mathbb{C}[\boldsymbol{x}]$. The parameter $\boldsymbol{x}$ is taken small to fulfill the conditions stated in Definition 2.1. In what follows, we recall the definition of the generating function of the homogeneous (a.k.a. complete) symmetric polynomials $h_n(x_1, x_2, \ldots, x_m)$ [36]

$$\frac{1}{(1-x_1t)(1-x_2t)\cdots(1-x_mt)} = \sum_{n\geq 0} h_n(x_1, x_2, \ldots, x_m)t^n. \tag{2.3}$$

In contrast to (2.2), the most difficult expressions to consider are those having non-factored denominators along with powers of λ and λ^{-1}. Indeed, compare [1, Theorem 2.1] with [1, Lemma 2.1] and see [27].

The next lemma shows that it is quite simple to eliminate Omega variables in (2.2) with a factored polynomial $P(\boldsymbol{x})$.

Lemma 2.3. *Let $n \geq 0$. Then we have*

$$\underset{=}{\overset{\lambda}{\Omega}} \frac{\lambda^n}{(1-x_1/\lambda)(1-x_2/\lambda)\cdots(1-x_m/\lambda)} = \begin{cases} 1 & \text{if } n = 0, \\ h_n(x_1, x_2, \ldots, x_m) & \text{if } n > 0. \end{cases} \tag{2.4}$$

Proof. The proof is straightforward from (2.3). ∎

We will use throughout this work the terminology Omega free for the expression obtained after the elimination of the Omega variable. For example, the right-hand side of (2.4) is an example of an Omega free expression.

Another nice feature of OMC is that under the Omega operator we can represent a matrix function in terms of another matrix function. Indeed, if

$$F(\boldsymbol{X}) = \sum_{\boldsymbol{a}\in S} f_{\boldsymbol{a}} \boldsymbol{X}^{\boldsymbol{a}} \quad \text{and} \quad G(\boldsymbol{X}) = \sum_{\boldsymbol{a}\in S} g_{\boldsymbol{a}} \boldsymbol{X}^{\boldsymbol{a}}$$

for some set S provided the conditions in Definition 2.1 are valid, then we have the next lemma.

Lemma 2.4. *The following identity holds:*

$$G(\boldsymbol{X}) = \underset{=}{\overset{\boldsymbol{\lambda}}{\Omega}} \sum_{\boldsymbol{a}\in S} \frac{g_{\boldsymbol{a}}}{f_{\boldsymbol{a}}} \boldsymbol{\lambda}^{\boldsymbol{a}} F\left(\frac{\boldsymbol{X}}{\boldsymbol{\lambda}}\right).$$

Proof. Observe that

$$\underset{=}{\overset{\lambda}{\Omega}} \sum_{\boldsymbol{a}\in S} \frac{g_{\boldsymbol{a}}}{f_{\boldsymbol{a}}} \boldsymbol{\lambda}^{\boldsymbol{a}} F\left(\frac{\boldsymbol{X}}{\boldsymbol{\lambda}}\right) = \sum_{\boldsymbol{a},\boldsymbol{b}\in S} \frac{g_{\boldsymbol{a}}}{f_{\boldsymbol{a}}} f_{\boldsymbol{b}} \boldsymbol{X}^{\boldsymbol{b}} \underbrace{\underset{=}{\overset{\lambda}{\Omega}} \boldsymbol{\lambda}^{\boldsymbol{a}-\boldsymbol{b}}}_{=\prod_{i=1}^{n} \delta_{a_i,b_i}} = \sum_{\boldsymbol{a}\in S} g_{\boldsymbol{a}} \boldsymbol{X}^{\boldsymbol{a}} = G(\boldsymbol{X})$$

with the usual Kronecker delta $\delta_{a,b}$. ■

2.2. Auxiliary results

Let

$$P(x) = \det(x\boldsymbol{I} - \boldsymbol{A}) = \prod_{i=1}^{r} (x - \alpha_i)^{m_i} \tag{2.5}$$

with $m_i \geq 1$ and $\sum_{i=1}^{r} m_i = N$ be the characteristic polynomial of $\boldsymbol{A}$. It follows from the Cayley–Hamilton theorem that P is an example of an annihilating polynomial; that is, a polynomial P such that $P(\boldsymbol{A}) = \boldsymbol{O}$. The annihilating polynomial of the smallest possible degree d is called the minimal polynomial [3, 21, 29, 33]

$$Q(x) = \prod_{i=1}^{r} (x - \alpha_i)^{n_i} = x^d + c_{d-1}x^{d-1} + \cdots + c_1 x + c_0 \tag{2.6}$$

with $1 \leq n_i \leq m_i$.

It follows from the existence of the annihilating polynomial that analytic matrix functions can be represented by a finite sum. In particular, we have the representation for the matrix exponential

$$\exp(t\boldsymbol{A}) = \sum_{k=0}^{d-1} x_{k+1}(t) \boldsymbol{A}^k. \tag{2.7}$$

We also recall that the coefficients $x_{k+1}(t)$ are unique using [13, Proposition 2]. We use this result to prove the next lemma which is equivalent to [40, Theorem 1] apart from the fact that the minimal polynomial $Q(x)$ in (2.6) is used instead of the characteristic polynomial $P(x)$ in (2.5). For other finite sum representations of the matrix exponential and other matrix function definitions, we refer the reader to [5–7, 38] and [28], respectively.

Lemma 2.5. *Let $\boldsymbol{A} \in \mathbb{C}^{N\times N}$. Then we have*

$$\exp(t\boldsymbol{A}) = \sum_{k=0}^{d-1} x_{k+1}(t) \boldsymbol{A}^k,$$

where

$$\boldsymbol{x}(t) = \boldsymbol{B}\,\boldsymbol{y}(t) \tag{2.8}$$

with $\boldsymbol{x}(t) = (x_1(t), \dots, x_d(t))^\mathsf{T}$,

$$\boldsymbol{B} = \begin{pmatrix} c_1 & c_2 & \cdots & c_{d-1} & 1 \\ c_2 & c_3 & \cdots & 1 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ c_{d-1} & 1 & \cdots & 0 & 0 \\ 1 & 0 & \cdots & 0 & 0 \end{pmatrix},$$

and $\boldsymbol{y}(t) = (y(t), y'(t), \dots, y^{(d-1)}(t))^\mathsf{T} \in \mathbb{C}^d$ *such that*

$$y^{(d)}(t) + c_{d-1}y^{(d-1)}(t) + \cdots + c_1 y'(t) + c_0 y(t) = 0 \tag{2.9}$$

with the coefficients of the ODE in (2.9) *determined by* $Q(x)$ *in* (2.6) *and satisfying the initial conditions*

$$y(0) = y'(0) = \cdots = y^{(d-2)}(0) = 0 \quad \text{and} \quad y^{(d-1)}(0) = 1. \tag{2.10}$$

Proof. Observe that

$$\sum_{k=0}^{d-1} x_{k+1}(t)\boldsymbol{A}^{k+1} = \boldsymbol{A}\exp(t\boldsymbol{A}) = \sum_{k=0}^{d-1} x'_{k+1}(t)\boldsymbol{A}^k \tag{2.11}$$

and by the uniqueness of the expansion in (2.11); that is, the corresponding coefficients in the left-hand side and right-hand side of (2.11) are equal. Thus, we obtain

$$x'_{k+1}(t) = x_k(t) - c_k x_d(t) \tag{2.12}$$

using

$$\begin{aligned} \sum_{k=0}^{d-1} x_{k+1}(t)\boldsymbol{A}^{k+1} &= \sum_{k=0}^{d-2} x_{k+1}(t)\boldsymbol{A}^{k+1} + x_d(t)\boldsymbol{A}^d \\ &= \sum_{k=0}^{d-2} x_{k+1}(t)\boldsymbol{A}^{k+1} - x_d(t)\sum_{i=0}^{d-1} c_i\boldsymbol{A}^i, \end{aligned}$$

which follows from the fact that the minimal polynomial in (2.6) is annihilating. We can easily show that (2.8) is equivalent to (2.12) since $x_d(t) = y(t)$. The initial condition in (2.10) is similarly proved by setting $t = 0$ in (2.11). ■

Concerning $\boldsymbol{y}(t) = (y(t), y'(t), \dots, y^{(d-1)}(t))^\mathsf{T}$ in (2.8); note that we can write

$$y(t) = \sum_{i=1}^{r}\sum_{j=0}^{n_i-1} c_{ij}t^j\exp(\alpha_i t), \tag{2.13}$$

where the coefficients c_{ij} in (2.13) are such that (2.10) is satisfied. Therefore, to determine $x_{k+1}(t)$, all we need is the solution of the most elementary IVP: an ODE with constant coefficients in (2.9) and the initial conditions in (2.10)!

An exact formula for c_{ij} in (2.13) is given in the next lemma.

Lemma 2.6. *The following identity holds:*

$$c_{ij} = \frac{1}{(j+1)!(n_i-j-1)!}\partial_\lambda^{n_i-j-1}\left(\frac{(\lambda-\alpha_i)^{n_i}}{\prod_{k=1}^r(\lambda-\alpha_k)^{n_k}}\right)\Bigg|_{\lambda=\alpha_i}. \tag{2.14}$$

Proof. We first show that

$$y^{(i-1)}(t) = \underset{=}{\overset{\lambda}{\Omega}}\frac{\exp(\lambda t)\lambda^i}{\prod_{k=1}^r(\lambda-\alpha_k)^{n_k}}. \tag{2.15}$$

Note that the expression for $y(t) = y^{(0)}(t)$ satisfies the IVP given in (2.9) and (2.10). Indeed, we have

$$\sum_{i=1}^{d+1} c_{i-1}y^{(i-1)}(t) = \underset{=}{\overset{\lambda}{\Omega}}\lambda\exp(\lambda t)\underbrace{\frac{\left(\sum_{i=1}^{d+1}c_{i-1}\lambda^{i-1}\right)}{\prod_{k=1}^r(\lambda-\alpha_k)^{n_k}}}_{\overset{(2.6)}{=}1} = \underset{=}{\overset{\lambda}{\Omega}}\lambda\exp(\lambda t) = 0$$

with the convention $c_d \equiv 1$. Regarding the initial conditions, note that

$$y^{(i-1)}(0) = \underset{=}{\overset{\lambda}{\Omega}}\frac{\lambda^i}{\prod_{k=1}^r(\lambda-\alpha_k)^{n_k}} = \underset{=}{\overset{\lambda}{\Omega}}\frac{\lambda^{i-d}}{\prod_{k=1}^r(1-\alpha_k/\lambda)^{n_k}} = \begin{cases}0, & 1\le i<d,\\ 1, & i=d.\end{cases}$$

Finally, using partial fraction decomposition, we have

$$\frac{1}{\prod_{k=1}^r(\lambda-\alpha_k)^{n_k}} = \sum_{i=1}^r\sum_{j=0}^{n_i-1}\frac{j!b_{ij}}{(\lambda-\alpha_i)^{j+1}} \tag{2.16}$$

with b_{ij} given by the right-hand side of (2.14). The result follows if we can show that $c_{ij} \equiv b_{ij}$. Indeed, observe that

$$\begin{aligned} y(t) &\overset{(2.15)}{=} \underset{=}{\overset{\lambda}{\Omega}}\frac{\lambda\exp(\lambda t)}{\prod_{k=1}^r(\lambda-\alpha_k)^{n_k}} \overset{(2.16)}{=} \sum_{i=1}^r\sum_{j=0}^{n_i-1} j!b_{ij}\underset{=}{\overset{\lambda}{\Omega}}\frac{\lambda\exp(\lambda t)}{(\lambda-\alpha_i)^{j+1}}\\ &= \sum_{i=1}^r\sum_{j=0}^{n_i-1} b_{ij}\partial_{\alpha_i}^j\underbrace{\underset{=}{\overset{\lambda}{\Omega}}\frac{\exp(\lambda t)}{1-\alpha_i/\lambda}}_{=\exp(\alpha_i t)} = \sum_{i=1}^r\sum_{j=0}^{n_i-1} b_{ij}t^j\exp(\alpha_i t)\end{aligned}$$

from the uniqueness of the solution of the IVP in (2.9) and (2.10); that is, we have $b_{ij} \equiv c_{ij}$ given in (2.13). ∎

3. Omega matrix calculus and time-dependent perturbation theory

Let us consider

$$\boldsymbol{H}(t) = \boldsymbol{H}_0 + \gamma \boldsymbol{V}(t), \tag{3.1}$$

where $\boldsymbol{H}_0$ is a time-independent Hamiltonian and $\gamma \boldsymbol{V}(t)$ represents a time-dependent interaction term. Throughout this work, we assume that the spectrum of $\boldsymbol{H}_0$ is given by a countable (discrete) set. We will be interested in the IVP (1.1) with $\boldsymbol{H}(t)$ given by (3.1) and $\boldsymbol{\psi}(t)$ in (1.2) determined by the time-dependent perturbation theory of the evolution operator

$$\boldsymbol{U}(t, t_0) = \sum_{n \geq 0} \gamma^n \boldsymbol{U}^{(n)}(t, t_0), \tag{3.2}$$

where $\boldsymbol{U}^{(0)}(t, t_0) = \exp(-\imath(t - t_0)\boldsymbol{H}_0)$ and

$$\boldsymbol{U}^{(n)}(t, t_0) = (-\imath)^n \exp(-\imath t \boldsymbol{H}_0) \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \\ \times \int_{t_0}^{t_{n-1}} dt_n \boldsymbol{V}_I(t_1)\boldsymbol{V}_I(t_2) \cdots \boldsymbol{V}_I(t_n) \exp(\imath t_0 \boldsymbol{H}_0)$$

if $n \geq 1$ with $\boldsymbol{V}_I(t) \equiv \exp(\imath \boldsymbol{H}_0 t)\boldsymbol{V}(t) \exp(-\imath \boldsymbol{H}_0 t)$. Here the subscript I stands for the interaction picture [15]. The associated Dyson series is given by

$$\boldsymbol{U}_I(t, t_0) = \sum_{n \geq 0} \gamma^n \boldsymbol{U}_I^{(n)}(t, t_0)$$

with $\boldsymbol{U}_I(t, t_0) = \exp(\imath t \boldsymbol{H}_0)\boldsymbol{U}(t, t_0) \exp(-\imath t_0 \boldsymbol{H}_0)$. For the convergence of the aforementioned series see, e.g., [41, Theorem 69] and [30]. It turns out that for our purposes it is sufficient to consider an interaction term of the form

$$\boldsymbol{V}(t) = \sum_{q=1}^{p} \exp((\imath \omega_q + \varepsilon)t)\boldsymbol{V}_q. \tag{3.3}$$

Indeed, if

$$\boldsymbol{V}(t) = \sum_{q=1}^{p} f_q(t)\boldsymbol{V}_q \tag{3.4}$$

with analytic f_q in a neighborhood of 0 so that we have locally

$$f_q(t) = \sum_{n \geq 0} \partial_t^n f_q(0) t^n / n!,$$

then we can use Lemma 2.4 with $F \to \exp$ and $G \to f$. More precisely, we have

$$\boldsymbol{V}(t) = \sum_{q=1}^{p} f_q(t)\boldsymbol{V}_q = \lim_{m \to \infty} \sum_{l \leq m} \sum_{q=1}^{p} \partial^l f_q(0) \underset{=}{\overset{\lambda}{\Omega}} \lambda^l \exp(t/\lambda)\boldsymbol{V}_q$$

such that the dependence on t of f_q is transferred to the exponential function. The potentials considered in [24, 31] are all of type (3.4). The time-dependent potential in (3.3) goes to zero as $t \to -\infty$ with a small parameter $\varepsilon > 0$. This class of potentials appears in time-dependent perturbation theory for bound states using adiabatic switching. See, e.g., [34, (104) and (106)].

To justify the use of the Neumann series in the following theorem, we introduce a complex parameter z small to ensure the convergence. Therefore, whenever we write

$$\left(\boldsymbol{I} - \frac{\boldsymbol{X}}{\lambda}\right) = \sum_{n\geq 0}\left(\frac{\boldsymbol{X}}{\lambda}\right)^n,$$

we actually mean

$$\left(\boldsymbol{I} - \frac{z\boldsymbol{X}}{\lambda}\right) = \sum_{n\geq 0}\left(\frac{z\boldsymbol{X}}{\lambda}\right)^n$$

making the replacement $\lambda \to \lambda/z$ everywhere. Since the final result (after the elimination of the Omega variable λ) does not depend on z, we omit this parameter for simplicity. Recall that only null powers of λ survive the action of the Omega operator resulting in the cancellation of all the factors containing the parameter z. This strategy was used before in the context of OMC [16–19].

We are now ready to state our main results.

Theorem 3.1. *Assume that $\boldsymbol{H}(t) \in \mathbb{C}^{N\times N}$ $(N < \infty)$ or $\boldsymbol{H}(t)$ is a restriction of (3.1) to a subspace of $\mathcal{H}$ of finite dimension. Then we have the basis- and integral-free Omega representation*

$$\boldsymbol{U}^{(n)}(t,t_0) = \exp(\imath t_0(\Omega_{\boldsymbol{q}_n} - \imath n\varepsilon))(-\imath)^n \sum_{q_1=1}^{p}\cdots\sum_{q_n=1}^{p} \underset{=}{\overset{\mu}{\Omega}} e^{\mu(t-t_0)}\mu \boldsymbol{R}_{\boldsymbol{q}_0}(\mu,\varepsilon)$$
$$\times \boldsymbol{V}_{q_1}\boldsymbol{R}_{\boldsymbol{q}_1}(\mu,\varepsilon)\boldsymbol{V}_{q_2}\cdots \boldsymbol{R}_{\boldsymbol{q}_{n-1}}(\mu,\varepsilon)\boldsymbol{V}_{q_n}\boldsymbol{R}_{\boldsymbol{q}_n}(\mu,\varepsilon),$$

where $\boldsymbol{H}_{0\boldsymbol{q}_i}(\varepsilon) = \boldsymbol{H}_0 - (\Omega_{\boldsymbol{q}_i} - i\imath\varepsilon)\boldsymbol{I}$,

$$\boldsymbol{R}_{\boldsymbol{q}_i}(\mu,\varepsilon) = (\mu\boldsymbol{I} + \imath\boldsymbol{H}_{0\boldsymbol{q}_i}(\varepsilon))^{-1}, \tag{3.5}$$

and

$$\Omega_{\boldsymbol{q}_i} \equiv \sum_{1\leq j\leq i} \omega_{q_j}$$

with the convention $\Omega_{\boldsymbol{q}_0} \equiv 0$. Furthermore, we have the alternative representation

$$\boldsymbol{R}_{\boldsymbol{q}_i}(\mu,\varepsilon) = \lim_{m\to\infty}\sum_{l\leq m}\sum_{k=0}^{d-1} l!\underset{=}{\overset{\nu}{\Omega}}\frac{\nu^l}{\mu}x_{k+1}\left(\frac{1}{\mu\nu}\right)(-\imath)^k \boldsymbol{H}_{0\boldsymbol{q}_i}^k(\varepsilon) \tag{3.6}$$

for the resolvent in (3.5) with $x_{k+1}(t)$ given in Lemma 2.5 with $\boldsymbol{A} \to -\imath\boldsymbol{H}_{0\boldsymbol{q}_i}(\varepsilon)$.

Proof. First, we observe that

$$\begin{aligned}\sum_{i=1}^{n}(\omega_{q_i}-\imath\varepsilon)t_i &= (\omega_{q_1}-\imath\varepsilon)(t_1-t_2)+(\omega_{q_1}+\omega_{q_2}-2\imath\varepsilon)t_2+\cdots+(\omega_{q_n}-\imath\varepsilon)t_n\\ &= (\omega_{q_1}-\imath\varepsilon)(t_1-t_2)+(\omega_{q_1}+\omega_{q_2}-2\imath\varepsilon)(t_2-t_3)\\ &\quad+(\omega_{q_1}+\omega_{q_2}+\omega_{q_3}-3\imath\varepsilon)t_3+\cdots+(\omega_{q_n}-\imath\varepsilon)t_n=\cdots\\ &= \sum_{i=1}^{n}(\underbrace{\omega_{q_1}+\cdots+\omega_{q_i}}_{=\Omega_{\boldsymbol{q}_i}}-i\imath\varepsilon)(t_i-t_{i+1})\end{aligned}$$

with the convention $t_{n+1}\equiv 0$. Therefore, a typical contribution to $\boldsymbol{U}^{(n)}(t,t_0)$ reads as follows:

$$\begin{aligned}&\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\cdots\int_{t_0}^{t_{n-1}}dt_n\exp(-\imath(t-t_1)\boldsymbol{H}_{0\boldsymbol{q}_0}(\varepsilon))\\ &\quad\times\boldsymbol{V}_{q_1}\exp(-\imath(t_1-t_2)\boldsymbol{H}_{0\boldsymbol{q}_1}(\varepsilon))\boldsymbol{V}_{q_2}\exp(-\imath(t_{n-1}-t_n)\boldsymbol{H}_{0\boldsymbol{q}_{n-1}}(\varepsilon))\cdots\\ &\quad\times\boldsymbol{V}_{q_n}\exp(-\imath(t_n-t_0)\boldsymbol{H}_{0\boldsymbol{q}_n}(\varepsilon))\exp(\imath t_0(\Omega_{\boldsymbol{q}_n}-\imath n\varepsilon))\end{aligned}$$

using

$$\boldsymbol{H}_0\equiv\boldsymbol{H}_{0\boldsymbol{q}_n}(\varepsilon)+(\Omega_{\boldsymbol{q}_n}-\imath n\varepsilon)\boldsymbol{I}.$$

The result now follows using a strategy similar to the proof of [17, Proposition 3.4]. Using the Neumann series

$$\mu\boldsymbol{R}_{\boldsymbol{q}_0}(\mu,\varepsilon)=\left(\boldsymbol{I}+\imath\frac{\boldsymbol{H}_{0\boldsymbol{q}_i}(\varepsilon)}{\mu}\right)^{-1}=\sum_{m_i\geq 0}\left(-\imath\frac{\boldsymbol{H}_{0\boldsymbol{q}_i}(\varepsilon)}{\mu}\right)^{m_i},\tag{3.7}$$

we obtain

$$\begin{aligned}&\underset{=}{\overset{\mu}{\Omega}}e^{\mu(t-t_0)}\mu\boldsymbol{R}_{\boldsymbol{q}_0}(\mu,\varepsilon)\frac{\boldsymbol{V}_{q_1}}{\mu}\mu\boldsymbol{R}_{\boldsymbol{q}_1}(\mu,\varepsilon)\frac{\boldsymbol{V}_{q_2}}{\mu}\cdots\mu\boldsymbol{R}_{\boldsymbol{q}_{n-1}}(\mu,\varepsilon)\frac{\boldsymbol{V}_{q_n}}{\mu}\mu\boldsymbol{R}_{\boldsymbol{q}_n}(\mu,\varepsilon)\\ &=\sum_{\boldsymbol{m}\geq\boldsymbol{0}_{n+1}}(-\imath)^{|\boldsymbol{m}|}\boldsymbol{H}_{0\boldsymbol{q}_0}^{m_0}(\varepsilon)\boldsymbol{V}_{q_1}\boldsymbol{H}_{0\boldsymbol{q}_1}^{m_1}(\varepsilon)\boldsymbol{V}_{q_2}\cdots\boldsymbol{H}_{0\boldsymbol{q}_{n-1}}^{m_{n-1}}(\varepsilon)\boldsymbol{V}_{q_n}\boldsymbol{H}_{0\boldsymbol{q}_n}^{m_n}(\varepsilon)\\ &\qquad\times\underset{=}{\overset{\mu}{\Omega}}\frac{e^{\mu(t-t_0)}}{\mu^{|\boldsymbol{m}|+n}}\\ &=\sum_{\boldsymbol{m}\geq\boldsymbol{0}_{n+1}}(-\imath)^{|\boldsymbol{m}|}\frac{\boldsymbol{H}_{0\boldsymbol{q}_0}^{m_0}(\varepsilon)\boldsymbol{V}_{q_1}\boldsymbol{H}_{0\boldsymbol{q}_1}^{m_1}(\varepsilon)\boldsymbol{V}_{q_2}\cdots\boldsymbol{H}_{0\boldsymbol{q}_{n-1}}^{m_{n-1}}(\varepsilon)\boldsymbol{V}_{q_n}\boldsymbol{H}_{0\boldsymbol{q}_n}^{m_n}(\varepsilon)}{(|\boldsymbol{m}|+n)!}\\ &\qquad\times(t-t_0)^{|\boldsymbol{m}|+n}\end{aligned}$$

with $\boldsymbol{m}=(m_0,\ldots,m_n)$ and $|\boldsymbol{m}|=\sum_{k=0}^{n}m_k$. On the other hand, by expanding the matrix exponentials in $\boldsymbol{U}^{(n)}(t,t_0)$ and applying repeatedly (a slight extension of) the incomplete beta function identity

$$\int_{t_0}^{t} (s-t_0)^k (t-s)^l \, ds = \frac{k!l!}{(k+l+1)!}(t-t_0)^{k+l+1}, \tag{3.8}$$

we obtain the desired result. Identity (3.8) can be easily obtained by showing that the left-hand side and right-hand side of (3.8) satisfy the same IVP:

$$\partial_t \phi_{k,l}(t,t_0) = l\phi_{k,l-1}(t,t_0) \quad \text{and} \quad \phi_{k,l}(t_0,t_0) = 0$$

using Leibniz rule for differentiating definite integrals. Note the symmetry

$$\phi_{k,l}(t,t_0) = (-1)^{k+l+1}\phi_{k,l}(t_0,t).$$

We now turn to the alternative expression for the resolvent in (3.5). We have

$$\boldsymbol{R}_{\boldsymbol{q}_i}(\mu,\varepsilon) = \lim_{m\to\infty} \sum_{l\le m} l! \underset{=}{\overset{\nu}{\Omega}} \frac{\nu^l}{\mu} \exp\Big(-\imath\frac{\boldsymbol{H}_{0\boldsymbol{q}_i}(\varepsilon)}{\mu\nu}\Big)$$

using the Neumann series in (3.7) and Lemma 2.4 with $F(\boldsymbol{X}) = \exp(\boldsymbol{X})$ and $G(\boldsymbol{X}) = (\boldsymbol{I}-\boldsymbol{X})^{-1}$ so that

$$(\boldsymbol{I}-\boldsymbol{X})^{-1} = \lim_{m\to\infty} \sum_{l\le m} l! \underset{=}{\overset{\nu}{\Omega}} \nu^l \exp\Big(\frac{\boldsymbol{X}}{\nu}\Big).$$

Finally, the result follows by recalling the representation given in Lemma 2.5. ■

Using Theorem 3.1, we can easily obtain an Omega free generating function which gives *exact expressions* for the n-term of the perturbation series (3.2).

Corollary 3.2. *Let $\boldsymbol{H}_0$ be diagonal with simple spectrum; that is, all the eigenvalues of $\boldsymbol{H}_0$ have multiplicity one. Then we have the Omega free representation*

$$\begin{aligned}(\boldsymbol{U}^{(n)}(t,t_0))_{ij} &= \exp(\imath t_0(\Omega_{\boldsymbol{q}_n} - \imath n\varepsilon)) \sum_{q_1=1}^{p} \cdots \sum_{q_n=1}^{p} \sum_{i_1} \cdots \sum_{i_{n-1}} \sum_{m\ge n} \frac{(-\imath(t-t_0))^m}{m!} \\ &\quad \times h_{m-n}(\alpha_i, \alpha_{i_1}, \ldots, \alpha_{i_{n-1}}, \alpha_j)(\boldsymbol{V}_{q_1})_{ii_1} \cdots (\boldsymbol{V}_{q_n})_{i_{n-1}j}\end{aligned}$$

with $\alpha_{i_j} = \epsilon_{i_j} - \Omega_{\boldsymbol{q}_j} + j\imath\varepsilon$ such that $i_0 \equiv i$ and $i_n \equiv j$ and an eigenvalue ϵ_i of $\boldsymbol{H}_0$.

Proof. It follows directly from Theorem 3.1 with the resolvent representation in (3.5) that

$$\begin{aligned}(\boldsymbol{U}^{(n)}(t,t_0))_{ij} &= \exp(\imath t_0(\Omega_{\boldsymbol{q}_n} - \imath n\varepsilon))(-\imath)^n \sum_{q_1=1}^{p} \cdots \sum_{q_n=1}^{p} \sum_{i_1} \cdots \sum_{i_{n-1}} \underset{=}{\overset{\mu}{\Omega}} \frac{e^{\mu(t-t_0)}}{\mu^n} \\ &\quad \times \Big(1+\imath\frac{\alpha_i}{\mu}\Big)^{-1}\Big(1+\imath\frac{\alpha_{i_1}}{\mu}\Big)^{-1} \cdots \Big(1+\imath\frac{\alpha_{i_{n-1}}}{\mu}\Big)^{-1}(1+\imath\frac{\alpha_j}{\mu})^{-1} \\ &\quad \times (\boldsymbol{V}_{q_1})_{ii_1} \cdots (\boldsymbol{V}_{q_n})_{i_{n-1}j},\end{aligned}$$

which gives the desired result after using Lemma 2.3 and observing that

$$h_{m-n}(-\imath\alpha_i, -\imath\alpha_{i_1}, \ldots, -\imath\alpha_{i_{n-1}}, -\imath\alpha_j) = (-\imath)^{m-n} h_{m-n}(\alpha_i, \alpha_{i_1}, \ldots, \alpha_{i_{n-1}}, \alpha_j)$$

holds. ∎

It is possible to extend the result stated in Corollary 3.2 to include degeneracy as we now show, but the resulting expression is more involved in comparison to Corollary 3.2. Indeed, under the presence of degeneracy $x_{k+1}(t)$ in (2.13) carries besides an exponential factor in t also a monomial in t resulting in a more involved expression after the elimination of the Omega variables.

Theorem 3.3. *Let $\sigma(\boldsymbol{H}_0) \equiv \{\epsilon_1, \ldots, \epsilon_r\}$ with an eigenvalue ϵ_i of $\boldsymbol{H}_0$ of multiplicity n_i and $i \in [r]$ such that $n_1 + \cdots + n_r = d$, where d is the degree of the minimal polynomial of $\boldsymbol{H}_0$. We have the Omega free representation of the n-term in time-dependent perturbation theory*

$$\begin{aligned}\boldsymbol{U}^{(n)}(t, t_0) = {} & \exp(\imath t_0(\Omega_{\boldsymbol{q}_n} - \imath n\varepsilon)) \sum_{q_1=1}^{p} \cdots \sum_{q_n=1}^{p} \sum_{\boldsymbol{i}_0} \cdots \sum_{\boldsymbol{i}_n} A_{\boldsymbol{i}_0} \cdots A_{\boldsymbol{i}_n} \\ & \times \sum_{m \geq |\boldsymbol{j}-\boldsymbol{m}|+n} \frac{(-\imath(t-t_0))^m}{m!} h_{m-|\boldsymbol{j}-\boldsymbol{m}|-n}(\boldsymbol{\alpha}_{i_0}, \ldots, \boldsymbol{\alpha}_{i_n}) \\ & \times \boldsymbol{H}_{0\boldsymbol{q}_0}^{k_0}(\varepsilon) \boldsymbol{V}_{q_1} \cdots \boldsymbol{V}_{q_n} \boldsymbol{H}_{0\boldsymbol{q}_n}^{k_n}(\varepsilon),\end{aligned}$$

where $|\boldsymbol{j} - \boldsymbol{m}| \equiv \sum_{k=0}^{n}(j_k - m_k)$, $\boldsymbol{\alpha}_{i_k} = (\alpha_{i_k}, \ldots, \alpha_{i_k}) \in \mathbb{C}^{j_k - m_k + 1}$, $\alpha_{i_j} = \epsilon_{i_j} - \Omega_{\boldsymbol{q}_j} + j\imath\varepsilon$,

$$\sum_{\boldsymbol{i}} = \sum_{i,j,k,l,m} \equiv \sum_{i=1}^{r} \sum_{j=0}^{n_i-1} \sum_{k=0}^{d-1} \sum_{l=k+1}^{d} \sum_{m=0}^{l-k-1}, \tag{3.9}$$

and

$$A_{\boldsymbol{i}} = A_{ijklm} \equiv c_{ij} \alpha_i^{l-k-m-1} c_l \, j! \binom{l-k-1}{m}$$

if $n_i > 1$ and set $j \equiv 0 \equiv m$ if $n_i = 1$.

Proof. We have

$$\begin{aligned}x_{k+1}(t) = {} & \sum_{l=k+1}^{d} c_l \partial_t^{l-k-1} y(t) = \sum_{i=1}^{r} \sum_{j=0}^{n_i-1} \sum_{l=k+1}^{d} c_{ij} c_l \partial_t^{l-k-1} (t^j \exp(-\imath\alpha_i t)) \\ = {} & \underbrace{\sum_{i=1}^{r} \sum_{j=0}^{n_i-1} \sum_{l=k+1}^{d} \sum_{m=0}^{l-k-1}}_{\equiv \sum_{i,j,l,m}} \underbrace{c_{ij}(-\imath\alpha_i)^{l-k-m-1} c_l \frac{j!}{(j-m)!} \binom{l-k-1}{m}}_{\equiv A_{ijklm}/(j-m)!} \\ & \times t^{j-m} \exp(-\imath\alpha_i t)\end{aligned} \tag{3.10}$$

if $n_i > 1$ with the convention that $c_d \equiv 1$ and using Leibniz rule for the derivative of the product. If $n_i = 1$, then $j \equiv 0 \equiv m$. In our case, a typical contribution to $x_{k+1}(t)$ reads as $t^j \exp(-\imath\alpha_i t)$ and a simple expression is obtained after eliminating the variable ν. Note that the following identity holds:

$$\lim_{m\to\infty}\sum_{l\le m} l!\overset{\nu}{\underset{=}{\Omega}}\frac{\nu^l}{\mu}(\mu\nu)^{-j}\exp\Bigl(-\frac{\imath\alpha_i}{\mu\nu}\Bigr) = \frac{j!}{\mu^{j+1}}\frac{1}{(1+\imath\alpha_i/\mu)^{j+1}}.$$

Indeed, we have

$$\begin{aligned}\lim_{m\to\infty}\sum_{l\le m} l!\overset{\nu}{\underset{=}{\Omega}}\frac{\nu^l}{\mu}(\mu\nu)^{-j}\exp\Bigl(-\frac{\imath\alpha_i}{\mu\nu}\Bigr) &= \imath^j\partial^j_{\alpha_i}\lim_{m\to\infty}\sum_{l\le m} l!\overset{\nu}{\underset{=}{\Omega}}\frac{\nu^l}{\mu}\exp\Bigl(-\frac{\imath\alpha_i}{\mu\nu}\Bigr)\\ &= \frac{\imath^j}{\mu}\partial^j_{\alpha_i}\lim_{m\to\infty}\sum_{l\le m}\sum_{n\ge 0}\frac{l!}{n!}\Bigl(-\frac{\imath\alpha_i}{\mu}\Bigr)^n\underbrace{\overset{\nu}{\underset{=}{\Omega}}\nu^{l-n}}_{=\delta_{l,n}}\\ &= \frac{\imath^j}{\mu}\partial^j_{\alpha_i}\frac{1}{1+\imath\alpha_i/\mu},\end{aligned}$$

which implies the identity. Note that only polynomials in the variable $1/\mu$ appear. As a consequence, we obtain

$$\begin{aligned}\boldsymbol{R}_{\boldsymbol{q}_n}(\mu,\varepsilon) &= \lim_{m\to\infty}\sum_{l\le m}\sum_{k=0}^{d-1} l!\overset{\nu}{\underset{=}{\Omega}}\frac{\nu^l}{\mu}x_{k+1}\Bigl(\frac{1}{\mu\nu}\Bigr)(-\imath)^k\boldsymbol{H}^k_{0\boldsymbol{q}_n}(\varepsilon)\\ &= \sum_{i,j,k,l,m}\frac{A_{ijklm}}{\mu^{j-m+1}(1+\imath\alpha_i/\mu)^{j-m+1}}(-\imath)^k\boldsymbol{H}^k_{0\boldsymbol{q}_n}(\varepsilon)\end{aligned}$$

using (3.9). The result now follows from Theorem 3.1 with the resolvent representation in (3.6) after observing that

$$\begin{aligned}&\overset{\mu}{\underset{=}{\Omega}}e^{\mu(t-t_0)}\mu\frac{1}{\mu^{j_0-m_0+1}(1+\imath\alpha_{i_0}/\mu)^{j_0-m_0+1}}\cdots\frac{1}{\mu^{j_n-m_n+1}(1+\imath\alpha_{i_n}/\mu)^{j_n-m_n+1}}\\ &\quad=\sum_{m\ge|\boldsymbol{j}-\boldsymbol{m}|+n}\frac{(t-t_0)^m}{m!}h_{m-|\boldsymbol{j}-\boldsymbol{m}|-n}(-\imath\boldsymbol{\alpha}_{i_0},\dots,-\imath\boldsymbol{\alpha}_{i_n})\end{aligned}$$

using the notation $\boldsymbol{\alpha}_{i_k} = (\alpha_{i_k},\dots,\alpha_{i_k}) \in \mathbb{C}^{j_k-m_k+1}$ and Lemma 2.3.

Finally, we justify the presence of the factor $(-\imath)^m$. We list the terms and corresponding contributing factors

$$\begin{aligned}\boldsymbol{U}^{(n)}(t,t_0) &\to (-\imath)^n, & c_{ij} &\to (-\imath)^{j_i+1-d},\\ (-\imath\alpha_i)^{l_i-k_i-m_i-1} &\to (-\imath)^{l_i-k_i-m_i-1}, & c_l &\to (-\imath)^{d-l_i},\\ (-\imath)^{k_i}\boldsymbol{H}^{k_i}_{0\boldsymbol{q}_i}(\varepsilon) &\to (-\imath)^{k_i}, & h_{m-|\boldsymbol{j}-\boldsymbol{m}|-n} &\to (-\imath)^{m-|\boldsymbol{j}-\boldsymbol{m}|-n}.\end{aligned}$$

Altogether, we have

$$(-\imath)^n(-\imath)^{l_i-k_i-m_i-1}\frac{(-\imath)^{d-l_i}}{(-\imath)^{d-j_i-1}}(-\imath)^{k_i}(-\imath)^{m-|\boldsymbol{j}-\boldsymbol{m}|-n}=(-\imath)^{m-|\boldsymbol{j}-\boldsymbol{m}|+j_i-m_i}$$

and the result follows taking the product

$$(-\imath)^{m-|\boldsymbol{j}-\boldsymbol{m}|}\prod_{i=0}^{n}(-\imath)^{j_i-m_i}=(-\imath)^m,$$

which enters the expression for $\boldsymbol{U}^{(n)}(t,t_0)$. ■

For clearness, since the expression for $\boldsymbol{U}^{(n)}(t,t_0)$ in the presence of degeneracy stated in Theorem 3.3 is involved, it is instructive to work out an explicit expression for $\boldsymbol{U}^{(n)}(t,t_0)$ for a particular case. From now on, we set $\boldsymbol{U}^{(n)}(t,0)\equiv\boldsymbol{U}^{(n)}(t)$. Let us take $n=2$, $p=1$ such that $\boldsymbol{V}(t)=\exp((\imath\omega+\varepsilon)t)\boldsymbol{V}$ in (3.3), $r=3$, $n_1=1$, $n_2=2$, and $n_3=3$, so that $d=n_1+n_2+n_3=6$, to obtain

$$\begin{aligned}\boldsymbol{U}^{(2)}(t)=&\sum_{i_0,j_0,k_0,l_0,m_0}\ \sum_{i_1,j_1,k_1,l_1,m_1}\ \sum_{i_2,j_2,k_2,l_2,m_2}\ \sum_{m\geq\sum_{k=0}^{2}(j_k-m_k)+2}\frac{(-\imath t)^m}{m!}\\&\times A_{i_0,j_0,k_0,l_0,m_0}A_{i_1,j_1,k_1,l_1,m_1}A_{i_2,j_2,k_2,l_2,m_2}\\&\times h_{m-\sum_{k=0}^{2}(j_k-m_k)-2}(\boldsymbol{\alpha}_{i_0},\boldsymbol{\alpha}_{i_1},\boldsymbol{\alpha}_{i_2})\boldsymbol{H}_{0\boldsymbol{q}_0}^{k_0}(\varepsilon)\boldsymbol{V}\boldsymbol{H}_{0\boldsymbol{q}_1}^{k_1}(\varepsilon)\boldsymbol{V}\boldsymbol{H}_{0\boldsymbol{q}_2}^{k_2}(\varepsilon),\end{aligned}$$

where

$$\sum_{i_p,j_p,k_p,l_p,m_p}\equiv\sum_{i_p=1}^{3}\sum_{j_p=0}^{n_{i_p}-1}\sum_{k_p=0}^{5}\sum_{l_p=k_p+1}^{6}\sum_{m_p=0}^{l_p-k_p-1}$$

with $p=0,1,2$. We also have $\boldsymbol{\alpha}_{i_p}=(\alpha_{i_p},\ldots,\alpha_{i_p})\in\mathbb{C}^{j_p-m_p+1}$ with

$$\begin{gathered}\alpha_{i_0}=\epsilon_{i_0},\qquad\alpha_{i_1}=\epsilon_{i_1}-\omega+\imath\varepsilon,\qquad\alpha_{i_2}=\epsilon_{i_2}-2\omega+2\imath\varepsilon,\\\boldsymbol{H}_{0\boldsymbol{q}_0}(\varepsilon)=\boldsymbol{H}_0,\quad\boldsymbol{H}_{0\boldsymbol{q}_1}(\varepsilon)=\boldsymbol{H}_0-(\omega-\imath\varepsilon)\boldsymbol{I},\quad\boldsymbol{H}_{0\boldsymbol{q}_2}(\varepsilon)=\boldsymbol{H}_0-2(\omega-\imath\varepsilon)\boldsymbol{I}.\end{gathered}$$

In the rest of this section, we establish contact with previous work. First, it is clear that Theorem 3.1 provides a genuine generalization of Putzer's representation, because upon setting $-\imath\boldsymbol{H}\to\boldsymbol{H}$ we obtain

$$\begin{aligned}\exp(\boldsymbol{H}_0t)=\boldsymbol{U}(t)|_{\gamma=0}=\boldsymbol{U}^{(0)}(t)&=\underset{=}{\overset{\mu}{\Omega}}e^{\mu t}\mu\boldsymbol{R}_{\boldsymbol{q}_0}(\mu,0)\\&=\lim_{m\to\infty}\sum_{l\leq m}\sum_{k=0}^{d-1}\underset{=}{\overset{\mu,\nu}{\Omega}}e^{\mu t}\nu^l x_{k+1}\left(\frac{1}{\mu\nu}\right)\boldsymbol{H}_0^k\\&=\sum_{k=0}^{d-1}x_{k+1}(t)\boldsymbol{H}_0^k,\end{aligned}\tag{3.11}$$

where the last equality follows from the uniqueness of the coefficients in (2.7). Anyway, for clearness, we confirm by an explicit calculation that this is indeed the case

$$\lim_{m\to\infty}\sum_{l\leq m} l!\overset{\mu,\nu}{\underset{=}{\Omega}} e^{\mu t}\frac{\nu^l}{(\mu\nu)^n} = \lim_{m\to\infty}\sum_{l\leq m} l!\underbrace{\overset{\mu}{\underset{=}{\Omega}}\frac{e^{\mu t}}{\mu^n}}_{=t^n/n!}\underbrace{\overset{\nu}{\underset{=}{\Omega}}\nu^{l-n}}_{=\delta_{l,n}} = t^n.$$

In other words, the term containing $(\mu\nu)^{-n}$ in $x_{k+1}(1/(\mu\nu))$ goes to t^n under the action of the Omega operators. From the above, we see that once the time dependence of $\boldsymbol{H}(t)$ is set to zero (by taking $\gamma \equiv 0$ in (3.1)), we recover the original Putzer formulation in [40]. Therefore, our work extends Putzer representation to the time-dependent setting.

Likewise, we can show that Theorem 3.3 is a generalization of Lemma 2.6. Indeed, we have

$$\boldsymbol{U}^{(0)}(t) = \sum_{i,j,k,l,m} c_{ij}\alpha_i^{l-k-m-1}c_l\, j!\binom{l-k-1}{m}\sum_{n\geq j-m}\frac{t^n}{n!}h_{n-j+m}(\boldsymbol{\alpha}_i)\boldsymbol{H}_0^k$$

with $\boldsymbol{\alpha}_i = (\alpha_i,\ldots,\alpha_i) \in \mathbb{C}^{j-m+1}$. Result (3.11) with $x_{k+1}(t)$ given by Lemma 2.6 now follows by observing that

$$h_{n-j+m}(\boldsymbol{\alpha}_i) = \frac{n(n-1)\cdots(n-j+m+1)}{(j-m)!}\alpha_i^{n-j+m}$$

and comparing with (3.10). We can easily show that this identity holds using the generating function in (2.3) by setting $m = 1$, taking ∂_t^{j-m} on both sides of (2.3), and comparing the final result with (2.3) by setting $m \to j-m+1$ with $x_i = x$ for $i \in \{1,\ldots,j-m+1\}$.

Next, we show that our work is associated with the representation of [31]. To achieve this goal we give another proof Theorem 3.1 by introducing a basis for the time-independent Hamiltonian $\boldsymbol{H}_0$ and using the approach via divided differences described in [31]. We will see that exactly the same result follows via this route and another one taking as the starting point Theorem 3.1. Let us first review some definitions and basic identities of [31]. We write

$$f[x_0,\ldots,x_n] = \sum_{k=0}^{n}\frac{f(x_k)}{\prod_{j\neq k}(x_k-x_j)}$$

for the divided differences of a function f. In particular, we have

$$\exp(-\imath t[\alpha_0,\ldots,\alpha_n]) = \sum_{m\geq 0}\frac{(-\imath t)^{m+n}[\alpha_0,\ldots,\alpha_n]^{m+n}}{(m+n)!} \tag{3.12}$$

with

$$[\alpha_0,\ldots,\alpha_n]^{m+n} = \begin{cases} 0, & m < 0, \\ 1, & m = 0, \\ h_m(\alpha_0,\ldots,\alpha_n), & m > 0. \end{cases}$$

Note that

$$\exp(-\imath t[\alpha_0,\ldots,\alpha_n]) = \exp(-\imath t[\alpha_{\varsigma(0)},\ldots,\alpha_{\varsigma(n)}])$$

for any permutation ς. We also need [31, Appendix B, Identities 1 and 2]. More precisely, we have

$$\begin{aligned}(-\imath)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \exp(-\imath(\alpha_1 t_1 + \cdots + \alpha_n t_n)) \\ = \exp(-\imath t[\beta_0,\ldots,\beta_{n-1},0]),\end{aligned} \tag{3.13}$$

where $\beta_i = \sum_{j=1}^{n-i} \alpha_j$ and

$$\exp(-\imath t[\alpha_0,\ldots,\alpha_n]) = \exp(-\imath t\beta)\exp(-\imath t[\beta_0,\ldots,\beta_n]), \tag{3.14}$$

where $\beta_i = \alpha_i - \beta$. Equations (3.13) and (3.14) stand for Identities 1 and 2 of [31], respectively.

Now let us consider the representation of $\boldsymbol{U}^{(n)}(t)$ in the basis of the eigenvectors of $\boldsymbol{H}_0$ with $\{\epsilon_0,\ldots,\epsilon_n\} \subseteq \sigma(\boldsymbol{H}_0)$. Therefore, we are left with the integral to be determined using the usual iterated-integral representation of the time-dependent perturbation series

$$\begin{aligned}\int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \exp(-\imath(\epsilon_1 - \epsilon_0 - \omega_1)t_1) \\ \times \exp(-\imath(\epsilon_2 - \epsilon_1 - \omega_2)t_2) \cdots \exp(-\imath(\epsilon_n - \epsilon_{n-1} - \omega_n)t_n) \\ = \exp\left(-\imath\left[\epsilon_n - \epsilon_0 - \sum_{i=1}^{n} \omega_i, \epsilon_{n-1} - \epsilon_0 - \sum_{i=1}^{n-1} \omega_i, \ldots, \epsilon_1 - \epsilon_0 - \omega_1, 0\right]\right),\end{aligned}$$

which follows from (3.13). Using (3.14), we get

$$\begin{aligned}\exp(-\imath t\epsilon_0) \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \exp(-\imath(\epsilon_1 - \epsilon_0 - \omega_1)t_1) \\ \times \exp(-\imath(\epsilon_2 - \epsilon_1 - \omega_2)t_2) \cdots \exp(-\imath(\epsilon_n - \epsilon_{n-1} - \omega_n)t_n) \\ = \exp\left(-\imath t\left[\epsilon_n - \sum_{i=1}^{n} \omega_i, \epsilon_{n-1} - \sum_{i=1}^{n-1} \epsilon_i, \ldots, \epsilon_1 - \omega_1, \epsilon_0\right]\right).\end{aligned}$$

Now we show that exactly the same result follows directly from Theorem 3.1, but this time instead of the iterated integrals we use the Omega operator representation of $\boldsymbol{U}^{(n)}(t)$ given in Theorem 3.1. Again, by passing to a representation in the basis of eigenvectors of $\boldsymbol{H}_0$, we obtain

$$\underset{=}{\overset{\mu}{\Omega}} \frac{e^{\mu t}}{\mu^n} \frac{1}{1+\imath\alpha_0/\mu} \frac{1}{1+\imath\alpha_1/\mu} \cdots \frac{1}{1+\imath\alpha_{n-1}/\mu} \frac{1}{1+\imath\alpha_n/\mu}$$
$$= \sum_{m\geq n} \frac{(-\imath t)^m}{m!} h_{m-n}(\alpha_n, \dots, \alpha_0) = \sum_{m\geq 0} \frac{(-\imath t)^{m+n}}{(m+n)!} h_m(\alpha_n, \dots, \alpha_0)$$
$$\overset{(3.12)}{=} \exp(-\imath t[\alpha_n, \dots, \alpha_0])$$

with $\alpha_k = \epsilon_k - \sum_{i=1}^{k} \omega_i$ using the convention $\sum_{i=1}^{0} \equiv 0$.

We are now ready to explore Theorem 3.3 in applications in the next section.

4. Examples

As noted in [31], even simple Hamiltonians have complicated terms in the time-dependent perturbation series if the integral representation is used, but the representation using OMC or divided differences turns out to be rather simple. To exemplify this point, let us revisit [31, Example 1]. We consider the (non-Hermitian) Hamiltonian

$$\boldsymbol{H}(t) = \boldsymbol{H}_0 + \gamma e^{\imath E t} \boldsymbol{F},$$

where $\boldsymbol{F}$ is a permutation operator of the eigenvectors of $\boldsymbol{H}_0$ with $\boldsymbol{F}|z_i\rangle = |z_f\rangle$, where $|z_i\rangle$ and $|z_f\rangle$ are eigenvectors of $\boldsymbol{H}_0$ with associated eigenvalues ϵ_i and ϵ_f, respectively. In this case we have $p = 1$, $\omega_1 = E$, and $\boldsymbol{V}_1 = \boldsymbol{F}$. Using Corollary 3.2, we have

$$\langle z_f|\boldsymbol{U}^{(n)}(t)|z_i\rangle$$
$$= \sum_{i_1,\dots,i_{n-1}} \frac{(-\imath t)^m}{m!} h_{m-n}(\alpha_{i_0}, \alpha_{i_1}, \dots, \alpha_{i_{n-1}}, \alpha_{i_n})(\boldsymbol{F})_{i_0,i_1} \cdots (\boldsymbol{F})_{i_{n-1},i_n}$$
$$= \sum_{m\geq n} \frac{(-\imath t)^m}{m!} h_{m-n}(\epsilon_f, \epsilon_i - E, \dots, \epsilon_f - (n-1)E, \epsilon_i - nE)$$
$$= \exp(-\imath t[\epsilon_i - nE, \epsilon_f - (n-1)E, \dots, \epsilon_i - E, \epsilon_f])$$

if n is odd and zero otherwise. We used that $\alpha_{i_j} = \epsilon_{i_j} - jE$, and the representation of $\boldsymbol{F}$ using the basis $\{|z_i\rangle, |z_f\rangle\}$ is

$$\boldsymbol{F} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Therefore, in this case $i_0 = 2$ and $i_n = 1$. Note that in the context of our framework the expression for $\langle z_f|\boldsymbol{U}^{(n)}(t)|z_i\rangle$ is straightforward and agrees with the corresponding expression given in [31] apart from a minor typo in [31, (19)]. The corrected expression is given above.

Now let us consider a time oscillating two-level Hamiltonian

$$\boldsymbol{H}(t) = \omega_0 \boldsymbol{\sigma}_z + g\cos(\omega t)\boldsymbol{\sigma}_x$$

with the Pauli matrices

$$\boldsymbol{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{and} \quad \boldsymbol{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

In this case, we have $|z\rangle \equiv |s\rangle$ with $s = 0, 1$, $p = 2$, $\gamma = g/2$, $\omega_1 = \omega = -\omega_2$, and $\boldsymbol{V}_1 = \boldsymbol{\sigma}_x = \boldsymbol{V}_2$. From Corollary 3.2, we have

$$\begin{aligned}
&\langle s|\boldsymbol{U}^{(n)}(t)|s\rangle \\
&\quad = \sum_{m\geq n}\sum_{\boldsymbol{q}} \frac{(-\imath t)^m}{m!} h_{m-n}((-1)^{s+n}\omega_0, \ldots, (-1)^{s+1}\omega_0 - \Omega_{\boldsymbol{q}_{n-1}}, (-1)^s\omega_0 - \Omega_{\boldsymbol{q}_n}) \\
&\quad = \sum_{\boldsymbol{q}} \exp(-\imath t[(-1)^s\omega_0 - \Omega_{\boldsymbol{q}_n}, (-1)^{s+1}\omega_0 - \Omega_{\boldsymbol{q}_{n-1}}, \ldots, (-1)^{s+n}\omega_0]),
\end{aligned}$$

where $\Omega_{\boldsymbol{q}_i} = -\omega\sum_{j=1}^{i}(-1)^{q_j}$ with even n and $\sum_{\boldsymbol{q}} \equiv \sum_{q_1,\ldots,q_n}$. A similar formula holds for $\langle s|\boldsymbol{U}^{(n)}(t)|1-s\rangle$ with odd n. Finally, we obtain

$$\boldsymbol{U}(t) = \begin{pmatrix} a_0(t) & b_1(t) \\ b_0(t) & a_1(t) \end{pmatrix},$$

where

$$\begin{aligned}
a_s(t) &= \sum_{n\geq 0}\sum_{\boldsymbol{q}} \left(\frac{g}{2}\right)^{2n} \exp\big(-\imath t[(-1)^s\omega_0 - \Omega_{\boldsymbol{q}_{2n}}, \ldots, (-1)^{s+2n}\omega_0]\big), \\
b_s(t) &= \sum_{n\geq 0}\sum_{\boldsymbol{q}} \left(\frac{g}{2}\right)^{2n+1} \exp\big(-\imath t[(-1)^s\omega_0 - \Omega_{\boldsymbol{q}_{2n+1}}, \ldots, (-1)^{s+2n+1}\omega_0]\big),
\end{aligned}$$

which agrees with [31, (C3)].

Next, we consider the time oscillating infinite-dimensional Hamiltonian

$$\boldsymbol{H}(t) = \omega\Big(\boldsymbol{a}^\dagger\boldsymbol{a} + \frac{1}{2}\Big) + \frac{\Gamma}{4}\cos(\Omega t)\Big(\frac{1}{2m\omega}\Big)^2(\boldsymbol{a}^\dagger + \boldsymbol{a})^4.$$

In this case, we have $|z\rangle \equiv |n\rangle$ with $n \in \mathbb{N}_0 \equiv \mathbb{N} \cup \{0\}$, $p = 10$, $\gamma = \Gamma/(32m^2\omega^2)$, $\omega_{1,2,3,4,5} = \Omega = -\omega_{6,7,8,9,10}$, and

$$\boldsymbol{V}_q = \sum_{n\geq 0} c_q(n)|n + 2q - 6\rangle\langle n|$$

such that $\boldsymbol{V}_{q+5} \equiv \boldsymbol{V}_q$ for $q \in \{1, 2, 3, 4, 5\}$ with

$$c_1(n) = \sqrt{n(n-1)(n-2)(n-3)}, \qquad c_2(n) = \sqrt{n(n-1)}(4n-2),$$
$$c_3(n) = 3(2n^2 + 2n + 1), \qquad c_4(n) = \sqrt{(n+1)(n+2)}(4n+6),$$
$$c_5(n) = \sqrt{(n+1)(n+2)(n+3)(n+4)}.$$

The decomposition above is obtained by expanding $(\boldsymbol{a}^\dagger + \boldsymbol{a})^4$ and collecting terms with four annihilation operators (one term), three annihilation operators (four terms), two annihilation operators (six terms), one annihilation operator (four terms), and no annihilation operator (one term). Therefore, we can write

$$\frac{\Gamma}{4} \cos(\Omega t) \Big(\frac{1}{2m\omega} \Big)^2 (\boldsymbol{a}^\dagger + \boldsymbol{a})^4 = \gamma \Big(\exp(\imath \Omega t) \sum_{q=1}^{5} \boldsymbol{V}_q + \exp(-\imath \Omega t) \sum_{q=1}^{5} \boldsymbol{V}_q \Big).$$

From Corollary 3.2, we obtain

$$\begin{aligned} \langle m | \boldsymbol{U}^{(1)}(t) | n \rangle &= \sum_{q=1}^{5} \sum_{m \geq 1} c_q(n) h_{m-1}(\epsilon_{n+2q-6}, \epsilon_n - \Omega) \delta_{m,n+2q-6} + (\Omega \to -\Omega) \\ &= \sum_{q=1}^{5} c_q(n) \exp(-\imath t [\epsilon_{n+2q-6}, \epsilon_n - \Omega]) \delta_{m,n+2q-6} + (\Omega \to -\Omega) \end{aligned}$$

with $\epsilon_n = \omega(n + 1/2)$. Again our expression agrees with [31, (24)], apart from another minor correction: $D_{\pm 2, \pm 4}$ should be replaced by $D_{\mp 2, \mp 4}$ in [31, (22)]. To show the correspondence, recall that $E_n = \omega(n + 1/2)$ and use (3.14) in [31, (24)].

Therefore, we have shown that all the examples considered in [31] are special cases of Corollary 3.2. Furthermore, the closed form expression in Theorem 3.3 can also be represented as follows:

$$\begin{aligned} \boldsymbol{U}^{(n)}(t) = \sum_{q_1=1}^{p} \cdots \sum_{q_n=1}^{p} \sum_{\boldsymbol{i}_0} \cdots \sum_{\boldsymbol{i}_n} A_{\boldsymbol{i}_0} \cdots A_{\boldsymbol{i}_n} \\ \times \exp(-\imath t [\boldsymbol{\alpha}_{\boldsymbol{i}_0}, \ldots, \boldsymbol{\alpha}_{\boldsymbol{i}_n}]) \boldsymbol{H}_{\boldsymbol{0}\boldsymbol{q}_0}^{k_0}(\varepsilon) \boldsymbol{V}_{q_1} \cdots \boldsymbol{V}_{q_n} \boldsymbol{H}_{\boldsymbol{0}\boldsymbol{q}_n}^{k_n}(\varepsilon) \end{aligned} \qquad (4.1)$$

using divided differences. The closed form expression (4.1) is an Omega free generating function encompassing all the examples considered in this section and therefore generalizes and unifies all the examples presented in [31]. We remark that it is easy to obtain all the examples considered in this section starting directly with the Omega free expression given in (4.1) by observing that

$$A_{ijklm} \equiv A_{i0kl0} = c_{i0} \alpha_i^{l-k-1} c_l$$

with

$$c_{i0} = \frac{1}{\prod_{k \neq i}(\alpha_i - \alpha_k)}$$

using Lemma 2.6 and

$$c_l = (-1)^{d-l} \sum_{1 \leq i_1 < \cdots < i_{d-l} \leq d} \alpha_{i_1} \cdots \alpha_{i_{d-l}}.$$

It is worth mentioning that the exponential in (3.12) which appears in (4.1) can be calculated efficiently with polynomial complexity in n [26].

Finally, we consider $\boldsymbol{V}(t) = e^{\varepsilon t}\boldsymbol{V}$ and take $t_0 \to -\infty$ before setting $\varepsilon \to 0$. We are interested in analyzing (in a non-rigorous way) the difficulties met under the presence of degeneracy in the context of our framework. We first consider $\boldsymbol{H}_0$ with simple spectrum. In what follows, we have $\alpha_i = \epsilon_i$ and $\alpha_j = \epsilon_j + \imath\varepsilon$. From Corollary 3.2, we obtain

$$\begin{aligned}
&(\boldsymbol{U}_I^{(1)}(t,t_0))_{ij} \\
&\quad = e^{\varepsilon t_0} e^{\imath\epsilon_i t} e^{-\imath\epsilon_j t_0} (\boldsymbol{V})_{ij} \sum_{m \geq 1} \frac{(-\imath(t-t_0))^m}{m!} h_{m-1}(\alpha_i, \alpha_j) \\
&\quad = e^{\varepsilon t_0} e^{\imath\epsilon_i t} e^{-\imath\epsilon_j t_0} (\boldsymbol{V})_{ij} \sum_{m \geq 1} \frac{(-\imath(t-t_0))^m}{m!} \overset{\lambda}{\underset{=}{\Omega}} \frac{\lambda^{m-1}}{(1-\alpha_i/\lambda)(1-\alpha_j/\lambda)} \\
&\quad = e^{\varepsilon t_0} e^{\imath\epsilon_i t} e^{-\imath\epsilon_j t_0} \frac{(\boldsymbol{V})_{ij}}{\alpha_i - \alpha_j} \sum_{m \geq 1} \frac{(-\imath(t-t_0))^m}{m!} \overset{\lambda}{\underset{=}{\Omega}} \left(\frac{\lambda^m}{1-\alpha_i/\lambda} - \frac{\lambda^m}{1-\alpha_j/\lambda} \right) \\
&\quad = e^{\varepsilon t_0} e^{\imath\epsilon_i t} e^{-\imath\epsilon_j t_0} \frac{(\boldsymbol{V})_{ij}}{\alpha_i - \alpha_j} \overset{\lambda}{\underset{=}{\Omega}} \left(\frac{\exp(-\imath(t-t_0)\lambda)}{1-\alpha_i/\lambda} - \frac{\exp(-\imath(t-t_0)\lambda)}{1-\alpha_j/\lambda} \right) \\
&\quad = e^{\varepsilon t_0} e^{\imath\epsilon_i t} e^{-\imath\epsilon_j t_0} (\boldsymbol{V})_{ij} \frac{\exp(-\imath(t-t_0)\alpha_i) - \exp(-\imath(t-t_0)\alpha_j)}{\alpha_i - \alpha_j} \\
&\quad = -\imath(\boldsymbol{V})_{ij} \left(\frac{\exp(\varepsilon t + \imath(\epsilon_i - \epsilon_j)t)}{\varepsilon + \imath(\epsilon_i - \epsilon_j)} - (t \to t_0) \right)
\end{aligned}$$

using Lemma 2.3 to get the second equality. Therefore, we have

$$\begin{aligned}
(\boldsymbol{U}_I^{(1)}(t,-\infty))_{ij} &= \lim_{t_0 \to -\infty} (\boldsymbol{U}_I^{(1)}(t,t_0))_{ij} \\
&= -\imath(\boldsymbol{V})_{ij} \frac{\exp(\varepsilon t + \imath(\epsilon_i - \epsilon_j)t)}{\varepsilon + \imath(\epsilon_i - \epsilon_j)}.
\end{aligned}$$

This is a well-known calculation.

Now we turn our attention to $\boldsymbol{H}_0$ including degeneracy using Theorem 3.3. We will see that the situation is much more subtle due to the presence of $\boldsymbol{j}, \boldsymbol{m} \neq \boldsymbol{0}_{n+1}$. The intricate nature of the presence of degeneracy of $\boldsymbol{H}_0$ in adiabatic switching was already noticed before. See, e.g., [11,12] and references therein. In this way, following the same route outlined above, we obtain

$$\begin{aligned}
&h_{m-|\boldsymbol{j}-\boldsymbol{m}|-1}(\boldsymbol{\alpha}_i,\boldsymbol{\alpha}_j)\\
&\quad= \underset{=}{\overset{\lambda}{\Omega}} \frac{\lambda^{m-|\boldsymbol{j}-\boldsymbol{m}|-1}}{(1-\alpha_i/\lambda)^{j_0-m_0+1}(1-\alpha_j/\lambda)^{j_1-m_1+1}}\\
&\quad= \frac{\partial_{\alpha_i}^{j_0-m_0}}{(j_0-m_0)!}\frac{\partial_{\alpha_j}^{j_1-m_1}}{(j_1-m_1)!}\underset{=}{\overset{\lambda}{\Omega}}\frac{\lambda^{m-1}}{(1-\alpha_i/\lambda)(1-\alpha_j/\lambda)}\\
&\quad= \frac{\partial_{\alpha_i}^{j_0-m_0}}{(j_0-m_0)!}\frac{\partial_{\alpha_j}^{j_1-m_1}}{(j_1-m_1)!}\Big(\frac{1}{\alpha_i-\alpha_j}\underset{=}{\overset{\lambda}{\Omega}}\Big(\frac{\lambda^m}{1-\alpha_i/\lambda}-\frac{\lambda^m}{1-\alpha_j/\lambda}\Big)\Big)\\
&\quad= \frac{\partial_{\alpha_i}^{j_0-m_0}}{(j_0-m_0)!}\frac{\partial_{\alpha_j}^{j_1-m_1}}{(j_1-m_1)!}\Big(\frac{\alpha_i^m-\alpha_j^m}{\alpha_i-\alpha_j}\Big)\\
&\quad= \frac{\partial_{\alpha_i}^{j_0-m_0}}{(j_0-m_0)!}\frac{\alpha_i^m}{(\alpha_i-\alpha_j)^{j_1-m_1+1}}+\frac{\partial_{\alpha_j}^{j_1-m_1}}{(j_1-m_1)!}\frac{\alpha_j^m}{(\alpha_j-\alpha_i)^{j_0-m_0+1}}
\end{aligned}$$

using again Lemma 2.3 to get the first equality. We have

$$\begin{aligned}
&\partial_{\alpha_j}^{j_1-m_1}\frac{\alpha_j^m}{(\alpha_j-\alpha_i)^{j_0-m_0+1}}\\
&\quad= \sum_{n_1=0}^{j_1-m_1}\binom{j_1-m_1}{n_1}(\partial_{\alpha_j}^{n_1}\alpha_j^m)(\partial_{\alpha_j}^{j_1-m_1-n_1}(\alpha_j-\alpha_i)^{-j_0+m_0-1}).
\end{aligned}$$

Going back to $(\boldsymbol{U}_I^{(1)}(t,t_0))_{ij}$ and using Theorem 3.3, we note that

$$\lim_{t_0\to-\infty} e^{\varepsilon t_0}e^{\imath\epsilon_i t}e^{-\imath\epsilon_j t_0}\sum_{m\geq|\boldsymbol{j}-\boldsymbol{m}|+1}\frac{(-\imath(t-t_0))^m}{m!}\partial_{\alpha_i}^{j_0-m_0}\frac{\alpha_i^m}{(\alpha_i-\alpha_j)^{j_1-m_1+1}}=0,$$

but

$$\begin{aligned}
&\lim_{t_0\to-\infty} e^{\varepsilon t_0}e^{\imath\epsilon_i t}e^{-\imath\epsilon_j t_0}\sum_{m\geq|\boldsymbol{j}-\boldsymbol{m}|+1}\frac{(-\imath(t-t_0))^m}{m!}\partial_{\alpha_j}^{n_1}\alpha_j^m\\
&\quad= \lim_{t_0\to-\infty} e^{\varepsilon t_0}e^{\imath\epsilon_i t}e^{-\imath\epsilon_j t_0}\\
&\qquad\times\sum_{m\geq|\boldsymbol{j}-\boldsymbol{m}|+1}\frac{(-\imath(t-t_0))^m}{m!}m(m-1)\cdots(m-n_1+1)\alpha_j^{m-n_1}\\
&\quad= \lim_{t_0\to-\infty} e^{\varepsilon t_0}e^{\imath\epsilon_i t}e^{-\imath\epsilon_j t_0}\sum_{m\geq|\boldsymbol{j}-\boldsymbol{m}|+1}\frac{(-\imath(t-t_0))^m}{(m-n_1)!}\alpha_j^{m-n_1}\\
&\quad= \lim_{t_0\to-\infty}(-\imath(t-t_0))^{n_1}e^{\varepsilon t_0}e^{\imath\epsilon_i t}e^{-\imath\epsilon_j t_0}\sum_{m\geq 0}\frac{(-\imath(t-t_0))^m}{m!}\alpha_j^m
\end{aligned}$$

$$= \lim_{t_0 \to -\infty} (-\imath(t-t_0))^{n_1} e^{\varepsilon t_0} e^{\imath \epsilon_i t} e^{-\imath \epsilon_j t_0} \exp(-\imath \alpha_j (t-t_0))$$
$$= \exp(\varepsilon t + \imath(\epsilon_i - \epsilon_j)t) \lim_{t_0 \to -\infty} (-\imath(t-t_0))^{n_1},$$

which is not finite if $n_1 > 0$. Recall that $0 \leq n_1 \leq j_1 - m_1$.

5. Concluding remarks

We introduced a new and simple combinatorial approach based on OMC to compute the terms in the time-dependent perturbation expansion of the quantum-evolution operator $\boldsymbol{U}(t, t_0)$. To determine $\boldsymbol{U}^{(n)}(t, t_0)$ all we need is the elimination of the Omega variables involving the most simple case handled in Lemma 2.3 along with the solution of the IVP given by (2.9) and (2.10). We have shown that our approach implies as special cases Putzer's representation [40, Theorem 1] of the matrix exponential and the integral-free approach to compute the time-dependent perturbation series using divided differences put forward recently in [31]. After the elimination of the Omega variables, we showed that all the examples considered in [31] are special cases of Corollary 3.2. Note also that in contrast to the representation given in [31] our is basis-free; that is, the eigenvectors of $\boldsymbol{H}_0$ are not assumed to be known a priori. Furthermore, in the context of OMC, we have the additional feature of using Lemma 2.4 in order to transfer the matrix dependence of one function to the other. This feature was a key step in order to generalize Putzer's representation to the time-dependent setting and in obtaining the closed form expression given in Theorem 3.3, which unifies and generalizes all the perturbation calculations exemplified in [31]. We also show that degeneracy associated with $\boldsymbol{H}_0$ in the context of adiabatic switching is a subtle problem which already appears in the first order of perturbation theory. We believe that due to the simplicity (yet furnishing us with non-trivial results) and versatility of the approach discussed here that other interesting applications will appear besides those considered here. For example, as time-dependent perturbation theory is connected with Feynman operational calculus [30, Chapters 14–19] we think it would be interesting to explore Feynman method to disentangle the exponential of operators using OMC.

Acknowledgments. We thank the referee for the constructive and helpful remarks.

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Communicated by Frédéric Patras

Received 1 January 2022; revised 5 May 2022.

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