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Iterative approach to the exponential representation of the time–displacement operator

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Abstract

An iterative method due to Voslamber is reconsidered. It provides successive approximations for the logarithm of the time–displacement operator in quantum mechanics. The procedure may be interpreted, *a posteriori*, as an infinite resummation of terms in the so-called Magnus expansion. A recursive generator for higher terms is obtained. From two illustrative examples, a detailed comparative study is carried out between the results of the iterative method and those of the Magnus expansion.

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1. Introduction

More than 50 years ago Wilhelm Magnus in a much celebrated article [1] proposed an exponential representation for the solution to the linear matrix non-autonomous differential equation $\dot{X} = A(t)X$. The main difficulty in achieving this aim arises from the fact that the matrices A evaluated at different values of t are, in general, non-commuting. Since then, the issue has become increasingly popular. In quantum mechanics, the time-evolution operator $U(t, 0)$ satisfies an equation of that type and then we can look for its exponential representation $U(t, 0) = \exp \Omega(t, 0)$. Usually Ω is expanded in a series $\sum \Omega_n$, where Ω_n is of order n in the Hamiltonian, a reason why this Magnus expansion is sometimes named *exponential perturbation theory*. Its most prized feature is probably that it exactly preserves the unitary character of the evolution operator to any order of approximation. In the general case when the evolution is ruled by a time-dependent Hamiltonian the exponent Ω is given in terms of multiple integrals of nested commutators of the Hamiltonian.

Over the years, the Magnus expansion has been applied to a wide range of problems in quantum mechanics from atomic to high energy physics, or nuclear magnetic resonance[1]. It

[1] A list of applications of the Magnus expansion can be found, for instance, in [3, 13].

has also been used for the determination of the evolution operator in an algebraic setting of classical mechanics [2]. The more mathematical questions on existence and convergence of Magnus expansion have also witnessed recent progress [3–5]. More recently, the Magnus idea has extended its domain of applications and has originated very interesting algorithms in the field of geometric integration of differential equations in numerical analysis [6, 7].

Apart from the Magnus expansion, and more or less directly related to it, one can find in the literature other exponential-like representations of U. Thus, in the Wilcox infinite-product representation $U = \mathrm{e}^{W_1}\,\mathrm{e}^{W_2}\cdots$ [8, 9], every term W_n is of order n. Instead, in the Fer infinite-product representation of $U = \mathrm{e}^{F_1}\,\mathrm{e}^{F_2}\cdots$ [9, 10], every contribution F_n is obtained from F_{n-1} and H, and contains terms of order 2^{n-1} and higher (with the exception of F_1, which is of first order).

In this paper, we explore a different approach to the approximate determination of Ω. The basic idea we shall use appears in an interesting, but surprisingly unnoticed, paper by Voslamber [11]. In it, the exponent Ω in U is obtained by an iterative algorithm built from Magnus expansion. To properly appreciate the distinguishing traits of the Voslamber proposal some comments are in order. The most conventional approach to the solution of the matrix differential equation $\dot{X} = A(t)X$ by power series expansion proceeds in two steps: first write it as an integral equation and second iterate to the desired order. From the point of view of this paper two facts should be noted. The iterative (Picard) method is linear, i.e. the output for a linear combination of two inputs is the linear combination of the corresponding outputs. This procedure gives rise to the common perturbation theory. Furthermore, when the iteration is carried out to a certain finite order essential qualitative properties of the exact solution are lost, e.g., the unitary character of the evolution operator. At variance with that situation, Voslamber method uses a nonlinear iterative algorithm which will automatically include in each step higher order terms. At the same time because it deals with the exponent Ω, it keeps the unitary character at any order of approximation. How all this is achieved will be explained in section 2, where Voslamber approach is reviewed and the basic equations are obtained in a different way. The connection with Magnus expansion is also reported. In section 3, we will present a recursive algorithm for the calculation of the main ingredient of the method, an issue only tangentially touched upon in Voslamber original paper. In section 4, application to two simple problems in quantum mechanics will be considered to assess the performance of the method. In particular, both modulus and relative phase of the matrix elements of the evolution operator as given by Voslamber and Magnus methods will be compared with the exact solution.

2. The method

Consider the time-dependent Schrödinger equation

$$\dot{U}(t,0) = \tilde{H}(t)U(t,0) \qquad U(0,0) = I \tag{1}$$

where $\tilde{H} \equiv H/\mathrm{i}\hbar$ is anti-Hermitian. $H(t)$ is the Hamiltonian of the system and $U(t,0)$ stands for the unitary time-evolution operator.

Following the usual setting to derive Magnus expansion [1, 8], we introduce the exponential representation $U(t,0) = \exp\Omega(t,0)$ (with the initial condition $\Omega(0,0) = 0$) of the time–displacement operator into (1). In the present case Ω is anti-Hermitian. This will provide the corresponding differential equation for Ω. To this end, we use the Wilcox formula [8] for the derivative of the exponential of an operator

$$\frac{\partial}{\partial t}\,\mathrm{e}^{\Omega} = \int_0^1 \mathrm{e}^{x\Omega}\dot{\Omega}\,\mathrm{e}^{(1-x)\Omega}\,\mathrm{d}x = \int_0^1 \mathrm{e}^{(1-x)\Omega}\dot{\Omega}\,\mathrm{e}^{x\Omega}\,\mathrm{d}x. \tag{2}$$

The new variable $y = \frac{1}{2} - x$ in the integrals above and equation (1) yields the new result

$$\int_{-1/2}^{1/2} \mathrm{e}^{-y\Omega}\,\mathrm{e}^{\Omega/2}\dot{\Omega}\,\mathrm{e}^{-\Omega/2}\,\mathrm{e}^{y\Omega}\,\mathrm{d}y = \tilde{H}. \tag{3}$$

Note that both forms in Wilcox's formula lead to the very same equation after some elementary simplifications. Next, let us define what we call the *dressed derivative* of Ω:

$$\Gamma \equiv \mathrm{e}^{\Omega/2}\dot{\Omega}\,\mathrm{e}^{-\Omega/2}. \tag{4}$$

We will use the well-known Baker–Hausdorff formula [8]

$$\mathrm{e}^{X}Y\mathrm{e}^{-X} = \sum_{n=0}^{\infty}\frac{1}{n!}\,\mathrm{ad}_X^n Y, \tag{5}$$

where the adjoint operator is defined in terms of the commutator as $\mathrm{ad}_X Y \equiv [X, Y]$, and $\mathrm{ad}_X^n = \mathrm{ad}_X(\mathrm{ad}_X^{n-1}Y)$, $\mathrm{ad}_X^0 Y = Y$. Then equation (3) becomes

$$\sum_{k=0}^{\infty}\frac{1}{(2k+1)!2^{2k}}\mathrm{ad}_\Omega^{2k}\Gamma = \frac{\sinh(\mathrm{ad}_{\Omega/2})}{\mathrm{ad}_{\Omega/2}}\Gamma = \tilde{H}. \tag{6}$$

Consequently,

$$\Gamma = \frac{\mathrm{ad}_{\Omega/2}}{\sinh(\mathrm{ad}_{\Omega/2})}\tilde{H} = \sum_{k=0}^{\infty}\frac{B_k(1/2)}{k!}\mathrm{ad}_\Omega^k\tilde{H}, \tag{7}$$

where use has been made of the Taylor series

$$\frac{t\,\mathrm{e}^{xt}}{\mathrm{e}^t - 1} = \sum_{k=0}^{\infty}\frac{B_k(x)}{k!}t^k \tag{8}$$

in terms of Bernoulli polynomials $B_k(x)$ [12]. Taking into account the connection with Bernoulli numbers $B_k(1/2) = -(1 - 2^{1-k})B_k$, equation (7) becomes

$$\Gamma = \sum_{k=0}^{\infty}\frac{2^{1-k}-1}{k!}B_k\mathrm{ad}_\Omega^k\tilde{H} = \sum_{n=0}^{\infty}\frac{2^{1-2n}-1}{(2n)!}B_{2n}\mathrm{ad}_\Omega^{2n}\tilde{H}. \tag{9}$$

This expression has been derived by Voslamber in a rather different way [11] (we note in passing his unconventional notation for Bernoulli numbers). The dressed derivative Γ is the central element in what follows, whereas the conventional Magnus expansion proceeds instead with $\dot{\Omega}$. As a matter of fact, if we introduce definition (4) for Γ in either (7) or (9) then, after some algebra, we obtain right the differential equation for the operator Ω involved in the Magnus method

$$\dot{\Omega} = \frac{\mathrm{ad}_\Omega}{\exp(\mathrm{ad}_\Omega) - 1}\tilde{H}, \tag{10}$$

as expected.

Suppose that H is of first order in a parameter λ, which we make explicit by writing λH instead of H. Suppose also that Ω and Γ can be developed in power series of λ for some finite time interval and sufficiently small λ, i.e., $\Omega(t) = \sum_{n=1}^{\infty}\lambda^n\Omega_n(t)$, just as in the Magnus expansion, and $\Gamma(t) = \sum_{n=1}^{\infty}\lambda^n\Gamma_n(t)$, with the initial condition $\Omega_n(0) = 0$. Introducing both expansions into (9) and gathering terms with the same λ powers we obtain Γ_k as a function of Ω_n with $n \leqslant k-2$. The first four terms in the Γ power expansion read

$$\Gamma_1 = \tilde{H} \tag{11}$$

$$\Gamma_2 = 0 \tag{12}$$

$$\Gamma_3 = -\tfrac{1}{24}[\Omega_1, [\Omega_1, \tilde{H}]] \tag{13}$$

$$\Gamma_4 = -\tfrac{1}{24}([\Omega_1, [\Omega_2, \tilde{H}]] + [\Omega_2, [\Omega_1, \tilde{H}]]). \tag{14}$$

In the next section, we will dwell on the practical calculation of the terms Γ_k.

If we introduce the power series expansions for Ω and Γ into equation (4), use the Baker-Hausdorff formula and the explicit expressions for Γ_k, it is also possible to obtain the various terms Ω_n in Magnus expansion which constitutes simply a consistency check. However, the idea here is to use equation (4) otherwise by building up an iterative procedure. From definition (4), we write

$$\dot{\Omega} = \mathrm{e}^{-\Omega/2}\Gamma\,\mathrm{e}^{\Omega/2}. \tag{15}$$

Once the terms Γ_k are known in terms of nested commutators of Ω_n ($n \leqslant k-2$) with $\tilde{H}$, we arrange the following iterative procedure. For the sake of simplicity in the notation, we shall occasionally write $U(t) \equiv U(t,0), \Omega(t) \equiv \Omega(t,0)\cdots$. The nth level approximant $\Omega^{[n]}$ is defined by

$$\Omega^{[n]} = \int_0^t \exp[-\Omega^{[n-1]}(t')/2]\Gamma^{[n]}(t')\exp[\Omega^{[n-1]}(t')/2]\,\mathrm{d}t', \qquad n = 1, 2, \ldots \tag{16}$$

with $\Gamma^{[n]} = \sum_1^n \lambda^n \Gamma_n$ and the seed $\Omega^{[0]} = 0$. The two first approximants read explicitly

$$\Omega^{[1]}(t) = \Omega_1(t) = \int_0^t \tilde{H}(t')\,\mathrm{d}t' \tag{17}$$

$$\Omega^{[2]}(t) = \int_0^t \mathrm{e}^{-\Omega_1(t')/2}\tilde{H}(t')\,\mathrm{e}^{\Omega_1(t')/2}\,\mathrm{d}t'. \tag{18}$$

Thus, the time–displacement operator is approximated in the Magnus expansion as $U \simeq \exp\left(\sum_{k=1}^n \Omega_k\right)$, and the Voslamber iterative algorithm approximates $U \simeq \exp\Omega^{[n]}$. In view of the Baker–Hausdorff formula (5), $\Omega^{[n]}$ gets contributions from an infinity of orders in λ, whereas Ω_n is strictly of order λ^n. This behaviour for $\Gamma^{[n]}$ is a direct consequence of the nonlinear character of the iterative procedure (16). The iterate $\Omega^{[n]}$ contains $\sum_1^n \lambda^k \Omega_k$ exactly. It also contains higher powers $\lambda^m (m > n)$ but the contribution of order λ^m is only part of that in Ω_m for $m > n$.

One could rightly ask whether the iterates (16) tend to a fixed point when $n \to \infty$, which should be the exact solution of the Magnus equation (10). To this respect we can only give a formal answer by pointing out that since $\Omega^{[n]}$ contains $\sum_1^n \lambda^k \Omega_k$, then in the limit $n \to \infty$, $\Omega^{[n]}$ should tend to Ω, provided it exists.

The issue to be analysed then is whether this arrangement will result in an improved approximate time–displacement operator with respect to the Magnus expansion. In a summarized way, we conclude that $\Omega^{[n]}$ may be interpreted as a re-summation of the Magnus expansion, as the result of the iterative procedure. Its net effect on the approximate solution remains to be analysed.

3. Recursive generation of higher order terms Γ_n

We turn now our attention to the more practical question of how to calculate Γ_k, which are the building blocks of the process. The terms Ω_n appearing in the computation of Γ_k are right those determined by the Magnus expansion, and may be obtained by well-established methods. Using the notation $\tilde{H}(t_i) \equiv \tilde{H}_i$, the first four orders read

(i) $\dot{\Omega}_1 = \tilde{H}$ so that

$$\Omega_1(t, t_0) = \int_{t_0}^{t} \mathrm{d}t_1 \tilde{H}_1. \tag{19}$$

(ii) $\dot{\Omega}_2 = -\frac{1}{2}[\Omega_1, \tilde{H}]$. Thus,

$$\Omega_2(t, t_1) = \frac{1}{2} \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 [\tilde{H}_1, \tilde{H}_2]. \tag{20}$$

(iii) $\dot{\Omega}_3 = -\frac{1}{2}[\Omega_2, \tilde{H}] + \frac{1}{12}[\Omega_1, [\Omega_1, \tilde{H}]]$. After some work and using the formula

$$\int_0^{\alpha} \mathrm{d}x \int_0^{x} f(x, y)\, \mathrm{d}y = \int_0^{\alpha} \mathrm{d}y \int_y^{\alpha} f(x, y)\, \mathrm{d}x \tag{21}$$

we obtain

$$\Omega_3(t, t_0) = \frac{1}{6} \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \int_{t_0}^{t_2} \mathrm{d}t_3 \{[\tilde{H}_1, [\tilde{H}_2, \tilde{H}_3]] + [[\tilde{H}_1, \tilde{H}_2], \tilde{H}_3]\}. \tag{22}$$

(iv) $\dot{\Omega}_4 = -\frac{1}{2}[\Omega_3, \tilde{H}] + \frac{1}{12}[\Omega_2, [\Omega_1, \tilde{H}]] + \frac{1}{12}[\Omega_1, [\Omega_2, \tilde{H}]]$, which yields

$$\begin{aligned}\Omega_4(t, t_0) = \frac{1}{12} \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \int_{t_0}^{t_2} \mathrm{d}t_3 \int_{t_0}^{t_3} \mathrm{d}t_4 \{&[[[\tilde{H}_1, \tilde{H}_2], \tilde{H}_3]\tilde{H}_4] \\ &+ [\tilde{H}_1, [[\tilde{H}_2, \tilde{H}_3], \tilde{H}_4]] + [\tilde{H}_1, [\tilde{H}_2, [\tilde{H}_3, \tilde{H}_4]]] + [\tilde{H}_2, [\tilde{H}_3, [\tilde{H}_4, \tilde{H}_1]]]\}.\end{aligned} \tag{23}$$

A recursive procedure for obtaining Γ_k, provided the Magnus expansion terms are known, follows next.

The recursive generator for Γ_n, turns out to be similar to that of the Magnus expansion for $\dot{\Omega}_n$ [13], and may be easily built up. Substituting the dressed derivative series $\Gamma = \sum_{j=1}^{\infty} \lambda^j \Gamma_j$ and the Magnus series $\Omega = \sum_{j=1}^{\infty} \lambda^j \Omega_j$ into equation (7) and equating terms of the same order one gets

$$\begin{aligned}&\Gamma_1 = \tilde{H} \\ &\Gamma_n = \sum_{j=1}^{n-1} \frac{B_j(1/2)}{j!} S_n^{(j)}, \qquad n \geqslant 2,\end{aligned} \tag{24}$$

where we have defined

$$S_n^{(k)} = \sum \big[\Omega_{i_1}, \big[\cdots \big[\Omega_{i_k}, \tilde{H}\big] \cdots\big]\big], \qquad (i_1 + \cdots + i_k = n - 1). \tag{25}$$

Note that in the last equation the order n in $\tilde{H}$ has been explicitly reckoned, whereas k represents the number of Ω's. The newly defined operators $S_n^{(k)}$ can again be calculated recursively. The recurrence relations are given by

$$\begin{aligned}&S_n^{(j)} = \sum_{m=1}^{n-j} \big[\Omega_m, S_{n-m}^{(j-1)}\big], \qquad 2 \leqslant j \leqslant n-1 \\ &S_n^{(1)} = [\Omega_{n-1}, \tilde{H}], \qquad\qquad S_n^{(n-1)} = \mathrm{ad}_{\Omega_1}^{n-1} \tilde{H}.\end{aligned} \tag{26}$$

4. Illustrative examples

For the sake of illustration of the method we shall apply the iterative procedure and the Magnus expansion to two simple examples frequently encountered in the literature. As a first instance of application, we shall consider the linearly driven harmonic oscillator, for which it is well known [14] that the Magnus expansion reduces to two terms, namely $\Omega = \Omega_1 + \Omega_2$, and provides the exact time-evolution operator U. The second example we shall consider is a particle of spin $1/2$ in a constant magnetic field (double Stern–Gerlach experiment).

The Hamiltonian of the driven harmonic oscillator is

$$H(t) = \hbar\omega a^\dagger a + f(t)(a^\dagger + a), \qquad [a, a^\dagger] = 1 \tag{27}$$

where $f(t)$ is an unspecified function of time and $a^\dagger, a$ are the usual raising and lowering operators. In the Dirac interaction picture the Hamiltonian reads

$$H_I(t) = f(t)(\mathrm{e}^{\mathrm{i}\omega t}a^\dagger + \mathrm{e}^{-\mathrm{i}\omega t}a). \tag{28}$$

In this particular case the fact that the commutator $[a, a^\dagger]$ is a c number greatly simplifies the procedure. Magnus series terminates ($\Omega_n = 0, n > 2$). Correspondingly the fixed point of the iteration (16) is $\Omega^{[2]}$. Either the iterate or the second-order approximation both leads to the exact solution

$$U_I(t) = \mathrm{e}^{\Omega^{[2]}} = \mathrm{e}^{\Omega_1+\Omega_2} = \mathrm{e}^{-\mathrm{i}\eta}\,\mathrm{e}^{-\mathrm{i}\alpha a^\dagger - \mathrm{i}\alpha^* a} \tag{29}$$

where

$$\alpha(t) \equiv \frac{1}{\hbar}\int_0^t f(t')\,\mathrm{d}t', \tag{30}$$

$$\eta(t) \equiv \frac{1}{\hbar^2}\int_0^t \mathrm{d}t_2 \int_0^{t_2} f(t_1) f(t_2) \sin[\omega(t_1 - t_2)]\,\mathrm{d}t_1. \tag{31}$$

In the second example, we consider the two-level system described by the Schrödinger equation (1) with Hamiltonian

$$H = -\tfrac{1}{2}\hbar\omega\sigma_z + f(t)\,\sigma_x \tag{32}$$

where $f(t)$ describes a rectangular mound: $f(t) = 0$ for $t < 0$ and $f(t) = V_0$ for $t > 0$; $\hbar\omega$ is the energy difference between the two levels and $\sigma_x, \sigma_y, \sigma_z$ are Pauli matrices. As is well known, this system admits the exact solution

$$U(t, 0) = \exp\left[\mathrm{i}\left(\frac{\omega}{2}\sigma_z - \frac{V_0}{\hbar}\sigma_x\right)t\right] \tag{33}$$

for $t > 0$.

The Dirac interaction picture is defined here by the explicit integration of the diagonal piece in the Hamiltonian, which can be carried out with the factorization

$$U = \exp(\mathrm{i}\omega\sigma_z t/2)U_I, \tag{34}$$

where U_I stands for the time–displacement operator in the Dirac picture and obeys

$$\dot{U}_I = \tilde{H}_I U_I, \qquad U_I(0, 0) = I \tag{35}$$

with

$$H_I = f(t)(\sigma_x \cos\omega t + \sigma_y \sin\omega t). \tag{36}$$

Our purpose is to obtain approximate expressions for U_I based on both the iterative approach and the Magnus expansion. As a first test, we shall compute the transition probability

$P(t)$ from an initial state with spin up to a state with spin down (or vice versa), in the interaction picture, given by

$$P(t) = |\langle -|U_I(t)|+\rangle|^2 \tag{37}$$

where $|\pm\rangle$ are the normalized eigenvectors of σ_z, with eigenvalues ± 1. The expression (37) will be computed on assuming: $U_I \simeq \exp \Omega^{[1]} = \exp \Omega_1$, $U_I \simeq \exp(\Omega_1 + \Omega_2)$ and $U_I \simeq \exp \Omega^{[2]}$, and the results compared with the exact analytical solution from (33)

$$P(t) = \left[\frac{2\rho}{\gamma} \sin \frac{\xi\gamma}{2}\right]^2, \qquad \gamma \equiv \sqrt{1+4\rho^2}, \tag{38}$$

where $\rho = V_0/\hbar\omega$ and $\xi = \omega t$.

The transition probability above provides a test about the modulus of U_I matrix elements. Instead, an observable like $|\langle x|U_I(t)|+\rangle|^2$, with $|x\rangle \equiv (|+\rangle + |-\rangle)/\sqrt{2}$ an eigenstate of σ_x, involves relative phases among matrix elements. Thus, we compute $\varphi_{21} - \varphi_{11}$, with the notation $(U_I)_{jk} = |u_{jk}| \exp(\mathrm{i}\varphi_{jk})$, as a second test. The exact solution furnishes the result

$$\varphi_{21} - \varphi_{11} = \xi - \frac{\pi}{2} - \tan^{-1}\left(\frac{1}{\gamma} \tan \frac{\xi\gamma}{2}\right). \tag{39}$$

The first iterate and the first-order Magnus expansion coincide, $\Omega_1 = \Omega^{[1]}$, and from (17) they read

$$\Omega_1 = \Omega^{[1]} = -\mathrm{i}\rho[\sigma_x \sin\xi + \sigma_y(1-\cos\xi)]. \tag{40}$$

For the second-order Magnus operator Ω_2 one has from (20)

$$\Omega_2 = -\mathrm{i}\rho^2(\sin\xi - \xi)\sigma_z. \tag{41}$$

The corresponding second-order Magnus approximation to the transition probability is then

$$P_M = \left[\frac{2}{\beta} \sin(\xi/2) \sin(\rho\beta)\right]^2, \tag{42}$$

with $\beta^2 \equiv 4\sin^2(\xi/2) + \rho^2(\sin\xi - \xi)^2$. The transition probability up to first order of approximation may be obtained removing the terms proportional to ρ^2 in (42). For relative phases we have $\xi - \frac{\pi}{2}$ for the first-order approximations and the following result:

$$\xi - \frac{\pi}{2} - \tan^{-1}\left[\frac{\rho}{\eta}(\xi - \sin\xi)\tan(\rho\eta)\right], \tag{43}$$

with $\eta^2 \equiv 4\sin^2\xi + \rho^2(\sin\xi - \xi)^2$, for the second-order Magnus approximation.

Finally, the second iterate is obtained from equation (18)

$$\begin{aligned}\Omega^{[2]}(t) = -\mathrm{i}\rho \int_0^{\omega t} &\{[\sin^2(\Delta) + \cos^2(\Delta)\cos\xi]\sigma_x \\ &+ \cos^2(\Delta)\sin\xi\sigma_y - \sin(2\Delta)\sin(\xi/2)\sigma_z\}\,\mathrm{d}\xi\end{aligned} \tag{44}$$

where $\Delta \equiv \rho|\sin(\xi/2)|$. Since it does not seem possible to derive an analytical expression for $\Omega^{[2]}$, the corresponding matrix elements have been computed numerically.

In figure 1, the various approximated transition probabilities as well as the exact result (38) have been plotted as a function of ξ (i.e., the dimensionless width of the rectangular mound) for a fixed value of the product $\xi\rho = 1.3$ (i.e., for a fixed area of the mound). We observe that the second iterate keeps the trend of the exact solution in a better way than the second-order Magnus approximation does. In contrast to this, note that the second-order correction fades with increasing ξ.

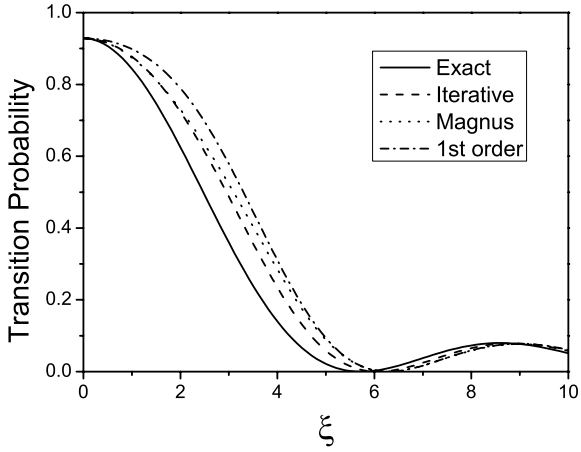

Figure 1. Transition probability in the two-level system as a function of ξ, for $\rho\xi = 1.3$: exact result (solid line), second iterate (dashed line), second-order Magnus expansion (dotted line) and first iterate (or order in Magnus expansion) (dashed–dotted line).

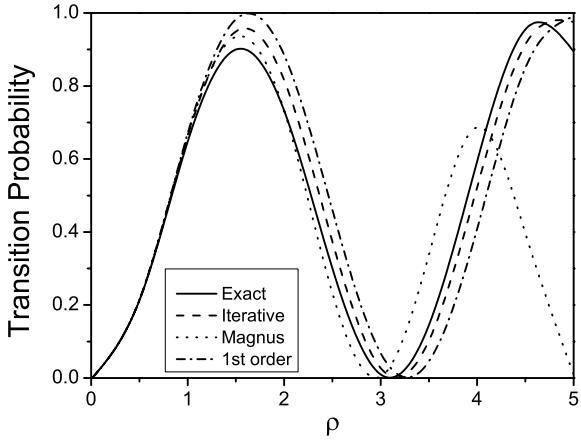

Figure 2. Transition probability in the two-level system as a function of ρ, for $\xi = 1$. Lines are coded as in figure 1.

In figure 2, we have plotted the corresponding transition probabilities versus ρ for fixed value $\xi = 1$. Although locally the second-order Magnus approximation may be more accurate, it seems that the trend of the exact solution is mimicked for a longer ρ interval by the second iterate.

As is well known, the Magnus expansion works the better the more sudden the perturbation. Thus, the re-summation involved in the iterative method somewhat improves that issue.

In figures 3 and 4, we have plotted the cosine of the different relative phases between matrix elements u_{21} and u_{11} of U_I. As their computation involves the multi-valued function arctan discontinuities may appear when representing φ as a function of either ρ or ξ. We have chosen to impose continuity of phases rather than use the principal value of arctan. This choice makes easier the comparison of results. In figure 3, the relative phase is represented versus ξ, keeping fixed the value $\xi\rho = 1.3$, just as in figure 1. In figure 4, the relative phase

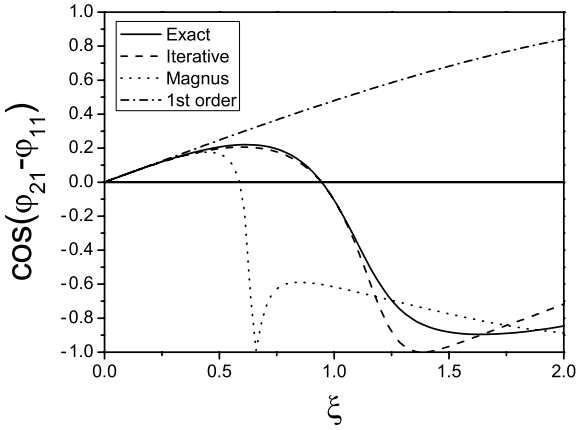

Figure 3. Relative phase in the two-level system as a function of ξ, for $\rho\xi = 1.3$. Lines are coded as in figure 1.

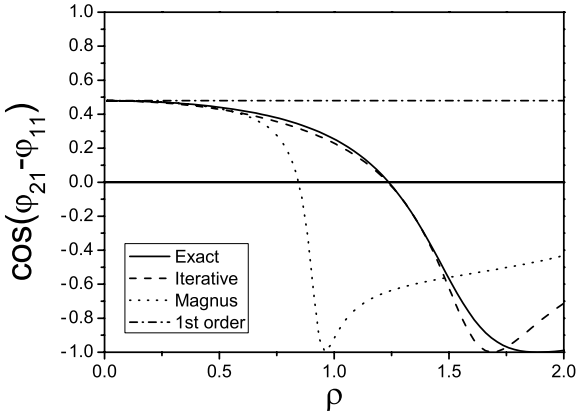

Figure 4. Relative phase in the two-level system as a function of ρ, for $\xi = 1$. Lines are coded as in figure 1.

is plotted versus ρ with a fixed value $\xi = 1$, just as in figure 2. First of all, we observe in both plots that the approximation of phases is a more delicate issue than that of modulus. We see that the iterative approach provides a remarkable improvement with respect to the Magnus expansion.

5. Conclusions

In this paper, the iterative algorithm proposed more than 30 years ago by Voslamber has been analysed in view of the recent revived interest in Magnus expansion. Concerning the general properties of the iterative method, a recursive procedure for its main ingredient, what we have called a dressed derivative, has been given. It has also been pointed out that the iteration includes automatically partial sums of higher order terms from Magnus expansion, of course at the expense of much more computational effort. The examples we have worked out allow a detailed comparison between the iterative and Magnus schemes. The results for the two-level system indicate that the iterative algorithm improves the efficiency of the approximation. For

Table 1. Schematic relationship among the four exponential-like representations of U. First column indicates the type: single or infinite product of exponentials. *BCH* refers to the Baker-Campbell-Hausdorff formula.

$U(t)$	Exponential perturbation theory	Iterative scheme	Approximation stays in:
$e^{\Omega(t)}$	Magnus	Voslamber	Lie algebra
	$\updownarrow$	$\updownarrow$	$\downarrow$
	via *BCH*	$\times$	exp
	$\updownarrow$	$\updownarrow$	$\downarrow$
$\prod_1^\infty e^{\Lambda_k(t)}$	Wilcox	FER	Lie group

the forced harmonic oscillator, the second order of the Magnus expansion is known to yield the exact result and the same is true for the iterative method.

Although not considered here, the extension of the iterative method to more general linear systems should not present huge difficulties.

The Voslamber iterative method could be added to a list of three exponential-like expansions named after Magnus, Wilcox and Fer, in the literature. Some comparison or parallelism may be established among these four. Thus, whereas Magnus and Voslamber algorithms work with the exponent of a single exponential to represent the time-evolution operator, the Wilcox and Fer methods operate with an infinite product of exponentials. Furthermore, the Magnus and Wilcox expansions can be formally connected via the repeated use of the Baker–Campbell–Hausforff formula [9], which combines the product of two exponentials into a single one, and are to be properly considered as true *exponential perturbation theories*. Instead, the Voslamber and Fer methods, being both iterative in nature, do not proceed order by order in the expansion parameter as it progresses. These ideas are collected in table 1, in which we explain the type of representation for U that the various methods use as well as the connections one can establish among them. Observe that in the Magnus and Voslamber schemes we approximate the exponent by either a truncation of a series or stopping the iteration, respectively. In both cases we move in a Lie algebra, which after exponentiation leads us to the corresponding Lie group. Instead, in the Wilcox and Fer schemes we approximate the infinite-product representation of U by a finite number of factors, which means that we are already in the Lie group. These facts are reflected in the last column of the table.

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