New analytic approximations based on the Magnus expansion

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Abstract

The Magnus expansion is a frequently used tool to get approximate analytic solutions of time-dependent linear ordinary differential equations and in particular the Schrödinger equation in quantum mechanics. However, the complexity of the expansion restricts its use in practice only to the first terms. Here we introduce new and more accurate analytic approximations based on the Magnus expansion involving only univariate integrals which also shares with the exact solution its main qualitative and geometric properties.

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1 The Magnus expansion

Non-autonomous systems of linear ordinary differential equations of the form

$$Y' = A(t)Y, \qquad Y(0) = I \tag{1}$$

appear frequently in many branches of science and technology. Here $A(t)$, Y are $n \times n$ matrices and, as usual, the prime denotes derivative with respect to time.

In a much celebrated paper [14], Magnus proposed to represent the solution of (1) as

$$Y(t) = \exp(\Omega(t)), \qquad \Omega(0) = 0, \tag{2}$$

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where the exponent $\Omega(t)$ is given by an infinite series

$$\Omega(t) = \sum_{m=1}^{\infty} \Omega_m(t) \tag{3}$$

whose terms are linear combinations of integrals and nested commutators involving the matrix A at different times. In particular, the first terms read explicitly

$$\begin{aligned}
\Omega_1(t) &= \int_0^t A(t_1)\ \mathrm{d}t_1, \\
\Omega_2(t) &= \frac{1}{2}\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2\ \ [A(t_1), A(t_2))] \\
\Omega_3(t) &= \frac{1}{6}\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_3\ \ ([A(t_1),[A(t_2),A(t_3)]] + [A(t_3),[A(t_2),A(t_1)]])
\end{aligned} \tag{4}$$

where $[X, Y] \equiv XY - YX$ is the commutator of X and Y. Equations (2) and (3) constitute the so-called *Magnus expansion* for the solution of (1), whereas the infinite series (3) is known as the *Magnus series*.

An intuitive way of interpreting the Magnus approach could be the following. Given the matrix linear system (1), we know that $Y(t) = \exp(\Omega_1(t))$ is the exact solution wherever A commutes with its time integral $\Omega_1(t) = \int_0^t A(s)ds$. In the general case, however, if one insists in having an exponential solution, then one needs to 'correct' the exponent. The successive terms $\Omega_m(t)$, $m > 1$, in (3) stand precisely for this correction.

Magnus proposal has the appealing feature of providing approximations which preserve important qualitative properties of the exact solution at any order of truncation. Such properties include, in particular, the unitary character of the evolution operator when dealing with quantum mechanical problems. It is perhaps for this reason that, since the 1960s the Magnus expansion has been successfully applied as an analytic tool in numerous areas of physics and chemistry, from atomic and molecular physics to quantum electrodynamics (see [1, 2] for a list of references). Nevertheless, only the first terms in the series (3) have been usually considered, not least due to the increasing complexity of evaluating the expressions appearing in Ω_m for $m > 2$ (e.g., eq. (4)).

An important issue of the Magnus expansion as an analytic tool concerns its convergence. In other words, given a certain $A(t)$, the problem is to determine the time interval where the operator $\Omega(t)$ in (2) can be obtained as the sum of the series (3). This issue has been extensively treated in the literature and here we will present some of the most recent developments in the field, as well as their implications when the Magnus approach is applied in practice.

Despite the long history and multiple applications of the expansion, the explicit time dependency of each term Ω_k is an aspect that has only been recently analyzed, in particular the order of approximation in time to the exact solution when the series (3) is truncated. This has been done in a systematic way by Iserles and Nørsett in [10] with the aim of constructing numerical integration algorithms for equation (1). These constitute prototypical examples of *geometric integrators*: numerical methods for discretizing differential equations which preserve their known qualitative features, such as invariant quantities and geometric structure [8]. By sharing such properties with the exact solution, these methods provide numerical approximations which are more accurate and more stable for important classes of differential equations, for instance those evolving on Lie groups [11]. If the differential equation (1) is defined in a Lie group $\mathcal{G}$, then the approximation (2) obtained when the series (3) is truncated also stays in $\mathcal{G}$, and thus qualitative properties linked to this fact are automatically preserved by the approximation. For instance, if the Lie group is $\mathrm{SU}(n)$, then unitarity is preserved along the evolution, as long as $\exp(\Omega)$ is conveniently approximated.

In nuclear magnetic resonance (NMR) in general and solid-state NMR in particular, it is of paramount interest to obtain the spin evolution and the final state of the density matrix leading to the spectral response. This requires, of course, to solve the time-dependent Schrödinger equation. The Magnus expansion is commonly applied in this setting, thus leading to the so-called average Hamiltonian theory (AHT) [7]. To carry out certain triple-resonance experiments it is necessary to correct a non-linear Bloch-Siegert phase-shift, and so the first step is to compute this phase-shift, which is usually done analytically with AHT or the Magnus series, but only up to the second term [23] due to the complexity of the expansion. It is clear that in this and other settings, having a systematic procedure for constructing the relevant terms appearing at higher orders could be advantageous when carrying out analytic computations.

In this paper we propose to use new analytic approximate solutions of equation (1) involving terms Ω_m with $m \geq 3$ which are more feasible to compute in practical applications. The new approximations are then illustrated on some examples involving 2×2 and 4×4 matrices in comparison with other standard perturbative procedures.

The paper is organized as follows. In section 2 we review the main features of the Magnus expansion, including its convergence. In section 3 we obtain the new analytic approximations and analyze their main features in connection with time dependent perturbation theory. Additional illustrative examples are collected in section 4. Finally, section 5 contains some concluding remarks. The reader is referred to [2] for a comprehensive review of the mathematical treatment and physical applications of the Magnus expansion.

2 Magnus series and its convergence

Although explicit formulae for Ω_m of all orders in the series (3) have been obtained in [10] by using graph theory, in practice it is much more convenient to construct recursive procedures to generate the successive terms. The one proposed in [12] is particularly well suited for carrying out computations up to high order:

$$S_m^{(1)} = [\Omega_{m-1}, A], \qquad S_m^{(j)} = \sum_{n=1}^{m-j} [\Omega_n, S_{m-n}^{(j-1)}], \quad 2 \leq j \leq m-1$$

$$\Omega_1 = \int_0^t A(t_1) dt_1, \qquad \Omega_m = \sum_{j=1}^{m-1} \frac{B_j}{j!} \int_0^t S_m^{(j)}(t_1) dt_1, \quad m \geq 2 \tag{5}$$

where B_j stand for Bernoulli numbers. Notice that this formalism can be directly applied to obtain approximate solutions of the time-dependent Schrödinger equation, since it constitutes a particular example of equation (1). In this setting it is some times called exponential perturbation theory. There is one important difference with the usual time-dependent perturbation theory: whereas in the later approach the truncated evolution operator is no longer unitary, the Magnus expansion furnishes by construction unitary approximations, no matter where the series is truncated.

A critical issue in this setting is, of course, to establish the range of validity of the Magnus series or, in other words, the convergence domain of the expansion: one expects that within this domain higher order terms in the Magnus series will provide more accurate approximations.

It is clear that if

$$\left[A(t), \int_0^t A(s) ds \right] = 0$$

identically for all values of t, then $\Omega_k = 0$ for $k > 1$, so that $\Omega = \Omega_1$. In general, the Magnus series does not converge unless A is small in a suitable sense. Several improved bounds to the actual radius of convergence in terms of A have been obtained along the years [18, 1, 15, 17]. In this respect, the following result is proved in [6]:

Theorem 2.1 *Let the equation $Y' = A(t)Y$ be defined in a Hilbert space $\mathcal{H}$, $2 \leq \dim(\mathcal{H}) \leq \infty$, with $Y(0) = I$. Let $A(t)$ be a bounded operator on $\mathcal{H}$. Then, the Magnus series $\Omega(t) = \sum_{m=1}^{\infty} \Omega_m(t)$, with Ω_m given by (5), converges in the interval $t \in [0, T)$ such that*

$$\int_0^T \|A(s)\| \, ds < \pi$$

and the sum $\Omega(t)$ satisfies $\exp \Omega(t) = Y(t)$.

This theorem, in fact, provides the optimal convergence domain, in the sense that π is the largest constant for which the result holds without any further restrictions on the operator $A(t)$. Nevertheless, it is quite easy to construct examples for which the bound estimate $r_c = \pi$ is still conservative: the Magnus series converges indeed for a larger time interval than that given by the theorem. Consequently, condition $\int_0^T \|A(s)\| ds < \pi$ is *not* necessary for the convergence of the expansion.

A more precise characterization of the convergence can be obtained in the case of $n \times n$ complex matrices $A(t)$. More specifically, in [6] the connection between the convergence of the Magnus series and the existence of multiple eigenvalues of the fundamental solution $Y(t)$ has been analyzed. Let us introduce a new parameter $\varepsilon \in \mathbb{C}$ and denote by $Y_t(\varepsilon)$ the fundamental matrix of $Y' = \varepsilon A(t)Y$. Then, if the analytic matrix function $Y_t(\varepsilon)$ has an eigenvalue $\rho_0(\varepsilon_0)$ of multiplicity $l > 1$ for a certain ε_0 such that: (a) there is a curve in the ε-plane joining $\varepsilon = 0$ with $\varepsilon = \varepsilon_0$, and (b) the number of equal terms in $\log \rho_1(\varepsilon_0)$, $\log \rho_2(\varepsilon_0)$, $\ldots, \log \rho_l(\varepsilon_0)$ such that $\rho_k(\varepsilon_0) = \rho_0$, $k = 1, \ldots, l$ is less than the maximum dimension of the elementary Jordan block corresponding to ρ_0, then the radius of convergence of the series $\Omega_t(\varepsilon) \equiv \sum_{k\geq 1} \varepsilon^k \Omega_{t,k}$ verifying $\exp \Omega_t(\varepsilon) = Y_t(\varepsilon)$ is precisely $r = |\varepsilon_0|$. Notice that this obstacle to convergence is due just to the logarithmic function. If $A(t)$ itself has singularities in the complex plane, then they also restrict the convergence of the procedure.

In addition to these estimates on the convergence of the expansion, it is also important for practical applications to have bounds on the individual terms Ω_m of the Magnus series, in particular for estimating errors when the series is truncated. Thus, it can be shown [16] that

$$\|\Omega_m(t)\| \leq \frac{f_m}{2} \left(2 \int_0^t \|A(s)\| ds \right)^m, \tag{6}$$

where f_m are the coefficients of

$$G^{-1}(x) = \sum_{m\geq 1} f_m \, x^m = x + \frac{1}{4}x^2 + \frac{5}{72}x^3 + \frac{11}{576}x^4 + \cdots,$$

the inverse function of

$$G(s) = \int_0^s \frac{1}{2 + \frac{t}{2}(1 - \cot \frac{t}{2})} \, dt.$$

To improve the accuracy and the bounds on the convergence domain of the Magnus series for a given problem, it is quite common to consider first a linear transformation on the system in such a way that the resulting equation is more appropriate in a certain sense. The idea is to choose a transformation $Y_0(t)$ and factorize the solution of (1) as $Y(t) = Y_0(t)Y_I(t)$, where the unknown Y_I satisfies the equation

$$Y_I' = A_I(t)Y_I,$$

with $A_I(t)$ depending on $A(t)$ and $Y_0(t)$. A typical example is the transformation to the interaction picture in quantum mechanics. In the context of the Magnus expansion, this general transformation is useful if $\|A_I(t)\| < \|A(t)\|$, since then the convergence domain provided by Theorem 2.1 can be enlarged.

To illustrate all these features we next analyze two simple examples.

Example 1. As a first case, we take equation (1) and $A(t) = A_0 + tA_1$, with

$$A_0 = \begin{pmatrix} -117 & -168 \\ 80 & 115 \end{pmatrix}, \qquad A_1 = \begin{pmatrix} -202 & -294 \\ 140 & 204 \end{pmatrix}. \tag{7}$$

As a matter of fact, this system has been recently used to check how different analytic and numerical approximations behave in practice [21, 23]. Applying recurrence (5) we get

$$\Omega_1(t) = tA_0 + \frac{1}{2}t^2 A_1, \qquad S_2^{(1)} = [\Omega_1(t), A(t)] = 0$$

since A_0 and A_1 commute. In consequence, $\Omega_k = 0$ for $k \geq 2$ and the Magnus series terminates just at the first term. In other words, $\exp(\Omega_1(t))$ already provides the exact solution of the problem:

$$Y(t) = \exp(\Omega_1(t)) = \begin{pmatrix} 15\,\mathrm{e}^{-(5+3t)t} - 14\,\mathrm{e}^{(3+4t)t} & 21\,(\mathrm{e}^{-(5+3t)t} - \mathrm{e}^{(3+4t)t}) \\ -10\,(\mathrm{e}^{-(5+3t)t} - \mathrm{e}^{(3+4t)t}) & -14\,\mathrm{e}^{-(5+3t)t} + 15\,\mathrm{e}^{(3+4t)t} \end{pmatrix}.$$

Example 2. Let us compute now the Magnus series in a simple physical model: the quantum two-level system described by the Hamiltonian

$$H(t) = H_0 + H_1 = \frac{1}{2}\hbar\,\omega_0\,\sigma_3 + f(t)\,\sigma_1 \tag{8}$$

in terms of the Pauli matrices, with $f = 0$ for $t < 0$ and $f = V_0$ for $t \geq 0$. The corresponding Schrödinger equation for the evolution operator,

$$i\hbar\frac{dU}{dt} = H(t)U(t), \qquad U(0) = I$$

can be recast in the form (1) with coefficient matrix $A(t) = -\frac{i}{\hbar}H(t)$. For this problem the exact solution reads

$$U(t,0) = \exp\left(-i\left(\frac{\omega_0}{2}\sigma_3 + \frac{V_0}{\hbar}\sigma_1\right)t\right), \tag{9}$$

whence one can compute the transition probability between eigenstates $|+\rangle \equiv (1,0)^T$ and $|-\rangle \equiv (0,1)^T$ of $H_0 = (\hbar/2)\omega_0\sigma_3$ as

$$P_{ex} = \frac{4\gamma^2}{4\gamma^2+\xi^2}\sin^2\sqrt{\gamma^2+\xi^2/4} \tag{10}$$

in terms of $\gamma \equiv V_0 t/\hbar$ and $\xi \equiv \omega_0 t$.

A simple calculation shows that the estimate given by Theorem 2.1 for the convergence of the Magnus expansion is

$$\int_0^t \left\| -\frac{i}{\hbar}H(s)\right\| ds = \sqrt{\gamma^2 + \frac{\xi^2}{4}} < \pi.$$

In addition, by analyzing the eigenvalues of the exact solution, it can be shown that this estimate is optimal, i.e., the boundary of the convergence domain corresponds exactly to $\sqrt{\gamma^2+\xi^2/4} = \pi$.

Since H_0 is diagonal, an obvious linear transformation to be done here is defined by the explicit integration of H_0, so that we factorize

$$U = U_0\,U_I = \exp(-i\xi\sigma_3/2)\,U_I. \tag{11}$$

This is nothing but the usual Interaction Picture in quantum mechanics, with U_I denoting the time evolution operator in the new picture and obeying

$$U_I' = -\frac{i}{\hbar} H_I(t)\, U_I, \qquad U_I(0) = I \tag{12}$$

with

$$H_I(t) = U_0^{-1} H_1(t) U_0 = f(t)(\sigma_1 \cos\xi - \sigma_2 \sin\xi). \tag{13}$$

Now the transition probability between eigenstates is just $P(t) = |\langle + | U_I(t) | - \rangle|^2$.

For the Hamiltonian (13) it is quite straightforward to implement the recurrence (5) in a symbolic algebra package and compute any term in the Magnus series corresponding to $U_I(t) = \exp(\Omega(t))$, solution of (12). The truncation $\Omega^{(p)}(t) \equiv \sum_{m=1}^{p} \Omega_m(t)$ can be written as

$$\Omega^{(p)}(t) = i\, \boldsymbol{\omega}^{(p)}(t) \cdot \boldsymbol{\sigma} \tag{14}$$

in terms of the vector $\boldsymbol{\omega}^{(p)}(t) = (\omega_1, \omega_2, \omega_3)$ and $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$, so that the corresponding transition probability is given by

$$P_M^{(p)} = \left(\frac{\sin\omega}{\omega} \right)^2 \left(\omega_1^2 + \omega_2^2 \right), \tag{15}$$

where $\omega \equiv \|\boldsymbol{\omega}^{(p)}\|$.

On the other hand, since $\|H_I(t)\| = |f(t)|$, then $\int_0^t \|(-i/\hbar) H_I(s)\|\, ds = \gamma$, and thus Theorem 2.1 guarantees that the Magnus expansion in the Interaction Picture is convergent if $\gamma < \pi$. Notice that a change of picture allows us to improve a great deal the convergence of the expansion.

How these features manifest in practice? We have computed with *Mathematica* the first 16 terms in the Magnus series and then formed the approximants $\Omega^{(p)}(\gamma, \xi)$, $p = 1, \ldots, 16$ in order to determine the corresponding transition probabilities with eq. (15). Finally, we have compared with the exact result (10) and represented the error as a function of p for several values of the parameters. In this way we have obtained Figure 1, where this error is depicted in logarithmic scale for $\gamma = 0.5, 1.5, 3.5$ and $\xi = 1$. For reader's convenience, the corresponding code can be found at the website `www.gicas.uji.es/Research/Magnus.html`.

Observe that for small values of γ in the convergence domain, the error in the transition probability decreases rapidly with the number of terms included in the Magnus approximation. For higher values of γ (e.g., $\gamma = 1.5$) one needs more terms to get a similar accuracy, whereas for $\gamma > \pi$ the error is approximately constant with p.

Next we analyze the rate of convergence of the Magnus series for the Hamiltonian (13). To do that we determine the norm of each term Ω_m for $m = 1, \ldots, 16$ and compare with the theoretical estimate (6), which in this case reads

$$\|\Omega\|_m \leq \pi \left(\frac{\gamma}{r_c} \right)^m$$

with $r_c = G(2\pi)/2 = 1.08686869\ldots$

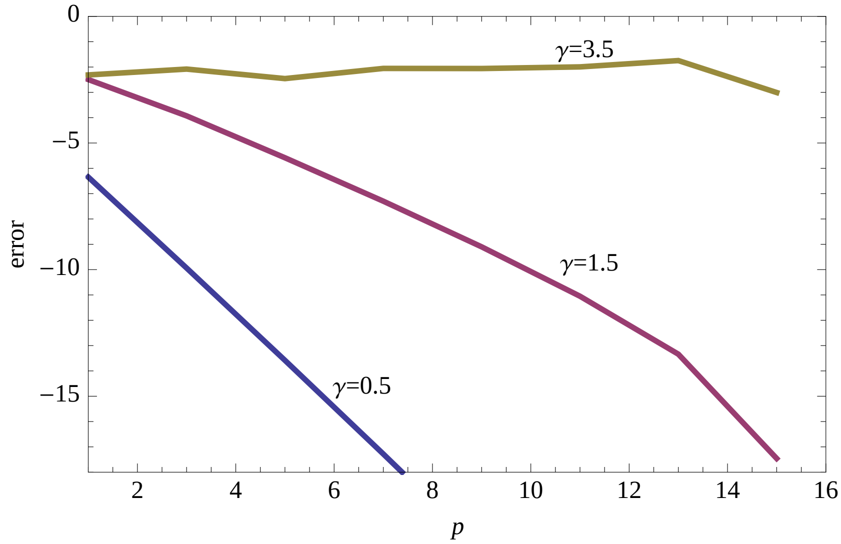

Figure 1: Error in the transition probability (in logarithmic scale) obtained by the truncated Magnus series $\Omega^{(p)} = \sum_i^p \Omega_i$ for the 2-level quantum system with rectangular step and $\xi = 1$.

Since, according with our previous comments, each Ω_m can be expressed as $\Omega_m(\gamma,\xi) = i\,\boldsymbol{\omega}_m(\gamma,\xi)\cdot\boldsymbol{\sigma}$, we represent in Figure 2 $\|\boldsymbol{\omega}_m\|$ (in logarithmic scale) as a function of m for the values of γ considered in Figure 1. In this case the norm is taken as the maximum value obtained for each γ in the interval $1 \leq \xi \leq 15$. Dashed curves correspond to the estimate (6) for $\gamma = 0.5, 1.5$. Notice how the rate of convergence varies with γ within the convergence domain, whereas for $\gamma = 3.5$ there is no convergence at all. The conservative character of the theoretical bound (6) is evident from this figure.

These examples clearly show that (a) the Magnus expansion leads in some cases to the exact solution of the problem (1); (b) it provides an accurate approximation within its convergence domain; (c) the rate of convergence is quite remarkable, and thus it is not necessary to compute many terms in the Magnus series for practical perturbative calculations.

3 Analytic approximations for the Magnus series

3.1 Approximations in terms of univariate integrals

Although the Magnus expansion has been extensively used as a perturbative tool, only the first terms have usually been considered, due to the increasingly intricate structure of Ω_m in the Magnus series. This is already evident from the first terms in (4): unless the elements of A and its commutators are polynomial or trigonometric functions, there is little hope that the terms of the Magnus series can be explicitly and exactly computed for $m > 2$. In this sense, some procedure designed to approximate the multivariate integrals and reduce the complexity of the expression would be of great help.

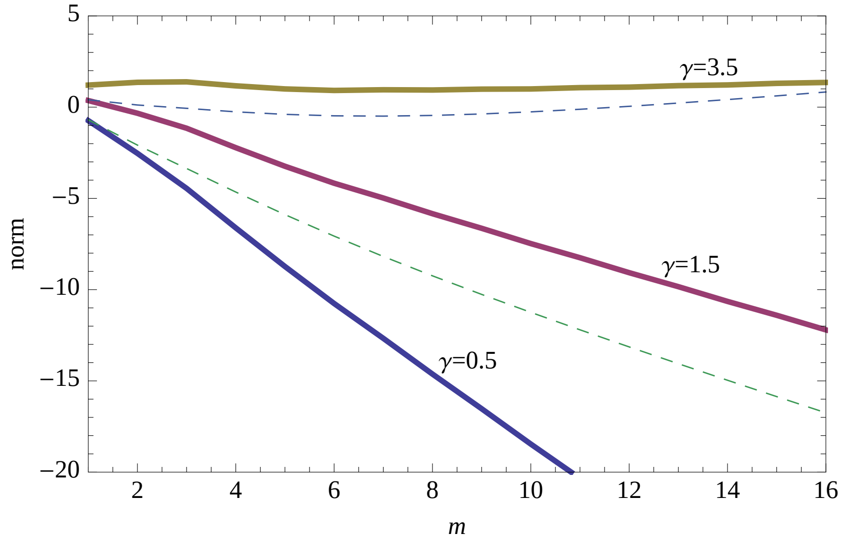

Figure 2: Maximum value of $\|\Omega_m\|$ (in logarithmic scale) for several γ in the interval $1 \leq \xi \leq 15$ for the first 16 terms of the Magnus expansion applied to the problem (12)-(13). Dashed curves correspond to the corresponding theoretical estimate (6) (only for $\gamma = 0.5$ and $\gamma = 1.5$).

Our aim in this section consists precisely in replacing the multivariate integrals appearing in the formalism by conveniently chosen univariate integrals involving only the matrix A. We also reduce the number of commutators to a minimum, so that the new expressions can be applied even the time dependency in $A(t)$ is non-trivial and the resulting approximations are consistent with the truncated Magnus series.

The first step is of course to analyze the time dependence of each term in the Magnus series. This can be achieved, in particular, by considering the Taylor expansion of the coefficient matrix $A(t)$ and then applying the recurrence (5) to get the successive terms Ω_m of the series. To take advantage of the time-symmetry of the expansion, it is more convenient to expand $A(t)$ around the midpoint $t_{1/2} = t_f/2$ of the time integration interval $[0, t_f]$, so that

$$A(t_{1/2} + t) = a_1 + a_2 t + a_3 t^2 + \cdots \tag{16}$$

where $a_i = \dfrac{1}{(i-1)!} \dfrac{d^{i-1}A(t)}{dt^{i-1}}\Big|_{t=t_{1/2}}$, and insert this expression into (5). Thus we get

$$\begin{aligned}
\Omega_1 &= \alpha_1 + \frac{1}{12}\alpha_3 + \frac{1}{80}\alpha_5 \\
\Omega_2 &= \frac{-1}{12}[\alpha_1, \alpha_2] - \frac{1}{80}[\alpha_1, \alpha_4] + \frac{1}{240}[\alpha_2, \alpha_3] \\
\Omega_3 &= \frac{1}{360}[\alpha_1, \alpha_1, \alpha_3] - \frac{1}{240}[\alpha_2, \alpha_1, \alpha_2] \\
\Omega_4 &= \frac{1}{720}[\alpha_1, \alpha_1, \alpha_1, \alpha_2]
\end{aligned} \tag{17}$$

up to order t^6, whereas $\Omega_5 = \mathcal{O}(t^7)$, $\Omega_6 = \mathcal{O}(t^7)$ and $\Omega_7 = \mathcal{O}(t^9)$. Here $\alpha_i \equiv t^i a_i$ and $[\alpha_{i_1}, \alpha_{i_2}, \ldots, \alpha_{i_{l-1}}, \alpha_{i_l}] \equiv [\alpha_{i_1}, [\alpha_{i_2}, [\ldots, [\alpha_{i_{l-1}}, \alpha_{i_l}] \ldots]]]$.

Next we introduce the averaged (or generalized momentum) matrices

$$A^{(i)}(t) = \frac{1}{t^i}\int_0^t (s - t/2)^i A(s) ds, \qquad i = 0, 1, \ldots, s-1. \tag{18}$$

Notice that $A^{(0)} = \Omega_1$ and, from the definition, $A^{(i)}(-t) = (-1)^{i+1} A^{(i)}(t)$. By inserting (16) into (18) we find (neglecting higher order terms)

$$A^{(i)} = \sum_{j=1}^{s} \left(T^{(s)}\right)_{ij} \alpha_j \;\equiv\; \sum_{j=1}^{s} \frac{1-(-1)^{i+j}}{(i+j)2^{i+j}} \alpha_j, \qquad 0 \le i \le s-1. \tag{19}$$

If this relation is inverted we can express α_i in terms of the univariate integrals $A^{(i)}$ as $\alpha_i = \sum_{j=1}^{s} \left(R^{(s)}\right)_{ij} A^{(j-1)}$, where $R^{(s)} = (T^{(s)})^{-1}$. Specifically, for $s = 2$ and $s = 3$ one has

$$R^{(2)} \equiv (T^{(2)})^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & 12 \end{pmatrix}, \qquad R^{(3)} = \begin{pmatrix} \frac{9}{4} & 0 & -15 \\ 0 & 12 & 0 \\ -15 & 0 & 180 \end{pmatrix} \tag{20}$$

respectively. In consequence we can write $\Omega(t)$ in terms of the univariate integrals (18) and construct the desired approximation to Ω up to order $2s$. In particular,

$$\begin{aligned} \Omega^{[4]}(t) &\equiv A^{(0)} - [A^{(0)}, A^{(1)}] \\ Y(t) &= \exp(\Omega^{[4]}(t)) + \mathcal{O}(t^5) \end{aligned} \tag{21}$$

provides a 4th-order approximation to the exact solution of (1), whereas the scheme

$$\begin{aligned} C_1 &= [\alpha_1, \alpha_2], \\ C_2 &= -\frac{1}{60}[\alpha_1, 2\alpha_3 + C_1] \\ \Omega^{[6]}(t) &\equiv A^{(0)} + \frac{1}{240}[-20\alpha_1 - \alpha_3 + C_1, \alpha_2 + C_2], \end{aligned} \tag{22}$$

with

$$\begin{aligned} \alpha_1 &= \frac{9}{4}A^{(0)} - 15A^{(2)} \\ \alpha_2 &= 12A^{(1)} \\ \alpha_3 &= -15A^{(0)} + 180A^{(2)} \end{aligned} \tag{23}$$

verifies that $\Omega^{[6]}(t) = \Omega(t) + \mathcal{O}(t^7)$. In other words, $\Omega^{[6]}(t)$ reproduces exactly the sum $\sum_{m=1}^{4} \Omega_m$ collected in (17) up to order t^6 (even the term $-\frac{1}{80}[\alpha_1, \alpha_4]$) when $A^{(0)}$, $A^{(1)}$ and $A^{(2)}$ are evaluated exactly, and thus $Y(t) = \exp(\Omega^{[6]}(t)) + \mathcal{O}(t^7)$.

Notice that the approximation (22) only requires the computation of three commutators, instead of the eight commutators present in (17). This is in fact the minimum number [4].

At this stage some comments are in order. First, although it has been assumed that $A(t)$ is sufficiently regular so that its Taylor expansion is well defined, it is clear that the final expressions, both for the Magnus series and for the approximations in terms of univariate integrals we have constructed, are still valid even if $A(t)$ is only integrable. Second, we have considered an expansion around the midpoint $t_{1/2}$ only for the shake of simplicity. The same results follow if one expands around $t = 0$. Third, when the exact evaluation of the univariate integrals $A^{(i)}$ is not possible, a numerical quadrature may be used instead. In this way, several numerical integration methods especially well adapted to equation (1) can be designed [3, 4].

3.2 Applicability in perturbation theory

In time perturbation theory in Quantum Mechanics one usually ends up with an equation of the form (1) where the matrix A is replaced by εA, for some (small) parameter $\varepsilon > 0$. For instance, if the Hamiltonian of the system is $H(t) = H_0 + \varepsilon H_1(t)$ and the dynamics corresponding to H_0 can be solved, then a transformation to the interaction picture is carried out, so that the new equation to be solved is (12), with $H_I(t) = \varepsilon\, \mathrm{e}^{-\frac{i}{\hbar} H_0 t}\, H_1(t)\, \mathrm{e}^{\frac{i}{\hbar} H_0 t}$.

When the Magnus expansion is applied to this equation, it is clear that each term $\Omega_m(t)$ in the series (3) is of order ε^m, and thus the approximate solution obtained by taking only into account the first p terms of the Magnus series has error of order ε^{p+1}. Since the previous analytic approximations in terms of univariate integrals can obviously also be applied in perturbation theory, it makes sense to analyze their dependence on the perturbation parameter ε.

Let us start with the approximation $\Omega^{[4]}$ given by (21) when the functions (18) are taken into account. Since $A^{(0)}(t) = \Omega_1(t)$, then

$$\Omega^{[4]}(t) = A^{(0)}(t) - [A^{(0)}(t), A^{(1)}(t)] = \Omega_1(t) + \tilde{\Omega}_2(t), \tag{24}$$

with

$$\tilde{\Omega}_2(t) = \Omega_2(t) + \mathcal{O}(t^5).$$

In other words, the difference between the exact solution $Y_{\mathrm{ex}}(t, \varepsilon)$ and the approximation obtained by considering (24) is a double asymptotic series in ε and t whose first terms read

$$Y_{\mathrm{ex}}(t, \varepsilon) - \mathrm{e}^{\Omega^{[4]}(t)} = \varepsilon^2 (u_{25}^{[4]} t^5 + u_{26}^{[4]} t^6 + \cdots) + \varepsilon^3 (u_{35}^{[4]} t^5 + u_{36}^{[4]} t^6 + \cdots) + \mathcal{O}(\varepsilon^4 t^5).$$

With respect to the approximation $\Omega^{[6]}$ given by (22) with (23) and (18), we get analogously

$$\Omega^{[6]}(t) = \Omega_1(t) + \sum_{i=2}^{4} \tilde{\Omega}_i(t) = \sum_{i=1}^{4} \Omega_i(t) + \mathcal{O}(\varepsilon^2 t^7),$$

so that

$$Y_{\mathrm{ex}}(t, \varepsilon) - \mathrm{e}^{\Omega^{[6]}(t)} = \varepsilon^2 (u_{27}^{[6]} t^7 + \cdots) + \varepsilon^3 (u_{37}^{[6]} t^7 + \cdots) + \varepsilon^4 (u_{47}^{[6]} t^7 + \cdots) + \mathcal{O}(\varepsilon^5 t^7)$$

for certain error coefficients $u_{ij}^{[6]}$. In general, for an approximation of order t^{2p} in terms of the functions (18) one has

$$\Omega^{[2p]}(t) = \Omega_1(t) + \sum_{i=2}^{2p-2} \tilde{\Omega}_i(t) = \sum_{i=1}^{2p-2} \Omega_i(t) + \mathcal{O}(\varepsilon^2 t^{2p+1}) \equiv \Omega^{(2p)}(t) + \mathcal{O}(\varepsilon^2 t^{2p+1})$$

and thus

$$Y_{\mathrm{ex}}(t,\varepsilon) - \mathrm{e}^{\Omega^{[2p]}(t)} = \varepsilon^2 (u_{2,2p+1}^{[2p]} t^{2p+1} + \cdots) + \varepsilon^3 (u_{3,2p+1}^{[2p]} t^{2p+1} + \cdots) + \mathcal{O}(\varepsilon^4 t^{2p+1}). \tag{25}$$

Notice that since in general $\tilde{\Omega}_2(t)$ does not reproduce the whole expression of $\Omega_2(t)$ there is always an error term of order ε^2. By contrast, when the expression of $\Omega^{(2p-2)}(t)$ is computed exactly one has instead

$$\begin{aligned} Y_{\mathrm{ex}}(t,\varepsilon) - \mathrm{e}^{\Omega^{(2p-2)}(t)} &= \varepsilon^{2p-1} \left(w_{2p-1,2p+1}^{(2p-2)} t^{2p+1} + w_{2p-1,2p+2}^{(2p-2)} t^{2p+2} + \cdots \right) + \\ & \quad \varepsilon^{2p} \left(w_{2p,2p+1}^{(2p-2)} t^{2p+1} + w_{2p,2p+2}^{(2p-2)} t^{2p+2} + \cdots \right) + \cdots \end{aligned} \tag{26}$$

In any case, for small values of the parameter ε relative to t, one expects that the previous analytic approximations be fairly accurate in the convergence domain of the Magnus expansion.

To put these results in perspective, let us briefly review the approach commonly used in standard time-dependent perturbation theory to solve the corresponding problem (1) with εA. When Dyson perturbation series is applied, the solution is given by

$$Y(t,\varepsilon) = I + \sum_{n=1}^{\infty} P_n(t,\varepsilon), \tag{27}$$

where P_n is the multivariate integral

$$P_n(t,\varepsilon) = \varepsilon^n \int_0^t dt_1 \ldots \int_0^{t_{n-1}} dt_n A(t_1)\, A(t_2) \ldots A(t_n). \tag{28}$$

The series (27) is convergent for any $t > 0$, but it only shares the qualitative properties of the exact solution when all the infinite terms are taken into account. In particular, for the Schrödinger equation (12), any truncation of the series provides a solution which is no longer unitary, in contrast with the Magnus expansion or any of the analytic approximations considered previously.

If a power series for $A(t)$ is considered, then clearly

$$P_n(t,\varepsilon) = \varepsilon^n \sum_{i \geq n} p_{ni}\, t^i,$$

so that, by denoting

$$Y^{(p)}(t,\varepsilon) \equiv I + \sum_{i=1}^{p} P_n(t,\varepsilon)$$

one has

$$Y_{\rm ex}(t,\varepsilon)-Y^{(p)}(t,\varepsilon) = \varepsilon^{p+1}(x_{1,p+1}t^{p+1}+x_{1,p+2}t^{p+2}+\cdots)+\varepsilon^{p+2}(x_{2,p+2}t^{p+2}+\cdots)+\cdots \tag{29}$$

for certain coefficients x_{ij}. Thus, in particular, if an approximation to the exact solution up to order, say, t^5 is desired within this framework, one has to compute all the integrals involved in P_n, $n = 1,\ldots,4$ and form $Y^{(4)}(t,\varepsilon)$, since in that case $Y_{\rm ex}(t,\varepsilon) - Y^{(4)}(t,\varepsilon) = \mathcal{O}(\varepsilon^5 t^5)$. Notice that for achieving the same order of approximation in t only the first two terms in the Magnus series have to be considered, according to (26) and the simpler expression $\mathrm{e}^{\Omega^{[4]}(t)}$ may be used for this purpose.

It is in fact possible to establish a connection between Magnus and Dyson series, as shown in [5, 20]. For the first terms one gets explicitly

$$\begin{aligned} P_1 &= \Omega_1, \\ P_2 &= \Omega_2 + \frac{1}{2!}\Omega_1^2, \\ P_3 &= \Omega_3 + \frac{1}{2!}(\Omega_1\Omega_2 + \Omega_2\Omega_1) + \frac{1}{3!}\Omega_1^3 \end{aligned} \tag{30}$$

and so on. The general term reads

$$\Omega_n = P_n - \sum_{j=2}^{n} \frac{1}{j} Q_n^{(j)}, \qquad n \geq 2, \tag{31}$$

where $Q_n^{(j)}$ can be obtained recursively from

$$\begin{aligned} Q_n^{(j)} &= \sum_{m=1}^{n-j+1} Q_m^{(1)} Q_{n-m}^{(j-1)}, \\ Q_n^{(1)} &= \Omega_n, \qquad\qquad Q_n^{(n)} = \Omega_1^n. \end{aligned} \tag{32}$$

Based on this relationship it is possible, in particular, to derive new, simpler expressions for P_i in terms of the univariate integrals appearing in the approximations to Ω_k considered here.

4 Illustrative examples

The purpose of this section is to illustrate the applicability of our technique to obtain new analytic approximations in time dependent perturbation theory. In particular, we integrate the Schrödinger equation with two different Hamiltonians.

4.1 Example 1: Two-level system in a rotating field

Our first problem is defined by the Hamiltonian

$$H(t) = \frac{1}{2}\hbar\omega_0\sigma_3 + \beta(\sigma_1 \cos\omega t + \sigma_2 \sin\omega t), \tag{33}$$

where β is a coupling constant, playing here the role of the perturbation parameter ε. This system constitutes a truncation in state space of a more general one, namely an atom or freely rotating molecule in a circularly polarized radiation field [19, 13].

The exact time-evolution operator can be obtained in closed form by transforming into a rotating frame. Specifically, one has ($\hbar = 1$)

$$U(t) = \exp\left(-\frac{1}{2} i\omega t\sigma_3\right) \exp\left(-it\left(\frac{1}{2}(\omega_0 - \omega)\sigma_3 + \beta\sigma_1\right)\right), \tag{34}$$

so that the quantum mechanical transition probability is given by

$$|(U(t))_{21}| = \left(\frac{2\beta}{\omega'} \sin\frac{\omega' t}{2}\right)^2 \tag{35}$$

in terms of $\omega' = \sqrt{(\omega_0 - \omega)^2 + 4\beta^2}$.

It has been rigorously established that the Magnus expansion converges for $t < 2\pi/\omega_0$ and diverges otherwise [6]. For this example we compute the error in the transition probability obtained by the truncated Magnus series $\Omega^{(m)}(t)$ with $m = 2, 4, 8$, thus providing approximations of the exact solution up to order 4, 6 and 10, respectively and then compare with the corresponding schemes involving only the univariate integrals (18). We plot in Figure 3 these errors as functions of time for $\omega = 4$, $\omega_0 = 1$ and $\beta = 0.4$. For clarity, we have collected only the results achieved by the 4th- and 6th-order schemes with $\Omega^{[4]}$ and $\Omega^{[6]}$ computed with the integrals (18) (dashed curves). From the figure it is clear that the relative error committed when replacing the exact expression of $\Omega^{(2p-2)}(t)$ by $\Omega^{[2p]}(t)$ is fairly small, as expected from our analysis. This is so although we have carried out all the computations without previously transforming the system to the interaction picture. Again, the file containing the computation can be downloaded from `www.gicas.uji.es/Research/Magnus.html`.

4.2 Example 2: A 4×4 matrix

For our second problem we take the following 4×4 matrix:

$$H(t) = \begin{pmatrix} t+1 & \delta & 0 & 0 \\ \delta & 3-t & 2 & 0 \\ 0 & 2 & t-3 & 1 \\ 0 & 0 & 1 & h_{44}(t) \end{pmatrix}$$

with $h_{44}(t) = -4 + \cos((2t-1)\pi/2)$ and the parameter δ is fixed to 0.1 (although the results do not change very much with the particular value of δ).

Theorem 2.1 (with $A(t) = -iH(t)$) guarantees that the Magnus expansion converges for $t < t_c \approx 0.79273$. For this example we compare the evolution with time of the norm of the $(4, 4)$ element of the solution matrix obtained with: (i) $\Omega^{(4)}(t)$, i.e., the first four terms of the Magnus series computed exactly (M6 curve in Figure 4); (ii) $\Omega^{[6]}(t)$, i.e., the new analytical approximation in terms of univariate integrals, which is exact up to $\mathcal{O}(t^6)$ (M6-approx), and (iii) the first six terms in the Dyson expansion (27) (P6). We have also included the

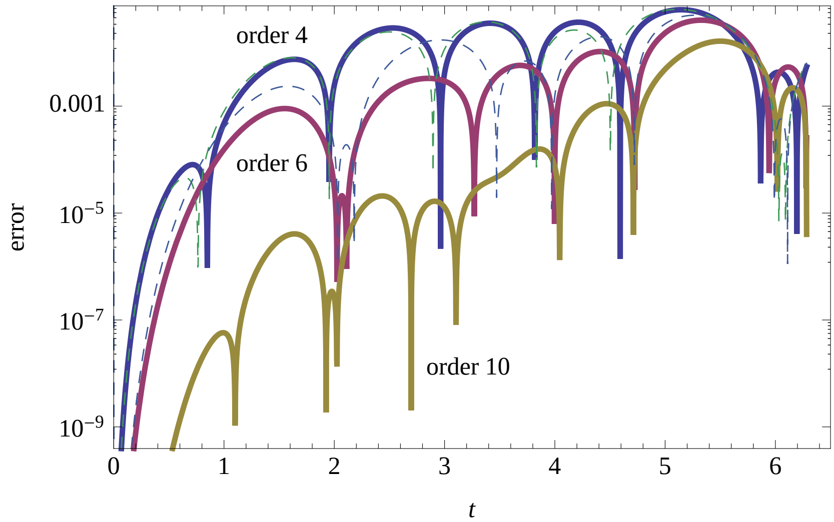

Figure 3: Error in the transition probability for the Hamiltonian (33) with $\omega = 4$, $\omega_0 = 1$ and $\beta = 0.4$ obtained with the truncated Magnus series up to order 4, 6 and 10 (thick curves) and the new analytic approximations of order 4 and 6 (dashed curves). The Magnus expansion converges for $t < 2\pi$.

result provided by a direct numerical integration carried out by the function `NDSolve` of *Mathematica*, which we take as the exact solution (Ex).

Observe in Figure 4 how standard perturbation theory, although with the same order of precision in time, fails to provide an accurate description of the evolution (the norm of the corresponding approximation $Y^{(6)}$ is already 1.00103 for $t = 0.3$), whereas the result obtained by $\exp(\Omega^{(4)}(t))$ (M6) coincides with the exact solution for the whole range of times considered. On the other hand, the new analytic approximation $\exp(\Omega^{[6]}(t))$ in terms of univariate integrals only differs from both the exact result and M6 at times larger than the convergence domain, and it is much simpler to compute. It is also work noticing that $\Omega^{(2)}(t) = \Omega^{[4]}(t)$ for this example.

5 Concluding remarks

The Magnus expansion was initially intended as a tool to get analytic approximation to the solution of linear systems of differential equations. Although since its conception it has been widely used in the perturbative treatment of numerous problems appearing in physics and chemistry, certain aspects related with its convergence and the approximation in time once the series is truncated have been addressed only during the last years. Although, as we have shown here, taking more terms in the Magnus series provides more accurate approximations within the convergence domain, in practical applications only the first terms in the expansion are usually computed, due to the increasing complexity of the successive terms.

In this work we have shown how it is possible to design new analytic ap-

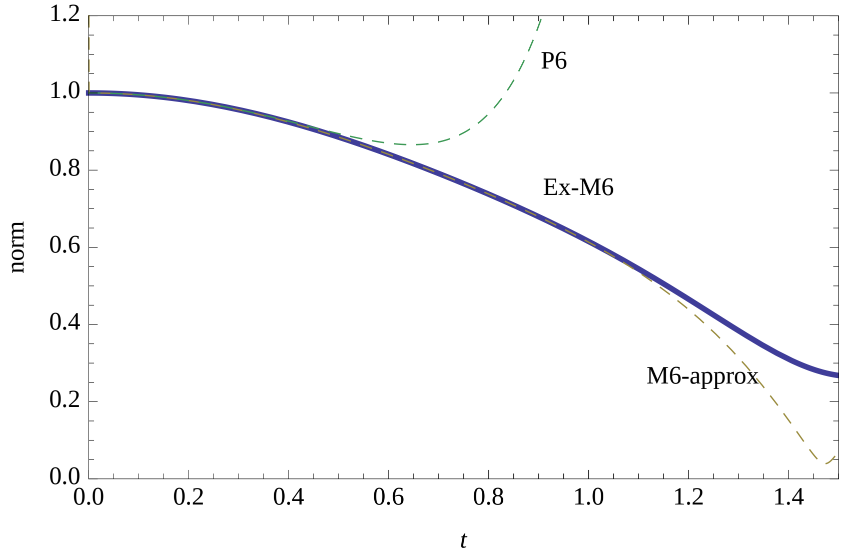

Figure 4: Norm of the $(4,4)$ element of the solution of Example 2 with $\delta = 0.1$ computed with standard perturbation theory (P6), the first 4 terms in the Magnus series (M6) and the new analytical approximation (M6-approx). The curve corresponding to the exact result (Ex) is over-imposed to M6. The Magnus expansion converges at least for $t < 0.79273$.

proximations based on generalized momenta of the coefficient matrix which incorporate more contributions of the expansion. They only require the evaluation of unidimensional integrals and thus are quite affordable to compute for general matrices $A(t)$, the only requisite being that $A(t)$ has to be an integrable function. In addition, in the convergence domain of the Magnus series, they furnish good approximations to both the exact terms of the series and the exact solution. We have studied where the series has to be truncated to get the required order of approximation and we have illustrated how the these new approximations behave in practice in comparison with the exact terms in the expansion and the standard time dependent perturbation theory. One important feature is that this scheme provides by construction closed form approximations which preserve the main qualitative properties of the exact solution.

This convergence domain of the Magnus expansion is affected both by the singularities of the $A(t)$ matrix in the complex plane and by the peculiarities of the logarithm of a matrix function in a way we have summarized here. As a matter of fact, the analysis of the effects of complex singularities of $A(t)$ on the exact dynamics of the differential system constitutes a fascinating subject by itself [9, 22], and remains largely an open problem in the particular case of the Magnus expansion and the analytical approximations considered here.

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