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Magnus and Fer expansions for matrix differential equations: the convergence problem

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Abstract. Approximate solutions of matrix linear differential equations by matrix exponentials are considered. In particular, the convergence issue of Magnus and Fer expansions is treated. Upper bounds for the convergence radius in terms of the norm of the defining matrix of the system are obtained. The very few previously published bounds are improved. Bounds to the error of approximate solutions are also reported. All results are based just on algebraic manipulations of the recursive relation of the expansion generators.

1. Introduction and general survey

The initial value problem for the matrix $X(t)$ given by the linear differential equation

$$\frac{\mathrm{d}X}{\mathrm{d}t} = A(t)X \tag{1}$$

with initial condition $X(0) = I$ appears very often in many branches of science. Here $A(t)$ stands for a sufficiently smooth matrix function to ensure the existence of solutions and the equation is, at least in principle, easily solved by iteration: expanding

$$X(t) = I + \sum_{k=1}^{\infty} P_k(t) \tag{2}$$

with $P_k(0) = 0$ and then substituting into equation (1) one is able to deduce in the usual way the recursive algorithm

$$\frac{\mathrm{d}}{\mathrm{d}t} P_k = A(t) P_{k-1} \qquad P_0 \equiv I. \tag{3}$$

The above scheme is named differently depending on the context: Neumann series, perturbation theory, Dyson expansion and so on. The series in equation (2) converges for all values of t for bounded $A(t)$ no matter how large its norm [1]. One drawback of the method is that its convergence is too slow and furthermore its truncation generally misses some special property of the exact solution: a point much stressed currently as will be discussed later. Note that although, for definiteness, we have stated the problem in matrix

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terms it could be, and in many applications has been, framed in a more abstract operator algebra setting.

In the following we address our interest toward two alternative methods to compute approximate expressions for $X(t)$, namely, Magnus [2] and Fer [3] expansions. The first (hereafter referred to as ME) yields a representation of the matrix X in terms of a unique exponential

$$X(t) = \mathrm{e}^{\Omega(t)} \tag{4}$$

where Ω is obtained as an infinite series

$$\Omega(t) = \sum_{k=1}^{\infty} \Omega_k(t). \tag{5}$$

From a practical point of view explicit formulae for Ω_k are available in terms of nested commutators of $A(t)$ and multiple integrals up to fourth [1, 4, 5] and fifth order [6]. Very recently explicit formulae for Ω_k of all orders have been given in [7]. The important feature for the purposes of the present work is that Ω_k can be obtained in a recursive way [4]. Moreover, recursive generation of Ω_k from P_k's of a Dyson expansion is also possible [4, 8].

Fer's expansion (FE from here on) furnishes an exponential infinite-product expansion of $X(t)$

$$X(t) = \prod_{k=1}^{\infty} \mathrm{e}^{F_k(t)} = \mathrm{e}^{F_1(t)}\, \mathrm{e}^{F_2(t)} \ldots . \tag{6}$$

Here the F_k's are also recursively built up [3, 9].

Before we state the profound reasons for the unique interest of these exponential algorithms and present their convergence problems, in the following two paragraphs we gather some references to different physical systems where ME and FE have been applied.

• *Magnus Expansion.* When tracing back citations to the paper of Magnus [2], the work by Robinson [10] seems to be the first application of the ME to a physical problem. Since then, the ME became rapidly popular and we quote just a few examples of its applications. It has been used in quantum mechanics to study time-dependent problems [1], semiclassical atomic collisions theory [11], the behaviour of molecular systems in intense laser fields [5], multiphoton excitation of molecules [12], pulsed magnetic resonance spectra [13, 14], spectral line broadening [15], infrared divergences in QED [16], the solar neutrino problem (MSW effect) [17], high-resolution NMR spectroscopy in terms of average Hamiltonians [8, 18], and a trajectories solution of the Hamilton equations in classical mechanics [19]. On the mathematical side, new horizons seem to have been opened for the algorithm used as an efficient numerical integrator [7].

• *Fer's Expansion.* In contrast to the ME, much less attention has been paid to solutions of equation (1) in the form of an infinite product of matrix exponentials and the FE has had a peculiar history. To the best of our knowledge, the proposal made by Fer in [3] was never used to solve physical problems until recently. Wilcox, in his fundamental paper [20] in this field, associated Fer's name with an interesting alternative infinite-product expansion which actually was a novelty by itself but definitely different from the FE. Since the ME is sometimes called the continuous analogue of the Baker–Campbell–Hausdorff formula, Wilcox expansion turns out to be the continuous analogue of the Zasenhauss formula. It is worth mentioning that Fer's paper is occasionally misquoted as a reference for the ME [11, 21]. This situation was clarified in [9] and some applications of the FE

to quantum mechanics were carried out for the first time. An adaptation of the algorithm to the particular context of classical mechanics in terms of Lie operators was elaborated in [22], where a comparison with Dragt–Finn factorization [23] is carried out. Application of Fer's factorization as a symplectic integrator [24] and as a tool for solving certain linear partial differential equations [25] has lately been developed by one of the present authors. In numerical analysis the FE was rediscovered by Iserles [26] and is now being intensively investigated as a powerful tool to treat both linear and nonlinear differential equations on Lie groups and other manifolds [27].

Needless to say, equation (1) could also be treated by any of the general purpose algorithms to solve differential equations. The important point to be emphasized here is that the main reason for the usefulness of the exponential algorithms we are discussing lies in the fact that, when truncated, they still preserve structural intrinsic properties of the exact solution. We quote just two instances of this fact: if equation (1) refers to the quantum mechanical evolution operator, $X(t)$ has to be unitary. If, on the other hand, we deal with the evolution operator of a classical Hamiltonian system it has to be symplectic. These are group theoretical properties which the ME and FE guarantee when stopped at any finite order because the special role the exponential mapping plays in group theory.

To end this brief survey, let us turn our attention towards the less studied aspects of these schemes, namely those questions referring to the convergence of the algorithms. This will be our main concern in this paper.

There are two correlated problems with respect to the Magnus solution: (i) When does X admit the exponential representation equation (4)?; (ii) Where (in t-domain) does the series in equation (5) converge? The first question was analysed by Magnus in his classical celebrated paper [2], and revisited by Wei [28]. Much less is known about the convergence question. As far as we know only Pechukas and Light [1] in the mid 1960s and very recently Iserles and Nørsett [7] have touched on this problem in the general case. Constraints on the convergence of the ME for some common decompositions of matrix $A(t)$ can be found in the literature [29]–[34]. However, this is a different and less general question which we are not concerned with here, since we do not require any particular knowledge of $A(t)$.

In this paper, by appropriately dealing with the recursive procedure for the generation of higher-order terms in the ME proposed in [4], we will be able to enlarge the convergence domain. We mention in passing that by a similar technique the often forgotten result quoted in the appendix of [1] can also be recovered.

Concerning the FE, the convergence of the algorithm was already considered in the original paper by Fer. We improve the argument and consequently widen the convergence region [35]. If some additional property is assumed for $A(t)$ it can be further enlarged.

The knowledge of bounds for the convergence of both the ME and FE is a result interesting in itself. When the ME and FE are used as a mathematical tool to obtain analytical approximations to $X(t)$ any information on the extension of the convergence region is of great interest. On the other hand, if the algorithms have to be useful for massive and precise numerical integration, the knowledge for such bounds is important. In both types of applications the need for bounds on the error of an approximate solution is something which hardly needs to be emphasized, so this important practical question will also be touched upon.

In order to make the paper self-contained, in section 2 make we shall report briefly on the recursive generation of the ME prior to analysing its convergence properties. The same scheme will be followed for the FE in section 3. In section 4 we draw our conclusions and consider the future developments.

2. Analysis of the Magnus series expansion

2.1. The algorithm

The Magnus proposal to solve equation (1) is to take $X(t)$ in the form $X = \mathrm{e}^{\Omega}$. If this is substituted in the original equation we obtain the nonlinear matrix differential equation [2, 4, 10, 20]

$$\dot{\Omega} = \sum_{j=0}^{\infty} \frac{B_j}{j!} \{\Omega^j, A\} \qquad \Omega(0) = 0. \tag{7}$$

Here the dot stands for time derivative, the curly brackets denote a nested commutator with Ω entering j times

$$\begin{aligned} &\{\Omega^j, A\} \equiv \{\Omega^{j-1}, [\Omega, A]\} = [\Omega, [\ldots[\Omega, A]\ldots]] \\ &\{\Omega^0, A\} \equiv A \end{aligned} \tag{8}$$

with $[\Omega, A] \equiv \Omega A - A\Omega$, and B_j are Bernoulli numbers [36].

Substituting Magnus series $\Omega = \sum_{j=1}^{\infty} \Omega_j$ into equation (7) one gets [4]

$$\begin{aligned} &\dot{\Omega}_1 = A \\ &\dot{\Omega}_n = \sum_{j=1}^{n-1} \frac{B_j}{j!} S_n^{(j)} \qquad n \geqslant 2 \end{aligned} \tag{9}$$

with the recurrence relation

$$\begin{aligned} &S_n^{(j)} = \sum_{m=1}^{n-j} [\Omega_m, S_{n-m}^{(j-1)}] \qquad 2 \leqslant j \leqslant n-1 \\ &S_n^{(1)} = [\Omega_{n-1}, A] \qquad S_n^{(n-1)} = \{\Omega_1^{n-1}, A\}. \end{aligned} \tag{10}$$

After integration we reach the final result

$$\begin{aligned} &\Omega_1 = \int_0^t A(\tau)\, \mathrm{d}\tau \\ &\Omega_n = \sum_{j=1}^{n-1} \frac{B_j}{j!} \int_0^t S_n^{(j)}(\tau)\, \mathrm{d}\tau \qquad n \geqslant 2. \end{aligned} \tag{11}$$

Connection between the Magnus series and Dyson perturbative series starts from the identity

$$\sum_{j=1}^{\infty} \Omega_j = \ln\left(I + \sum_{j=1}^{\infty} P_j\right). \tag{12}$$

As stated by Burum [4, 8]

$$\Omega_n = P_n - \sum_{j=2}^{n} \frac{(-1)^n}{j} R_n^{(j)} \qquad n \geqslant 2 \tag{13}$$

where $R_n^{(j)}$ may be obtained recursively from

$$\begin{aligned} &R_n^{(j)} = \sum_{m=1}^{n-j+1} R_m^{(1)} R_{n-m}^{(j-1)} \\ &R_n^{(1)} = P_n \qquad R_n^{(n)} = P_1^n. \end{aligned} \tag{14}$$

2.2. Convergence of the Magnus expansion

In order to study the convergence of the Magnus series we now substitute equation (11) into equation (10) to get

$$S_n^{(j)}(t) = \left[\int_0^t A(\tau)\,\mathrm{d}\tau, S_{n-1}^{(j-1)}(t)\right] + \sum_{m=2}^{n-j}\sum_{p=1}^{m-1}\frac{B_p}{p!}\left[\int_0^t S_m^{(p)}(\tau)\,\mathrm{d}\tau, S_{n-m}^{(j-1)}(t)\right]. \tag{15}$$

Let the matrix $A(t)$ be bounded, with $\|A(t)\|$ a piecewise continuous function which we assume is bounded above by the scalar function $k(t)$, $\|A(t)\| \leqslant k(t)$. If we denote $K(t) \equiv \int_0^t k(t')\,\mathrm{d}t'$, we will have $\|\Omega_1(t)\| \leqslant K(t)$ and equation (15) implies

$$\|S_n^{(j)}(t)\| \leqslant 2K(t)\|S_{n-1}^{(j-1)}(t)\| + 2\sum_{m=2}^{n-j}\sum_{p=1}^{m-1}\frac{|B_p|}{p!}\left(\int_0^t \|S_m^{(p)}(\tau)\|\,\mathrm{d}\tau\right)\|S_{n-m}^{(j-1)}(t)\|. \tag{16}$$

It is straightforward to show by induction that

$$\|S_n^{(j)}(t)\| \leqslant (K(t))^{n-1}\,k(t)\,f_n^{(j)} \tag{17}$$

provided the coefficients $f_n^{(j)}$ obey the many-term recurrence relation

$$f_n^{(j)} = 2\sum_{m=1}^{n-j}\sum_{p=0}^{m-1}\frac{|B_p|}{p!m}f_m^{(p)}\,f_{n-m}^{(j-1)} \tag{18}$$

with $f_1^{(0)} = 1$, $f_n^{(0)} = 0$, for $n > 1$. Consequently, if we define

$$b_n = \frac{1}{n}\sum_{p=1}^{n-1}\frac{|B_p|}{p!}f_n^{(p)} \tag{19}$$

we have

$$\|\Omega_n(t)\| \leqslant b_n(K(t))^n. \tag{20}$$

We conclude then that absolute convergence of Magnus series is ensured if

$$K(t)\lim_{n\to\infty}\frac{b_{n+1}}{b_n} < 1. \tag{21}$$

Numerical investigation of this condition clearly indicates that we will have convergence for t values which make

$$K(t) < \xi \equiv 1.086\,869. \tag{22}$$

Clearly this bound could be improved if the inequalities leading to equation (20) could be sharpened.

In the particular case of $k(t) = \rho t^\lambda$, $\lambda \in \mathbb{Z}^+$, $\rho \in \mathbb{R}^+$, considered in [7] we have

$$t < \left[\frac{(1+\lambda)\xi}{\rho}\right]^{1/(1+\lambda)}. \tag{23}$$

Our value $\xi = 1.086\,869$ has to be compared with the value 0.125 given by Iserles and Nørsett. This means that we have neatly enlarged the convergence domain.

A similar procedure going through equations (13) and (14) leads to

$$\|R_n^{(j)}\| \leqslant (K(t))^n g_n^{(j)} \tag{24}$$

provided $g_n^{(j)}$ is generated by the recurrence relation

$$g_n^{(j)} = \sum_{m=1}^{n-j+1} \frac{1}{m!} g_{n-m}^{(j-1)} \qquad j > 1$$
$$g_1^{(1)} = 1. \tag{25}$$

A numerical investigation now yields the following bound for convergence of the Magnus series

$$K(t) < \ln 2 = 0.693\,147 \tag{26}$$

which reproduces the result quoted by Pechukas and Light [1] for a constant upper bound $k(t) = \rho$.

We consider equation (26) a check that confirms the validity of the procedure followed in this section and (22), in turn, a significant improvement of the bound for the convergence region.

2.3. Order analysis and error bounds

Let us suppose now that $A(t) = \mathrm{O}(t^\lambda)$. Then, obviously, $\Omega_1(t) = \mathrm{O}(t^{\lambda+1})$, whereas, from equations (10) and (11), we have

$$\Omega_2(t) = -\frac{1}{2}\int_0^t [\Omega_1(\tau), A(\tau)]\,\mathrm{d}\tau = \mathrm{O}(t^{2\lambda+3}) \tag{27}$$

because the leading term in the expansion of $A(t)$ commutes with that corresponding to $\Omega_1(t)$. It is easy to show by induction that $\Omega_n(t) = \mathrm{O}(t^{n(\lambda+1)+1})$ for $n \geqslant 2$. Therefore, when the Magnus series for $\Omega(t)$ is truncated at the nth term and the approximation $\Omega^{[n]}(t) \equiv \sum_{j=1}^{n} \Omega_j(t)$ is considered, then $\Omega(t) - \Omega^{[n]}(t) = \mathrm{O}(t^{(n+1)(\lambda+1)+1})$, so that in terms of matrices

$$X(t) - X^{[n]}(t) \equiv \mathrm{e}^{\Omega(t)} - \mathrm{e}^{\Omega^{[n]}(t)} = \mathrm{O}(t^{(n+1)(\lambda+1)+1})$$

which is the result obtained in [7].

In the general case, if we write $K = \alpha\xi$, with $0 < \alpha < 1$, the estimate in equation (20) leads to $\|\Omega_{n+1}\| \leqslant \alpha^{n+1}\xi^{n+1}b_{n+1}$, whereas

$$\|\Omega(t) - \Omega^{[n]}(t)\| \leqslant \sum_{i=n+1}^{\infty} \alpha^i \xi^i b_i.$$

As an illustration, if $\alpha = 1/2$ and $n = 4$, then $\|\Omega - \Omega^{[n]}\| < 0.0065$.

3. Analysis of the Fer product expansion

3.1. The algorithm

Fer's algorithm approximates the solution $X(t)$ to equation (1) by a product of matrix exponentials. The expansion is generated by the following recursive scheme:

$$X = \mathrm{e}^{F_1}\,\mathrm{e}^{F_2}\ldots\mathrm{e}^{F_n}X_n$$
$$\dot{X}_n = A_n(t)X_n \qquad X_n(0) = I \qquad n = 1, 2, 3\ldots \tag{28}$$

with $F_n(t)$ and $A_n(t)$ given by

$$F_{n+1}(t) = \int_0^t A_n(t')\,\mathrm{d}t' \qquad A_0(t) = A(t) \qquad n = 0, 1, 2\ldots$$

$$\begin{aligned} A_{n+1} &= \mathrm{e}^{-F_{n+1}} A_n\, \mathrm{e}^{F_{n+1}} - \int_0^1 \mathrm{d}x\, \mathrm{e}^{-xF_{n+1}} A_n\, \mathrm{e}^{xF_{n+1}} \\ &= \int_0^1 \mathrm{d}x \int_0^x \mathrm{d}u\, \mathrm{e}^{-(1-u)F_{n+1}} [A_n, F_{n+1}]\, \mathrm{e}^{(1-u)F_{n+1}} \\ &= \sum_{j=1}^{\infty} \frac{(-)^j\ j}{(j+1)!} \{F_{n+1}^j, A_n\} \qquad n = 0, 1, 2\ldots \end{aligned} \tag{29}$$

where the notation of the previous section has been used.

When after n steps we impose $X_n = I$ we are left with an approximation $X^{[n]}(t)$ to the exact solution $X(t)$.

3.2. Convergence of the Fer expansion

To study the convergence of the Fer expansion we look for conditions on $A(t)$ which insure $F_n \to 0$ as $n \to \infty$. As in the previous section, we take $A(t)$ to be a bounded matrix with $\|A(t)\| \leqslant k(t) \equiv k_0(t)$. Fer's algorithm, equations (28) and (29), provides then a recursive relation among corresponding bounds $k_n(t)$ for $\|A_n(t)\|$. If we denote $K_n(t) \equiv \int_0^t k_n(t')\,\mathrm{d}t'$, we can write this relation in the generic form

$$k_{n+1} = f(k_n, K_n) \tag{30}$$

which after integration gives

$$K_{n+1} = M(K_n). \tag{31}$$

The question now is: When will $K_n \to 0$ as $n \to \infty$? This will certainly be so if zero is a stable fixed point for the iteration of the mapping M and K_0 is within its basin of attraction. To see when this is the case we have to solve the equation $\xi = M(\xi)$ to find where the next fixed point lies. Let us do it explicitly. By taking norms in the recursive scheme of equations (29) we have

$$\|A_{n+1}\| \leqslant \int_0^1 \mathrm{d}x \int_0^x \mathrm{d}u\, \mathrm{e}^{2(1-u)K_n} \|[A_n, F_{n+1}]\| \tag{32}$$

which can be written in the form $\|A_{n+1}\| \leqslant k_{n+1}$, with

$$k_{n+1} = \frac{1 - \mathrm{e}^{2K_n}(1 - 2K_n)}{2K_n} \frac{\mathrm{d}K_n}{\mathrm{d}t} \tag{33}$$

and consequently K_{n+1} is given by equation (31) with

$$M(K_n) = \int_0^{K_n} \frac{1 - \mathrm{e}^{2x}(1 - 2x)}{2x}\,\mathrm{d}x. \tag{34}$$

That is the mapping we have to iterate. It is clear that $\xi = 0$ is a stable fixed point of M. The next, unstable, fixed point is $\xi = 0.860\,4065$. So we can conclude that we have a convergent Fer expansion for values of time t such that

$$\int_0^t \|A(t')\|\,\mathrm{d}t' \leqslant K_0(t) < 0.860\,4065. \tag{35}$$

This result widens the range $K_0(t) < 0.628$ originally given by Fer [3] using a slightly different argument.

We point out that additional properties of $A(t)$ allow an improvement of this result. For example, if $A(t)$ happens to be skew-Hermitian then $\xi = 2$.

Notice also that whenever for a particular value $n = n_0$ another bound $\tilde{k}_{n_0} < k_{n_0}$ for $\|A_{n_0}\|$ is found, then the iteration process given by equation (31) can be started from $\tilde{K}_{n_0} = \int_0^t \tilde{k}_{n_0}(t')\,\mathrm{d}t'$. This could provide a wider convergence t-domain. In the next subsection we emphasize the importance of enlarging this region because of its effect on the error bounds of approximate solutions.

3.3. Error bounds

We want now to bound $\|X - X^{[n]}\|$ where $X^{[n]}$ is the nth order Fer approximation and let us write $X = X^{[n]}X_n$. Then, if we introduce $D_n = X_n - I$, we have $\mathcal{E}_n \equiv X - X^{[n]} = X^{[n]}D_n$.

To bound $\|\mathcal{E}_n\|$ we are going to bound both D_n and $X^{[n]}$. To this end we start by writing D_n in the form

$$D_n(t) = \int_0^t \mathrm{d}t'\, A_n(t')X_n(t'). \tag{36}$$

From equation (28) we get $\|X_n\| \leqslant \exp[\int_0^t \|A_n\|\,\mathrm{d}t'] \leqslant \mathrm{e}^{K_n}$, and so

$$\|D_n\| \leqslant \int_0^t \|A_n\|\|X_n\|\,\mathrm{d}t' \leqslant \mathrm{e}^{K_n}\int_0^t \|A_n\|\,\mathrm{d}t' \leqslant K_n\,\mathrm{e}^{K_n}. \tag{37}$$

As far as $X^{[n]}$ is concerned, we observe that

$$\|X^{[n]}\| = \|XX_n^{-1}\| \leqslant \|X\|\|X_n^{-1}\| \leqslant \mathrm{e}^{K_0}\,\mathrm{e}^{K_n}. \tag{38}$$

Finally, we have

$$\|\mathcal{E}_n\| \leqslant K_n\,\mathrm{e}^{K_0+2K_n} \tag{39}$$

where K_n is given recursively by equation (34) starting with the initial value K_0. As we have already noticed

$$K_0 < 0.860\,4065 \Rightarrow K_n \underset{n\to\infty}{\to} 0 \Rightarrow \|\mathcal{E}_n\| \underset{n\to\infty}{\to} 0 \tag{40}$$

and this allows us to find error bounds for the Fer approximate solutions.

We have already pointed out the importance of enlarging the region where, for a given value of t, $K_0(t)$ may lie and still after iteration originate $K_n \to 0$ as $n \to \infty$. If ξ bounds this region (here $\xi = 0.860\,4065$ for a general A) we can always write $K_0 = \alpha\xi$, with $0 < \alpha < 1$, and thus

$$\|\mathcal{E}_n\| \leqslant \alpha^{2^n}\xi\,\mathrm{e}^{\xi(\alpha+2\alpha^{2^n})}. \tag{41}$$

So, in general, the larger the bound ξ, the smaller the coefficient α and the better the error bounds.

Again, as already mentioned above, for skew-Hermitian A equation (39) can be refined to $\|\mathcal{E}_n\| \leqslant 2(K_0/2)^{2^n}$.

4. Conclusions and outlook

As we have sketched in the introduction, the ME and FE have deserved very different attention in the literature. From the point of view of physical applications, the ME has been extensively used in a variety of issues, while the FE has been either ignored or misquoted until recently. As regards convergence, an upper bound appears already in Fer's original work. This is in contrast to the situation for the ME.

The rate of convergence of the FE is faster than that of the ME in the sense that, for a prescribed precision, one needs more Ω_k's than F_k's even if from the computational point of view the latter could require more work than the former. Thus, the characteristics of the problem at hand might ultimately dictate the method to be used.

The analysis reported in this paper has been based directly on the original form of the differential matrix equation (1). Convenient transformations based on a more detailed knowledge of the A matrix can originate better performances of both the ME and FE. An analysis in this sense along the lines of [37] is in progress. We emphasize also that our results may be of some utility in the construction and implementation of numerical integrators, a question that we will analyse in the forthcoming future.

The two algorithms discussed so far are by no means mutually exclusive. They can be combined in a mixed way. Thus one can for instance leave the ME after a few steps and go on with the FE, a procedure already suggested in [9] and implemented in its lowest orders in [35].

In conclusion, we think that the various bounds we have obtained here, equations (22) and (35), contribute to a deeper understanding of Magnus and Fer expansions. We encourage an efficient incorporation of the present results to avoid a rather blind application of these schemes.

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References

[1] Pechukas P and Light J C 1966 On the exponential form of time-displacement operators in quantum mechanics *J. Chem. Phys.* **44** 3897–912

[2] Magnus W 1954 On the exponential solution of differential equations for a linear operator *Commun. Pure Appl. Math.* **7** 649–73

[3] Fer F 1958 Résolution de l'equation matricielle $\dot{U} = pU$ par produit infini d'exponentielles matricielles *Bull. Classe Sci. Acad. Roy. Bel.* **44** 818–29

[4] Klarsfeld S and Oteo J A 1989 Recursive generation of higher-order terms in the Magnus expansion *Phys. Rev.* A **39** 3270–3

[5] Milfeld K F and Wyatt R E 1983 Study, extension and application of Floquet theory for quantum molecular systems in an oscillating field *Phys. Rev.* A **27** 72–94

[6] Prato D and Lamberti P W 1997 A note on Magnus formula *J. Chem. Phys.* **106** 4640–3

[7] Iserles A and Nørsett S P 1997 On the solution of linear differential equations in Lie groups DAMTP tech. report 1997/NA3, University of Cambridge
Iserles A and Nørsett S P 1997 Linear ODEs in Lie groups DAMTP tech. report 1997/NA9, University of Cambridge

[8] Burum D P 1981 Magnus expansion generator *Phys. Rev.* B **24** 3684–92

[9] Klarsfeld S and Oteo J A 1989 Exponential infinite-product representations of the time displacement operator *J. Phys. A: Math. Gen.* **22** 2687–94

[10] Robinson D W 1963 Multiple Coulomb excitations of deformed nuclei *Helv. Phys. Acta* **36** 140–54

[11] Baye D and Heenen P H 1973 A theoretical study of fast proton-atomic hydrogen scattering *J. Phys. B: At. Mol. Phys.* **6** 105–13

[12] Schek I, Jortner J and Sage M L 1981 Application of the Magnus expansion for high-order multiphoton excitation *Chem. Phys.* **59** 11–27

[13] Evans W A B 1968 On some application of Magnus expansion in nuclear magnetic resonance *Ann. Phys.* **48** 72–93
[14] Waugh J S 1982 Theory of broadband spin decoupling *J. Magn. Reson.* **50** 30–49
[15] Cady W A 1974 Rotational spectral line broadening of OCS by noble gases *J. Chem. Phys.* **60** 3318–23
[16] Dahmen H D, Scholz B and Steiner F 1982 Infrared dynamics of QED and the asymptotic behavior of the electron form factor *Nucl. Phys.* B **202** 365–81
[17] D'Olivo J C and Oteo J A 1990 Magnus expansion and the two-neutrino oscillations in matter *Phys. Rev.* D **42** 256–9
D'Olivo J C and Oteo J A 1996 Nonadiabatic three-neutrino oscillations in matter *Phys. Rev.* D **54** 1187–93
[18] Ernst R R, Bodenhausen G and Wokaun A 1986 *Principles of NMR in One and Two Dimensions* (Oxford: Clarendon)
[19] Oteo J A and Ros J 1991 The Magnus expansion for classical Hamiltonian systems *J. Phys. A: Math. Gen.* **24** 5751–62
[20] Wilcox R M 1967 Exponential operators and parameter differentiation in quantum physics *J. Math. Phys.* **8** 962–82
[21] Wei J and Norman E 1963 Lie algebraic solution of linear differential equations *J. Math. Phys.* **4** 575–81
[22] Casas F, Oteo J A and Ros J 1991 Lie algebraic approach to Fer's expansion for classical Hamiltonian systems *J. Phys. A: Math. Gen.* **24** 4037–46
[23] Dragt A J and Finn J M 1976 Lie series and invariant functions for analytic symplectic maps *J. Math. Phys.* **17** 2215–27
[24] Casas F 1996 Fer's factorization as a symplectic integrator *Num. Math.* **74** 283–303
[25] Casas F 1996 Solution of linear partial differential equations by Lie algebraic methods *J. Comp. Appl. Math.* **76** 159–70
[26] Iserles A 1984 Solving linear ordinary differential equations by exponentials of iterated commutators *Num. Math.* **45** 183–99
[27] Zanna A 1996 The method of iterated commutators for ordinary differential equations on Lie groups DAMTP tech. report 1996/NA12, University of Cambridge
[28] Wei J 1963 Note on global validity of the Baker–Hausdorff and Magnus theorems *J. Math. Phys.* **4** 1337–41
[29] Klarsfeld S and Oteo J A 1989 The Baker–Campbell–Hausdorff formula and the convergence of Magnus expansion *J. Phys. A: Math. Gen.* **22** 4565–72
[30] Klarsfeld S and Oteo J A 1989 Analytic properties for the Magnus operator for two solvable hamiltonians *Phys. Lett.* **142A** 393–7
[31] Fel'dman E B 1984 On the convergence of the Magnus expansion for spin systems in periodic magnetic fields *Phys. Lett.* **104A** 479–81
[32] Salzman W R 1987 New criterion for convergence of exponential perturbation theory in the Schrödinger representation *Phys. Rev.* A **36** 5074–6
[33] Maricq M M 1987 Convergence of Magnus expansion for time-dependent two-level systems *J. Chem. Phys.* **86** 5647–51
[34] Fernández F M 1990 Convergence of the Magnus expansion *Phys. Rev.* A **41** 2311–14
[35] Blanes S 1994 Evolución de sistemas dinámicos: desarrollos de Magnus y Fer *Master Thesis* University of Valencia
[36] Abramowitz M A and Stegun I A 1965 *Handbook of Mathematical Functions* (New York: Dover)
[37] Casas F, Oteo J A and Ros J 1994 Linear time-dependent Hamiltonian systems beyond the adiabatic limit *J. Phys. A: Math. Gen.* **27** 4325–39