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Floquet theory: exponential perturbative treatment

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Abstract

We develop a Magnus expansion well suited for Floquet theory of linear ordinary differential equations with periodic coefficients. We build up a recursive scheme to obtain the terms in the new expansion and give an explicit sufficient condition for its convergence. The method and formulae are applied to an illustrative example from quantum mechanics.

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1. Introduction

One of the outstanding results in the theory of linear systems of differential equations with periodic coefficients is contained in Floquet theorem [1]. It applies to matrix linear differential equations of the form

$$\frac{dZ}{dt} = A(t)Z \quad Z(0) = I \quad (1)$$

where A is a complex n by n matrix-valued function and its matrix elements are integrable periodic functions of t with period T . Here I represents the identity matrix of dimension n . Floquet theorem states that the solution $Z(t)$ has a very precise structure [1, 2]:

$$Z(t) = P(t) \exp(tF) \quad (2)$$

where F and P are n by n matrices, $P(t) = P(t+T)$ for all t and F is constant. Thus, albeit a solution of (1) is not, in general, periodic, the departure from periodicity is determined by (2). This result, when applied in quantum mechanics, is referred to as Bloch wave theory [3]. It is widely used in problems of solid state physics, where space-periodic potentials are quite common. In nuclear magnetic resonance this structure is exploited as far as either time-dependent periodic magnetic fields or sample spinning are involved [4]. Asymptotic stability of the solution $Z(t)$ is dictated by the nature of the eigenvalues of F , the so-called characteristic exponents of the original periodic system. Also, the matrix $P(t)$ is the starting point for some perturbative analyses [5].

An alternative manner of interpreting equation (2) is to consider the piece $P(t)$, provided it is invertible, to perform a transformation of the solution in such a way that the coefficient matrix corresponding to the new representation has all its matrix entries given by constants. Thus the piece $\exp(tF)$ in (2) may be considered as an exact solution of the system (1) previously moved to a representation where the coefficient matrix is the constant matrix F . The t -dependent change of representation is carried out by $P(t)$. In other words, (1) with $A(t+T) = A(t)$ is a reducible system in the sense of Lyapunov by means of a periodic matrix $P(t)$ [6, 7]. Of course, Floquet theorem by itself gives no practical information about this procedure. It just states that such a representation does exist. In fact, a serious difficulty in the study of differential equations with periodic coefficients is that no general method to compute either the matrix $P(t)$ or the eigenvalues of F is known.

Mainly two ways of exploiting the above structure of $Z(t)$ are found in the literature [8]. The first one consists in performing a Fourier expansion of the formal solution, leading to an infinite system of linear differential equations with constant coefficients. Thus, the t -dependent finite system is replaced with a constant one at the price of handling infinite dimension. Resolution of the truncated system furnishes an approximate solution. The second approach is of perturbative nature. It deals directly with the form (2) by expanding

$$P(t) = \sum_{n=1}^{\infty} P_n(t) \quad F = \sum_{n=1}^{\infty} F_n. \quad (3)$$

Every term F_n in (3) is fixed so as to ensure $P_n(t) = P_n(t+T)$, which in turn guarantees the Floquet structure (2) at any order of approximation.

In this paper we investigate an alternative way to ascertain the explicit form of the transformation $P(t)$. By incorporating the so-called Magnus expansion into Floquet theory we propound a recursive and convergent scheme which has the salient feature of preserving additional geometric properties of the solution.

An intuitive way of introducing the conventional Magnus expansion [9] (hereafter referred to as the ME) is the following. Recall that the solution corresponding to the initial-value problem (1) with constant matrix A reads $Z(t) = \exp(At)$. It seems then natural to propound a solution of equation (1) in the true exponential form

$$Z(t) = \exp(\Omega(t)) \quad \Omega(0) = 0 \quad (4)$$

and then to study its possible advantages. The ME is obtained by expanding

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

which justifies the name *exponential perturbation theory* coined for the Magnus expansion in some contexts. The relevant point for the usefulness of such an exponential representation is that in many cases any truncation of (5) leads to an approximation for $Z(t)$ which necessarily preserves intrinsic properties of the exact solution associated with the geometric or algebraic structure of the problem. Hence the interest of the ME as regards quantum mechanics perturbation theory [10] of the time evolution operator and its connection with more standard procedures in quantum field theory [11]. The property of ME just quoted is also at the basis of its more recent use in numerical analysis as a geometric integrator [12, 13].

ME is successfully used in a number of periodic time-dependent systems. For instance, in NMR spectroscopy one finds the so-called *average Hamiltonian theory* [4] in which the quantum system is supposed to be observed stroboscopically with period T and no further measurement at intermediate times. This theory is built up on the basis of the conventional ME to find F by computing $\Omega(t=T)$. An extension of the theory allowing intermediate computations could be of experimental interest.

Substituting equation (4) into (1) one obtains the nonlinear differential equation for Ω (see for instance [9, 14, 15]):

$$\dot{\Omega} = \frac{\text{ad}_{\Omega}}{\exp(\text{ad}_{\Omega}) - 1} A = \sum_{j=0}^{\infty} \frac{B_j}{j!} (\text{ad}_{\Omega})^j A \quad \Omega(0) = 0 \quad (6)$$

where ad_{Ω} is the adjoint operator: $\text{ad}_{\Omega} A = [\Omega, A] \equiv \Omega A - A \Omega$, $(\text{ad}_{\Omega})^0 A = A$, $\text{ad}_{\Omega}^n A = \text{ad}_{\Omega}(\text{ad}_{\Omega}^{n-1} A)$. Here the dot represents the time derivative and B_j are Bernoulli numbers [16].

Our purpose here is to extend the use of the ME to perturbatively solve for $P(t)$ and F in (2). More specifically we explain how to efficiently replace the perturbative expansion for $P(t)$ in (3) with an exponential ansatz, so that in (2) we try approximate solutions in the form

$$Z(t) = \exp(\Lambda(t)) \exp(Ft). \quad (7)$$

We shall show how the computation of Λ and F is carried out perturbatively, preserving at the same time Floquet decomposition at every order of approximation.

The plan of the paper is the following. In section 2 we recall a recursive procedure for the determination of Ω_k in the conventional ME and also report on sufficient conditions for the convergence of the series. In section 3 we setup the equations for the exponential perturbative Floquet expansion, which constitutes a novelty as far as ME is concerned. The reader might think of the method as a kind of *constrained Magnus expansion*. Our recursive procedure for determining this constrained expansion is given in section 4. An analysis of its convergence is carried out in section 5. The results and formulae are eventually illustrated on a simple problem, well known in time-dependent quantum mechanics, in section 6.

2. Recursive generation for conventional Magnus expansion

There are several ways to obtain the successive contributions to the series in (5). For instance, in [12] a technique based on binary trees, which presents very interesting features, is completely developed. We shall be concerned here with the recursive scheme initiated in [14], which we sketch for the sake of completeness.

Introducing Magnus series (5) into (6) and gathering terms of the same order one obtains

$$\Omega_n = \sum_{j=0}^{n-1} \frac{B_j}{j!} \int_0^t S_n^{(j)}(\tau) d\tau \quad n \geq 1 \quad (8)$$

where $S_n^{(j)}(t)$ is obtained recursively

$$\begin{aligned} S_n^{(j)} &= \sum_{m=1}^{n-j} [\Omega_m, S_{n-m}^{(j-1)}] \quad (1 \leq j \leq n-1) \\ S_1^{(0)} &= A \quad S_n^{(0)} = 0 \quad (n > 1). \end{aligned} \quad (9)$$

Particular cases are $S_n^{(1)} = [\Omega_{n-1}, A]$ and $S_n^{(n-1)} = (\text{ad}_{\Omega_1})^{n-1} A$. The generic structure of $S_n^{(j)}$ is as follows:

$$S_n^{(j)} = \sum [\Omega_{i_1}, [\dots [\Omega_{i_k}, A] \dots]] \quad (i_1 + \dots + i_k = n-1) \quad (10)$$

where k represents the number of Ω s. This recurrence may be programmed with a symbolic language. Of course, the effective order of computation one reaches does depend on the particular structure of A .

Assume there exists a non-negative scalar function $k(t)$ such that $\|A(t)\| \leq k(t)$ and denote $K(t) = \int_0^t k(\tau) d\tau$. The matrix norm appearing in the expression above is as yet unspecified

but has to satisfy the *consistency condition* or *submultiplicative property* $\|AB\| \leq \|A\|\|B\|$, so that $\|[A, B]\| \leq 2\|A\|\|B\|$ is implied.

Suppose now

$$\begin{aligned}\|\Omega_n(t)\| &\leq b_n K^n(t) \\ \|S_n^{(j)}(t)\| &\leq f_n^{(j)} K^{n-1}(t)k(t)\end{aligned}\quad (11)$$

for some unspecified coefficients $b_n, f_n^{(j)}$. Equation (9) implies

$$\|S_n^{(j)}(t)\| \leq 2 \sum_{m=1}^{n-j} b_m f_{n-m}^{(j-1)} K^{n-1}(t)k(t) \quad (12)$$

and hence

$$f_n^{(j)} = 2 \sum_{m=1}^{n-j} b_m f_{n-m}^{(j-1)} \quad (1 \leq j \leq n-1) \quad (13)$$

with $f_1^{(0)} = 1, f_n^{(0)} = 0$ for $n > 1$. A similar bounding on equation (8) yields

$$\|\Omega_n(t)\| \leq \frac{1}{n} \sum_{j=0}^{n-1} \frac{|B_j|}{j!} f_n^{(j)} K^n(t) \quad (14)$$

and therefore

$$b_n = \frac{1}{n} \sum_{j=0}^{n-1} \frac{|B_j|}{j!} f_n^{(j)} \quad (n \geq 1). \quad (15)$$

Equations (13) and (15) give recursively the coefficients b_n , which allows the study of the convergence of the series $\sum b_n K(t)^n$ through the D'Alembert criterion. According to the extant studies an explicit sufficient condition for existence of an exponential solution [17] and for the convergence of the series expansion (5) [18] reads

$$\int_0^t \|A(s)\| ds \leq K(t) \leq \xi = 1.086\,869 \quad (16)$$

establishing a constraint between t and $\|A\|$ for convergence of the conventional Magnus expansion. A more involved proof on convergence bounds, no longer based on recurrences, has been recently reported [19], yielding $\xi = 2$.

3. Floquet–Magnus expansion

When the Floquet form (2) is introduced in our differential equation (1) the evolution equation for P is obtained:

$$\dot{P}(t) = A(t)P(t) - P(t)F \quad P(0) = I. \quad (17)$$

The constant matrix F is also unknown and we will determine it so as to ensure $P(t+T) = P(t)$. Now we replace the usual perturbative scheme in equation (3) with the exponential ansatz

$$P(t) = \exp(\Lambda(t)) \quad \Lambda(0) = 0. \quad (18)$$

Obviously, $\Lambda(t+T) = \Lambda(t)$ so as to preserve periodicity. Now equation (17) conveys

$$\frac{d}{dt} \exp(\Lambda) = A \exp(\Lambda) - \exp(\Lambda)F. \quad (19)$$

Since $\dot{\Lambda}$ does not commute in general with Λ we use the well known formula [15]

$$\frac{d}{dt} \exp(\Lambda(t)) = \int_0^1 \exp(x\Lambda) \dot{\Lambda} \exp((1-x)\Lambda) dx = \int_0^1 \exp((1-x)\Lambda) \dot{\Lambda} \exp(x\Lambda) dx. \quad (20)$$

Eventually equation (19) becomes

$$\int_0^1 \exp(y\Lambda) \dot{\Lambda} \exp(-y\Lambda) dy = A - \exp(\Lambda) F \exp(-\Lambda). \quad (21)$$

Now taking into account the operator identity (sometimes referred to as the Baker–Hausdorff formula) [15]

$$e^X Y e^{-X} = \sum_{k=0}^{\infty} \frac{1}{k!} (\text{ad}_X)^k Y = \exp(\text{ad}_X) Y \quad (22)$$

we obtain

$$\sum_{k=0}^{\infty} \frac{1}{(k+1)!} (\text{ad}_\Lambda)^k \dot{\Lambda} = A - \sum_{k=0}^{\infty} \frac{1}{k!} (\text{ad}_\Lambda)^k F. \quad (23)$$

We are interested in obtaining an explicit differential equation for Λ . With this in mind let us define the function

$$\varphi(x) = \frac{e^x - 1}{x} = \sum_{k=1}^{\infty} \frac{1}{k!} x^{k-1} \quad (24)$$

and correspondingly

$$(\varphi(x))^{-1} = \frac{x}{e^x - 1} = \sum_{k=0}^{\infty} \frac{B_k}{k!} x^k. \quad (25)$$

Then equation (23) gives

$$\varphi(\text{ad}_\Lambda) \dot{\Lambda} = A - \exp(\text{ad}_\Lambda) F \quad (26)$$

which yields

$$\dot{\Lambda} = (\varphi(\text{ad}_\Lambda))^{-1} A - ((\varphi(\text{ad}_\Lambda))^{-1} + \text{ad}_\Lambda) F. \quad (27)$$

The series expansion (25) leads finally to

$$\dot{\Lambda} = \sum_{k=0}^{\infty} \frac{B_k}{k!} (\text{ad}_\Lambda)^k (A + (-)^{k+1} F). \quad (28)$$

This equation is now, in the Floquet context, the analogue of the Magnus equation (6). Notice that if we put $F = 0$ then (6) is recovered. The next move is to consider the series expansions for Λ and F

$$\Lambda(t) = \sum_{k=1}^{\infty} \Lambda_k(t) \quad F = \sum_{k=1}^{\infty} F_k \quad (29)$$

with $\Lambda_k(0) = 0$, for all k . Equating terms of the same order in (28) one obtains the successive contributions to the series (29). Therefore, the explicit ansatz we are propounding reads

$$Z(t) = \exp\left(\sum_{k=1}^{\infty} \Lambda_k(t)\right) \exp\left(t \sum_{k=1}^{\infty} F_k\right).$$

It seems quite natural to us to name this method the Floquet–Magnus expansion.

4. Recursive generation for Floquet–Magnus expansion

The point now is how to compute the different terms in the expansion (29). As is the case for conventional ME, one possibility would be to use graph theory to embrace the analysis of the more general equation (28). Instead, we simply generalize the recursive procedure expounded in section 2 for the conventional ME.

Substituting the expansions of equation (29) into (28) and equating terms of the same order one can write

$$\dot{\Lambda}_n = \sum_{j=0}^{n-1} \frac{B_j}{j!} (W_n^{(j)}(t) + (-)^{j+1} T_n^{(j)}(t)) \quad (n \geq 1). \quad (30)$$

The terms $W_n^{(j)}(t)$ may be obtained by a similar recurrence to that given in equation (9)

$$\begin{aligned} W_n^{(j)} &= \sum_{m=1}^{n-j} [\Lambda_m, W_{n-m}^{(j-1)}] \quad (1 \leq j \leq n-1) \\ W_1^{(0)} &= A \quad W_n^{(0)} = 0 \quad (n > 1) \end{aligned} \quad (31)$$

whereas the terms $T_n^{(j)}(t)$ obey the recurrence relation

$$\begin{aligned} T_n^{(j)} &= \sum_{m=1}^{n-j} [\Lambda_m, T_{n-m}^{(j-1)}] \quad (1 \leq j \leq n-1) \\ T_n^{(0)} &= F_n \quad (n > 0). \end{aligned} \quad (32)$$

Every F_n is fixed by the condition $\Lambda_n(t+T) = \Lambda_n(t)$. As a matter of fact, this constraint renders our initial-value problem a boundary-value problem. An outstanding feature is that F_n can be determined independently of $\Lambda_n(t)$ as the solution $Z(t) = P(t) \exp(tF)$ shrinks to $Z(T) = \exp(TF)$. Consequently, the conventional Magnus expansion $Z(t) = \exp(\Omega(t))$ computed at $t = T$ must furnish

$$F_n = \frac{\Omega_n(T)}{T} \quad \forall n \quad (33)$$

which in turn can be obtained from equation (8). The first contributions to the Floquet–Magnus expansion read explicitly

$$\begin{aligned} \Lambda_1(t) &= \int_0^t A(x) dx - tF_1 \\ F_1 &= \frac{1}{T} \int_0^T A(x) dx \\ \Lambda_2(t) &= \frac{1}{2} \int_0^t [A(x) + F_1, \Lambda_1(x)] dx - tF_2 \\ F_2 &= \frac{1}{2T} \int_0^T [A(x) + F_1, \Lambda_1(x)] dx. \end{aligned} \quad (34)$$

5. Convergence of Floquet–Magnus expansion

From the recurrence relations in the preceding section it is possible to obtain a sufficient condition on $K(T)$ such that convergence of the series $\sum \Lambda_n$ is guaranteed in the whole interval $t \in [0, T]$.

We commence by combining equations (11) and (33), which yields

$$\|F_n\| \leq b_n \frac{1}{T} K^n(T). \quad (35)$$

With this bound in mind, we can prove similar inequalities for the terms appearing in Λ_n . They are given in the following.

Lemma. *The following bounds hold:*

- (i) $\|W_n^{(j)}(t)\| \leq h_n^{(j)} K^{n-1}(T)k(t)$;
- (ii) $\|T_n^{(j)}(t)\| \leq g_n^{(j)} \frac{1}{T} K^n(T)$;
- (iii) $\|\Lambda_n(t)\| \leq (b_n + c_n) K^n(T)$

for non-negative coefficients $h_n^{(j)}$, $g_n^{(j)}$ and c_n , which can be recursively determined.

Notice that the above bounds do depend on T , a fact to be considered as a consequence of the boundary condition $P(t) = P(t + T)$.

Proof. By induction on n .

- (i) $\|W_n^{(j)}(t)\| \leq 2 \sum_{m=1}^{n-j} \|\Lambda_m\| \|W_{n-m}^{(j-1)}\| \leq 2 \sum_{m=1}^{n-j} (b_m + c_m) h_{n-m}^{(j-1)} K^{n-1}(T)k(t)$ and thus

$$h_n^{(j)} = 2 \sum_{m=1}^{n-j} (b_m + c_m) h_{n-m}^{(j-1)} \quad (n > 1, 1 \leq j \leq n-1) \quad (36)$$

provided

$$h_1^{(0)} = 1 \quad h_n^{(0)} = 0 \quad (n > 1). \quad (37)$$

- (ii) $\|T_n^{(j)}(t)\| \leq 2 \sum_{m=1}^{n-j} \|\Lambda_m\| \|T_{n-m}^{(j-1)}\| \leq 2 \sum_{m=1}^{n-j} (b_m + c_m) g_{n-m}^{(j-1)} \frac{1}{T} K^n(T)$, so that

$$g_n^{(j)} = 2 \sum_{m=1}^{n-j} (b_m + c_m) g_{n-m}^{(j-1)} \quad (n > 1, 1 \leq j \leq n-1) \quad (38)$$

provided

$$g_n^{(0)} = b_n \quad \forall n. \quad (39)$$

- (iii) The recurrence for Λ_n can be written as

$$\Lambda_n(t) = \int_0^t G_n(\tau) d\tau - t F_n \quad (n \geq 1) \quad (40)$$

where

$$\begin{aligned} G_1(\tau) &= A(\tau) \\ G_n(\tau) &= \sum_{j=1}^{n-1} \frac{B_j}{j!} (W_n^{(j)}(\tau) - (-1)^j T_n^{(j)}(\tau)) \quad (n \geq 2). \end{aligned} \quad (41)$$

Therefore

$$\|\Lambda_n(t)\| \leq \|F_n\| T + \int_0^T \|G_n(\tau)\| d\tau \quad \forall n. \quad (42)$$

For $n \geq 2$,

$$\|\Lambda_n(t)\| \leq b_n K^n(T) + \sum_{j=1}^{n-1} \frac{|B_j|}{j!} (h_n^{(j)} + g_n^{(j)}) K^n(T) \equiv (b_n + c_n) K^n(T) \quad (43)$$

whereas for $n = 1$, $\|\Lambda_1(t)\| \leq 2K(T)$, so that $c_1 = 1$. \square

Then, we have the definition

$$c_n = \sum_{j=1}^{n-1} \frac{|B_j|}{j!} (h_n^{(j)} + g_n^{(j)}) \quad (n > 1) \quad (44)$$

which together with equations (36)–(39) allows the use of the D'Alembert criterion to study the convergence of the series $\sum (b_n + c_n) K^n(t)$. We conclude then that absolute convergence of the Floquet–Magnus series is ensured if

$$K(T) \lim_{n \rightarrow \infty} \frac{b_{n+1} + c_{n+1}}{b_n + c_n} < 1.$$

Numerical study of this condition suggests that $(b_{n+1} + c_{n+1})/(b_n + c_n) \rightarrow 4.778\,97$ as $n \rightarrow \infty$, so the series converges if

$$\int_0^T \|A(t)\| dt \leq K(T) < \xi_F \equiv 0.209\,25. \quad (45)$$

This is then a sufficient condition for the absolute convergence of our procedure. Notice that convergence of the series $\sum F_n$ is already guaranteed by (33) and the discussion in section 4.

6. An illustrative example

Some readers may be not particularly interested in formal technical details but rather in the applicability of the method. Next we sketch a solvable example from quantum mechanics where the infinite expansions, obtained from Floquet–Magnus recurrences, are completely summed. Comparison with the exact solution illustrates the feasibility of the method.

The time evolution of a quantum system, defined by a periodic Hamiltonian $H(t)$, may be described by a unitary operator $U(t)$ satisfying the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} U = H U \quad U(0) = I \quad (46)$$

which is a particular operator realization of equation (1). Next, the case of a periodically driven harmonic oscillator is treated with the present formalism. Computations were carried out programming section 4 recurrences via symbolic languages.

The Hamiltonian for a linearly driven harmonic oscillator is given by (with $\hbar = 1$)

$$H = \frac{1}{2}\omega_0(p^2 + q^2) + f(t)q \quad (47)$$

where q, p are dimensionless coordinate and momentum operators satisfying $[q, p] = i$, $f(t)$ is a real function of time and ω_0 gives the energy level spacing in the absence of the perturbation $f(t)q$. Alternatively

$$H = \omega_0 \left(a^\dagger a + \frac{1}{2} \right) + \frac{f(t)}{\sqrt{2}} (a^\dagger + a) \quad (48)$$

where $a = (q + ip)/\sqrt{2}$, with $[a, a^\dagger] = 1$. As is well known this is an exactly solvable problem, irrespective of the form of $f(t)$. The conventional ME yields the exact solution, by solving first in the interaction picture [20]. It reads

$$U(t) = \exp \left(-\frac{1}{2}i\omega_0 t(p^2 + q^2) \right) \exp \left(-i(q \operatorname{Re} \phi + p \operatorname{Im} \phi) - \frac{1}{2}i\psi \right) \quad (49)$$

$$\phi = \int_0^t dt_1 f(t_1) \exp(i\omega_0 t_1) \quad (50)$$

$$\psi = \int_0^t dt_2 \int_0^{t_2} dt_1 f(t_1) f(t_2) \sin[\omega_0(t_1 - t_2)]. \quad (51)$$

Let us particularize $f(t) = \beta \cos \omega t$. The integrals in equations (50) and (51) can be easily calculated, although the Floquet structure of the solution is not apparent. The remarkable feature of this example is that the infinite Floquet–Magnus expansion may be solved and closed expressions for F and Λ obtained.

Once the recurrences for the Floquet–Magnus expansion in section 4 are explicitly computed for several orders, their general term is guessed by inspection. For the Floquet operator we obtain

$$F = -i \left[\frac{\omega_0}{2} (p^2 + q^2) - \beta \frac{\omega_0}{\omega} \sum_{k=0}^{\infty} \left(\frac{\omega_0}{\omega} \right)^k q + \beta^2 \frac{\omega_0}{4\omega^2} \sum_{k=0}^{\infty} (2k+1) \left(\frac{\omega_0}{\omega} \right)^k \right] \quad (52)$$

and the associated transformation results from

$$\Lambda(t) = i\beta^2 \frac{\omega_0}{\omega^3} \left[\sin(\omega t) \sum_{k=0}^{\infty} (k+1) \left(\frac{\omega_0}{\omega} \right)^k - \frac{\omega t}{2} \sum_{k=0}^{\infty} \left(\frac{\omega_0}{\omega} \right)^k \right] \\ - i [\sin(\omega t) q + \omega_0 (\cos(\omega t) - 1) p] \frac{\beta}{\omega} \sum_{k=0}^{\infty} \left(\frac{\omega_0}{\omega} \right)^k. \quad (53)$$

The resulting series may be summed in closed form and the Floquet operator reads eventually

$$F = -i \frac{\omega_0}{2} \left[\left(q - \frac{\beta}{\omega_0(\rho^2 - 1)} \right)^2 + p^2 \right] - i \frac{\beta^2}{4\omega_0(\rho^2 - 1)} \quad (54)$$

with $\rho \equiv \omega/\omega_0$; its eigenvalues are the so-called *Floquet eigenenergies* [21]

$$E_n = \omega_0 \left(n + \frac{1}{2} \right) + \frac{\beta^2}{4\omega_0(\rho^2 - 1)}. \quad (55)$$

The corresponding Λ transformation is

$$\Lambda(t) = i \frac{\beta/\omega_0}{1 - \rho^2} \left[(\rho \sin \omega t) q + (\cos \omega t - 1) p + \left(\frac{2\rho^2}{1 - \rho^2} + \cos \omega t \right) \frac{\beta \sin \omega t}{4\omega} \right]. \quad (56)$$

Notice that both operators are antihermitian and reproduce the exact solution of the problem, as they should.

7. Conclusions

The matrix initial-value problem $\dot{Z} = A(t)Z$, $Z(0) = I$ we have considered in this paper has, notwithstanding its apparent simplicity, a long history concerning both its mathematical structure and its applications to control the evolution of many and varied physical systems. There are two aspects of the differential equation which have deserved special attention.

The first aspect we want to comment on refers to the geometric structure of the solutions when $A(t)$ belongs to a Lie algebra and we want $Z(t)$ to evolve in the corresponding Lie group. If, as is most often the case, we have to be content with approximate solutions, special care is needed not to spoil that algebraic property. Magnus expansion provides such a guarantee.

The second particular item concerns the case when the coefficient matrix $A(t)$ is periodic in t . Then further information is available on the structure of the solution as is given by the time-honoured Floquet theorem, which ensures the factorization of the solution in a periodic part and a purely exponential factor. This is an existence theorem with no constructive hint and again special procedures have to be followed to keep the prescribed form.

Our main purpose in this paper has been to fuse together the two important aspects of the problem. This has been achieved by properly adapting the recursive analysis of Magnus expansion to the Floquet-dictated structure. Consequently the solution has the required form and evolves in the desired group no matter what the order of truncation. The whole procedure has been given an algorithmic formulation which already allows direct implementation. A

different question, not touched upon here, is the possibility of enhanced performance of the method, which certainly deserves further attention.

The always elusive problem of the convergence of the proposed algorithm has been analysed and a sufficient condition for convergence given. The bound ξ_F in the periodic Floquet case turns out to be smaller than the corresponding bound ξ in the conventional Magnus expansion. At first sight this could be understood as an impoverishment of the result. However it has to be recalled that, due precisely to the Floquet theorem, once the condition is fulfilled in one period convergence is assured for any value of time. In contrast in the general Magnus case the bound always gives a running condition.

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References

- [1] Floquet M G 1883 Sur les équations différentielles linéaires à coefficients périodiques *Ann. École Norm. Sup.* **2** 47–89
- [2] Coddington E A and Levinson N 1955 *Theory of Ordinary Differential Equations* (New York: McGraw-Hill)
- [3] Kittel C 1995 *Introduction to Solid State Physics* (New York: Wiley)
- [4] Ernst R R, Bodenhausen G and Wokaun A 1986 *Principles of NMR in One and Two Dimensions* (Oxford: Clarendon Press)
- [5] Wiesel W E and Pohlen D J 1994 Canonical Floquet theory *Celest. Mech. Dyn. Astron.* **58** 81–96
- [6] Nemytskii V V and Stepanov V V 1989 *Qualitative Theory of Differential Equations* (New York: Dover)
- [7] Yakubovich V A and Starzhinskii V M 1975 *Linear Differential Equations with Periodic Coefficients* (New York: Wiley)
- [8] Levante T O, Baldus M, Meier B H and Ernst R R 1995 Formalized quantum mechanical Floquet theory and its applications to sample spinning in nuclear magnetic resonance *Mol. Phys.* **86** 1195–212
- [9] Magnus W 1954 On the exponential solution of differential equations for a linear operator *Commun. Pure Appl. Math.* **7** 649–73
- [10] Pechukas P and Light J C 1966 On the exponential form of time-displacement operators in quantum mechanics *J. Chem. Phys.* **44** 3897–912
- [11] Oteo J A and Ros J 2000 From time-ordered products to Magnus expansion *J. Math. Phys.* **41** 3268–77 and references therein
- [12] Iserles A and Nørsett S P 1999 On the solution of linear differential equations in Lie groups *Phil. Trans. R. Soc. A* **357** 983–1019
- [13] Blanes S, Casas F and Ros J 2000 Improved high order integrators based on the Magnus expansion *BIT* **40** 434–50
- [14] Klarsfeld S and Oteo J A 1989 Recursive generation of higher-order terms in the Magnus expansion *Phys. Rev. A* **39** 3270–3
- [15] Wilcox R M 1967 Exponential operators and parameter differentiation in quantum physics *J. Math. Phys.* **8** 962–82
- [16] Abramowitz M A and Stegun I A 1965 *Handbook of Mathematical Functions* (New York: Dover)
- [17] Moan P C, Oteo J A and Ros J 1999 On the existence of the exponential solution of linear differential systems *J. Phys. A: Math. Gen.* **32** 5133–9
- [18] Blanes S, Casas F, Oteo J A and Ros J 1998 Magnus and Fer expansions for matrix differential equations: the convergence problem *J. Phys. A: Math. Gen.* **31** 259–68
- [19] Moan P C and Oteo J A 2001 Convergence of the exponential Lie series *J. Math. Phys.* **42** 501–8
- [20] Klarsfeld S and Oteo J A 1989 Analytic properties of the Magnus operator for two solvable Hamiltonians *Phys. Lett. A* **142** 393–7
- [21] Lefebvre R and Palma A 1997 The harmonic Floquet oscillator *J. Mol. Struct. (Theochem)* **390** 23–32