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Lie algebraic approach to Fer's expansion for classical Hamiltonian systems

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Abstract. The so-called Fer's expansion is proposed as a solution for the time-evolution operator of classical time-dependent Hamiltonian systems. The quadratic Hamiltonians treated as examples show that, under very different regimes, the second-order approximation already gives extremely good results.

1. Introduction

The time evolution of a classical Hamiltonian system can be described by a one-parameter group of canonical transformations acting on the initial values of phase space variables. If we adopt this point of view then the purpose of dynamics is to compute the action of this group for a given Hamiltonian. It is accomplished by solving the evolution equation for the operators that carry out the transformation. Such an equation is equivalent to the usual Hamiltonian equations of motion for which a number of approximate methods have been devised over the years. One possible resolution scheme is to seek explicitly time-dependent canonical transformations in terms of infinite products of exponentials of Lie operators. This type of approach has been applied to different topics in the literature [1]. In particular, it has been extensively used to solve beam dynamics in particle accelerators [2]. However, the arguments in these exponentials correspond to a unique power of the expansion parameter (or any equivalent label). Thus, it can actually be considered as an exponential perturbation theory.

In the present study we elaborate an adaptation of the so-called Fer's expansion [3, 4] to classical Hamiltonian systems. Unlike the previously mentioned approach the arguments of the exponentials contain an infinity of orders in the expansion parameter. The interest of Fer's iterative expansion has been emphasized for quantum mechanical time-dependent problems [4]. We shall see that its classical version also gives very good results, even with a few iterations. The analysis is performed by means of Lie transform techniques. The use of Lie operators in the context of classical dynamics already has a long history [5]. These tools enable one to transform Poisson brackets of functions into commutators of operators, and *vice versa*. As a consequence the procedure can benefit from well established results in quantum mechanics.

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In section 2 we set up the notation concerning Lie transforms and derive Fer's expansion for classical systems. In section 3 we apply the method to some physical examples given by quadratic Hamiltonians. Finally, section 4 contains the conclusions.

2. Fer's expansion for classical Hamiltonian systems

Let us consider a phase space Γ of dimension $2N$. Introduce the vector $\boldsymbol{\xi}$ whose $2N$ components are the generalized coordinates and momenta: $(q_1,\ldots,q_N,p_1,\ldots,p_N) = (\xi_1,\ldots,\xi_{2N})$. The set of regular real-valued time-dependent functions on the phase space is an infinite-dimensional Lie algebra under the Poisson bracket composition law which we denote by $\mathcal{O}$. We consider two elements of $\mathcal{O}$ to be equivalent if their difference is a function of time only. Then $\mathcal{O}$ is divided into equivalence classes, $\{C_f,\ f\in\mathcal{O}\}$, which form the quotient set $\hat{\mathcal{O}}$. Now with each element $C_f\in\hat{\mathcal{O}}$ we associate the Lie operator $:f:$ from $\mathcal{O}$ to $\mathcal{O}$ defined by

$$:f:=\sum_{i=1}^{N}\frac{\partial f}{\partial q_i}\frac{\partial}{\partial p_i}-\frac{\partial f}{\partial p_i}\frac{\partial}{\partial q_i}=\sum_{i,j=1}^{2N}\frac{\partial f}{\partial \xi_i}J_{ij}\frac{\partial}{\partial \xi_j}. \tag{2.1}$$

Here we follow the notation of [2]. What we call the Lie operator $:f:$ is also known as the Lie derivative generated by f and denoted by L_f. J is the symplectic $2N\times 2N$ matrix $\left(\begin{smallmatrix}0 & I\\ -I & 0\end{smallmatrix}\right)$. Then, the action of $:f:$ on any function $g\in\mathcal{O}$ is $:f:g=[f,g]$, where the square bracket stands for the Poisson bracket of classical mechanics. It is clear that $:f:$ is independent of the representative element of C_f considered. Besides, the commutator of two Lie operators, $\{:f:,:g:\}$, equals the Lie operator associated with the Poisson bracket of both functions, i.e. $\{:f:,:g:\}=:[f,g]:$.

It is also important to realize that as an operator on $\mathcal{O}$ $:f:$ inherits the linear character of the derivative operators in equation (2.1), $:f:(ag_1+bg_2)=a:f:g_1+b:f:g_2$; but as a new element of $\mathcal{O}$, $(:f:g)$ is in general by no means a linear function on Γ.

Let $H(\boldsymbol{\xi},t)$ be an explicitly time-dependent Hamiltonian and $\mathcal{M}(t,t_0)$ the symplectic map that generates the trajectories $\boldsymbol{\xi}(t)$ in phase space starting from the initial conditions $\boldsymbol{\xi}(t_0)$, namely

$$\boldsymbol{\xi}(t)=\mathcal{M}(t,t_0)\boldsymbol{\xi}(t_0). \tag{2.2}$$

This symplectic map is governed by the evolution equation [6]:

$$\dot{\mathcal{M}}=-\mathcal{M}:H: \qquad \mathcal{M}(t_0,t_0)=\exp:c(t_0):. \tag{2.3}$$

The dot stands for the time derivative. The initial condition guarantees $\mathcal{M}$ to be continuously connected with the identity operator provided c is any function of time, independent of q and p. A formal solution to equation (2.3) may be given in terms of *Dyson's chronological product* but we shall *not* deal with this topic. An alternative method based on the Magnus expansion [7] has been proposed in [8]. There, the solution is written as a single exponential of a unique Lie operator.

When $\{\int_{t_0}^{t}:H(\tau):\,\mathrm{d}\tau,:H(t):\}=0$, then $\mathcal{M}=\exp[-\int_{t_0}^{t}:H(\tau):\,\mathrm{d}\tau]$, and this is clearly the case if H is time-independent. In classical mechanics one can always avoid explicitly time-dependent problems by increasing the number of degrees of freedom by one and appropriately changing the Hamiltonian. However this can complicate the algebraic structure of the problem.

We proceed in another way. Let us suppose that the exponential is a good approximation and that a solution can be written in the form

$$\mathcal{M} = \mathcal{M}_1 \mathrm{e}^{:F_1:} \tag{2.4}$$

where $:F_1: = -\int_{t_0}^{t} :H(\tau): \,\mathrm{d}\tau$ whereas the transformation $\mathcal{M}_1$ describes the difference between the approximation and the exact mapping, with $\mathcal{M}_1(t_0, t_0) = \exp :c(t_0):$. The question is to find the evolution equation satisfied by $\mathcal{M}_1$. Let us substitute equation (2.4) into (2.3). Taking into account [9] that

$$\frac{\partial}{\partial t}\mathrm{e}^{:F_1:} = \int_0^1 \mathrm{e}^{x:F_1:} :\dot{F}_1: \mathrm{e}^{(1-x):F_1:}\,\mathrm{d}x \tag{2.5}$$

we obtain

$$\dot{\mathcal{M}}_1 = -\mathcal{M}_1 :H_1: \tag{2.6}$$

where $:H_1:$, the Lie operator associated with the transformed Hamiltonian H_1, reads

$$:H_1: =: [\mathrm{e}^{F_1}, H]: - \int_0^1 \mathrm{d}x :[\mathrm{e}^{xF_1}, H]:. \tag{2.7}$$

Here $[\mathrm{e}^{F_1}, H]$ stands for the Taylor series of iterated Poisson brackets: $[\mathrm{e}^{F_1}, H] = \sum_{k=0}^{\infty} [F_1^k, H]/k!$, with

$$[F_1^k, H] \equiv \underbrace{[F_1, [F_1, \ldots, [F_1, H] \ldots]]}_{k \text{ times}} \qquad [F_1^0, H] \equiv H. \tag{2.8}$$

The procedure can be repeated with equation (2.6) which gives rise to the following recursive scheme:

$$\begin{aligned}
&\mathcal{M} = \mathcal{M}_n \mathrm{e}^{:F_n:} \ldots \mathrm{e}^{:F_1:} \\
&\dot{\mathcal{M}}_n = -\mathcal{M}_n :H_n: \qquad \mathcal{M}_n(t_0, t_0) = \mathrm{e}^{:c(t_0):} \\
&:F_{n+1}: = -\int_{t_0}^{t} :H_n(\tau): \,\mathrm{d}\tau \qquad :H_0: \equiv :H: \\
&:H_{n+1}: =: [\mathrm{e}^{F_{n+1}}, H_n]: - \int_0^1 \mathrm{d}x :[\mathrm{e}^{xF_{n+1}}, H_n]: = \sum_{k=1}^{\infty} \frac{k}{(k+1)!} :[F_{n+1}^k, H_n]:
\end{aligned} \tag{2.9}$$

this is what we call Fer's expansion for the classical evolution operator.

Suppose that we replace H by ϵH, where ϵ is a small expansion parameter. Then, by virtue of the preceding equations, F_n (with $n \geqslant 1$) contains an infinite number of powers of ϵ beginning with $\epsilon^{2^{n-1}}$, which greatly favours the rate of convergence of the expansion. This fact somehow suggests [10] a connection with techniques for accelerating the convergence of perturbation series in the sense of Kolmogorov–Arnold–Moser which have also been considered from a Lie algebraic point of view [11].

When the functions involved in equation (2.8) (or the corresponding Lie operators) belong to a Poisson subalgebra of $\hat{\mathcal{O}}$ (or a subalgebra under commutation), then the calculation can be carried out with compact expressions. Under these circumstances a finite exponential product of Lie transforms could be attained. In a different context Wei and Norman [12] proved such a solution to exist, at least locally.

For the sake of completeness, we sketch the form of the infinite exponential product expansion quoted in the introduction. As a matter of fact, it can be thought of as a generalization of the Zassenhaus formula [9]. The method has been extensively worked out by Dragt and co-workers [2, 6]. For the type of Hamiltonian we shall study in the next section we do not need the full expansion but just a few terms. It is worthwhile noticing that in this situation the expansion coincides with that of Kumar [13] and a left-running version by Wilcox [9]. If we denote

$$\mathcal{M} = \ldots \mathrm{e}^{:K_2:}\mathrm{e}^{:K_1:} \tag{2.10}$$

then the first terms read

$$:K_1: =: F_1: \qquad :K_2: = \frac{1}{2}\int_{t_0}^{t} :[H(\tau), K_1(\tau)]: \, \mathrm{d}\tau. \tag{2.11}$$

Higher order terms can be found in [4, 9, 13]. As equation (2.11) already shows this expansion is characterized by the fact that K_n is order ϵ^n.

3. Illustrative examples

Hamiltonians defined by quadratic forms are of considerable interest in physics. It turns out that these Hamiltonians are, in general, especially simple to handle. We consider, in particular, the unidimensional parametrically driven harmonic oscillator given by

$$H = \tfrac{1}{2}(p^2 + q^2) + \phi(t)q^2 \tag{3.1}$$

where ϕ is a time function to be specified later. This simple, although not trivial, Hamiltonian will enable us to appreciate the performance of the method. We compute Fer's expansion up to second order and compare the obtained approximate trajectories with the exact numerical results. The scheme provided by equations (2.10) and (2.11) is also examined. The corresponding formulae for the generalized harmonic oscillator, $H(q, p, t) = A(t)p^2 + B(t)qp + C(t)q^2$, are collected in the appendix.

We suppose that at the initial time t_0 the system is in $q(t_0) = q_0$, $p(t_0) = p_0$. According to the formulae in section 2 we get

$$:F_1: = Tp\partial_q - (2\Phi + T)q\partial_p \tag{3.2}$$

where $\Phi = \int_{t_0}^{t} \phi(\tau)\, \mathrm{d}\tau$ and $T = t - t_0$. The Lie operator associated with the transformed Hamiltonian given by equation (2.7) yields

$$:H_1: = \frac{2(\Phi - T\phi)}{\mu^2}[(1 - \mu\sin\mu - \cos\mu)(p\partial_p - q\partial_q) + 2\left(\frac{\sin\mu}{\mu} - \cos\mu\right)((2\Phi + T)q\partial_p + Tp\partial_q)] \tag{3.3}$$

with $\mu = 2\sqrt{(2\Phi + T)T}$. Eventually, we need to know the action on q and p of a general exponential map $\mathcal{E} \equiv \exp[\alpha(p\partial_p - q\partial_q) + \beta q\partial_p + \gamma p\partial_q]$, with α, β and γ functions of time. The argument in the exponential is the most general element that we need since the operators $p\partial_p - q\partial_q$, $q\partial_p$, $p\partial_q$ (or, alternatively, the functions qp, $\frac{1}{2}q^2$, $\frac{1}{2}p^2$) span the SU(1,1) algebra. Then we get the canonical transformation

$$\begin{aligned} \mathcal{E}q &= \left(\cosh\eta - \frac{\alpha}{\eta}\sinh\eta\right) q + \frac{\gamma}{\eta}\sinh(\eta)p \\ \mathcal{E}p &= \left(\cosh\eta + \frac{\alpha}{\eta}\sinh\eta\right) p + \frac{\beta}{\eta}\sinh(\eta)q \end{aligned} \tag{3.4}$$

with $\eta^2 = \alpha^2 + \beta\gamma$.

The approximate trajectories up to second order furnished by

$$\xi_i(t) \simeq \mathrm{e}^{:F_2:}\mathrm{e}^{:F_1:}\xi_i(t_0) \qquad (i = 1,2) \tag{3.5}$$

are explicitly

$$\begin{aligned} q(t) &\simeq (c^- q_0 + s^+ p_0)\cos(\mu/2) + (c^+ p_0 + s^- q_0)\frac{2T}{\mu}\sin(\mu/2) \\ p(t) &\simeq (c^+ p_0 + s^- q_0)\cos(\mu/2) - (c^- q_0 + s^+ p_0)\frac{\mu}{2T}\sin(\mu/2). \end{aligned} \tag{3.6}$$

The following notation has been used

$$c^{\pm} \equiv \cosh\eta \pm \frac{\alpha}{\eta}\sinh\eta \qquad s^+ \equiv \frac{\gamma}{\eta}\sinh\eta \qquad s^- \equiv \frac{\beta}{\eta}\sinh\eta. \tag{3.7}$$

In our case the functions α, β and γ are integrals of the coefficients of the Lie operators appearing in equation (3.3)

$$\begin{aligned} \alpha &= -\int_{t_0}^{t} \frac{2(\Phi - T\phi)}{\mu^2}(1 - \mu\sin\mu - \cos\mu)\,\mathrm{d}t' \\ \beta &= -\int_{t_0}^{t} \frac{\Phi - T\phi}{T}\left(\frac{\sin\mu}{\mu} - \cos\mu\right)\,\mathrm{d}t' \\ \gamma &= -\int_{t_0}^{t} \frac{\Phi - T\phi}{2\Phi + T}\left(\frac{\sin\mu}{\mu} - \cos\mu\right)\,\mathrm{d}t' \end{aligned} \tag{3.8}$$

where $T = t' - t_0$ now.

Next we choose three particular forms of $\phi(t)$ and compare the second-order Fer's approximant with direct numerical integration of the equations of motion, namely $\ddot{q} + (1 + 2\phi)q = 0$; $p = \dot{q}$. In order to make the three perturbations comparable we fix $\phi(0)$ to have the same value in all cases. The results corresponding to equation (2.11) are also reported. The initial conditions are $t_0 = -1$, $q_0 = 1$, $p_0 = 1$, in all examples.

(i) As a first application we take the symmetrical pulse $\phi = (\epsilon/2)\mathrm{sech}(\zeta t)$. Adiabatic regimes correspond to sufficiently small values of ζ, whereas large values of ζ represent sudden perturbations. The parameter ϵ measures the strength of the perturbation. For up to $\epsilon \simeq 1$ our approximate trajectories and the exact numerical results are virtually indistinguishable both for small and large ($\simeq 1$) values of ζ. Although the global agreement is impressive there exists, however, a small time-lag between both the approximate and exact results which can be appreciated only for sufficiently large time intervals. The more sudden (or weak) the perturbation the smaller this time-lag.

The full curve on figure 1 corresponds to second-order Fer's approximation (and the indistinguishable exact trajectory) whereas the broken curve illustrates the alternative factorization of [5, 6, 9, 13], according to equations (2.10) and (2.11). The input values are $\zeta = 1$, $\epsilon = 0.5$ and the time interval considered is $-1 < t < 6$.

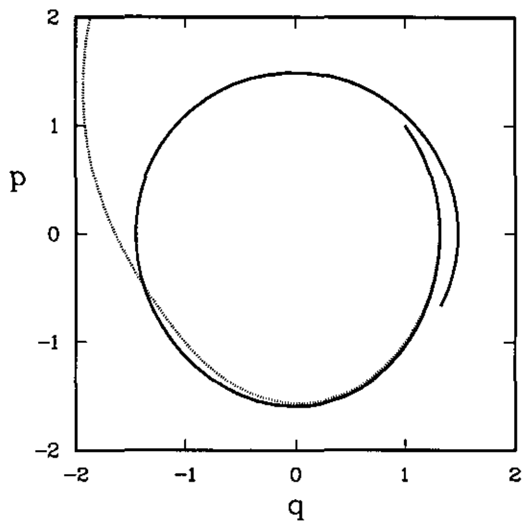

Figure 1. Comparison between the second-order Fer's approximate trajectory (full curve) and the alternative approach of [6] (broken curve) for the first example with $\epsilon = 0.5$, $\zeta = 1$. The plotted time interval is $-1 < t < 6$. The exact numerical result is indistinguishable from Fer's approximant.

(ii) As a second example we choose an asymmetric pulse: $\phi = (\epsilon/2)\exp(-\zeta t)$ for $t \geqslant 0$, and $\phi = 0$ for $t < 0$. Thus, after the perturbation is suddenly switched on we can control its effective duration by means of the parameter ζ. For the sake of illustration we show in figure 2 the exact (full curve) and second-order Fer's approximation (broken curve) trajectories for $-1 < t < 6$, $\epsilon = 0.5$ and $\zeta = 1$. Again, the only observable difference is a small time-lag at the end of the plotted path.

(iii) The third and last case that we analyse here corresponds to the periodic perturbation given by $\phi = (\epsilon/4)(1 + \cos\zeta t)$. Notice that, unlike the previous cases, this perturbation does not exhibit a decreasing tail. The corresponding equation of motion is of the Mathieu type which, as is well known, has been widely applied in many branches of physics and technology. We use this form of ϕ to check the long-time behaviour of Fer's approximate solution. Inputs in figure 3 are: $\epsilon = 0.9, \zeta = 1$ and lines are coded as in figure 2. The plotted time interval is $60 < t < 70$, therefore far away from the initial instant. The trajectories are drawn in a clockwise direction. Albeit the global agreement is worse than in preceding cases we emphasize the important feature that the approximation remains very close to the exact trajectory. If we change to $\epsilon = 0.4$ the results greatly improve as shown in figure 4.

On the other hand, the trajectories provided by secular perturbation theory move

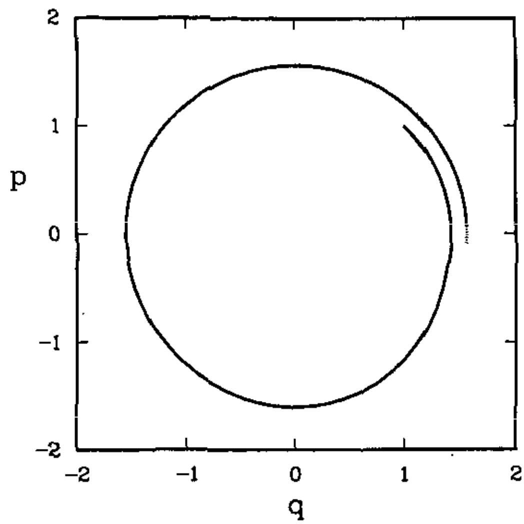

Figure 2. Exact (full curve) and second-order Fer's approximate (broken curve) trajectories for the second example. Input values are $\epsilon = 0.5$, $\zeta = 1$. The plotted time interval is $-1 < t < 6$.

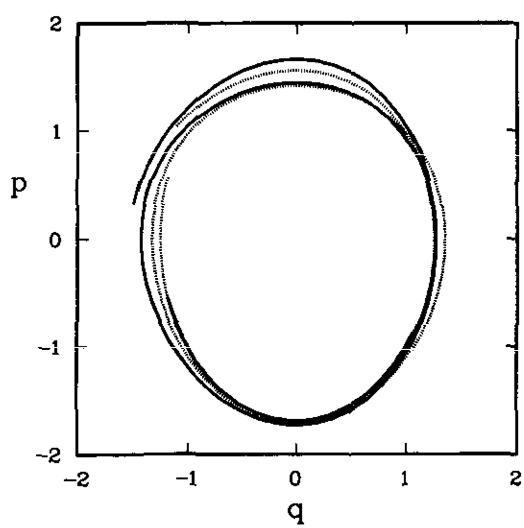

Figure 3. Trajectories corresponding to the periodic perturbation (third example). The exact (full curve) and second-order Fer's approximant (broken curve) are plotted in the interval $60 < t < 70$, with input values $\epsilon = 0.9$, $\zeta = 1$. The trajectories are drawn in a clockwise sense.

rapidly away from the exact solution. So, except for very short times, they are out of range of the figures. For this reason we have not plotted them.

4. Conclusions

We have built up Fer's expansion for the classical evolution operator. This infinite

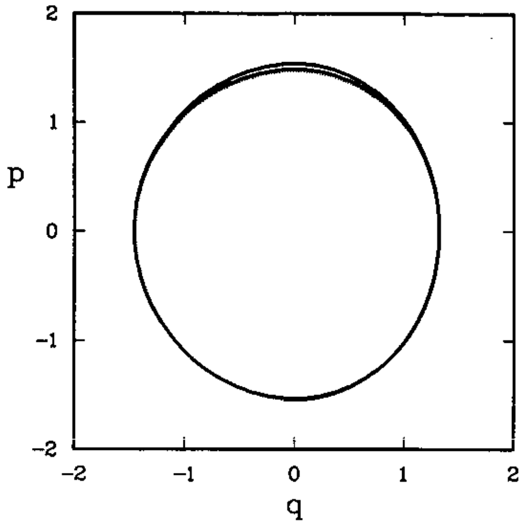

Figure 4. Same as in figure 3 except the input value $\epsilon = 0.4$.

repeated action of exponential Lie transformations seems to provide a very good representation of the time-evolution operator $\mathcal{M}$. The examples worked out clearly indicate that up to second order it gives better results than alternative proposals we know. In particular, compared to usual perturbative treatments this improvement could be associated with the fact that our expansion makes a high-order re-summation of the power series. The computation procedure is iterative.

The various examples have been chosen in order to embrace very different perturbative regimes, even with large coupling constants. The first one describes adiabatic as well as sudden situations, depending on the value of ζ. The second example corresponds to an everlasting decaying pulse suddenly introduced. The third case describes a periodic regime.

Albeit the visual agreement between the exact trajectories and that provided by the second Fer's approximant is very good we insist on the fact that the approximation suffers from a time-lag with respect to the exact solution. Due to the goodness of the fit it is quite difficult to visualize it directly on the plots unless ϵ is large enough. All the same, it constitutes an interesting effect that merits to be kept in mind: The point $(q(t), p(t))$ of an exact trajectory in phase space is amazingly well fitted by computing Fer's approximant at some different instant $t + \delta$, where $\delta = \delta(\epsilon, \zeta, t)$ varies in a smooth and uniform way along the trajectory. The full validity of this observation for Hamiltonians other than quadratic has to be confirmed.

In summary, Fer's expansion constitutes a new recipe to expand $\mathcal{M}$ as a composition of exponential mappings. The results in the examined examples show the fast convergence of the method. As regards multi-dimensional systems ($N > 1$) investigations are being carried out, as well as on some other class of Hamiltonians.

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Appendix

In this appendix we calculate the first and second orders of Fer's expansion for the generalized simple harmonic oscillator, whose Hamiltonian is given by

$$H(q,p,t) = A(t)p^2 + B(t)qp + C(t)q^2 \tag{A1}$$

with $A(t), B(t)$ and $C(t)$ arbitrary time-dependent functions. This system has received considerable attention recently in connection with the geometrical phase factor known in quantum mechanics as Berry's phase [14] and its classical analogue (Hannay's angle [15]).

For the Hamiltonian (A1) we get

$$:F_1: = -\beta(p\partial_p - q\partial_q) - 2\gamma q\partial_p + 2\alpha p\partial_q \tag{A2}$$

where, now,

$$\alpha(t) = \int_{t_0}^{t} A(\tau)\,\mathrm{d}\tau \qquad \beta(t) = \int_{t_0}^{t} B(\tau)\,\mathrm{d}\tau \qquad \gamma(t) = \int_{t_0}^{t} C(\tau)\,\mathrm{d}\tau. \tag{A3}$$

Let us define $\eta^2 \equiv \beta^2 - 4\alpha\gamma$. If we denote

$$\begin{aligned} f_{11}(t) &= \tfrac{1}{2}(\beta^2+\eta^2)A - \alpha\beta B + 2\alpha^2 C & f_{12}(t) &= -\beta A + \alpha B \\ f_{21}(t) &= 2(\beta\gamma A - 2\alpha\gamma B + \alpha\beta C) & f_{22}(t) &= 2(-\gamma A + \alpha C) \\ f_{31}(t) &= 2\gamma^2 A - \beta\gamma B + \tfrac{1}{2}(\beta^2+\eta^2)C & f_{32}(t) &= -\gamma B + \beta C \end{aligned} \tag{A4}$$

and

$$\begin{aligned} h_1(t) &= \frac{1}{\eta^2}\left(f_{21} - \frac{1}{2}f_{22}\right)\cosh 2\eta + \frac{1}{\eta}\left(f_{22} - \frac{1}{2\eta^2}f_{21}\right)\sinh 2\eta + \frac{1}{2\eta^2}f_{22} \\ h_2(t) &= \frac{1}{\eta^2}(2f_{31} - f_{32})\cosh 2\eta + \frac{1}{\eta}\left(2f_{32} - \frac{1}{\eta^2}f_{31}\right)\sinh 2\eta + \frac{1}{\eta^2}f_{32} \\ h_3(t) &= \frac{1}{\eta^2}(f_{12} - 2f_{11})\cosh 2\eta + \frac{1}{\eta}\left(\frac{1}{\eta^2}f_{11} - 2f_{12}\right)\sinh 2\eta - \frac{1}{\eta^2}f_{12} \end{aligned} \tag{A5}$$

then the Lie operator associated with the transformed Hamiltonian H_1 takes the compact form

$$:H_1: = h_1(p\partial_p - q\partial_q) + h_2 q\partial_p + h_3 p\partial_q. \tag{A6}$$

Whence we obtain the second-order Fer's approximant

$$:F_2: = -I_1(p\partial_p - q\partial_q) - I_2 q\partial_p - I_3 p\partial_q \tag{A7}$$

where

$$I_i(t) = \int_{t_0}^{t} h_i(\tau)\,\mathrm{d}\tau. \tag{A8}$$

The approximate trajectories given by equation (3.5) are explicitly

$$\begin{aligned} q(t) &\simeq (-m^+v^+ + u^+n^-)p_0 + (m^+n^+ - u^+v^-)q_0 \\ p(t) &\simeq (m^-n^- + u^-v^+)p_0 - (m^-v^- + u^-n^+)q_0. \end{aligned} \tag{A9}$$

Here we have used the following notation:

$$\begin{aligned} m^{\pm} &= \cosh\eta \pm \frac{\beta}{\eta}\sinh\eta \qquad n^{\pm} = \cosh\sigma \pm \frac{I_1}{\sigma}\sinh\sigma \\ u^+ &= \frac{2\alpha}{\eta}\sinh\eta \qquad v^+ = \frac{I_3}{\sigma}\sinh\sigma \\ u^- &= \frac{2\gamma}{\eta}\sinh\eta \qquad v^- = \frac{I_2}{\sigma}\sinh\sigma. \end{aligned} \tag{A10}$$

with $\sigma^2 \equiv I_1^2 + I_2 I_3$, $(\sigma \neq 0)$. These expressions are not valid when $\eta = 0$. In that case the calculation of the corresponding formulae is straightforward.

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