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Linear time-dependent Hamiltonian systems beyond the adiabatic limit

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Abstract. A classical version of the Magnus expansion well suited to studying adiabatic time-evolution is built up. The method improves the adiabatic approximation while being symplectic in character. It is shown that the first-order approximation is already accurate enough even far from the adiabatic limit. An analysis of the changes suffered by the adiabatic invariant of a linear Hamiltonian system along its time-evolution illustrates part of the above results. Asymptotic formulae for such changes are also obtained with explicit computation of pre-exponential factors.

1. Introduction

Explicitly time-dependent problems present special difficulties in classical mechanics. However, they deserve detailed study because very interesting properties emerge when, even for simple linear systems, some parameters are allowed to vary with time. For instance, particular recent interest has been devoted to systems in which adiabatic evolution originates geometric contributions to the action-angle variables [1–3] or to the motion of spinning neutral particles in inhomogeneous magnetic fields [4], just to quote a few examples.

In this paper we deal with the approximate computation of trajectories in phase space for time-dependent linear one-dimensional Hamiltonians as well as a related observable of physical interest: the adiabatic invariant. We develop a technique especially well suited to treating slow variation of external parameters of the system. The basic idea consists in applying the classical version of the Magnus expansion (ME) [5, 6] using a particular coordinate system. By solving the instantaneous Hamiltonian, a solution in the adiabatic limit is obtained which we will consider as a zero-order approximation. The first-order correction stems properly from the application of the ME and appears to be accurate enough in the intermediate regime, even far away from the adiabatic limit. The results are applied to the generalized harmonic oscillator (GHO) in one degree of freedom. The method may be viewed as a version for classical mechanics of the recently proposed *adiabatic Magnus expansion* [7] for quantum systems.

A particular aspect of the adiabatic evolution of classical systems that has received considerable attention in the literature is the subject of adiabatic invariants. As is well known an adiabatic invariant is exactly conserved only in the adiabatic limit, i.e. under the assumption that the variation of the external parameters during the evolution is infinitely slow. However, the ratio between the proper time of the system (which fixes the timescale) and the characteristic time of variation of parameters has actually a finite value. Consequently the adiabatic invariant does generally vary because the variation of the parameters takes place in a finite time-lapse. The way in which these changes occur

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has been the subject of many works over the years [8–11]. We shall show how our ME can help in computing this observable.

The method we propose furnishes the final results in terms of quadratures and, provided they converge, can be used either for finite or infinite time-intervals. If we are interested only in the later case then the integrations can be approximated by asymptotic methods, leading, in general, to analytical results. In this paper we carry out the application of asymptotic methods to such quadratures. Besides, we also employ an alternative method based on the usual asymptotic analysis of the differential equations of motion. As a sequel, we obtain a new improved formula to describe asymptotic changes in the adiabatic invariant which, incidentally, has a component with geometrical character. The so-called pre-exponential factors are also explicitly obtained. We note in passing the interest recently raised up about the computation of such prefactors in the context of quantum mechanics [12, 13].

The paper organizes as follows. In section 2 we introduce the *adiabatic classical Magnus expansion* (henceforth referred to as ACME), define the adiabatic approximation and find the first-order correction to the adiabatic trajectories. Notation and concepts concerning the adiabatic invariant are given in section 3. It also includes ACME corrections to the computation of the variation of this observable up to first order. In section 4 an asymptotic evaluation of such first-order result is given, as well as an alternative treatment based on the asymptotic analysis of the differential equations of motion. Section 5 contains a number of illustrative examples allowing a comparison between various approximate results and the exact numerical solutions. Our conclusions are contained in section 6.

2. The ACME

Let us characterize the state of a Hamiltonian dynamical system by the $2N$-dimensional vector $\xi = (q, p)$ whose components are the generalized coordinates and momenta and let $H(\xi, t)$ be the corresponding Hamiltonian function. The trajectories in phase space can be viewed as the result of a time-dependent transformation acting on initial values,

$$\xi(\tau) = \mathcal{M}(\tau, \tau_0, \xi(\tau_0)) \,. \tag{1}$$

We have introduced the new variable $\tau = \epsilon t$, where $1/\epsilon$ is the timescale. The equations of motion for ξ can be formally expressed as an evolution equation for the symplectic map $\mathcal{M}$, namely

$$\frac{\mathrm{d}\mathcal{M}}{\mathrm{d}\tau} = \frac{1}{\epsilon}\mathcal{M}L_{-H} \tag{2}$$

where L_{-H} is the Lie operator associated to the function $-H(\xi(\tau_0), t)$. This (in general nonlinear) evolution operator $\mathcal{M}$ is the starting point in some formulations of classical mechanics based on Lie series [14].

What identifies a linear system is the fact that the map $\mathcal{M}$ can be represented by a $2N \times 2N$ matrix $\mathbf{M}$. The time evolution is then governed by the differential equation

$$\dot{\mathbf{M}} = \frac{1}{\epsilon}\mathbf{S}\mathbf{M} \qquad \mathbf{M}(\tau_0, \tau_0) = \mathbf{I} \,. \tag{3}$$

where $\mathbf{S}$ is a matrix obtained from Hamilton equations, I is the $2N \times 2N$ identity matrix and the dot stands for derivative with respect to τ. For linear systems the above equation is equivalent to (2). It is worthwhile noting that an explicit time-dependence in the Hamiltonian can always be dropped out by increasing the number of degrees of freedom. However, the dynamics expressed in this $2(N+1)$-dimensional phase space becomes nonlinear in general.

Magnus expansion in the standard form [5] proceeds to find a solution to (3) of the form $\mathbf{M}(\tau, \tau_0) = \exp \Omega(\tau, \tau_0)$ with $\Omega(\tau_0, \tau_0) = 0$. In the general case, the time-evolution map reads $\mathcal{M} = \exp L_\Omega$, in terms of the Lie operator L_Ω associated with the Magnus observable Ω. We have employed the same notation (Ω) for both situations. Yet in the first case Ω is a matrix whose matrix elements are functions of τ but not of the phase-space coordinates ξ and in the second one it stands for an observable, i.e. a function defined in phase space: $\Omega = \Omega(\xi, \tau)$ Both, Ω and L_Ω satisfy their own differential equation which is solved in the form of series: $\Omega = \sum \Omega_i$. The first two terms in that expansion read

$$\Omega_1(\tau, \tau_0) = \frac{1}{\epsilon} \int_{\tau_0}^{\tau} \mathrm{d}x\, \mathbf{S}(x) \qquad \Omega_2(\tau, \tau_0) = \frac{1}{2\epsilon^2} \int_{\tau_0}^{\tau} \mathrm{d}x \int_{\tau_0}^{x} \mathrm{d}y\, [\mathbf{S}(x), \mathbf{S}(y)]\,. \tag{4}$$

Square brackets stand for the usual commutator: $[A, B] = AB - BA$. Similar equations hold for the general case where the corresponding Lie operators replace matrices. Higher-order terms are given in form of multiple commutators and can be computed by recursive procedures [15]. Notice the important fact that the symplectic character in $\mathbf{M}$ is always kept no matter the number of terms retained in the series for Ω. It is a salient feature of the exponential representation for $\mathbf{M}$.

Direct application of the ME in (3) turns out to be very appropriate when H presents sudden time dependence. As a matter of fact, in the sudden limit the ME to first-order furnishes the exact solution. The situation is different for the adiabatic regime and henceforth we focus our attention on this aspect of the time-evolution.

Let us consider a non-singular time-dependent transformation $\xi_R(\tau) = \mathbf{R}^{-1}\xi(\tau)$ which brings the state of the system $(q(\tau), p(\tau))$ into new variables $(q_R(\tau), p_R(\tau))$. If $\mathbf{M}(\tau, \tau_0)$ governs the evolution of $\xi(\tau)$ then the evolution of the system in terms of the new variables is given by $\mathbf{M}_R(\tau, \tau_0) = \mathbf{R}^{-1}(\tau)\mathbf{M}(\tau, \tau_0)\mathbf{R}(\tau_0)$, so that

$$\xi_R(\tau) = \mathbf{M}_R(\tau, \tau_0)\xi_R(\tau_0)\,. \tag{5}$$

It is straightforward to verify that $\mathbf{M}_R$ obeys the equation

$$\dot{\mathbf{M}}_R = \mathbf{S}_R\mathbf{M}_R \qquad \mathbf{M}_R(\tau_0, \tau_0) = I \tag{6}$$

with

$$\mathbf{S}_R = \frac{1}{\epsilon}\mathbf{R}^{-1}\mathbf{S}\mathbf{R} - \mathbf{R}^{-1}\dot{\mathbf{R}}. \tag{7}$$

It is clear that an appropriate choice of $\mathbf{R}$ may render dynamics very much simpler than it was in the original coordinate system. Obviously, no systematic procedure exists to find such a transformation. But as far as we are interested in the adiabatic regime an obvious point of reference is the time-independent case. Then great simplification occurs if $\mathbf{S}$ is rendered diagonal. This suggests to take in the adiabatic regime $\mathbf{R}$ so as to instantaneously diagonalize the matrix $\mathbf{S}(\tau)$. The diagonal piece $\Delta \equiv (1/\epsilon)\mathbf{R}^{-1}\mathbf{S}\mathbf{R} - \mathrm{diag}(\mathbf{R}^{-1}\dot{\mathbf{R}})$ in (7) should then be much more important than the remainder term of $\mathbf{R}^{-1}\dot{\mathbf{R}}$. Mathematically, the above assertion, valid when the eigenvalues of $\mathbf{S}$ are purely imaginary, is based on the Riemman–Lebesgue lemma [7]. This procedure leads to interesting approximation schemes [16, 17].

It is worth noticing that the piece $\mathbf{R}^{-1}\dot{\mathbf{R}}$ in (7) has a pure geometrical origin for it depends just on the coordinate transformation $\mathbf{R}$ and not on the slowness parameter ϵ.

The diagonal piece Δ can be readily integrated by making the factorization

$$\mathbf{M}_R = \exp\left(\int_{\tau_0}^{\tau} \mathrm{d}x\, \Delta(x)\right)\mathbf{M}'_R\,. \tag{8}$$

Thus $\mathbf{M}'_R$ satisfies

$$\dot{\mathbf{M}}'_R = \mathbf{S}'_R \mathbf{M}'_R \qquad \mathbf{S}'_R = \exp\left(-\int_{\tau_0}^{\tau} \mathrm{d}x \Delta(x)\right)(\mathbf{S}_R - \Delta)\exp\left(\int_{\tau_0}^{\tau} \mathrm{d}x \Delta(x)\right). \tag{9}$$

Now, the simplest approximation one can do is $\mathbf{M}'_R = \mathbf{I}$, then

$$\mathbf{M}_R \simeq \exp \int_{\tau_0}^{\tau} \mathrm{d}x \Delta(x). \tag{10}$$

This is the well known adiabatic approximation (AA) which is exact in the limiting case of vanishing ϵ. Notice that the above map keeps the symplectic character of the approximate time-evolution.

The AA can be improved by taking into account the effects of non-diagonal terms, namely looking for more complete approximate solutions to (9). It is at this point that we introduce the ACME. As said above, in linear cases we have $\mathbf{M}'_R = \exp \Omega$, where $\Omega = \Omega_1 + \Omega_2 \ldots$. Explicitly,

$$\Omega_1 = \int_{\tau_0}^{\tau} \mathrm{d}x \mathbf{S}'_R(x). \tag{11}$$

Let us illustrate with the one-dimensional GHO the behaviour of phase-space approximate trajectories. The GHO Hamiltonian reads

$$H(q, p, \tau) = \tfrac{1}{2}[X(\tau)q^2 + 2Y(\tau)qp + Z(\tau)p^2]. \tag{12}$$

In the particular case when X, Y, Z are constant the orbits are ellipses for $XZ > Y^2$ and hyperbolae for $XZ < Y^2$. The special situation $XZ = Y^2$ corresponds to a bifurcation in parameter space and orbits are straight lines. Departures from the above behaviour appearing when a time-dependence occurs will be analysed with the ACME. In the following we shall assume that $X(\tau)$, $Y(\tau)$, $Z(\tau)$ are regular enough functions for all the following expressions to have a meaning. Futhermore, we take $X(\tau)Z(\tau) > Y^2(\tau)$ for all real τ although formal results can also be attained in the opposite case.

The matrix $\mathbf{S}$ now reads

$$\mathbf{S} = \begin{pmatrix} Y & Z \\ -X & -Y \end{pmatrix} \tag{13}$$

and can be diagonalized whenever $XZ \neq Y^2$ (i.e. provided no instantaneous bifurcation occurs) by the matrix

$$\mathbf{R}(\tau) = \mathbf{R}^{-1}(\tau) = \frac{1}{\sqrt{2\lambda(Y+\lambda)}} \begin{pmatrix} Y+\lambda & Z \\ -X & -Y-\lambda \end{pmatrix} \tag{14}$$

where $\lambda = \pm\sqrt{Y^2 - XZ}$ are the instantaneous eigenvalues of $\mathbf{S}(\tau)$. Hereafter we put $\lambda \equiv \mathrm{i}\omega$. It is straightforward to verify that

$$\mathbf{S}_R = \begin{pmatrix} \gamma(Z\dot{X} - X\dot{Z})/2 + \mathrm{i}\omega/\epsilon & \alpha \\ \beta & -\gamma(Z\dot{X} - X\dot{Z})/2 - \mathrm{i}\omega/\epsilon \end{pmatrix} \tag{15}$$

where we have defined the functions

$$\begin{aligned} \alpha &= \gamma[(i\dot{\omega} + \dot{Y})Z - (\mathrm{i}\omega + Y)\dot{Z}] \\ \beta &= \gamma[(i\dot{\omega} + \dot{Y})X - (\mathrm{i}\omega + Y)\dot{X}] \\ \gamma &= [2i\omega(\mathrm{i}\omega + Y)]^{-1}. \end{aligned} \tag{16}$$

Eventually we get

$$\mathbf{S}'_R = \begin{pmatrix} 0 & \alpha \mathrm{e}^{-2a} \\ \beta \mathrm{e}^{+2a} & 0 \end{pmatrix} \tag{17}$$

with

$$a(\tau,\tau_0)=\frac{1}{2}\log\frac{k(\tau_0)}{k(\tau)}+\mathrm{i}\int_{\tau_0}^{\tau}\mathrm{d}x\,\omega'(x) \tag{18}$$

$$\omega'(\tau)=\frac{\omega}{\epsilon}+\frac{Y\dot{Z}-Z\dot{Y}}{2\omega Z}\qquad k(\tau)=\left[\frac{(\omega-\mathrm{i}Y)X}{(\omega+\mathrm{i}Y)Z}\right]^{1/2} \tag{19}$$

so that $\mathbf{M}_R(\tau,\tau_0)=\exp\begin{pmatrix}a&0\\0&-a\end{pmatrix}\mathbf{M}'_R$. Now, since $\mathbf{M}'_R$ satisfies the evolution equation (9) we use the ME to approximate its solution

$$\mathbf{M}'_R\simeq\exp\Omega_1\qquad\Omega_1=\int_{\tau_0}^{\tau}\mathrm{d}x\mathbf{S}'_R(x)\,. \tag{20}$$

After straightforward calculation we obtain the following approximate expression for $\mathbf{M}_R$:

$$\mathbf{M}_R(\tau,\tau_0)\simeq\cosh\eta\begin{pmatrix}\mathrm{e}^{+a}&0\\0&\mathrm{e}^{-a}\end{pmatrix}+\frac{\sinh\eta}{\eta}\begin{pmatrix}0&h_1(\tau)\mathrm{e}^{+a}\\h_2(\tau)\mathrm{e}^{-a}&0\end{pmatrix} \tag{21}$$

where

$$h_1(\tau)=\int_{\tau_0}^{\tau}\mathrm{d}x\,\alpha(x)\,\mathrm{e}^{-2a(x,\tau_0)}\qquad h_2(\tau)=\int_{\tau_0}^{\tau}\mathrm{d}x\,\beta(x)\,\mathrm{e}^{+2a(x,\tau_0)}\qquad\eta^2=h_1(\tau)h_2(\tau)\,. \tag{22}$$

Notice that the AA is recovered from (21) taking formally the limit $\eta\to 0$, which in turn corresponds to $h_i\to 0$ $(i=1,2)$. The reason why h_1, h_2 tend to zero in the adiabatic limit stems from the oscillatory character of the integrand in (22).

Let us take a specific form of X, Y, Z in order to check the behaviour of the above trajectories in phase space. For the sake of simplicity we particularize the Hamiltonian in (12) to

$$X=1+\xi\,\mathrm{sech}(\tau)\qquad Y=0\qquad Z=1\,. \tag{23}$$

The corresponding H is then asymptotically ($\tau\to\pm\infty$) a simple harmonic oscillator of unit frequency. The parameter ξ controls the intensity of the perturbation. We shall study the modifications introduced by a time-dependence whose characteristic timescale is given by $T=1/\epsilon$. Our goal is to compare the trajectories in phase space obtained with the first-order ACME and those obtained by exact numerical integration as well as in the AA, for different values of the parameters.

As a first case we take $T=10$, $\xi=0.9$. We note in passing that the intensity of the *perturbation* is 90% of the non-perturbed problem. In figure 1 we have plotted the exact trajectories (full curve), the AA (dash-dotted curve) and the first-order ACME trajectories (dashed curve). In the time interval represented by $(-1<t<10)$ the three lines match each other. A comparison between the characteristic time T and the natural period of the non-perturbed system indicates that the case at hand is *a priori* only a moderately adiabatic situation. Even so, the AA is already a good approximation and therefore the ACME correction is not properly necessary. Yet it is a first verification of our scheme.

Figure 2 is similar to figure 1 except that now $T=1$. This situation is far from adiabaticity. Consequently, the AA should fail. It is what we observe in figure 2. Instead, the first order ACME fits pretty well the exact trajectory. The same trend holds even for higher values of T^{-1} although, as could be expected, the agreement progressively worsens.

These are representative examples of results we obtain by means of the ACME. This method to approximate the solution of time-dependent problems allows one to improve the AA in the sense that the results computed are good not only in the adiabatic regime but for intermediate situations too.

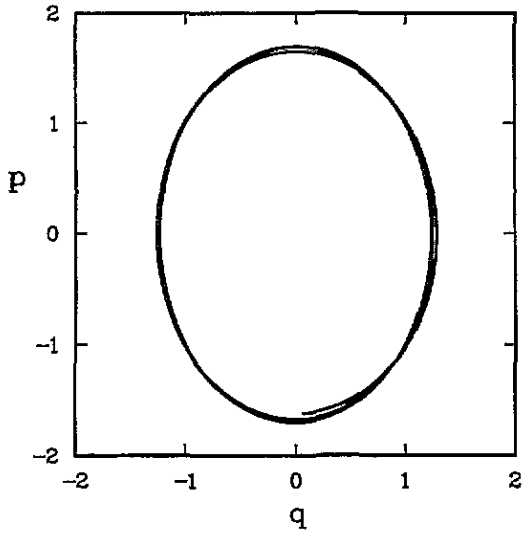

Figure 1. Trajectories in phase space for the GHO given in (23). Here $T = 10, \xi = 0.9$. The exact result (full curve), first order of ACME (dotted curve) and the adiabatic approximation (dash-dotted curve) are almost on the same track in the present case.

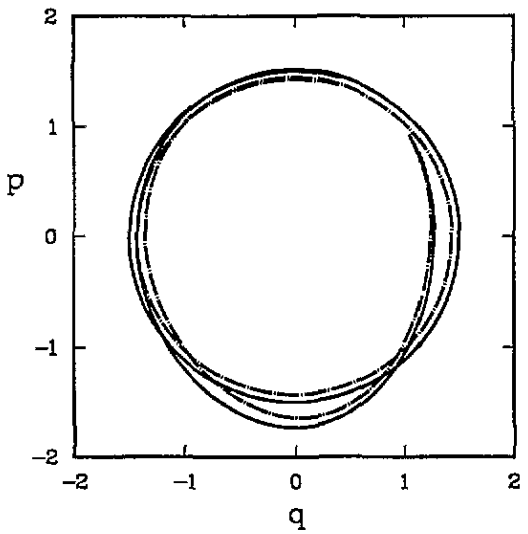

Figure 2. Same as in figure 1 except $T = 1$.

3. Adiabatic invariant

In the following sections we will focus our attention on the accuracy of the conservation of the adiabatic invariant for the GHO. This is a subject extensively treated in the literature. Since the papers by Lewis [18] and Symon [19] we know how to compute an exact invariant by solving a certain nonlinear differential equation. However, analytical results are rare and therefore no information about the properties of the adiabatic invariant can be easily extracted. Direct analytical computations of the adiabatic invariant are possible just for

very few models. Hence, accurate analytical approximations will, certainly, be welcome. Our programme is then the following. First of all, we shall fit the ACME to perform such calculations for arbitrary time intervals. Then we shall discuss an asymptotic approach. Finally, we shall study the problem under the perspective of exponential asymptotic analysis of ordinary differential equations [20–26], i.e. without resorting to the ACME, in order to compare results.

Suppose given (12), the GHO Hamiltonian with one degree of freedom depending on the parameters X, Y, Z which vary slowly so that they tend sufficiently fast to definite limits as $\tau \equiv \epsilon t \to \pm\infty$. Then there exist the limit values $J(+\infty)$ and $J(-\infty)$ of the adiabatic invariant $J(\tau) \equiv H(\tau)/\omega(\tau)$, and we can speak about the increment of J

$$\Delta J = J(+\infty) - J(-\infty) \tag{24}$$

over the infinite time interval $]-\infty, +\infty[$. For instance, for the simple linear oscillator

$$\ddot{x} = -\omega^2(\epsilon t)x \qquad \omega(\pm\infty) = \omega_\pm \tag{25}$$

with analytic frequency $\omega(\epsilon t) > \text{const} > 0$, this increment is an exponentially small quantity in $1/\epsilon$ [27]. Furthermore, it is possible to compute explicitly the leading term in the asymptotic expansion of ΔJ when $\epsilon \to 0$ [11, 20, 24, 25]. Similar results have been obtained for linear systems with several degrees of freedom [23]. If the function $\omega(\epsilon t) \in C^\infty(-\infty, +\infty)$ then the asymptotic expansion for ΔJ is [9]

$$\Delta J = O(\epsilon^n) \qquad \text{for every } n$$

and thus in the limit $\epsilon \to 0$ this change decays faster than any power of ϵ.

Consider a finite time interval instead of an infinite one. Now we introduce $\delta J(\tau, \tau_0) = J(\tau) - J(\tau_0)$. We do know that the adiabatic invariant changes very little after a time of order $1/\epsilon$. We can pose the question about how much the instantaneous action variable changes after a time interval much longer than $1/\epsilon$. In the following we envisage giving a quantitative answer.

The instantaneous value $J(\tau)$ of the adiabatic invariant (or action variable) for the GHO is simply

$$J(\tau) = -\mathrm{i}p_R(\tau)q_R(\tau)\,. \tag{26}$$

Let us denote by m_{ij} $(i, j = 1, 2)$ the τ-dependent matrix elements of M'_R. Then, from (5), (8) and (26), it is clear that the exact expression for δJ is given by

$$\begin{aligned}\delta J(\tau, \tau_0) = -\mathrm{i}\big[&m_{11}(\tau)m_{21}(\tau)q_R^2(\tau_0) + m_{22}(\tau)m_{12}(\tau)p_R^2(\tau_0) \\ &+ (m_{11}(\tau)m_{22}(\tau) + m_{12}(\tau)m_{21}(\tau) - 1)q_R(\tau_0)p_R(\tau_0)\big]\,.\end{aligned} \tag{27}$$

For later usage we point out explicitly that according to (9) and (17) m_{ij} satisfy

$$\begin{aligned}&\dot{m}_{11} - \alpha\mathrm{e}^{-2a}m_{21} = 0 \qquad \dot{m}_{21} - \beta\mathrm{e}^{+2a}m_{11} = 0 \\ &\dot{m}_{22} - \beta\mathrm{e}^{+2a}m_{12} = 0 \qquad \dot{m}_{12} - \alpha\mathrm{e}^{-2a}m_{22} = 0\,.\end{aligned} \tag{28}$$

These equations are the starting point for studying non-adiabatic effects in the GHO without resorting to the Magnus expansion.

In view of (27) any method which improves the AA ($m_{11} = m_{22} = 1, m_{12} = m_{21} = 0$), leads in general to non-vanishing δJ. If we use (20) to compute approximately the functions $m_{ij}(\tau)$ $(i, j = 1, 2)$, we obtain the first-order ACME correction to the adiabatic invariant

$$\delta J(\tau, \tau_0) \simeq -\mathrm{i}\left\{\frac{\sinh 2\eta}{2\eta}\big[h_2(\tau)q_R^2(\tau_0) + h_1(\tau)p_R^2(\tau_0)\big] + 2(\sinh\eta(\tau))^2 q_R(\tau_0)p_R(\tau_0)\right\} \tag{29}$$

where h_1, h_2, η were already defined in (22). This is our new expression for the increment of the adiabatic invariant δJ along the interval $[\tau_0, \tau]$ in terms of quadratures, and it constitutes a valid approximation only if the integrals in (22) converge. In principle this scheme to compute δJ can be iterated: one can evaluate higher orders in the Magnus expansion of $\mathbf{M}'_R$ and subsequently obtain corresponding expressions for δJ. The accuracy of such a procedure rests on the convergence properties of the Magnus expansion, about which very little is known.

4. Asymptotic analysis of ΔJ

Often an asymptotic determination ($\epsilon \to 0$) of the quadratures in (22) is possible. If we are interested in infinite time-intervals, the leading contribution to integrals may sometimes be computed. Our purpose here is to study the behaviour of (29) under the above hypothesis.

For simplicity we consider the simple time-dependent harmonic oscillator, obtained from the GHO with parameters $X = \omega^2(\tau)$, $Y = 0$, $Z = 1$. In this case, equation (29) leads to

$$\Delta J \simeq \frac{\sinh 2|\mathcal{K}|}{2|\mathcal{K}|}\left[\omega_- \mathcal{K}^* q_R^2(-\infty) - \frac{1}{\omega_-}\mathcal{K} p_R^2(-\infty)\right] - 2\mathrm{i} q_R(-\infty) p_R(-\infty)\sinh^2|\mathcal{K}| \tag{30}$$

where ω_- was defined in (25) and

$$\mathcal{K} \equiv \int_{-\infty}^{+\infty} \mathrm{d}\tau \frac{\dot{\omega}(\tau)}{2\omega(\tau)} \exp\left[-\frac{2\mathrm{i}}{\epsilon}\Theta(\tau)\right] \qquad \Theta(\tau) = \int_0^\tau \omega(\tau_1)\mathrm{d}\tau_1 \tag{31}$$

i.e. first-order ACME gives ΔJ in terms of only one integral. Equation (31) has already been studied in the literature in connection with the above barrier one-dimensional scattering problem [28]. So here we will merely adopt the appropriate hypothesis for the frequency and subsequently will apply those results.

For complex τ the equation $\zeta = \Theta(\tau)$ defines a mapping from the τ-plane into the plane of the complex variable ζ. This transformation takes the integral $\mathcal{K}$ of (31) into

$$\mathcal{K} = \int_{-\infty}^{+\infty} \mathrm{e}^{-2\mathrm{i}\zeta/\epsilon}\, \chi(\zeta)\, \mathrm{d}\zeta \tag{32}$$

where

$$\chi(\zeta) = \frac{1}{2\omega}\frac{\mathrm{d}\omega}{\mathrm{d}\zeta} = \frac{1}{2\omega^2}\frac{\mathrm{d}\omega}{\mathrm{d}\tau}. \tag{33}$$

Now we assume [24] that $\omega(\tau)$ is analytic on a neighborhood $\mathcal{N}$ of the real τ-axis. A fundamental role in the asymptotic analysis is played by the set U of roots, isolated singular points and branch points (collectively called transition points) of such a type that

$$\omega(\tau) = \omega_0(\tau - \tau_c)^{\nu/2}\left[1 + \sum_{j=1}^{\infty}\omega_j(\tau - \tau_c)^j\right] \qquad \nu \in \mathcal{R} \quad \omega_0 \neq 0 \tag{34}$$

holds true in the vicinity of τ_c. Assuming that U has no limit point, $0 < \mathrm{glb}_U|\mathrm{Im}\,\zeta| = m$ and that no other boundary point of $\mathcal{N}$ has $|\mathrm{Im}\,\zeta| = m$, we can shift the path of integration of the Fourier integral (32) to the line $\mathrm{Im}\,\zeta = -m$. This line contains a finite number of transition points and $\nu > -2$ at each, because points with $\nu < -2$ in (34) are excluded from the domain of $\Theta(\tau)$.

For the simplest case of a root τ_c an analysis of the structure of $\chi(\zeta)$ near $\zeta_c = \Theta(\tau_c)$ and some additional hypothesis on its behaviour on the Stokes line $\mathrm{Im}\,\zeta = \mathrm{Im}\,\zeta_c = -m$, along which integration takes place, leads to [24, 25]

$$\mathcal{K} \sim -\mathrm{i}\frac{\nu\pi}{\nu+2}\mathrm{e}^{-2m/\epsilon}\exp\left(-\frac{2\mathrm{i}}{\epsilon}\mathrm{Re}\,\zeta_c\right) + \mathrm{o}(\mathrm{e}^{-2m/\epsilon}) \tag{35}$$

as $\epsilon \to 0$. Substitution of (35) into (30) immediately reveals the exponentially small character of ΔJ:

$$\Delta J \simeq \frac{\mathrm{i}\pi\nu}{\nu+2}\mathrm{e}^{-2m/\epsilon}\left[\omega_-\varphi q_R^2(-\infty) + \omega_-^{-1}\varphi^* p_R^2(-\infty)\right] + \mathrm{o}(\mathrm{e}^{-2m/\epsilon}) \tag{36}$$

where $\varphi \equiv \exp((2\mathrm{i}/\epsilon)\mathrm{Re}\,\zeta_c)$.

In the case of several transition points $\zeta_1, \zeta_2, \ldots, \zeta_k$ with $\mathrm{Im}\,\zeta_k = -m$, each transition point makes a separate, additive contribution to $\mathcal{K}$ given by (35), with the corresponding value of ν characterizing the particular point provided that $|\zeta_{l+1} - \zeta_l| \gg \epsilon$ [26].

The above result coincides with that obtained in first-order asymptotic perturbation theory, showing, at least partially, the consistency of the method. We expect that the performance of the present exponential perturbation theory holds beyond the extreme case $\epsilon \to 0$, unlike asymptotic perturbation theory.

Alternatively, more elaborated methods to compute ΔJ in the limit $\epsilon \to 0$ are available [24–26]. They proceed directly from the ordinary differential equations satisfied by m_{ij}, (28). Unlike the ACME, they work only for infinite time-intervals, and systematic improvement of their results is not possible at first. Here we present one of them in order to compare results in section 5 for some examples.

Assuming that $m_{11} = m_{22} = 1$; $m_{12}, m_{21} \ll 1$ in $\mathbf{M}'_R$, the first-order non-adiabatic corrections are obtained. Thus, we only need to look for the asymptotic form of m_{12} and m_{21} when $\tau \to +\infty$ to compute the asymptotic behaviour of ΔJ.

Standard asymptotic analysis for ordinary differential equations and the assumptions that X, Y, Z can be analytically continued into the complex τ–plane and that there exists a transition point τ_c of the type (34) for $\omega'(\tau)$ lead directly to [3, 20, 26]

$$\Delta J \simeq 2\mathrm{i}\cos\left(\frac{\pi}{2\pm\nu}\right)\mathrm{e}^{-2|\mathrm{Im}\,\zeta_c|}\left[k_-\mathrm{e}^{2\mathrm{i}\mathrm{Re}\,\zeta_c}q_R^2(-\infty) + k_-^{-1}\mathrm{e}^{-2\mathrm{i}\mathrm{Re}\,\zeta_c}p_R^2(-\infty)\right] + \mathrm{o}(\mathrm{e}^{-2|\mathrm{Im}\,\zeta_c|}) \tag{37}$$

where now $\zeta_c = \int_0^{\tau_c}\omega'(\tau)\mathrm{d}\tau$, $k_- = k(-\infty)$ and ω' is given in (19). The plus, minus signs correspond to the cases $\omega' = \omega/\epsilon$ (i.e. the simple harmonic oscillator), $\omega' \neq \omega/\epsilon$, respectively. According to the analysis by Meyer [24], in the first one we can take $\nu > -2$, whereas in the general case $-2 < \nu < 2$.

This asymptotic expression for ΔJ has the same structure as the one obtained previously in the literature [3, 11, 20–25] for the simple linear oscillator. However, as already noted elsewhere [3], for the GHO ζ includes a *geometric contribution* (i.e. explicitly independent on ϵ) besides the known dynamical one (which does depend explicitly on the time–scale). This feature is evident in the 'amplitude' factor ($\exp[-2|\mathrm{Im}\,\zeta_c|]$) as well as in the 'pre-exponential' factor.

5. Illustrative examples

In the present section we deal with three specific examples. They have been chosen in order to embrace very different behaviours of the frequency ω and our aim is to appreciate the performance of the Magnus method. We compute the change in the adiabatic invariant ΔJ

(a) by numerical integration of the equation of motion and (b) by applying the first-order ACME, (29). For one of the examples we include asymptotic results too.

In all cases we analyse an infinite time-interval but for computational reasons we must take finite values τ_+, τ_- as the limits in the integrals of (22). For the same reason, τ_- and τ_+ will be our initial and final times, respectively, when solving numerically the equations of motion. Numerical results show that for these examples the final value of $|\Delta J|$ does not depend on the particular election of τ_+, τ_- provided their absolute values are large enough.

The two first examples concern the GHO. The last one shows first-order ACME computations for the simple time-dependent harmonic oscillator.

Example 1

As a first application we choose the following definition for the parameters of the GHO:

$$\begin{aligned} X(\tau) &= \sqrt{a^2 + \frac{1}{\cosh\tau}} + \frac{b}{\cosh\tau} \\ Y(\tau) &= \sqrt{c^2 - \frac{b^2}{\cosh^2\tau}} \\ Z(\tau) &= \sqrt{a^2 + \frac{1}{\cosh\tau}} - \frac{b}{\cosh\tau} \end{aligned} \tag{38}$$

where a, b, c are constants such that $a \neq 0$, $a > c$. The frequency is given by

$$\omega(\tau) = \sqrt{a^2 - c^2 + \frac{1}{\cosh\tau}} \tag{39}$$

whence $\omega(\tau) > 0$ for all real τ and $\omega \to \omega_\pm = \sqrt{a^2 - c^2} > 0$ as $\tau \to \pm\infty$.

The function $\omega^2(\tau)$ is analytic in a strip along the real τ-axis. Its poles are located at $\tau_p = \mathrm{i}(2n+1)\pi/2$, $n = 0, \pm 1, \ldots$ and $\omega(\tau_c) = 0$ at points τ_c such that

$$\cosh\tau_c = \phi \equiv \frac{-1}{a^2 - c^2}. \tag{40}$$

We can distinguish two cases:

- if $|\phi| > 1$ then $\tau_c = \log(|\phi| \pm \sqrt{\phi^2 - 1}) + \mathrm{i}(2n+1)\pi$
- if $|\phi| \leqslant 1$ then $\tau_c = \begin{cases} \mathrm{i}(\beta_1 + 2n\pi) \\ \mathrm{i}(\beta_2 + 2n\pi) \end{cases}$ with $\cos\beta_l = -|\phi|$, $\sin\beta_1 = -\sin\beta_2 = \sqrt{1-\phi^2}$.

The full curves in figures 3 and 4 correspond to the exact numerically evaluated function $|\Delta J| = |\Delta J|(\epsilon)$ whereas the dotted curves illustrate the first-order adiabatic Magnus approximation to this function. Inputs in figure 3 are $a = 3$, $b = 0.1$, $c = 2$ ($|\phi| < 1$) and in figure 4 $a = 3$, $b = 0.1$, $c = 2.97$ ($|\phi| > 1$), so they are illustative of the two cases just quoted and show how the ϕ value affects the shape of the curves.

In figure 3 our approximate $|\Delta J|$ obtained with the ACME and the exact numerical result are virtually indistinguishable even for large values of ϵ. On the other hand, albeit the global agreement in figure 4 is worse than in the preceeding one, it is important to notice that the approximation remains very close to the exact result for all values of ϵ and not only in a neighbourhood of $\epsilon = 0$.

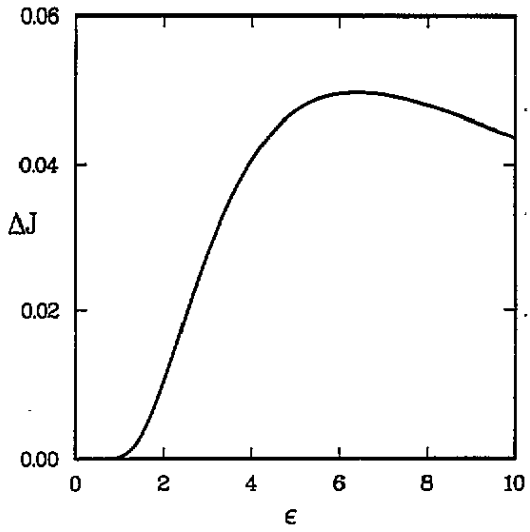

Figure 3. Change in the adiabatic invariant versus the slowness parameter ϵ for the GHO in example 1. Input values are $a = 3$, $b = 0.1$, $c = 2$. The full curve stands for the exact result. The dotted curve corresponds to the first order of ACME. In the present case both curves appear on the same track.

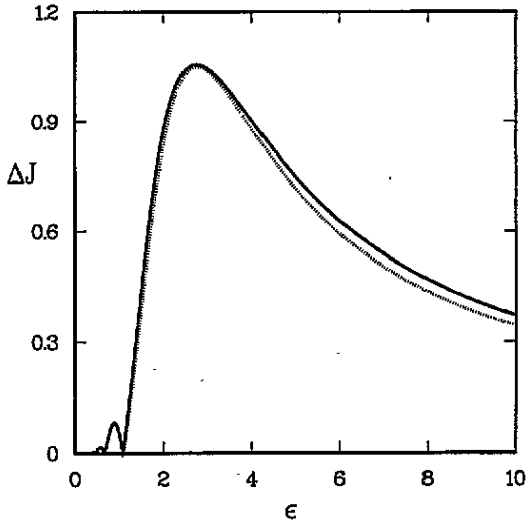

Figure 4. Same as in figure 1 except $c = 2.97$.

Example 2

The second example that we analyse is the GHO with parameters

$$X(\tau) = a + \frac{b}{\cosh \tau}$$
$$Y(\tau) = \sqrt{c^2 - \frac{b^2}{\cosh^2 \tau}} \tag{41}$$

$$Z(\tau) = a - \frac{b}{\cosh \tau}$$

where, again, a, b, c are constants such that $a \neq 0$, $a > c$. In this case $\omega = \sqrt{a^2 - c^2} = \text{const} > 0$ for all real or complex τ, i.e. no transition points exist at any value of τ. Results concerning this situation are illustrated in figures 5 and 6, where lines are coded as in figure 3. Input values in figure 5 are $a = 3$, $b = 0.1$, $c = 2$, whereas in figure 6 $a = 3$, $b = 0.1$, $c = 2.97$. Now there is no visible difference between both exact results and the approximate $|\Delta J|$ obtained with the ACME. It can be shown that the two values of $|\Delta J|$ agree up to the fourth decimal digit, irrespective of the ϵ considered.

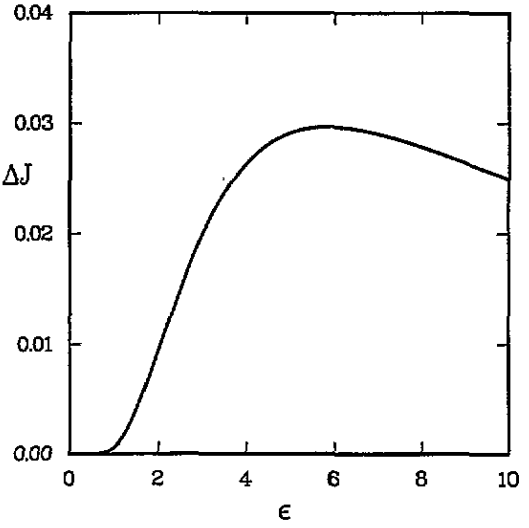

Figure 5. Change in the adiabatic invariant versus the slowness parameter ϵ for the GHO in example 2. Input values are the same as in figure 3. Curves are coded as in figure 3.

At this point some comments are in order. First, as figures 3 and 4 show, $|\Delta J| = |\Delta J|(\epsilon)$ does not obey an exponential law in $1/\epsilon$ for all plotted values of ϵ, so that expressions (36) and (37) for ΔJ must be understood as asymptotic results and only valid in the limit $\epsilon \to 0$. Secondly, this is not the case for (29) obtained *via* ACME since, as previous figures show, it gives very accurate results for ΔJ in a wide range of values of the parameter ϵ, and thirdly, even when the frequency ω is constant the change in the adiabatic invariant is different from zero in the GHO. This peculiarity is described very accurately by first-order ACME.

Example 3

Next we take a simple harmonic oscillator whose frequency is given by

$$\omega(\tau) = \left[1 + \frac{1}{1 + 2e^{-\tau}}\right]^{1/2}. \tag{42}$$

It was analysed by Wasow [25]. Clearly, $\omega(\tau) > 0$ for all real τ and its limits at infinity are $\omega_- = 1$, $\omega_+ = \sqrt{2}$. For complex τ one finds that ω^2 is meromorphic with simple zeros at $\tau_c = i(2n + 1)\pi$ and simple poles at $\tau_p = \log 2 + i(2n + 1)\pi$ with $n \in \mathbb{Z}$.

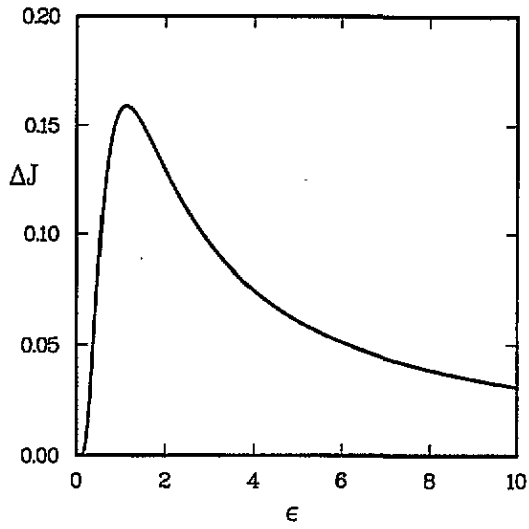

Figure 6. Same as in figure 5 except $c = 2.97$.

Then a straightforward calculation yields

$$\Theta(\tau_c) = \int_0^{\tau_c} \omega(\tau)\mathrm{d}\tau = \sqrt{2}\log\frac{\sqrt{6}-2}{\sqrt{6}+2} - \log\frac{2-\sqrt{3}}{2+\sqrt{3}} + \mathrm{i}(2n+1)\pi \qquad (43)$$

and one concludes that $\tau_c = -\mathrm{i}\pi$ is the transition point that satisfies all the properties enumerated in the sequel of (34). For this point $\nu = 1$ and $\mathrm{Im}\,\zeta_c = \mathrm{Im}\,\Theta(\tau_c) = -\pi$. We obtain as $\epsilon \to 0$

$$|\Delta J| \simeq P\,\mathrm{e}^{-2\pi/\epsilon} + \mathrm{o}(\mathrm{e}^{-2\pi/\epsilon}) \qquad (44)$$

where

$$P \equiv \rho\left|\varphi q_R^2(-\infty) + \varphi^* p_R^2(-\infty)\right| . \qquad (45)$$

The constant $\rho = \pi/3$ or 1 depending on whether (36) or (37) is used.

In figure 7 we show the 'prefactor' $\mathrm{e}^{2\pi/\epsilon}|\Delta J|$ as a function of ϵ. The full curve stands for the exact numerical computation. The dotted line represents our first order ACME (29). One can see the extremely good agreement between these two procedures. For the sake of comparison we have also plotted the asymptotic result P given by (equation 45) with both values of ρ. Initial conditions are $q_R(-\infty) = 1$, $p_R(-\infty) = 0$ in all cases.

6. Conclusions

We have constructed an adiabatic method based on the Magnus expansion which works as a symplectic integrator for the time evolution. The method is well adapted to linear time-dependent systems and its utility has been illustrated by calculating trajectories in phase space as well as changes in the adiabatic invariant. The different illustrative examples we have worked out tell us that the trajectories in phase space and the adiabatic invariant are pretty well fitted by ACME.

Here we have computed only the first-order ME albeit higher orders are, in principle, recursively calculable. Even so, we would enhance the impressive agreement reached between the exact numerical and approximate results shown in different figures where the

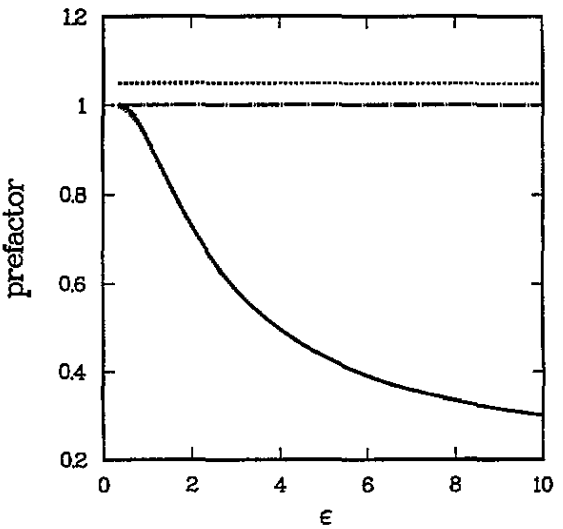

Figure 7. 'Prefactor' $e^{2\pi/\epsilon}|\Delta J|$ versus the slowness parameter ϵ for the simple harmonic oscillator in example 3. The full curve stands for the exact numerical result. The dotted line (almost coincident with the full curve) corresponds to first order of the ACME exactly computed (*cf equation (30)*). *Dashed and dash-dotted lines stand for (44) with* $\rho = \pi/3$ *and* $\rho = 1$, respectively.

range over which the slowness parameter runs is by no means small. If it is, the ACME may still work in intermediate regimes and not merely in the adiabatic one. Due to the difficulty in finding out analytical methods valid outside the adiabatic and sudden limits this feature constitutes by itself a novelty.

We think that the ACME for linear systems is henceforth well established and the degree of performance attained encourages extending the algorithm to nonlinear systems.

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