NON-ADIABATIC ASPECTS OF TIME-DEPENDENT HAMILTONIAN SYSTEMS

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1. INTRODUCTION

Extreme adiabatic behavior furnishes great simplification in the treatment of linear time-dependent Hamiltonian systems. But the actual time variation of the parameters is only finitely, rather than infinitely, slow. Then one is forced to consider corrections to the adiabatic limit.

In this contribution a practical algorithm for that purpose is proposed. It is based on the Magnus expansion for the classical evolution operator (Magnus, 1954; Oteo and Ros, 1991). In our approach this expansion is carried out after an appropriate coordinate transformation is implemented in order to make it useful in the adiabatic regime. The first order of the resulting expansion is then applied to the evaluation of the change of the so called adiabatic invariant.

2. THE ADIABATIC CLASSICAL MAGNUS EXPANSION

Let us consider a Hamiltonian dynamical system with one degree of freedom and let the two-dimensional vector $\vec{\xi} = (q,p)$ represents its state. Trajectories in phase space can be viewed as the action of the time-dependent evolution operator acting on the initial state: $\vec{\xi}(\tau) = \mathcal{M}(\tau,\tau_0,\vec{\xi}(\tau_0))$. Here we have introduced the new variable $\tau = \epsilon t$, where $1/\epsilon$ sets the time scale and $\epsilon \rightarrow 0$ in the adiabatic limit.

In this formalism a linear system is characterized by the fact that the map $\mathcal{M}$ can be represented by a 2×2 matrix M which satisfies the differential equation

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

where S is a 2×2 matrix obtained from the Hamiltonian, I is the identity matrix and the dot stands for derivative with respect to τ.

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Magnus expansion (ME) in the standard form (Magnus, 1954) gives a solution to Eq.(1) of the form $M(\tau,\tau_0) = \exp\Omega(\tau,\tau_0)$ with $\Omega(\tau_0,\tau_0) = 0$. Here Ω is a matrix whose matrix elements are functions of τ and τ_0 but not of the phase space coordinates $\vec{\xi}$. It satisfies its own differential equation which is solved in the form of a series: $\Omega = \sum \Omega_i$. The first term in that expansion is $\Omega_1(\tau,\tau_0) = \frac{1}{\epsilon}\int_{\tau_0}^{\tau} dx S(x)$. Higher order terms can be computed by recursive procedures.

Direct ME as a symplectic integrator for Eq.(1) has been shown (Oteo and Ros, 1991) to work particularly well when H presents sudden time dependence. The situation is different for the adiabatic regime we are now interested in. Here we propose to use still the same scheme but only after some phase space coordinate transformation has been carried out. In the new coordinates the dynamics is exactly solved in the adiabatic limit giving the Adiabatic Approximation (AA). Further corrections which take into account the finite rate at which H varies with time are then obtained via ME.

To see how this procedure works, let us perform a nonsingular time-dependent transformation $\vec{\xi}_R(\tau) = R^{-1}\vec{\xi}(\tau)$. The time evolution of the new coordinates will be governed by

$$\vec{\xi}_R(\tau) = M_R(\tau,\tau_0)\vec{\xi}_R(\tau_0). \tag{2}$$

Here $M_R(\tau,\tau_0) = R^{-1}(\tau)M(\tau,\tau_0)R(\tau_0)$ obeys the equation

$$\dot{M}_R = S_R M_R, \qquad M_R(\tau_0,\tau_0) = I, \tag{3}$$

with

$$S_R = \frac{1}{\epsilon}R^{-1}SR - R^{-1}\dot{R}. \tag{4}$$

We take in the adiabatic regime R so as to instantaneously diagonalize the matrix $S(\tau)$. The diagonal of S_R should then be the dominant term. As we are going to see this procedure leads to an interesting approximation scheme.

The diagonal part $\Delta \equiv \mathrm{diag}(S_R)$ can be easily integrated out by making the factorization

$$M_R = \exp\left(\int_{\tau_0}^{\tau} dx\Delta(x)\right) M_R'. \tag{5}$$

Thus M_R' satisfies

$$\dot{M}_R' = S_R' M_R', \quad S_R' = \exp\left(-\int_{\tau_0}^{\tau} dx\Delta(x)\right)(S_R - \Delta)\exp\left(\int_{\tau_0}^{\tau} dx\Delta(x)\right). \tag{6}$$

The AA amounts to take the simplest approximation $M_R' = I$. In order to improve this zero order step we apply ME to Eq.(6) introducing what we call Adiabatic Classical Magnus Expansion (hereafter referred to as ACME). Then $M_R' = \exp\Omega$, with $\Omega = \Omega_1 + \Omega_2 + \ldots$ In first order

$$\Omega_1 = \int_{\tau_0}^{\tau} dx S_R'(x). \tag{7}$$

As they will be needed in the next section we collect some explicit formulae for the case of the Generalized Harmonic Oscillator (GHO) with Hamiltonian

$$H(q,p,\tau) = \frac{1}{2}[X(\tau)q^2 + 2Y(\tau)qp + Z(\tau)p^2]. \tag{8}$$

The time-dependent functions X, Y, Z will supposed to be gentle (i.e., $C^\infty(-\infty,+\infty)$

with $L^1(-\infty,+\infty)$-derivatives of any order (Wasow, 1973)), and have finite limits as $\tau \to \pm\infty$. In the following we shall assume $X(\tau)Z(\tau) > Y^2(\tau)$ for real τ although formal results can also be obtained in the opposite case. We define $\omega(\tau) = \sqrt{XZ - Y^2}$.

A long but otherwise straightforward calculation allows one to write the matrix M_R to first order in the form:

$$M_R(\tau,\tau_0) = \cosh\eta \begin{pmatrix} e^{+a} & 0 \\ 0 & e^{-a} \end{pmatrix} + \frac{\sinh\eta}{\eta} \begin{pmatrix} 0 & h_1(\tau)e^{+a} \\ h_2(\tau)e^{-a} & 0 \end{pmatrix}. \tag{9}$$

where:

$$\begin{aligned} \eta^2 &= h_1(\tau)h_2(\tau), \\ h_1(\tau) &= \int_{\tau_0}^{\tau} dx\alpha(x)e^{-2a(x,\tau_0)}, \\ h_2(\tau) &= \int_{\tau_0}^{\tau} dx\beta(x)e^{+2a(x,\tau_0)}, \end{aligned} \tag{10}$$

with $\alpha = \gamma[(i\dot{\omega}+\dot{Y})Z-(i\omega+Y)\dot{Z}]$, $\beta = \gamma[(i\dot{\omega}+\dot{Y})X-(i\omega+Y)\dot{X}]$, $\gamma = [2i\omega(i\omega+Y)]^{-1}$, $k(\tau) = [(\omega - iY)X/(\omega + iY)Z]^{1/2}$ and

$$a(\tau,\tau_0) = \frac{1}{2}\log\frac{k(\tau_0)}{k(\tau)} + i\int_{\tau_0}^{\tau} dx \left(\frac{\omega}{\epsilon} + \frac{Y\dot{Z} - Z\dot{Y}}{2\omega Z}\right). \tag{11}$$

This scheme can be proved (Casas et al., 1993) to significantly improve the AA for computing trajectories pretty far from the adiabatic regime. Here, instead, we turn to the analysis of the adiabatic invariant.

3. ADIABATIC INVARIANT AND ITS VARIATION IN THE ACME APPROACH

Under the previous hypothesis for the parameters X, Y, Z of the GHO the action $J(\tau)$ is an adiabatic invariant, i.e. it is constant in the limit $\epsilon \to 0$. Its instantaneous value is $J(\tau) \equiv H(\tau)/\omega(\tau) = -ip_R(\tau)q_R(\tau)$. Furthermore there exist the limit values $J(+\infty)$ and $J(-\infty)$ so that we can define $\Delta J = J(+\infty) - J(-\infty)$ (Arnold et al., 1988). The asymptotic behavior of ΔJ has been profoundly studied over the years (Lenard, 1959; Keller and Mu, 1991). We can consider a finite time interval instead of an infinite one and introduce $\delta J(\tau,\tau_0) = J(\tau) - J(\tau_0)$. We do know that J changes very little over a period of order $1/\epsilon$ and pose the question of how much does it change during a much longer interval. We give here a quantitative answer in the scheme described in the previous section.

Let $m_{ij}(i,j = 1,2)$ be the τ-dependent matrix elements of M'_R. Then the exact expression for δJ is given by

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

We see from this expression that in the AA $m_{11} = m_{22} = 1, m_{12} = m_{21} = 0$ and correspondingly $\delta J = 0$, while any method which goes beyond the AA leads in general to nonvanishing values for δJ.

We want to study this question from the ACME we have just introduced . The previously given formulae allows one to write down the first order approximation for $\delta J(\tau,\tau_0)$, namely

$$\delta J(\tau,\tau_0) = -i\left\{\frac{\sinh 2\eta}{2\eta}\left[h_2(\tau)q_R^2(\tau_0)+h_1(\tau)p_R^2(\tau_0)\right]+2(\sinh\eta(\tau))^2 q_R(\tau_0)p_R(\tau_0)\right\}. \tag{13}$$

This expression is a valid approximation provided the integrals involved are convergent. In that case we can either solve them numerically or, in some cases, apply techniques from asymptotic analysis to extract the leading term in their asymptotic expansions.

An important aspect of our scheme worth emphasizing is its possibility to be iterated by evaluating higher order terms in the Magnus expansion for M_R' and the corresponding expressions for δJ. Of course, to rigorously proceed in this way would require a study of the convergence of the algorithm. This remains an open problem for the standard Magnus expansion. Nevertheless, in spite of that, the procedure has been heuristically used in different contexts in Physics and Chemistry.

When an asymptotic determination of the integrals is possible the ACME reproduces the exponentially small character of ΔJ as $\epsilon \to 0$ when $\omega(\tau)$ is an analytic function of τ. This has been discussed in (Casas et al., 1993) where other asymptotic analysis of ΔJ are also carried out.

4. EXAMPLES

To illustrate what has been said so far we present now the comparison between two ways of computing ΔJ: on the one side we do it by numerical integration of the equation of motion, on the other side we apply our first order formula from ACME given in Eq.(13). We treat three different examples. Two of them refer to the GHO while the other concerns the simple time-dependent harmonic oscillator. We think that the time variation of the parameters considered cover a wide spectrum of behavior. For computational reasons we have to take finite values $\tau_\pm$ as the limits in the 'infinite' time interval. But provided their absolute values are large enough ΔJ does not depend of the particular values chosen.

ACME for the Generalized Harmonic Oscillator

We treat a GHO with parameters given by:

$$\begin{aligned} X(\tau) &= \sqrt{a^2+\frac{s}{\cosh\tau}}+\frac{b}{\cosh\tau}, \\ Y(\tau) &= \sqrt{c^2-\frac{b^2}{\cosh^2\tau}}, \\ Z(\tau) &= \sqrt{a^2+\frac{s}{\cosh\tau}}-\frac{b}{\cosh\tau}, \end{aligned} \tag{14}$$

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

$$\omega(\tau) = \sqrt{a^2-c^2+\frac{s}{\cosh\tau}}. \tag{15}$$

The parameter s serves to distinguish the two cases we are considering: $s = 1$ and $s = 0$.

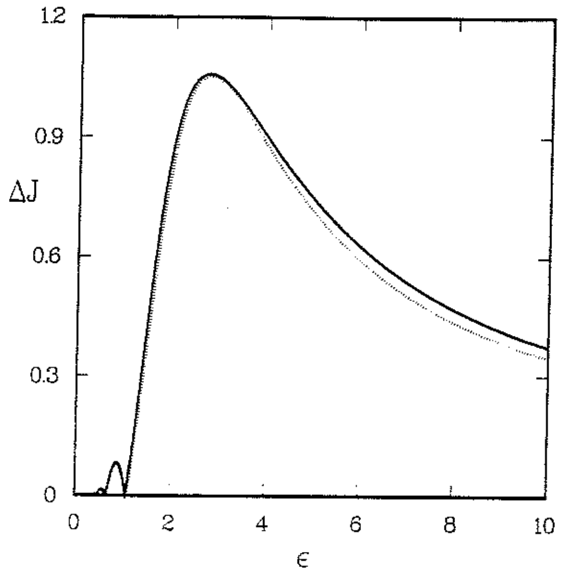

Figure 1. Change in the adiabatic invariant for the example Eq.(14) with $s = 1, a = 3, b = 0.1, c = 2.97$. Solid line corresponds to the exact value and dotted line to first-order ACME.

The asymptotic analysis depends strongly of the transition points of the function $\omega(\tau)$ i.e. of its roots, isolated singular points and branch points.

i) For $s = 1$, $\omega(\tau) > 0$ for 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 being located at $\tau_p = i(2n+1)\pi/2$, $n = 0, \pm 1, \ldots$. As for its zeros τ_c, if we introduce $\rho = 1/(c^2 - a^2)$, we can distinguish two cases:

- $|\rho| > 1$ then $\tau_c = \log\left(|\rho| \pm \sqrt{\rho^2 - 1}\right) + i(2n+1)\pi$
- $|\rho| \leq 1$ then $\tau_c = \begin{cases} i(\beta_1 + 2n\pi) \\ i(\beta_2 + 2n\pi) \end{cases}$

with $\cos\beta_i = -|\rho|$, $\sin\beta_1 = -\sin\beta_2 = \sqrt{1-\rho^2}$.

Numerical results for this example show that our first order adiabatic Magnus expansion reproduces extremely well the exact behaviour for $|\rho| < 1$. For $|\rho| > 1$ on the average $|\Delta J|$ takes higher values and the agreement worsens, but not dramatically. This can be seen in Figure 1, which corresponds to initial state $(q_R, p_R) = (1, 0)$ and parameters $(a, b, c) \doteq (3, 0.1, 2.97)$. Solid line represents exact values while dotted line (where visible) corresponds to our first order ACME. Furthermore we want to emphasize the fact that our corrections go clearly beyond the exponential asymptotic limit. This is seen by observing the non-exponential character of ΔJ over the whole range of ϵ explored. To the best of our knowledge this is a novel result.

ii) For $s = 0$ the frequency given by Eq.(15) is a constant $\omega = \sqrt{a^2 - c^2} > 0$ on the entire complex τ-plane and so no transition points exist. We have explored a wide range of values for the parameters a, b, c, ϵ and in all cases the exact value and the first order Magnus approximation for ΔJ agree up to the fourth decimal place. An interesting fact to observe here is that notwithstanding the constancy of $\omega(\tau)$, $\Delta J \neq 0$. Methods based on the analysis of singularities in the complex plane cannot cope with this situation. On the contrary, our ACME correction very accurately reproduces the exact behavior.

Asymptotic ACME and the Simple Harmonic Oscillator

Let us consider a simple harmonic oscillator ($X = \omega^2, Y = 0, Z = 1$) in Eq.(8)) with frequency

$$\omega(\tau) = \left[1 + \frac{1}{1 + 2e^{-\tau}}\right]^{1/2}, \tag{16}$$

which was analyzed by Wasow (Wasow, 1974). Now $\omega(\tau) > 0$ for real τ and its limits at $\pm\infty$ are $\omega_- = 1$, $\omega_+ = \sqrt{2}$. ω^2 is a meromorphic function with simple zeroes at $\tau_c = i(2n+1)\pi$ and simple poles at $\tau_p = \log 2 + i(2n+1)\pi$.

Now Eq.(13) simplifies to give

$$\Delta J = \frac{\sinh 2|K|}{2|K|}\left[\omega_- K^* q_R^2(-\infty) - \frac{1}{\omega_-}K p_R^2(-\infty)\right] - 2iq_R(-\infty)p_R(-\infty)\sinh^2|K|, \tag{17}$$

where

$$K \equiv \int_{-\infty}^{+\infty} d\tau \frac{\dot\omega(\tau)}{2\omega(\tau)} \exp\left[-\frac{2i}{\epsilon}\Theta(\tau)\right], \quad \Theta(\tau) = \int_{-\infty}^{\tau} \omega(x)dx. \tag{18}$$

Following the asymptotic analysis of the equation of motion by Wasow (1974) and Meyer (1975) we obtain (Casas et al., 1993) that as $\epsilon \to 0$

$$\Delta J \sim \frac{\pi}{6} e^{-2\pi/\epsilon}\left[\varphi p_R^2(-\infty) - \varphi^* q_R^2(-\infty)\right] + O\left(e^{-4\pi/\epsilon}\right). \tag{19}$$

Here φ is given in terms of $\Theta(\tau_c = -i\pi)$. We see from this equation that first order adiabatic Magnus expansion gives correctly the exponentially small character of ΔJ in the limit $\epsilon \to 0$ as well as an approximation to the much more elusive pre-exponential factor.

In Figure 2 we show the function $|\Delta J|(\epsilon)$ calculated a) by numerical integration of the equation of motion (solid line), b) from the Eq.(19) (broken line) and c) by application of ACME, Eq.(17) (dotted line). We take as initial conditions $q_R(-\infty) = 1, p_R(-\infty) = 0$. We conclude that for the values of the parameter ϵ considered the exact and ACME results practically coincide.

5. CONCLUSIONS

A previously proposed scheme for integrating the equations of motion for time-dependent linear Hamiltonian systems has been adapted to work in the adiabatic regime. It is based on the Magnus expansion and as such originates a practical algorithm which can be used as a symplectic integrator to determine the trajectories. Because it is recursive in nature it could be systematically improved by going to higher orders. The first order we have explicitly considered furnishes already extremely good results even far away of the strict adiabatic limit. Nevertheless higher order contributions should be studied to see if these results are confirmed. The scheme has been also applied to the analysis of the adiabatic invariant. As it is well known this magnitude is not strictly speaking a constant and the proposed form of the Magnus expansion reproduces the exponentially small behaviour of its variation. Besides that, however, our scheme gives a way to approximately evaluate ΔJ. We illustrate this point different time-dependences of the parameters of a one-dimensional Generalized Harmonic Oscillator.

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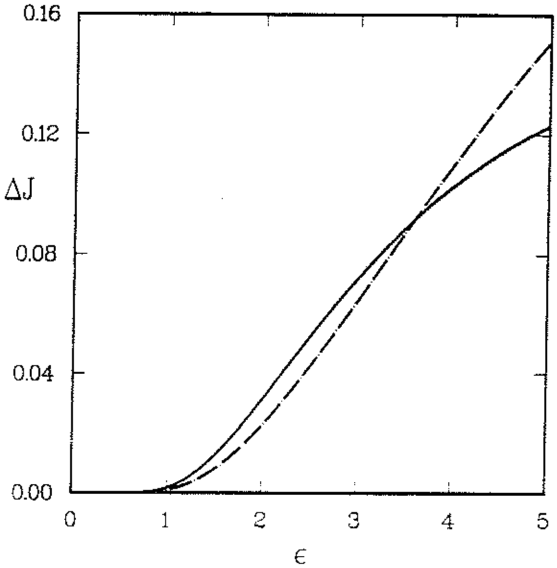

Figure 2. Change in the adiabatic invariant for the simple harmonic oscillator with frequency Eq.(16). Solid line correspond to an exact calculation, broken line to application of Eq.(19) and dotted line to ACME.

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