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Geometric factors in the adiabatic evolution of classical systems

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The adiabatic evolution of the classical time-dependent generalized harmonic oscillator in one dimension is analyzed in detail. In particular, we define the adiabatic approximation, obtain a new derivation of Hannay's angle requiring no averaging principle and point out the existence of a geometric factor accompanying changes in the adiabatic invariant.

The theory of adiabatic evolution in classical mechanics has received considerable attention through the years [1–7], mainly in connection with the subject of adiabatic invariants. Formal results have met in linear time-dependent Hamiltonian systems an especially well suited frame to assess their domain of validity [1,2]. More recently, increasing attention to these systems has been motivated by the discovery of the geometric contribution to the adiabatic evolution of angle variables [8,9].

In this Letter we study the so-called generalized harmonic oscillator (GHO) evolving adiabatically in time. In the first part we define the adiabatic approximation and determine the quantity that is conserved along the evolution in this approximation. Next for cyclic systems a novel derivation of Hannay's angle is obtained. Unlike the original construction [8] our procedure does not require any averaging principle [4].

Since the method follows closely the operator formulation of the quantum adiabatic theorem [10] the analogy between Hannay's angle and Berry's phase [11] is enhanced. Moreover, the formalism avoids explicit introduction of action–angle variables, a question always delicate when dealing with time-dependent Hamiltonians [4]. The price to be paid for this gain in the interpretation is that the formalism does not generalize easily to non-linear systems.

In the second part we study non-adiabatic effects. They induce changes in the abovementioned approximately conserved quantity that are exponentially small [12]. We find that, in general, this exponential factor contains, besides the known terms, also a geometric contribution. This result constitutes, in turn, the classical analogue to the geometric amplitude factor found [13,14] in adiabatic quantum transitions inherent to two-level systems which has recently been experimentally measured [15].

Introduce the vector $\boldsymbol{\xi}=(q,p)$, whose components are the generalized coordinate and momentum. The trajectories in phase space can be generated by means of a symplectic map $\mathscr{M}$ acting on initial values,

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

Here we have introduced the new variable $\tau=\epsilon t$, where $1/\epsilon$ fixes the time scale. The above equation is the starting point in formulations of classical mechanics based on Lie transformations [16]. The map $\mathscr{M}$ can be expressed as a matrix M whenever one deals with linear Hamiltonian systems. The GHO, whose Hamiltonian reads

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

is a particular one-dimensional realization of this class. Furthermore, we shall suppose a gentle dependence of X, Y, Z on the scaled time τ.

For the Hamiltonian in eq. (2) the time evolution of M is governed by the differential equation

$$\dot{M}=(1/\epsilon)SM\,,\quad M(\tau_0,\tau_0)=I\,, \tag{3}$$

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where the dot stands for derivative with respect to the scaled time τ,

$$S=\tfrac{1}{2}(Z-X)\sigma_1+\tfrac{1}{2}\mathrm{i}(Z+X)\sigma_2+Y\sigma_3\,,$$

in terms of Pauli matrices and I is the 2×2 identity matrix.

The (instantaneous) eigenvectors of the matrix $S(\tau)$ happen to be linearly independent for any value of τ provided $Y^2(\tau)\neq X(\tau)Z(\tau)$ and hence $S(\tau)$ can be rendered diagonal by the time-dependent matrix $R(\tau)$:

$$S(\tau)=R(\tau)S_{\mathrm{d}}(\tau)R^{-1}(\tau)\,, \tag{4}$$

where $S_{\mathrm{d}}(\tau)$ stands for the diagonal matrix (λ_+,λ_-) with $\lambda_+=-\lambda_-=\lambda\equiv\sqrt{Y^2-XZ}$, and R can be written as

$$R(\tau)=\frac{1}{2\sqrt{2\lambda(Y+\lambda)}}\times[(Z-X)\sigma_1+\mathrm{i}(Z+X)\sigma_2+2(Y+\lambda)\sigma_3]=R^{-1}(\tau)\,. \tag{5}$$

At this point it is useful to examine the characteristics of the motion when X, Y, Z are held fixed. For the parameter subspace where $XZ>Y^2$ the orbits are closed (elliptic) contours representing the foliation of the phase space in T^1-tori, $\lambda=\mathrm{i}\omega$ and $\omega=\sqrt{XZ-Y^2}$ is the constant rotation frequency. Otherwise, in the parameter region where $XZ<Y^2$, the orbits are hyperbolas. The case $XZ=Y^2$ corresponds to a bifurcation in parameter space and the orbits are straight lines. We point out that schemes based on the averaging principle need the introduction of action–angle variables which is only possible in the former case. At first, we restrict ourselves to this situation too. However, since our method formally applies in both parameter regions we shall indicate the corresponding results for the case $XZ<Y^2$ whenever possible.

Next we consider the following factorization for M:

$$M(\tau,\tau_0)=R(\tau)M_R(\tau,\tau_0)R^{-1}(\tau_0)\,. \tag{6}$$

This is equivalent to making the formal transformation $\boldsymbol{\xi}_R(\tau)\equiv R^{-1}(\tau)\boldsymbol{\xi}(\tau)$, taking us from $\boldsymbol{\xi}(\tau)$ to new variables $\boldsymbol{\xi}_R(\tau)=(q_R(\tau),\,p_R(\tau))$ in terms of which the new mapping reads

$$\boldsymbol{\xi}_R(\tau)=M_R(\tau,\tau_0)\boldsymbol{\xi}_R(\tau_0)\,, \tag{7}$$

and satisfies

$$\dot{M}_R=S_RM_R\,,\quad M_R(\tau_0,\tau_0)=I\,, \tag{8}$$

with

$$\begin{aligned}S_R&\equiv(1/\epsilon)S_{\mathrm{d}}-R^{-1}\dot{R}\\&=[\mathrm{i}\omega/\epsilon+\tfrac{1}{2}\gamma(Z\dot{X}-X\dot{Z})]\sigma_3\\&\quad+\tfrac{1}{2}[(\alpha+\beta)\sigma_1+\mathrm{i}(\alpha-\beta)\sigma_2]\,,\end{aligned} \tag{9}$$

in terms of the functions

$$\alpha=\gamma[(\mathrm{i}\dot{\omega}+\dot{Y})Z-(\mathrm{i}\omega+Y)\dot{Z}]\,,$$

$$\beta=\gamma[(\mathrm{i}\dot{\omega}+\dot{Y})X-(\mathrm{i}\omega+Y)\dot{X}]\,,$$

$$\gamma=[2\mathrm{i}\omega(\mathrm{i}\omega+Y)]^{-1},\quad S_{\mathrm{d}}=\mathrm{i}\omega\sigma_3\,.$$

There is a crucial difference between the two terms in S_R. Whereas the first term does depend explicitly on the time scale of the system the second one depends on ϵ only through the scaled time τ and so is geometric in character. As a matter of fact, the geometric character here is not related to the parameter space, but to the phase space itself. In this sense our interpretation resembles that of Aharonov–Anandan [17] for quantum systems.

If S_R were diagonal the solution to eq. (8) would be $M_R=\exp(a\sigma_3)$ where, after integrating exact differentials,

$$a(\tau,\tau_0)=\tfrac{1}{2}\log\frac{k(\tau_0)}{k(\tau)}+\mathrm{i}\int_{\tau_0}^{\tau}\left(\frac{\omega}{\epsilon}+\frac{Y\dot{Z}-\dot{Y}Z}{2\omega Z}\right)\mathrm{d}\tau\,, \tag{10}$$

with the following definition:

$$k(\tau)=[(\omega-\mathrm{i}Y)X/(\omega+\mathrm{i}Y)Z]^{1/2}\,.$$

This suggests introducing M'_R by

$$M_R=\exp(a\sigma_3)M'_R\,. \tag{11}$$

This new matrix M'_R accounts for the difference between the exact and diagonal approximate solutions. Its matrix elements m_{ij} $(i,j=1,2)$ obey

$$\dot{m}_{11}-\alpha\mathrm{e}^{-2a}m_{21}=0,\quad \dot{m}_{21}-\beta\mathrm{e}^{+2a}m_{11}=0\,, \tag{12}$$

$$\dot{m}_{22}-\beta\mathrm{e}^{+2a}m_{12}=0,\quad \dot{m}_{12}-\alpha\mathrm{e}^{-2a}m_{22}=0\,. \tag{13}$$

We shall come back to these equations later on.

Under adiabatic conditions, namely when the proper time of the system is much smaller than the time scale $(2\pi\epsilon\ll\omega)$, M'_R can be replaced in eq. (11)

by the identity matrix leading to the adiabatic approximation (AA). During evolution each component of $\boldsymbol{\xi}_R$ changes only by an exponential factor involving $a(\tau, \tau_0)$, which has both a real and imaginary part. Thus in this approximation the quantity $p_R q_R$ is exactly conserved. We note in passing that $J \equiv -\mathrm{i} p_R q_R = H/\omega$ is the usual expression for the adiabatic invariant [7], provided the constraint $XZ > Y^2$ is fulfilled.

For a time-independent system we have $M'_R = I$, and the quantity $\omega(t-t_0)$ is thereby the polar angle of the trajectory in the p_R–q_R plane. This idea may be extended to the more general case of a cyclic system in parameter space, i.e. a GHO Hamiltonian which at some instant τ_1 verifies $X(\tau_1)=X(\tau_0)$, $Y(\tau_1)=Y(\tau_0)$, $Z(\tau_1)=Z(\tau_0)$. In this case $a(\tau_1, \tau_0)$ is purely imaginary and the first term which survives,

$$\frac{1}{\epsilon}\int_{\tau_0}^{\tau_1} \omega(\tau)\, \mathrm{d}\tau ,$$

is called the dynamical angle whereas the remainder

$$\theta_{\mathrm{H}} \equiv \int_{\tau_0}^{\tau_1} [(Y\dot{Z} - \dot{Y}Z)/2\omega Z]\, \mathrm{d}\tau \tag{14}$$

is the Hannay angle and is considered of geometric character. If $XZ < Y^2$, angles become imaginary and their corresponding formulae are readily obtained by restoring $\omega = -\mathrm{i}\lambda$, $\lambda \in \mathbb{R}$, in all the above expressions. The generalization to GHO with N degrees of freedom is straightforward whenever the corresponding $S(\tau)$ matrix can be diagonalized.

It still remains a point to be clarified. As a matter of fact, the operator R is not uniquely determined because any non-singular diagonal transformation $Q(\tau)$ leads to a new matrix $R' \equiv RQ$ that also diagonalizes S. However, neither the dynamical phase not the Hannay angle are changed by this transformation. The former cannot change because of the uniqueness of the instantaneous eigenvalues. Moreover

$$(R'^{-1}\dot{R}')_{\mathrm{d}} = (Q^{-1}R^{-1}\dot{R}Q)_{\mathrm{d}} + Q^{-1}\dot{Q} ,$$

whence the difference,

$$(R'^{-1}\dot{R}')_{\mathrm{d}} - (R^{-1}\dot{R})_{\mathrm{d}} = Q^{-1}\dot{Q} ,$$

is just an exact differential. Thus, we can conclude that (at the AA level) the result of making the transformation Q is just adding an exact differential to the total angle which provides a vanishing contribution when the system is cyclic.

This completes the answer to the first question issued in the introduction.The remainder of this Letter is devoted to study asymptotic variations of J caused by non-adiabatic effects, i.e. because $M'_R \neq I$ in the general case.

Assume that X, Y, Z tend sufficiently fast to definite limits as $\tau \to \pm\infty$ and verify $X(\tau)Z(\tau) > Y^2(\tau)$ for all real τ. Thus, the limiting values of the adiabatic invariant $J(\pm\infty)$ do exist and we can properly define the quantity $\Delta J \equiv J(+\infty) - J(-\infty)$.

An asymptotic determination of ΔJ was first obtained by Dykhne [12] using the Hamiltonian in eq. (2) with $Z=1$, $Y=0$, and X depending analytically on τ. He got $\Delta J = \mathrm{O}(\exp(-c/\epsilon))$, $c=\text{const}>0$, a behaviour that has also been found in further analyses [6,18], even for non-linear one-dimensional systems [19,20]. What we shall see is that the more general Hamiltonian in eq. (2) leads to a geometric additional factor in ΔJ.

The exact expression for ΔJ is given by

$$\begin{aligned}\Delta J = -\mathrm{i}\{ & m_{11}(+\infty) m_{21}(+\infty) q_R^2(-\infty) \\ & + m_{22}(+\infty) m_{12}(+\infty) p_R^2(-\infty) \\ & + [m_{11}(+\infty) m_{22}(+\infty) \\ & + m_{12}(+\infty) m_{21}(+\infty) - 1] \\ & \times q_R(-\infty) p_R(-\infty)\} .\end{aligned} \tag{15}$$

Writing

$$M'_R = \begin{pmatrix} 1+\delta_{11} & m_{12} \\ m_{21} & 1+\delta_{22} \end{pmatrix},$$

with δ_{ii}, $m_{ij} \ll 1$, we get to first order in non-adiabatic corrections

$$\begin{aligned}\Delta J \simeq -\mathrm{i}[& m_{21}(+\infty) q_R^2(-\infty) \\ & + m_{12}(+\infty) p_R^2(-\infty)] ,\end{aligned} \tag{16}$$

and we have to look for the asymptotic form of m_{12} and m_{21}.

Let us assume that X, Y, Z can be analytically continued into the complex τ-plane and that a complex value τ_{c} exists at which $\omega(\tau_{\mathrm{c}}) = 0$, namely a complex point where the two eigenfrequencies become degenerate. The crossing or transition point τ_c is a singularity of S. For functions X, Y, Z of a reasonably common type, we assume that in a neighborhood of τ_c:

$$\omega^2 = \rho(\tau-\tau_c)^{\nu}[1+Q(\tau)] , \tag{17}$$

with real $\rho \neq 0$, $\nu > 0$, $Q(\tau)$ analytic at τ_c and $Q(\tau_c)=0$. The particular choice $Y=0$, $Z=1$, $\nu=1$ leads to Dykhne's singularity model.

As already stated before, each eigenvector acquires during its evolution only an exponential factor and so it corresponds always to the same eigenvalue. However, if instead of integrating eq. (3) along the real τ-axis we modify the circuit to circle the crossing then one eigenvector becomes the other yielding a non-vanishing contribution to ΔJ. As the difference with respect to AA evolution arises only from the circling of the singularity we have to analyze eqs. (12), (13) in a neighborhood of τ_c. The idea to be developed consists in solving there exactly eqs. (12), (13) and then joining this local solution to that provided by the AA [21,22]. Owing to the similarities between eqs. (12) and (13) we give details only for eq. (13). In the neighborhood of the transition point τ_c:

$$\dot m_{22} + \frac{\dot\omega k(\tau_0)}{2\mathrm{i}\omega} \exp\left(2\mathrm{i}\int_{\tau_0}^{\tau} \omega'(\tau')\,\mathrm{d}\tau'\right) m_{12} = 0 ,$$

$$\dot m_{12} - \frac{\dot\omega}{2\mathrm{i}\omega k(\tau_0)} \exp\left(-2\mathrm{i}\int_{\tau_0}^{\tau} \omega'(\tau')\,\mathrm{d}\tau'\right) m_{22} = 0 . \tag{18}$$

We have denoted

$$\omega' = \frac{\omega}{\epsilon} + \frac{Y\dot Z - \dot Y Z}{2\omega Z} . \tag{19}$$

Hereafter we set $\tau_0 \to -\infty$, $k_- \equiv k(-\infty)$, $\omega_\pm \equiv \omega(\pm\infty)$. Further we introduce the function

$$f(\tau) = \frac{1}{\sqrt{\omega'}}\left[m_{22}\exp\left(-\mathrm{i}\int^{\tau}\omega'\,\mathrm{d}\tau'\right) + \mathrm{i}k_- m_{12}\exp\left(\mathrm{i}\int^{\tau}\omega'\,\mathrm{d}\tau'\right)\right] , \tag{20}$$

where the lower integration limit is irrelevant to our purposes and its behaviour at $\tau \to -\infty$ is

$$f \sim \exp\left(-\mathrm{i}\int^{\tau}\omega'(\tau')\,\mathrm{d}\tau'\right) , \tag{21}$$

for $m_{12} \to 0$, $m_{22} \to 1$. Taking into account eq. (18) and dropping terms containing the difference $\dot\omega/\omega - \dot\omega'/\omega'$ (which is of order ϵ) the function f obeys the equation

$$\ddot f + \omega'^2 f = 0 . \tag{22}$$

The asymptotic form $(\tau \to +\infty)$ of $f(\tau)$ is

$$f \sim A\exp\left(-\mathrm{i}\int^{\tau}\omega'(\tau')\,\mathrm{d}\tau'\right) + B\exp\left(\mathrm{i}\int^{\tau}\omega'(\tau')\,\mathrm{d}\tau'\right) , \tag{23}$$

with A, B constant. Therefore, once the coefficients A, B have been determined, comparison between eqs. (20) and (23) immediately yields $m_{12}(+\infty)$.

The mathematical problem of finding the first asymptotic approximation to the ratio B/A from eq. (22) has already been tackled in the literature in connection with the above-barrier reflection of a quasi-classical particle [12,13,18,21–24]. The methods are essentially based on the manner in which analyticity of ω' breaks down at the point τ_c. If ω^2 has a zero of order ν then, owing to the presence of the geometric term, ω'^2 has a singularity:

$$\omega'^2 = \rho'(\tau-\tau_c)^{-\nu}[1+Q'(\tau)] , \tag{24}$$

with definitions for ρ', Q' similar to those in the sequel of eq. (17). As a consequence, analyses carried out for a particular ω^2 (whose zero has multiplicity ν) cannot be trivially extended to ω'^2 (which has a pole of multiplicity ν). This problem has been independently analyzed by Pokrovskii and Khalatnikov [21], and Meyer [23] yielding equivalent conclusions. Here we merely apply their asymptotic results which allow us to determine the ratio B/A. Eventually we get

$$m_{12}(+\infty) = 2k_-^{-1}\cos\left(\frac{\pi}{2\pm\nu}\right)\exp(2\mathrm{i}\zeta) ,$$

$$\zeta = \int_{\tau_r}^{\tau_c}\omega'(\tau)\,\mathrm{d}\tau , \tag{25}$$

where τ_r is any point on the real τ-axis and $\mathrm{Im}\,\zeta<0$. The bar means complex conjugation. The plus, minus signs correspond to the cases $\omega'=\omega/\epsilon$ (i.e., no geometric contribution), $\omega'\neq\omega/\epsilon$ respectively.

By the same token eq. (12) provides $m_{21}(+\infty)$ and a similar discussion holds. The result for the change in J is finally given by

$$\Delta J\simeq 2C\cos\left(\frac{\pi}{2\pm\nu}\right)\exp(2\,\mathrm{Im}\,\zeta)\,,$$

$$C=-\mathrm{i}[k_-q_R^2(-\infty)+k_-^{-1}p_R^2(-\infty)]\exp(2\mathrm{i}\,\mathrm{Re}\,\zeta)\,. \tag{26}$$

This expression for ΔJ has the same structure as the one obtained by Dykhne [12] by we want to emphasize that here ζ includes a geometric contribution besides the known dynamical one. This is so for both the "amplitude" factor $(\exp(2\,\mathrm{Im}\,\zeta))$ and the "pre-exponential" factor (C).

When ω has several complex zeroes $\{\tau_{c,i}\}$ the prescription consists in selecting the zero that leads to the least value of

$$\left|\mathrm{Im}\int_{\tau_r}^{\tau_{c,i}}\omega'\,\mathrm{d}\tau\right|,$$

which might be not the closest one to the real τ-axis. If various values $\tau_{c,i}$ fulfill the above condition then a summation extended to all of them has to be performed. Of course, when no crossing occurs the method does not apply.

In summary, we have developed a formalism that enables one to define clearly the adiabatic approximation for the GHO providing at the same time a simple derivation of Hannay's angle. Methods based on the averaging principle apply only in the parameter space region where $XZ>Y^2$ but are not valid if $XZ<Y^2$. On the contrary, our approach holds in both regimes. Finally, we have analyzed the exponentially small variations of the adiabatic invariant due to non-adiabatic effects. An analytic continuation procedure into the complex time plane generalizes some previous results and exhibits the appearance of a new factor, geometric in character. This constitutes the classical counterpart to the recently studied [13,14] geometric factor contributing to the quantum transition probability in two-level systems.

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