Quantum and Classical Connections and Topological Phases: A Study of a Perturbed Rotator†

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In this paper are discussed the quantum mechanical connection and its classical counterpart, as well as the quantum and classical topological angles. The two were calculated for a model system to see whether they show any resemblance. The most interesting result we found is that the quantum and the classical topological phases are each formed due to a single discontinuous jump that occurs at some time during the external cycle. However, whereas the quantum mechanical topological phase is formed in the usual adiabatic limit, we had to establish a new parameter which, by allowing it to approach its limiting value, forms the classical topological phase.

I. Introduction

In two recent publications, Baer et al.[1,2] studied a quantum mechanical model that describes the motion of an electron housed by a molecule driven by a *periodic* external perturbation. The study was done by solving the respective Schroedinger equation within the two-state approximation, with the aim of deriving the time-dependent phase of the electronic wave function related to the initially populated state. This phase is a sum of two terms: the dynamic phase, ϖt, and a residual phase termed *connection*. The connection was the main subject of the above-mentioned papers because, at the adiabatic limit, upon completion of a period of the external field, it becomes the topological (Berry) phase.[3] In the present paper the emphasis will be the classical analogue for the quantum connection function. In contrast to the quantum connection, which is a well-defined phase related to a wave function, the meaning of the classical connection is not self-evident. Hannay[4] and Berry[5] suggested identifying this phase with the changes of a periodic phase caused by a slowly oscillating external perturbation which affects the periodic system. Thus, if $q(t)$ is the phase of the unperturbed periodic system at time t, $0 \le t \le T$, where T is its period, and if $\theta(\tau)$ is the phase of the whole system at time τ, then the difference $\Delta\theta(\tau) = \theta(\tau) - q(\tau - nT)$, where $n = [\tau/T]$, in the adiabatic limit, will be termed the classical connection. Part of this paper is devoted to the analytic derivation of $\Delta\theta(\tau)$ in the adiabatic limit, and once this part is completed, we apply the formula to a perturbed rotator (which classically is identical to the above-mentioned model).

The paper is organized in the following way: In the next section the model, in the quantum framework, is introduced and a few numerical results for the connection function are presented. The third section is devoted to the classical approach and is divided into three parts. (a) In the first part, employing the action−angle variables, the general formula for the classical connection in the adiabatic limit is derived. (b) In the second part, the perturbed rotator is treated to some extent; this treatment is accompanied by a series of numerical results. (c) In the third part, the numerical findings are analyzed employing an approximate analytic treatment relevant for the low-frequency case (the only situation for which the classical connection becomes apparent). The conclusions are summarized in the fourth section.

II. Quantum Mechanical Treatment

We consider an electronic Hamiltonian closely related to the Jahn−Teller model[6] which is expressed in terms of the Mathieu equation,[1,2,6−11] namely

$$H = -\frac{1}{2}E_{\mathrm{el}}\frac{\partial^2}{\partial q^2} - G\cos(2q - \varphi) \tag{1}$$

Here q is an angular (periodic) electronic coordinate, E_{el} and G are constants, and φ is a periodic variable related to the external field and is assumed to change linearly with time, namely, $\varphi = \omega t$, where ω is the periodicity of the external field. We consider the equation ($\hbar = 1$)

$$\mathrm{i}(\partial\Psi/\partial t) = H\Psi \tag{2}$$

which will be solved within the first-order approximation in G/E_{el}, yielding the ground-state doublet only. In a space representation this doublet is described in terms of the electronic functions $\cos q$ and $\sin q$ (q is a characteristic electronic coordinate), and therefore Ψ can be expanded as[2,10]

$$\Psi = \chi_1(t)\cos q + \chi_2(t)\sin q \tag{3}$$

In what follows eq 2 will be solved for the initial conditions: $\chi_1(t{=}0) = 1$ and $\chi_2(t{=}0) = 0$. Replacing $\chi_1(t)$ and $\chi_2(t)$ by $\psi_+(t)$ and $\psi_-(t)$ defined as[10]

$$\psi_\pm(t) = \frac{1}{2}\exp\left(\mathrm{i}\frac{1}{2}E_{\mathrm{el}}t\right)(\chi_1 \pm i\chi_2) \tag{4}$$

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we get the corresponding equations for $\psi_+(t)$ and $\psi_-(t)$:

$$\mathrm{i}\frac{\partial\psi_+}{\partial t} = -\frac{1}{2}G\exp(\mathrm{i}\varphi)\psi_-$$
$$\mathrm{i}\frac{\partial\psi_-}{\partial t} = -\frac{1}{2}G\exp(-\mathrm{i}\varphi)\psi_+ \quad (5)$$

Next we eliminate ψ_- from eqs 5 to obtain a single, second-order equation for ψ_+:

$$\frac{\partial^2\psi_+}{\partial t^2} - \mathrm{i}\omega\frac{\partial\psi_+}{\partial t} + \frac{1}{4}G^2\psi_+ = 0 \quad (6)$$

Once eq 6 is solved, we can obtain $\chi_1(t)$ — the eigenfunction for the initially populated state — which is usually a fast oscillating function of t, where the oscillations are caused by the "dynamical phase" $(1/2)Gt$. In what follows we consider the "smoother" function $\eta(t)$ defined as

$$\eta(t) = \chi_1(t)\exp(-(1/2)\mathrm{i}Gt) \quad (7)$$

with the aim of studying the time dependence of the phase $\gamma(t)$ defined through the expression

$$\eta(t) = \rho(t)\exp(\mathrm{i}\gamma(t)) \quad (8)$$

Once $\eta(t)$ is derived, there are several ways to extract $\gamma(t)$; we shall use the following one:

$$\gamma(t) = \int_0^t\left(\frac{\partial\gamma}{\partial t'}\right)\mathrm{d}t' \quad (9a)$$

where

$$\frac{\partial\gamma}{\partial t} = F\left(\frac{\langle\eta(t)|(\partial\eta/\partial t)\rangle}{\langle\eta(t)|\eta(t)\rangle}\right) \quad (9b)$$

Here F stands for the imaginary part of the expression in the parentheses.

A special emphasis will be given to $\gamma(t)$ at $t = \tilde{T}$, where $\tilde{T}$ is the period of the external field ($\tilde{T} = 2\pi/\omega$). The case of an arbitrary $\tilde{T}$ will be discussed only briefly, and we will be mainly interested in the adiabatic limit where $\tilde{T}$ is large, namely, $\tilde{T} \gg G^{-1}$, for which $\gamma(t=\tilde{T})$ becomes the topological (Berry) phase β.

The solution of eq 6 (as well as the solution for a similar equation for $\psi_-(t)$) can be written in terms of exponential functions. Returning to the original χ functions, we get for $\chi_1(t)$ the following explicit expression:[2,7,10]

$$\chi_1(t) = \cos(kt)\cos\left(\frac{1}{2}\omega t\right) + \frac{\omega}{2k}\sin(kt)\sin\left(\frac{1}{2}\omega t\right) + \mathrm{i}\frac{G}{2k}\sin(kt)\cos\left(\frac{1}{2}\omega t\right) \quad (10)$$

where k, defined as

$$k = (1/2)(G^2 + \omega^2)^{1/2} \quad (11)$$

forms, together with ω, the two characteristic periodicities of the system. The function $\gamma(t)$ is calculated employing eqs 9 and 10, where $\partial\gamma/\partial t$ can be shown to be

$$\frac{\mathrm{d}\gamma}{\mathrm{d}t} = \frac{G}{2}\times$$
$$\left(1 - \frac{\left(\frac{\omega}{2k}\right)^2\sin^2(kt)\,(1-\cos(\omega t)) + \frac{\omega}{4k}\sin(2kt)\sin(\omega t)}{\cos^2\left(\frac{1}{2}\omega t\right) + \frac{\omega}{4k}\sin(2kt)\sin(\omega t) - \left(\frac{\omega}{2k}\right)^2\sin^2(kt)\cos(\omega t)}\right) \quad (12)$$

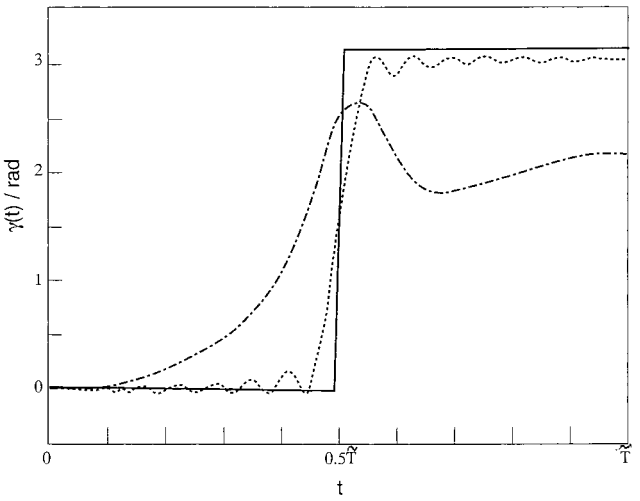

Figure 1. Quantum mechanical phase $\gamma(t)$ as calculated for $G = 0.01$ au: -·-, $\tilde{T} = 10^3$ au; ---, $\tilde{T} = 10^4$ au; —, $\tilde{T} = 10^6$ au.

In Figure 1 are shown several $\gamma(t)$ functions as calculated for a given value of G and three values of $\tilde{T}$. It is noticed that, as $\tilde{T}$ increases, namely, as the adiabatic limit is approached, $\gamma(t)$ tends to a step function and β reaches the value of π.

The behavior of $\gamma(t)$ in the adiabatic limit can also be obtained analytically. Following eq 8, we may write[2,10]

$$\gamma(t) = F\,(\ln(\eta(t))) \quad (13)$$

and consider the (adiabatic) case, namely, the case that $\tilde{T} \to \infty$ (or $\omega \to 0$). It can be shown, employing eqs 8 and 10, that $\gamma(t)$ takes the form[2,10]

$$\lim_{T\to\infty}(\gamma(t)) = \{F\,(\ln(\cos(\omega t/2) + O(\omega)\} \quad (14)$$

Having this expression, it is recognized that since $\cos(1/2)\omega t > 0$ for $t \le T/2$ and $\cos(1/2)\omega t < 0$ for $t \ge \tilde{T}/2$ it follows that $\gamma(t) \cong 0$ for $0 \le t \le \tilde{T}/2$ and $\gamma(t) \cong \pi$ for $\tilde{T}/2 \le t \le \tilde{T}$. This also implies that $\beta \cong \pi$. Thus, eq 14 describes a time-dependent step function where the step takes place at $t \approx \tilde{T}/2$ similarly to the step presented in Figure 1.

III. Classical Treatment

III.1. Action−Angle Variables. The classical treatment is based on the action−angle variables I and θ,[12] and the aim is to study the effect of a slowly varying (i.e., adiabatic) external field on the angle θ. The action variable I is defined as

$$I = (1/2\pi)\int_\Gamma^q p\,\mathrm{d}q \quad (15)$$

where q is the spatial coordinate, p is its conjugate momentum, and Γ is the closed path formed by the (p,q) trajectory. Since the system is affected by a time-dependent external field characterized by a parameter λ, it is expected that Γ will depend

on this parameter. Nevertheless, in case the system changes adiabatically, I is a constant of the motion.[12] The angle θ is the conjugate coordinate of I. The transformation $(p,q) \rightarrow (I,\theta)$ is done employing the generating function $F(q,I|\lambda)$ defined as

$$F(q,I|\lambda) = \int_{q_0}^{q(\lambda)} p \, dq \tag{16}$$

As a result of this transformation, a new Hamiltonian, $\tilde{H} = \tilde{H}(I,\theta)$, is formed, which is related to the old one as follows:

$$\tilde{H} = H + \frac{\partial F(q,I|\lambda)}{\partial t} = H + \frac{\partial F(q,I|\lambda)}{\partial \lambda}\frac{d\lambda}{dt}$$

or

$$\tilde{H} = H + p\frac{\partial q}{\partial \lambda}\frac{d\lambda}{dt} \tag{17}$$

Equation 17 is valid because of the two independent variables I and q; in the quasi-adiabatic situation, I is a constant of motion so that only q depends explicitly on time. Next we consider the equation of motion for θ. Thus

$$\frac{\partial \theta}{\partial t} = \frac{\partial \tilde{H}}{\partial I} = \frac{\partial H}{\partial I} + \frac{\partial}{\partial I}\left(p\frac{\partial q}{\partial \lambda}\frac{d\lambda}{dt}\right) \tag{18}$$

It is important to recognize that the second term yields the rate of change of θ for fixed values of p and q, due to the external field. Writing θ as

$$\theta(t) = \varpi t + \int_0^t \frac{\partial}{\partial I}\left(p(t')\frac{\partial q}{\partial \lambda}\frac{d\lambda}{dt}\bigg|_{t=t'}\right) dt' = \varpi t + \Delta\theta(t) \tag{19}$$

where ϖ stands for $\partial H/\partial I$ and is the periodicity of the system in case λ is fixed (in other words, it is the periodicity of the (p,q) trajectory, ignoring external perturbation) and $\Delta\theta(t)$ is the change of θ at time t caused by the external time-dependent perturbation. Being in the adiabatic situation where the system completes a cycle of time T $(=2\pi/\varpi)$, while the external field changes only slightly, we shall calculate $\Delta\theta(t)$ in the following way.

First is calculated the average value of $\Delta\theta(t)$ (see eq 19), namely, $\Delta\theta_{av}(\lambda)$ at a fixed given λ for one completed (fast) cycle:[11a]

$$\Delta\theta_{av}(\lambda) = \frac{1}{T}\int_0^T \Delta\theta_{pert}(t'|\lambda)\, dt' =$$

$$\frac{1}{T}\int_0^T \frac{\partial}{\partial I}\left(p(t')\frac{\partial q(\lambda)}{\partial \lambda}\frac{d\lambda}{dt}\bigg|_{t=t'}\right) dt' =$$

$$\frac{\partial}{\partial I}\left[\frac{1}{T}\int_0^T \left(p(t')\frac{\partial q(\lambda)}{\partial \lambda}\frac{d\lambda}{dt}\bigg|_{t=t'}\right) dt'\right]$$

or

$$\Delta\theta_{av}(\lambda) = \frac{\partial}{\partial I}\left\langle p(t)\frac{\partial q(\lambda)}{\partial \lambda}\frac{d\lambda}{dt}\right\rangle \tag{20}$$

It is important to emphasize that p is not explicitly dependent on λ. The only functions that are explicitly dependent on λ are q and I. To obtain $\Delta\theta(t)$, we perform the following integration:

$$\Delta\theta(t) = \int_0^t \Delta\theta_{av}(\lambda(\tau))\, d\tau \tag{21}$$

which takes the form

$$\Delta\theta(t) = \int_0^t \frac{\partial}{\partial I}\left\langle p(\tau)\frac{\partial q}{\partial \lambda}\frac{d\lambda}{dt'}\bigg|_{t'=\tau}\right\rangle d\tau$$

or

$$\Delta\theta(t) = \frac{\partial}{\partial I}\int_0^t \left\langle p\frac{\partial q(\lambda)}{\partial \lambda}\frac{d\lambda}{dt'}\bigg|_{t'=\tau}\right\rangle d\tau \tag{22}$$

If the external field is presented in terms of a periodic coordinate φ (making $\lambda(t) \equiv \varphi(t)$) so that

$$\varphi = t/\omega \tag{23}$$

where ω is the periodicity of this external field, then it follows from eq 22 that

$$\Delta\theta_{cc}(\phi) = \frac{\partial}{\partial I}\int_0^{\phi} \left\langle p(\varphi')\frac{\partial q(\varphi)}{\partial \varphi}\bigg|_{\varphi=\varphi'}\right\rangle d\varphi' \tag{24}$$

The index "cc" was added to remind us that eq 24 stands for the *classical* analogue of the quantum *connection* function. For $\phi = 2\pi$, eq 24 yields a phase which has been suggested to be considered as the classical analogue of the quantum topological phase.[4,5] In what follows this phase is termed the classical analogue of the topological phase.

III.2. Perturbed Rotator Model. We consider the following classical Hamiltonian:

$$H = E = (1/2)p^2 + G\cos(2q - \varphi) \tag{25}$$

where both the coupling coefficient G and the total energy E are expressed in units of E_{el} (see eq 1). Using this Hamiltonian, the two coupled equations of motion are

$$\partial q/\partial t = p$$
$$\partial p/\partial t = 2G\sin(2q - \varphi) \tag{26}$$

Equations 26 can be converted into a single second-order equation which is known to have an analytic solution.[13] However, we will solve eqs 26, just as they are, numerically. All results due to the present study are for positive values of the total energy E. Since in this case the range of the coordinate q is unlimited but with a 2π periodicity, we consider the following range of q: $q_0 \le q \le q_0 + 2\pi$, where q_0 has a given initial value of q. To calculate the topological phase, the calculations of $q(t)$ and $p(t)$ are repeated for a φ grid along the $(0,2\pi)$ range with fixed values of q_0. We found that nothing of interest happens unless E closely approaches the value of G (see eq 25). Consequently we introduce the parameter α defined as $\alpha = E/G$, and all results will be discussed as a function of α (>1).

In Figure 2a,b are presented the functions $p(t)$ and $q(t)$ and in Figure 2c is presented the function $p(q)$, all calculated for $\alpha = 1.01$, $q_0 = 0.5$ rad, and two values of φ, namely, $\varphi = 0.0$ and 0.5 rad. (The reason for choosing α to be so close to 1 will be discussed later.) The results presented so far (up to a shift) are dependent on neither φ nor q_0. The period of the trajectory can be calculated independently employing the explicit expression for I. According to eq 15, the action variable, I, for this model is given in the form

$$I = (1/\pi\sqrt{2})\int_0^{2\pi} [E - G\cos(2q - \varphi)]^{1/2}\, dq \tag{27}$$

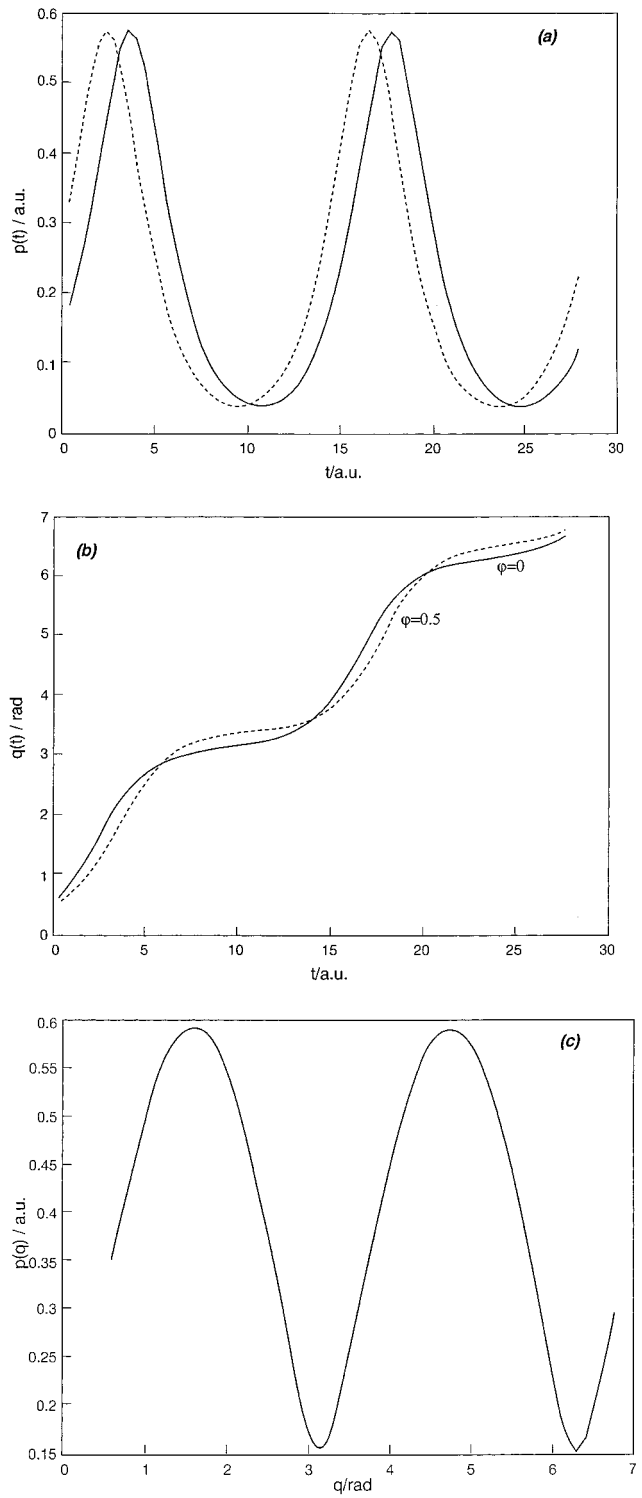

Figure 2. Trajectory calculations: (a) $p(t)$; (b) $q(t)$; (c) $p(q)$. Calculations are done for $\alpha = 1.01$ and $q_0 = 0.5$ rad. Key: —, results for $\varphi = 0.0$ rad; ---, results for $\varphi = 0.5$ rad.

and the corresponding rotator's frequency, ϖ, accordingly defined as

$$\varpi = \partial E/\partial I = (\partial I/\partial E)^{-1} \tag{28}$$

is equal to

$$\varpi = \pi(8G)^{1/2}\left[\int_0^{2\pi}(\alpha - \cos(2q - \varphi))^{-1/2}\,\mathrm{d}q\right]^{-1} \tag{29}$$

In eqs 28 and 29 it was assumed that $q_0 = 0$, but the results can be shown, analytically, to be independent of q_0. In the same way it can be shown that both I and ϖ are independent of φ.

Next we calculate $\Delta\theta_{cc}(\phi)$, applying eq 24 with a slight change: we replace $\partial/\partial I$ by $\varpi(\partial/\partial E)$ so that eq 23 becomes

$$\Delta\theta_{cc}(\phi) = \varpi\frac{\partial}{\partial E}\int_0^{f}\left\langle p\left.\frac{\partial q(\varphi')}{\partial\varphi'}\right|_{\varphi'=\varphi}\right\rangle \mathrm{d}\varphi \tag{30}$$

It is important to emphasize that in applying eq 30 *all* derivatives were calculated numerically. In particular we shall refer to the function $\Delta\theta_{av}(\lambda)$ as presented in eq 20, and it will now be written in the form

$$\Delta\theta_{av}(\varphi) = \varpi\frac{\partial}{\partial E}\left\langle p\frac{\partial q(\varphi)}{\partial\varphi}\right\rangle \tag{20′}$$

where, as before, $\partial/\partial I$ is replaced by $\varpi(\partial/\partial E)$. Two derivatives are involved in evaluating $\Delta\theta_{av}(\varphi)$, and both were carried out numerically. First, the derivative with respect to φ was calculated, and this was done as follows: For a fixed value of E we computed $p(t_j|\varphi)$ and $q(t_j|\varphi)$, where $j = 0, ..., N$ so that $t_0 = 0$ and $t_N = T$ and then a similar set for $\varphi + \Delta\varphi$. Next the following expression was derived:

$$\left\langle p\frac{q(\varphi)}{\partial\varphi}\right\rangle = \Delta t\sum_{j=0}^{N}\tilde{p}_j(\varphi)\frac{q_j(\varphi+\Delta\varphi) - q_j(\varphi)}{\Delta\varphi} \tag{31}$$

where

$$\tilde{p}_j(\varphi) = (1/2)(p_j(\varphi+\Delta\varphi) + p_j(\varphi))$$

and Δt is the time step. The differentiation with respect to E was done in a similar way, namely, performing the above calculation once for E and once for $E + \Delta E$ and then computing the derivative in the usual (numerical) way.

In Figure 3 are presented the functions $\Delta\theta_{cc}(\phi)$ as calculated for $\alpha = 1.01$ and 1.001. In each part are shown two curves, calculated for two different initial values of q, namely, $q_0 = 1.0$ and 2.0 rad. As can be seen, results are presented for α values close to 1. We intended, of course, to calculate $\Delta\theta_{cc}(\phi)$ for arbitrary values of α, but it was found that in cases that α was too large (in fact $\alpha > 1.1$) the functions $\Delta\theta_{cc}(\phi)$ exhibited, at most, a weak dependence on ϕ, and therefore, essentially, they were of no interest. It was only when $\alpha \to 1.0$ ($\alpha = 1.0$ is the lowest possible value for this version of our model) that the interesting features started to emerge. The region of $\alpha \approx 1.0$ is the region where the total energy of the system $E \approx G$, namely, the point where the potential reaches its maximal value and the kinetic energy of the rotator is ~0.0. It is also important to mention that in this situation T, the periodicity of the unperturbed rotator, is large.

The following are to be noticed.

(1) The functions $\Delta\theta_{cc}(\phi)$ are strongly dependent on ϕ (and on q_0). In particular, at a specific short range of ϕ a discontinuous step is formed. The sharpness of this sudden increase becomes more pronounced the closer α gets to 1 (we found that this unique shape disappears once α becomes larger than 1.1). It is seen that the discontinuous step occurs for ϕ values which fulfill

$$\phi = 2q_0$$

namely, for trajectories started at the separatrix (the separartrix is the location of the highest value of the periodic potential, in

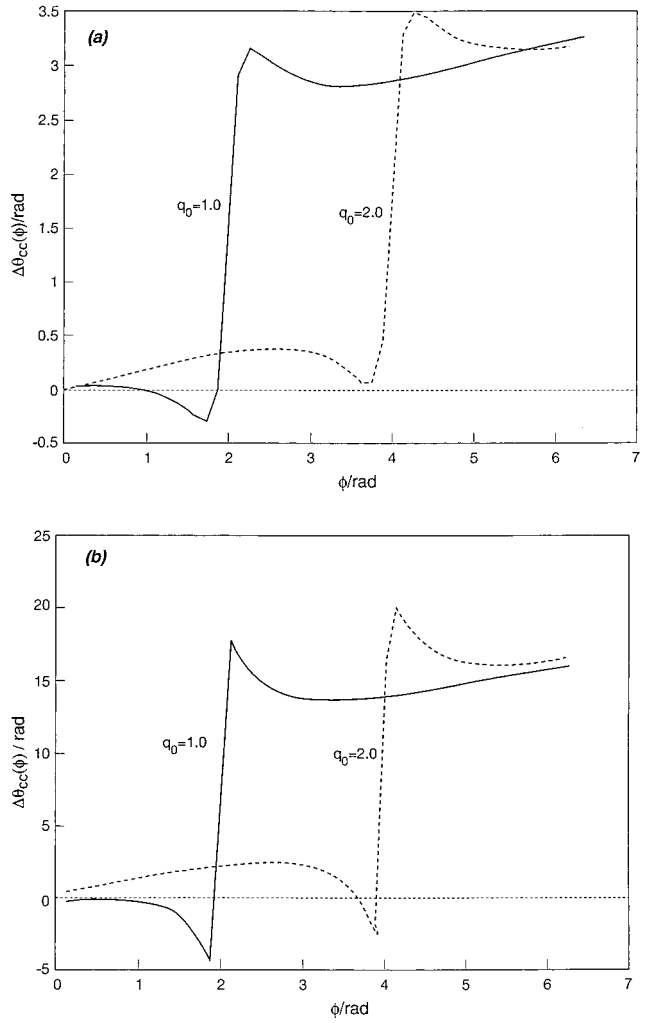

Figure 3. Classical connection function, $\Delta\theta_{cc}(\phi)$, as a function of ϕ: (a) results for $\alpha = 1.01$; (b) results for $\alpha = 1.001$. Key: —, $q_0 = 1$ rad; ---, $q_0 = 2$ rad.

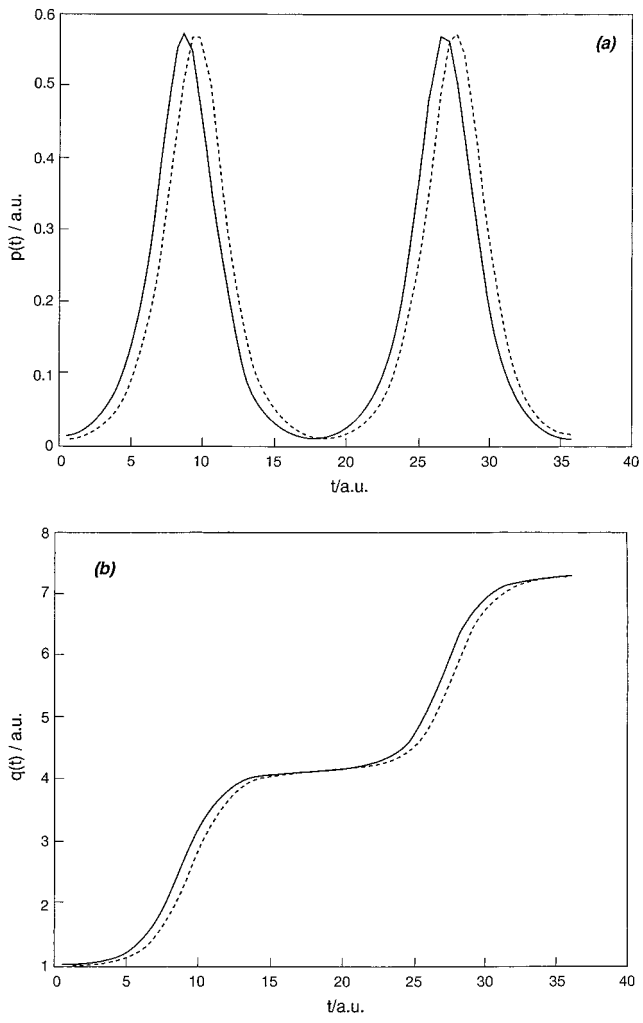

Figure 4. Trajectory calculations: (a) $p(t)$; (b) $q(t)$ Calculations are done for $\alpha = 1.001$ and $q_0 = 1$ rad. Key: —, results for $\varphi = 1.99$ rad; ---, results for $\varphi = 2.01$ rad.

other words, the location of the barrier). This case is analyzed in subsection III.3.

(2) As for the classical topological phase, namely, $\Delta\theta_{cc}(\phi{=}2\pi)$, the following is found: In the cases where α is not too close to 1 the value of $\Delta\theta_{cc}(\phi{=}2\pi)$ is of no significance, but once $\alpha \rightarrow 1.0$ this value increases rapidly. Thus, for $\alpha = 1.01$ the value of the topological phase is $\sim$3 rad, but for $\alpha = 1.001$ it is already $\sim$15 rad.

(3) Although $\Delta\theta_{cc}(\phi)$ is seen to be strongly dependent on q_0, the topological phase, $\Delta\theta_{cc}(\phi{=}2\pi)$, is not dependent on this parameter as one should expect.

To get some more insight we present, in Figure 4, the functions $p(t)$ and $q(t)$ as calculated for $\alpha = 1.001$ and for two values of φ (both close to the separatrix): one at $\varphi = 1.99$ rad, a value of φ just before the above-mentioned abrupt step takes place, and one at $\varphi = 2.01$ rad immediately after it (both calculations were done for $q_0 = 1$ rad). Although no unusual behavior is observed, still it can be seen that within the time interval $15.0 < t < 22.0$ au the two $p(t)$ functions approach zero and the $q(t)$ functions hardly change (in both cases their values are $\sim$4 rad; at this value $\cos(2q - \varphi) \approx \cos(0) \approx 1$; namely, at this value $E \approx G$; see eq 25) so that the kinetic energy of the (unperturbed) rotator is relatively small.

Since the $p(t)$ and $q(t)$ functions did not show any particularly unusual behavior, we decided to get a better understanding by presenting the integrand of $\Delta\theta_{cc}(\phi)$, namely, $\Delta\theta_{av}(\varphi)$, given in eq 20′, as a function of φ for the two values of q_0 (see Figure 5). In both cases the functions present a spiked shape reminiscent of a Dirac δ function at the respective points $\varphi = 2q_0$. Thus, we are left with a puzzle: What causes the connection function

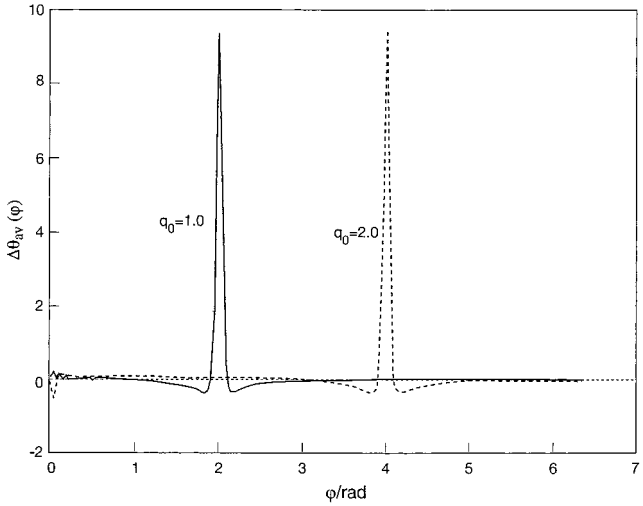

Figure 5. Average phase, $\Delta\theta_{av}(\varphi)$, of the perturbed rotator, calculated as a function of φ for $\alpha = 1.001$ and for two values of q_0: —, $q_0 = 1$ rad; ---, $q_0 = 2$ rad.

$\Delta\theta_{cc}(\phi)$ to become a step function, and what is the source of the large values of the respective topological phases, $\Delta\theta_{cc}(\phi=2\pi)$?

III.3. Analysis of the Classical Results. Inspecting the curves in Figures 3 and 5, it is noticed that the step takes place at $\varphi = 2q_0$. This means the following: Since a calculation of a trajectory starts at $q = q_0$ and since the trajectories are calculated for different φ values, we obtain the step for those trajectories that start at $q = q_0 = \varphi/2$. From eq 25 it is seen that in such a case $\cos(2q - \varphi) = 1$ so that the trajectory starts at the top of the (oscillatory) potential where the kinetic energy is close to zero (because then $E \approx G$). In what follows we consider the motion of the unperturbed rotator when a trajectory is started at that point (the approach to be utilized is reminiscent of studies of trapped trajectories in the transition region of reactive systems with barriers[14,15]). In the vicinity of this initial q value, we assume the potential to be approximated by

$$V(q|\varphi) = G\cos(2q - \varphi) = G(1 - (1/2)(2q - \varphi)^2) \qquad (32)$$

Having this form for the potential, the equations of motion can be solved analytically, and we get for q and p the following results:

$$q = \frac{\varphi}{2} + \left(\frac{\epsilon}{8G}\right)^{1/2}(e^{kt} - e^{-kt})$$

$$p = (\epsilon/2)^{1/2}(e^{kt} + e^{-kt}) \qquad (33)$$

where $\epsilon = E - G$ and $k = 2\sqrt{G}$. The corresponding frequency, ω_1 ($=2\pi k$), is $\omega_1 = 4\pi\sqrt{G}$. Equations 33 fulfill at $t = 0$ the condition that $q = \varphi/2$ and $p = (2\epsilon)^{1/2}$.

Next we refer to the integrand in eq 20, which we designate as $J(t,\varphi)$:

$$J(t,\varphi) = \varpi\frac{\partial}{\partial E}\left(p\frac{\partial q(\varphi)}{\partial\varphi}\right) \qquad (34)$$

where, as above, $\partial/\partial I$ is replaced by $\varpi(\partial/\partial E)$. We are interested in estimating the values of $J(t,\varphi)$ for the situation just described above. Thus, substituting eqs 33 into eq 34 yields for $J(t\approx 0,\varphi\approx 2q_0)$ the expression

$$J(t\approx 0,\varphi\approx 2q_0) = \varpi(1/32\epsilon)^{1/2}(e^{kt} + e^{-kt}) \qquad (35)$$

It is noticed that when $\epsilon \to 0$ (and this is the case when $\alpha \to 1$) the function $J(t\approx 0,\varphi\approx 2q_0)$ attains very large values. We continue by examining the integrand in eq 20′: As long as $\varphi < 2q_0$, the function $\Delta\theta_{av}(\varphi)$ remains almost unchanged because the integrand, $J(t,\varphi)$, never attains significant values. Once $\varphi \approx 2q_0$, the function $\Delta\theta_{av}(\varphi\approx 2q_0)$ attains large values, because of the significant contributions due to $J(t,\varphi\approx 2q_0)$ at $t \approx 0$. These contributions become larger the closer ϵ is to zero. Next we consider eq 30 (see also eq 21): As long as ϕ, the upper limit of the integral, does not reach $2q_0$, the values of $\Delta\theta_{cc}(\phi)$ are small and of no significance. However, once ϕ passes $2q_0$, the function $\Delta\theta_{cc}(\phi)$ gets contributions from the large values of $\Delta\theta_{av}(\varphi\approx 2q_0)$ so that it rapidly increases, thus building up its discontinuous step. The construction of this step is completed once ϕ passes this region (so that $\Delta\theta_{cc}(\phi)$ stays essentially constant), because of insignificant contributions along the rest of the ϕ interval.

IV. Discussion and Conclusions

In this paper are discussed the quantum and classical connections and their corresponding topological phases. The two types of approaches were applied for a model system to see whether the corresponding results show any resemblance. Before going into the analysis of the results, one major difference between the two approaches has to be emphasized: Whereas the periodicity, $\tilde{T}$, of the external perturbation plays an explicit role in the quantum treatment and therefore it is straightforward to expose the adiabatic limit, the classical treatment (based on the "adiabatic invariants" approximation) only implicitly depends on $\tilde{T}$ and therefore it is not simple to find the adiabatic limit. From previous quantum treatments[1,2] it is known that, for a given energy E, the system becomes more adiabatic the larger the product $\tilde{T}G$. In other words, for a given $\tilde{T}$ and E, increasing the value of G will enhance the adiabaticity of the system. It seems to us that, to a certain extent, a similar situation is encountered also within the classical treatment. However, since, for a given (total positive) energy E, the value of G cannot increase indefinitely, it is limited by the value of E and therefore $G \le E$ (see eq 25). From the numerical study we found indications that, indeed, the system becomes more adiabatic the closer G gets to E. The main outcome that supports this finding is the fact that both the quantum and the classical topological phases are formed due to a single *discontinuous jump* that occurs at some time during the external cycle (see Figure 1 for the quantum system and Figure 3 for the classical one).

Although the two frameworks seem to be similar for the main result, namely, being able to form topological phases at similar conditions, the two also differ from each other at least in one respect: Whereas the quantum topological phase converges systematically to π as $G \to \infty$ (for a given $\tilde{T}$), we do not encounter such a situation for the classical phase because this phase increases indefinitely as $\alpha \to 1$ (without showing any tendency to converge). The only way to limit this consistent increase is to impose some kind of (semiclassical) quantization to inhibit the system from reaching the separatrix. This cannot be achieved within single-coordinate models; however, it can be achieved within certain multicoordinate models. Therefore, it would be of interest to extend both the quantum and classical treatments to multicoordinate models.

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