

Aharonov-Anandan phase and the quasistationarity of driven quantum systems

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Abstract. – We derive necessary and sufficient conditions for the quasistationarity of time-dependent quantum systems and point out the relationship between the degree of quasistationarity, the Fubini-Study metric, and the Aharonov-Anandan phase. As an illustration, we analyze the dynamical localization of an electron in a double quantum well and the sustainability of field-induced orientation of polar molecules.

Introduction. – The capability of steering the quantum dynamics into predefined paths by external fields has profound implications for physical and (bio) chemical processes. *E.g.*, laser-orienting molecules is essential for molecular trapping, electron transfer reactions and laser-induced isomerization [1–3]. Major efforts are currently devoted to developing techniques and concepts for promoting a quantum system into a state for which at a certain time t_c , the expectation value of a given observable achieves a predefined (control) quantity [4]. The general question of how to maintain this desired value for a time lag t_s , *i.e.*, the dynamical sustainability of the control process, has not been addressed specifically. This issue is, however, of vital importance for applications. For instance, in a chemical reaction the observable of interest might be the reactants relative orientation that acts as the control parameter for the reaction yield. If the reaction takes place on a time scale t_{reac} , it is essential that the orientation persists for a time t_s larger than t_{reac} .

The purpose of the present work is to develop general concepts for determining the properties of the external, time-dependent driving fields that lead to a coherent control process sustainable in time. For a system residing in a known state at $t = 0$, one aims at steering with time-dependent external fields the expectation values $\langle O \rangle(t)$ of the observable O to attain the desired value $\langle O \rangle_c(t = t_c)$. Here, t_c is the duration of the control process and $\langle O \rangle(t)$, $\forall t$ are measured relative to $\langle O \rangle_0 = \langle O \rangle(t = 0)$. The question posed here is what are the necessary and sufficient conditions to sustain $\langle O \rangle(t > t_c)$ close to $\langle O \rangle_c$ for a given time lag t_s . Here we deal with non-stationary systems that are well describable in terms of pure states composed by a coherent superposition of a finite number N of unperturbed states.

Formulation of the problem. – It is instructive to introduce some general definitions.

Definition 1. A time-dependent observable is called a (field-induced) *quasistationary* observable if within $t_c \leq t \leq t_s$ the relation $|\langle O \rangle(t) - \langle O \rangle_c| < \eta$ applies, where $|\langle O \rangle_c| \gg \eta \in \mathcal{R}^+$. Thus, η characterizes the degree of quasistationarity of $\langle O \rangle(t)$ during $t \in [t_c, t_s]$.

Definition 2. A time-dependent observable is called *cyclic quasistationary* if it is quasistationary and its expectation value satisfies $\langle O \rangle(t_c + \mathcal{T}_k) = \langle O \rangle(t_c + \mathcal{T}_{k-1})$ ($k = 1, 2, \dots, n_c$), with $\mathcal{T}_0 = 0$, n_c is the number of cycles, and \mathcal{T}_k ($\mathcal{T}_k > 0$) is the duration of the k -th cycle.

Definition 3. A time-dependent observable is called *periodic quasistationary* (PQ) if it is quasistationary and there exists $\mathcal{T} > 0$ such that $\langle O \rangle(t_c + k\mathcal{T}) = \langle O \rangle(t_c)$ with $k = 1, 2, \dots, n_{pc}$. The quantity \mathcal{T} is then referred to as the period of the observable and n_{pc} is the number of periodic cycles. In general $n_c \geq n_{pc}$, for a periodic cycle may contain sub-cycles. Examples of PQ processes are the coherent suppression of tunnelling (CST) [5–7], dynamical localization [6, 8], and sustainable molecular orientation [9]. The CST occurs when a particle in a symmetric double quantum well (SDQW) attains at $t = t_c$ a state that is localized in one of the wells (say the left one). Applying an appropriate continuous-wave (CW) laser field (with a period T) the particle remains localized in the left well, meaning that the tunnelling is coherently suppressed [5–7]. To monitor the system one utilizes the time-dependent probability $P_L(t)$ of finding the particle in the left well. The CST occurs when $P_L(t_c + kT) \approx P_L(t_c)$ ($k = 1, 2, 3, \dots$) [5–7]. If for a given state $|\Psi(t)\rangle$ the expectation value of *any* observable is PQ, then the state is called a PQ state.

Quasistationarity and Aharonov-Anandan phase. – A *necessary* condition for a quantum state to be PQ is that the corresponding wave function possesses a periodic cyclic evolution, *i.e.*

$$|\Psi(t_c + k\mathcal{T})\rangle = e^{i\phi_k} |\Psi(t_c)\rangle, \quad k = 1, 2, \dots, n_{pc}, \quad (1)$$

where $\phi_k \in \mathcal{R}$ is the phase change within k periodic cycles and \mathcal{T} stands for the duration of each periodic cycle. The total phase ϕ ($\exp[i\phi] = \langle \Psi(t_c) | \Psi(t_c + k\mathcal{T}) \rangle$) acquired by the wave function during an evolution cycle can be written as $\phi_T = \phi_D + \phi_{AA}$, where ϕ_D and ϕ_{AA} represent the dynamical and the Aharonov-Anandan (AA) phases [10–13], respectively. For a given physical system the dynamical phase ϕ_D is not uniquely determined, since it is only defined up to a gauge transformation. The Aharonov-Anandan phase $\phi_{AA} = \phi_T - \phi_D$, however, is gauge invariant and constitutes a uniquely determined property of the physical system, *i.e.*, ϕ_{AA} is a geometric quantity in that it does not depend on the choice of the Hamiltonian as long as the Hamiltonians describe the same closed path in the projective space⁽¹⁾.

For a further progress we employ the Floquet formalism [6]. For a periodic external field with a period T and frequency $\omega = 2\pi/T$, the system state vector is expressible as

$$|\Psi(t)\rangle = \sum_{\lambda} A_{\lambda} e^{-i\varepsilon_{\lambda} t/\hbar} |\Phi_{\lambda}(t)\rangle. \quad (2)$$

The Floquet modes $|\Phi_{\lambda}(t)\rangle$ have the same periodicity as the external field and ε_{λ} are the corresponding quasienergies. According to conventional wisdom, the degeneracy of quasienergies is a necessary condition for the occurrence of CST [6] (CST is just a particular case of PQ). This general belief is not strictly correct and leaves open the possibility of achieving CST in the absence of quasienergy degeneracy: This can be seen in case of a two-level system (TLS) for which the state vector (2) at stroboscopic times is given by

$$|\Psi(t_c + kT)\rangle = e^{-\frac{i}{\hbar}\varepsilon_2 kT} \left[e^{-\frac{i}{\hbar}(\varepsilon_1 - \varepsilon_2)kT} A_1 e^{-\frac{i}{\hbar}\varepsilon_1 t_c} \Phi_1(t_c) + A_2 e^{-\frac{i}{\hbar}\varepsilon_2 t_c} \Phi_2(t_c) \right]. \quad (3)$$

⁽¹⁾The wave function of a time-dependent N -level system is expressible as a coherent superposition of the N stationary eigenstates of the unperturbed system. The coefficients of this expansion constitute the components of an N -dimensional complex vector in the N -dimensional complex space \mathbb{C}^N . The corresponding projective Hilbert space, usually denoted by $\mathbb{C}P^{N-1}$, is defined as the set of all complex lines in \mathbb{C}^N that pass through the origin (these lines are sometimes referred to as “rays”). Thus, all the vectors in \mathbb{C}^N that differ by only a multiplicative phase have the same image in the projective space $\mathbb{C}P^{N-1}$. Hence, trajectories in the Hilbert space corresponding to the evolution of a cyclic state project onto closed curves in the projective space.

ϵ_1 and ϵ_2 are the representatives of the two quasienergy classes in the first Brillouin zone. The state vector (3) turns periodic cyclic (cf. eq. (1)) if all the relevant Floquet states have the same phase (modulo 2π) at $t = t_c + \mathcal{T}$, *i.e.*, if one of the following conditions is fulfilled: a) If $\epsilon_1 - \epsilon_2 = n\hbar\omega$; ($n \in \mathcal{Z}$). b) If $A_1 = 0$ or $A_2 = 0$. c) If $(\epsilon_1 - \epsilon_2)l = m\hbar\omega$; ($l, m \in \mathcal{Z}$, $m/l \notin \mathcal{Z}$).

The condition a) corresponds to the degeneracy of quasienergies and leads to $\mathcal{T} = T$. The condition b) results in $\mathcal{T} = T$ and occurs when the wave function collapses into a Floquet state. The condition c) implies a periodic cyclic evolution with the duration of each periodic cycle being a multiple of the period of the field, *i.e.*, $\mathcal{T} = |l|T$. Notably, the conditions b) and c) *do not* require crossing of quasienergies. The conditions a), b), and c) can be regarded as *necessary* conditions for PQ. Generalization to N -level systems is readily performed along the same lines. Thus, prerequisites for the cyclic evolution of an N -level system are the conditions a), c), or their combinations have to occur repeatedly (*i.e.*, they have to be fulfilled for all the combinations of pairs of quasienergies corresponding to the Floquet modes that enter the expansion (2)). The generalization of condition b) is the requirement that all but one of the expansion coefficients A_λ must vanish. We stress, however, that conditions a), b), c), or their combinations are not *sufficient* for a state to be PQ, since only the periodicity of time-dependent observables is then guaranteed but not quasistationarity. To derive *necessary and sufficient* conditions for PQ we proceed as follows: Let λ_i ($i = 1, 2, \dots, N-1$) be the coordinates on the projective Hilbert space corresponding to an N -level system and let ϕ_G be the geometric phase (see [10] and references therein) acquired by the wave function through an arbitrary (but unitary) evolution. We introduce the N -dimensional space \mathcal{L}_ξ with points ξ determined by the set of coordinates $\xi_i = \lambda_i$; $\xi_N = 2\phi_G$ with a metric defined as $\tilde{g} = \begin{pmatrix} g & 0 \\ 0 & 1 \end{pmatrix}$. The $(N-1) \times (N-1)$ block matrix $g = (g_{ij})$, $g_{ij} = \text{Re}[\langle \partial_{\xi_i} \Psi | \partial_{\xi_j} \Psi \rangle] - \langle \partial_{\xi_i} \Psi | \Psi \rangle \langle \Psi | \partial_{\xi_j} \Psi \rangle$, ($i, j = 1, 2, \dots, N-1$) is the Fubini-Study metric [10, 11]. As ϕ_G is defined modulo 2π , we restrict the analysis to the region $0 \leq \xi_N \leq 4\pi$ of \mathcal{L}_ξ . The length of a path $C_{\mathcal{L}}$ with (nonorthogonal) end points $\xi_c = \xi(t_c)$ and $\xi' = \xi(t')$ in \mathcal{L}_ξ is given by (summation over repeated indexes is implied) $L(C_{\mathcal{L}}) = \int_{\xi_c}^{\xi'} (\tilde{g}_{\alpha\beta} d\xi_\alpha d\xi_\beta)^{1/2}$; $\alpha, \beta = 1, 2, \dots, N$. The length $L(C_{\mathcal{L}})$ constitutes a nondegenerate positive-definite functional, which is also a representation invariant. Stationary states are represented in \mathcal{L}_ξ by *stationary* points (*i.e.*, their coordinates are invariant with time) in the hyperplane $\xi_N = 0$ (point A in fig. 1). If $C_{\mathcal{L}}$ is such that $L(C_{\mathcal{L}}) \approx 0$ for $t' = t_s$ the system is quasistationary (curve B in fig. 1). Generally, the opposite is not true. For example, if the path $C_{\mathcal{L}}$ corresponds to multiple turns in the vicinity of ξ_c , the

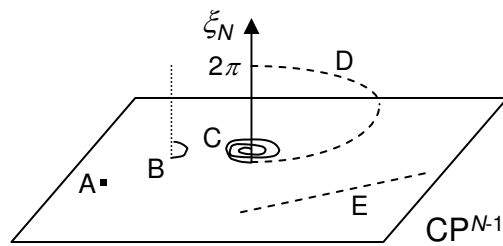


Fig. 1 – Different kinds of trajectories in \mathcal{L}_ξ . Point A represents a stationary state. Trajectories B and C correspond to cyclic quasistationary states with small and large lengths, respectively. D corresponds to a cyclic evolution far from quasistationarity. E represents a non-cyclic state evolving along a large geodesic. The dotted line perpendicular to the hyperplane $\xi_N = 0$ guides the eye.

length $L(C_{\mathcal{L}})$ may be rather long while the system is still quasistationary (curve C in fig. 1). Therefore, $L(C_{\mathcal{L}}) \approx 0$ (with $t' = t_s$) constitutes a *sufficient* condition for quasistationarity. This constraint is, however, too strong. A weaker condition is inferred by taking as a reference the path $C_{\mathcal{L}}^{free}$ corresponding to the evolution of the field-free system in the time interval $t_c \leq t \leq t_s$. The condition $L(C_{\mathcal{L}}) \ll L(C_{\mathcal{L}}^{free})$ for $t' = t_s$ serves thus as a *sufficient* condition for the quasistationarity of the driven system. It has been shown in ref. [11] that

$$\tilde{g}_{\alpha\beta} d\xi_{\alpha} d\xi_{\beta} = \left\langle \dot{\tilde{\Psi}}(t) | \dot{\tilde{\Psi}}(t) \right\rangle dt^2 \geq g_{ij} d\xi_i d\xi_j, \quad (4)$$

where $|\dot{\tilde{\Psi}}(t)\rangle = d|\tilde{\Psi}(t)\rangle/dt$ is the velocity vector in the Hilbert space \mathcal{H} of the curve $t \rightarrow |\tilde{\Psi}(t)\rangle$ at the time t along the path of evolution of $|\Psi(t)\rangle = \langle \Psi(t) | \Psi(t_c) \rangle / (|\langle \Psi(t) | \Psi(t_c) \rangle|) |\Psi(t)\rangle$ [11]. For paths lying on the hyperplane $\xi_N = 0$, (4) reduces to an equality. Such an equality is reached only when the left-hand side of (4) acquires an extremum value corresponding to the shortest paths (called geodesics) in \mathcal{L}_{ξ} . So all the paths lying in the hyperplane $\xi_N = 0$ are geodesics. The *geodesics* on \mathcal{L}_{ξ} can be found by extremizing $L(C_{\mathcal{L}})$ with fixed end points. Because of the structure of the metric \tilde{g} the geodesics on \mathcal{L}_{ξ} correspond to the geodesics determined by the Fubini-Study metric $g = (g_{ij})$ [12] with $\phi_G = 0$, *i.e.*, all the geodesics on \mathcal{L}_{ξ} lie on the hyperplane $\xi_N = 2\phi_G = 0$. Thus we deduce that if a system evolves through a geodesic on \mathcal{L}_{ξ} , then its evolution corresponds to a curve in the hyperplane $\xi_N = 0$ and vice versa [14] (fig. 1). For stationary states, the system evolution corresponds to geodesics of zero length. Assuming the wave functions at the fixed end points of the path to be in phase in the Pancharatnam sense, *i.e.*, if $\langle \Psi(t_c) | \Psi(t') \rangle$ is a positive real number, one finds that the geodesic on \mathcal{L}_{ξ} connecting ξ_c and ξ' is determined by the curve $C_{geo} = \{|\Psi(t)\rangle : t_c \leq t \leq t_c + \arccos[\langle \Psi(t_c) | \Psi(t') \rangle]\} \subset \mathcal{H}$ with

$$|\Psi(t)\rangle = |\Psi(t_c)\rangle \cos(t - t_c) + \left(\frac{|\Psi(t')\rangle - \frac{\langle \Psi(t_c) | \Psi(t') \rangle |\Psi(t_c)\rangle}{\sqrt{1 - \langle \Psi(t_c) | \Psi(t') \rangle^2}} \right) \sin(t - t_c). \quad (5)$$

For systems with cyclic evolution the wave function evolves along a cycle of duration \mathcal{T} to $|\Psi(t' = t_c + \mathcal{T})\rangle = |\Psi(t_c)\rangle$ (recall the wave functions at t_c and t' are in phase). From eq. (5) follows $\langle \Psi(t_c + \mathcal{T}) | \Psi(t_c) \rangle = \cos \mathcal{T} = 1$ and, consequently, $\mathcal{T} = 0$. This means that for a time cyclic system all the geodesics are of zero length [14]. For cyclic evolution the hyperplane $\xi_N = 0$ can thus be identified with the stationary states of the system. The deviation of the path on \mathcal{L}_{ξ} from the hyperplane $\xi_N = 0$ can then be regarded as a measure of the degree of stationarity of a time-dependent quantum system that evolves cyclically. Such a deviation is characterized by $\xi_N = 2\phi_G$. Taking into account that for the case of cyclic evolution ϕ_G reduces to the Aharonov-Anandan (AA) geometric phase ϕ_{AA} [10, 13], a *necessary* condition for the quasistationarity of a cyclic (in time) quantum system can be written as $\phi_{AA} \approx 0$ (for a periodic cycle with its subcycles). This condition is not sufficient, since for some cases in which $\xi(t_c)$ and $\xi(t')$ correspond to the ends of a long trajectory the system can evolve from $\xi(t_c)$ to $\xi(t')$ and back to $\xi(t_c)$ through approximately the same path [14] (note that in such cases the condition $\phi_{AA} \approx 0$ is fulfilled while the system is far from being quasistationary). In the most general situation, the necessary condition $\phi_{AA} \approx 0$ has to be complemented with the condition $L(C_{\mathcal{L}}) \approx 0$ to be sufficient for quasistationarity. Here we focus on the situation [14] where the condition $\phi_{AA} \approx 0$ is a necessary and “sufficient” condition for a cyclic quantum system to be quasistationary (from now on we only address this case). If any of the conditions a), b), c), or their combinations is augmented with the requirement that the corresponding AA geometric phases acquired during a periodic cycle and subcycles approach zero, then the

system is PQ. The degree of quasistationarity (*i.e.* the sustainability) of a cyclic system is quantified as follows: The smaller ϕ_{AA} , the stronger the quasistationarity of the system. This criterium is a consequence of the lack of cyclic geodesics on \mathcal{L}_ξ with nonzero length and is not viable for the case of noncyclic evolution, where a system with $\phi_G = 0$ can be far from quasistationarity if it evolves through a long geodesic (curve E in fig. 1).

So we conclude that parameters of external fields that are favorable for inducing PQ are determined as follows: 1) Find the set \mathcal{S} of the field parameters (frequency, field amplitude strength, ...) for which at least one of the conditions a), b), c) is fulfilled. 2) The optimal field parameters (for inducing PQ) are in the subset of \mathcal{S} with the smallest AA geometric phase.

Below we demonstrate the quasistationarity of two particular observables; we stress however that once the system is driven to a PQ state, any other observable will also be PQ.

Examples. – For an illustration we consider a TLS described by the Hamiltonian $H_{TLS} = -(\hbar\omega_0/2)\sigma_z + \mu V(t)\sigma_x$, where $\hbar\omega_0$ is the energy splitting between the two stationary states $|1\rangle$ and $|2\rangle$ and μ is the transition dipole. $\sigma_{z,x}$ are the Pauli matrices. The Hamiltonian H_{TLS} with $V(t) = V_0 \sin \omega t$ has been studied in the context of CST induced by a CW laser in a (SDQW) [5–7]. In this case, H_{TLS} is invariant under $(\mu \rightarrow -\mu; t \rightarrow t + \pi/\omega)$ and hence the Floquet modes have well-defined generalized parity. Accordingly, quasienergies cross when a system parameter is varied. At these crossing points the tunnelling of a state localized in the left well to the right well is suppressed. In contrast, when the SDQW is subject to an infinite train of unipolar kicks with amplitudes p and period T applied at $t = t_c$, *i.e.* when the interaction potential is $V_{\text{kick}}(t) = p \sum_{j=0}^{\infty} \delta(t - t_c - jT)$, H_{TLS} is no longer invariant under $(\mu \rightarrow -\mu; t \rightarrow t + T/2)$ and the Floquet modes do not have a well-defined generalized parity. According to the von Neumann-Wigner theorem [15], the existence of quasienergy crossings is then no longer guaranteed when a single system parameter is varied. In fact, the quasienergies exhibit typical avoided crossings. The periodically kicked TLS is solvable analytically (*cf.*, *e.g.*, [9, 16]) with quasienergies $\epsilon_{1,2}$ being $\epsilon_1 = -\hbar\omega/(2\pi) \arccos(\cos \varphi \cos \vartheta)$; $\epsilon_2 = -\epsilon_1$, where $\varphi = \mu p/\hbar$ and $\vartheta = \pi\omega_0/\omega$. Thus, when a single parameter is varied, say φ , the condition a), corresponding to the degeneracy of quasienergies is never met. The system, however, exhibits CST in the *absence of quasienergy degeneracy*, as demonstrated numerically [17]. Assuming the system to have been prepared in a time-dependent state $|\Psi(t)\rangle = c_1(t)|1\rangle + c_2(t)|2\rangle$ such that $c_{1,2}(0) = \pm 1/\sqrt{2}$, then at $t = 0$ the particle is localized in the left well. If no external field is applied for $t > 0$, then $P_L(t > 0) = (1 + \cos(\omega_0 t))/2$. Consequently, the particle oscillates from one well to the other with period $T_0 = 2\pi/\omega_0$ and the initial localization is not sustainable in time. To sustain the initial particle localization, a time-dependent field capable of inducing quasistationarity is required. Concerning the periodically kicked TLS we found that for $\varphi = (2n + 1)\pi/2$, $|\Psi(t)\rangle$ is cyclic regardless of the value of ϑ . For $t_c = T/2$ the condition b) is fulfilled and each periodic cycle is a single cycle with a duration $\mathcal{T} = T$. For $t_c < T/2$ the condition c) is fulfilled and each periodic cycle lasts $\mathcal{T} = 2T$ and encompasses two subcycles with durations $2t_c$ and $2(T - t_c)$. If $t_c = 0$, we find for each periodic cycle

$$\phi_{AA} = (\pi/2)(1 - \cos[\pi T/T_0]). \quad (6)$$

Thus, from the requirement $\phi_{AA} \approx 0$ we infer that for a periodic train of kicks with amplitudes such that $\varphi = (2n + 1)\pi/2$ (this guarantees periodicity) and a period such that $T \ll T_0/\pi$ (this ensures quasistationarity) the system is PQ. *I.e.*, a particle initially localized in one of the wells remains there while the pulse train is on. If the kicks amplitude is such that $\varphi = (2n + 1)\pi/2$ (with n an integer) then the kicked TLS is always cyclic regardless of the value of the period T of kicks. In such a situation, the dependence of the probability $P_L(t) = |\langle \Psi(t) | l \rangle|^2$ on the period T of the train of kicks can be mapped into a dependence

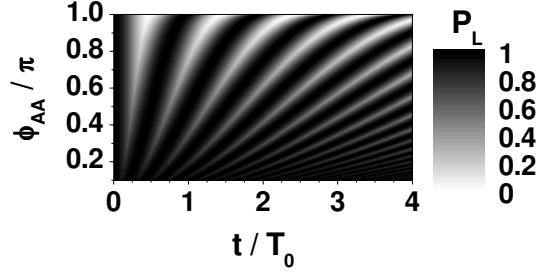


Fig. 2 – Periodically kicked TLS: Probability P_L of finding the particle in the left well as a function of the AA geometric phase ϕ_{AA} and the time. The strength of the kicks is chosen as $p = \hbar\pi/(2\mu)$.

on ϕ_{AA} , since each value of T is related to the phase ϕ_{AA} given by (6). Figure 2 shows $P_L(t) = |\langle \Psi(t) | l \rangle|^2$ for the case of the periodically kicked TLS as a function of ϕ_{AA} and the time (we choose $\varphi = \mu p / \hbar = \pi/2$). Figure 2 evidences that the degree of quasistationarity increases when the AA phase approaches zero. For $\phi_{AA} \approx \pi$ quasistationarity is absent and the particle oscillates from one well to the other with the field-free period T_0 .

We performed also numerical calculations for a periodically kicked four-level rotor (FLR) to describe the orientation of polar molecules induced by unipolar pulses [9]. Within the rigid-rotor approximation, the dynamics of a polar molecule subjected to a periodic train of short unipolar pulses is given by [9] $i\hbar\partial_t\Psi_{FLR}(\theta, \phi, t) = [L^2/(2I) - \mu_0 V_{\text{kick}}(t) \cos(\theta)]\Psi_{FLR}(\theta, \phi, t)$, where $I = mR_0^2$ is the moment of inertia at the internuclear equilibrium distance R_0 and m is the reduced mass of the nuclei. L stands for the angular momentum operator, μ_0 is the permanent dipole moment, θ represents the angle between the molecular axis and the applied field (polarized along the z -axis), ϕ specifies the corresponding azimuthal angle. Because of the cylindrical symmetry around the molecular axis, the projection of the angular momentum M_J onto the field polarization axis is conserved. Assuming the initial condition $M_J = 0$, the time-

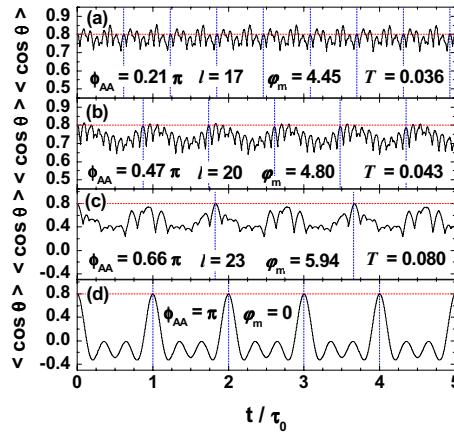


Fig. 3 – The molecular orientation parameter $\langle \cos \theta \rangle$ vs. time. τ_0 is the molecule rotational period. T and $p = \hbar\varphi_m/\mu_0$ are the period and the strength of the fields favorable for cyclic evolution. The smallest ϕ_{AA} (inset a) corresponds to the strongest sustainable orientation. Horizontal and vertical lines mark, respectively, the orientation control value $\langle \cos \theta \rangle(t_c) \approx 0.8$ and evolution cycle periods $T = lT$.

dependent wave function that describes the quantum dynamics of the molecule (within a four-level approximation) is expressed as $\Psi_{FLR}(\theta, \phi, t) = \sum_{J=0}^3 c_J(t) Y_{J,0}(\theta, \phi)$. Here $Y_{J,M}(\theta, \phi)$ are spherical harmonics and c_J are expansion coefficients obtained by solving for Ψ_{FLR} .

The observable of interest is $\langle \cos \theta \rangle(t) = \langle \Psi_{FLR}(\theta, \phi, t) | \cos \theta | \Psi_{FLR}(\theta, \phi, t) \rangle$, a quantity that characterizes the degree of the molecular axis orientation along the applied-field polarization direction. The orientation parameter varies in the interval $[-1, 1]$. Perfect orientation is achieved when $\langle \cos \theta \rangle(t)$ reaches extremal values. Assuming the molecule to be initially prepared such that $c_J(t_c) = 1/2$, then at $t = t_c$ the molecule is well oriented, with $\langle \cos \theta \rangle(t_c) \approx 0.8$. To show how quasistationarity is induced we performed numerical calculations for a NaI molecule following the same procedure as in [9]. In the absence of external fields NaI has a rotational period of $\tau_0 \approx 138$ ps. For a train of unipolar pulses we find several sets of field parameters within the range $0.036 \leq T \leq 0.1$ and $3 \leq \varphi_m = \mu_0 p / \hbar \leq 7$ that lead to the cyclic evolution of the system. Some of these situations are displayed in fig. 3. In all cases we find condition c) is responsible for the periodic cyclic evolution. The periodicity (with a period $\mathcal{T} = lT$) of $\langle \cos \theta \rangle$ is evident. Figure 3(a) corresponds to the smallest value of ϕ_{AA} . Therefore, the situation of fig. 3(a) is optimal (*i.e.*, it constitutes a sustainable strong molecular orientation). With increasing ϕ_{AA} the orientation is lost. For a field-free molecule (fig. 3(d)) $\phi_{AA} = \pi$ applies and the orientation parameter averaged over a rotational period vanishes, *i.e.* the initial value of the molecular orientation (~ 0.8) is not sustainable.

Conclusions. – In summary, we identified necessary and sufficient conditions for the quasistationarity of a non-equilibrium quantum system and pointed out the relationship between quasistationarity, the Fubini-Study metric, and the Aharonov-Anandan phase. We illustrated our findings by numerical results for the dynamical localization of an electron in a double quantum well and for the sustainability of field-induced orientation of polar molecules.

REFERENCES

- [1] DION C. M. *et al.*, *J. Chem. Phys.*, **105** (1996) 9083.
- [2] STAPELFELDT H. and SEIDEMAN T., *Rev. Mod. Phys.*, **75** (2003) 543.
- [3] AOIZ F. J. *et al.*, *Chem. Phys. Lett.*, **289** (1998) 132.
- [4] SCHIRMER S. G., FU H. and SOLOMON A. I., *Phys. Rev. A*, **63** (2001) 063410.
- [5] GROSSMANN F., DITTRICH T., JUNG P. and HÄNGGI P., *Phys. Rev. Lett.*, **67** (1991) 516.
- [6] GRIFONI M. and HÄNGGI P., *Phys. Rep.*, **304** (1998) 229.
- [7] BAVLI R. and METIU H., *Phys. Rev. A*, **47** (1993) 3299.
- [8] DUNLAP D. H. and KENKRE V. M., *Phys. Rev. B*, **34** (1986) 3625.
- [9] MATOS-ABIAGUE A. and BERAKDAR J., *Chem. Phys. Lett.*, **382** (2003) 475.
- [10] SHAPER E. and WILCZEK F. (Editors), *Geometric Phase in Physics* (World Scientific) 1989.
- [11] PATI A. K., *Phys. Rev. A*, **52** (1995) 2576.
- [12] MUKUNDA N. and SIMON R., *Ann. Phys. (N.Y.)*, **228** (1993) 205.
- [13] AHARONOV Y. and ANANDAN J., *Phys. Rev. Lett.*, **58** (1987) 1593.
- [14] We exclude the case of cyclic states evolving through accidentally reversed trajectories in which the system evolves from $\xi(t_c)$ to $\xi(t')$ and back to $\xi(t_c)$ through the same path. In such a situation, $\xi_N = 0$ and the corresponding trajectory is not necessarily a geodesic.
- [15] VON NEUMANN J. and WIGNER E., *Phys. Z.*, **30** (1929) 467.
- [16] GEISEL T., *Phys. Rev. A*, **41** (1990) 2989.
- [17] MATOS-ABIAGUE A. and BERAKDAR J., *Appl. Phys. Lett.*, **84** (2004) 2346.