Universal wave functions structure in mixed systems

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Abstract – When a regular classical system is perturbed, nonlinear resonances appear as prescribed by the KAM and Poincaré-Birkhoff theorems. Manifestations of this classical phenomena to the morphologies of quantum wave functions are studied in this letter. We reveal a systematic formation of a universal structure of localized wave functions in systems with mixed classical dynamics. Unperturbed states that live around invariant tori are mixed when they collide in an avoided crossing if their quantum numbers differ in a multiple of the order of the classical resonance. At the avoided crossing eigenstates are localized in the island chain or in the vicinity of the unstable periodic orbit corresponding to the resonance. The difference of the quantum numbers determines the excitation of the localized states which is revealed using the zeros of the Husimi distribution.

Introduction. – Hamiltonian classical systems have a variety of dynamical behaviors [1]. On one side there are integrable systems with conserved quantities as degrees of freedom resulting in constrained dynamics around invariant tori. On the other extreme, chaotic systems are characterized by properties of mixing and ergodicity. The phase space is dynamically filled and only constrained by the conservation of the energy. The quantum mechanics of these dynamical systems has been intensively studied in the last forty years and the correspondence between classical and quantum mechanics has been established with solid grounds [2,3].

It is unusual that a generic system belongs to those extreme cases as it would display mixed dynamics where chaos coexists with regions of regular motion. The dynamics of mixed systems are more subtle mainly because regular and chaotic regions are connected by fractal boundaries. A standard way to understand this complex dynamics is perturbing an integrable system. Its response to weak perturbations has been completely understood in terms of the celebrated Kolmogorov-Arnold-Moser (KAM) and the Poincaré-Birkhoff (PB) theorems [4,5]. The KAM theorem states that depending on the rationality of the frequencies of the motion, some of the invariant tori are deformed and survive while others are destroyed. The consequence of the fate of rational tori is the survival of an equal even number of stable (elliptic) and unstable (hyperbolic) periodic orbits (PB theorem). In the vicinity of a stable orbit, a chain of islands of regularity surrounded by a chaotic sea is developed [1]. These classical structures, usually called nonlinear resonances, have important influences in various phenomena from chemical systems, solid-state physics to nano optics [6–8].

Almost ubiquitous, the quantum mechanics of nearly regular and mixed systems is much less known than the integrable or chaotic cases. The relation between classical dynamics and avoided crossings (ACs) observed in the spectra of quantum systems has been a subject of several studies in the past. In chaotic systems, several aspects of ACs are well known [9,10]. In mixed systems, using a semiclassical approach, nonlinear resonances were shown to be responsible for energy levels approach each other closely, exhibiting avoided crossings, instead of crossings as happen in integrable systems [11–13]. More recently, Brodier, Schlageck, and Ullmo [14], have developed a semiclassical theory of resonance assisted tunneling showing the coupling interaction term between states localized in invariant tori. Interestingly enough, a selection rule emerges because the interaction only occurs between states with quantum numbers that differ in a multiple of the order of the resonance. So, it is expected that the appearance of a nonlinear resonance is revealed in the quantum spectra with series of ACs of states localized in tori with quantum numbers that fulfill the selection rule. In fact, this has been shown in ref. [15] when the multiple is equal to one.
In this letter we go one step forward and show such a systematic for ACs between states with quantum numbers that differ in a multiple greater than one. We compute the series of ACs corresponding to a resonance of a paradigmatic system of quantum chaos studies and show that the states in the center of AC have a surpassing structure: one is an excited state localized in the island chain and the other in the associated periodic orbit. This shows that a classical nonlinear resonance imprints clear signatures in the wave function morphologies. The excitations of the localized structure are related to the number of zeros in each island or in the vicinity of the unstable periodic orbit (PO) associated to the resonance.

The systematic of ACs generated by a nonlinear resonance is a fertile field to test the building block of the semiclassical theory of resonance assisted tunneling, that is, the interaction coupling term between states localized in invariant tori [14]. For these reasons, we have studied the behavior of the series of ACs varying the value of the Planck constant \( \hbar \). We clearly show an unexpected result that the semiclassical expression for the interaction coupling term works better in the deep quantum regime; seeing signs of an improvement of this theory seems necessary.

**The model.** We study the Harper map in the unit square as a model system,
\[
\begin{align*}
p_{n+1} &= p_n + k \sin(2\pi q_n) \quad (\text{mod } 1), \\
qu_{n+1} &= q_n - k \sin(2\pi p_{n+1}) \quad (\text{mod } 1),
\end{align*}
\]
where \( k \) is a parameter that measures the strength of the perturbation. This map can be understood as the stroboscopic version of the flow corresponding to the (kicked) Hamiltonian
\[
H(p, q, t) = -\frac{k}{2\pi} \cos(2\pi p) - \frac{k}{2\pi} \cos(2\pi q) \sum_n \delta(t-n). \tag{2}
\]

The Harper map comprises all the essential ingredients of mixed dynamics and is extremely simple from a numerical point of view. For very small \( k \), the dynamics described by the map is essentially regular, that is, the phase space is covered by invariant tori. As \( k \) gets bigger, nonlinear resonances (islands) start to appear following the KAM and PB theorems. The system presents a mixed dynamics with regions of regularity around the origin and the corners coexisting with chaos as shown in fig. 1(c) and 2(e) and (f). For \( k > 0.63 \) there are no remaining visible regular islands due to chaotic dynamics covering all the phase space.

The quantum mechanics of the Harper map is described by the unitary time-evolution operator [17,18]
\[
\hat{U}_k = \exp[iNk \cos(2\pi \hat{q})] \exp[iNk \cos(2\pi \hat{p})], \tag{3}
\]
with \( N = (2\pi \hbar)^{-1} \), that is, a Hilbert space of \( N \) dimensions for a fixed value of \( \hbar \). This is due to the quantization on the torus which implies that the wave function should be periodic in both position and momentum representations. The semiclassical limit is reached as \( N \) takes increasing values.
For a fixed value of \( N \), the spectrum of eigenphases \( \phi_i(k) \) and eigenfunctions \( |\psi_i(k)\rangle \) of the evolution operator of the quantum map are obtained by diagonalization of eq. (3). The characteristics of \( |\psi_i(k)\rangle \) are analyzed using the Husimi distribution [19]. The Husimi representation of an eigenstate of a quantum map is a quasiprobability distribution in phase space that has exactly \( N \) zeros in the unite square [16].

Eigenphases \( \phi_i(k) \) change linearly for very small strength of the perturbation \( k \) and the Husimi distribution of the eigenstates \( |\psi_i(k)\rangle \) is localized in the vicinity of invariant tori [16,18]. Eigenstates with negative slope are centered in \( (q,p) = (1/2,1/2) \) and in \( (q,p) = (0,0) \) for positive slope. A bigger absolute value of the slope implies that the state is nearer to the periodic point \( (q,p) = (1/2,1/2) \) or \( (q,p) = (0,0) \). The states with maximum absolute value of the slope resemble a Gaussian distribution centered in the mentioned periodic points and correspond to label 1 (negative slope) and \( N \) (positive slope). Excited states have \( n \) zeros inside the region of maximum probability, being \( n + 1 \) their label for negative slope and \( (N - (n + 1)) \) for positive slope.

**Method.** – The influence of a nonlinear resonance \( r:s \) to quantum maps is uncovered using the following numerical procedure. We consider a series of eigenstates \( |\phi_i(k)\rangle \) with \( i = 1,\ldots,i_{max} \) \((i_{max} < N/2)\) for a very small perturbation \( k = k_0 \) and we associate for each state \( i \) a perturbed one with \( k = k_0 + \delta k \), if the overlap \( \langle \phi_i(k_0)|\phi_j(k_0 + \delta k)\rangle \) is the maximum of all \( j \). Then, this procedure is repeated for perturbations \( k = k_0 + n\delta k \) with \( n = 2,\ldots,n_{max} \) an integer. Thus, we have associated a series of perturbed states and eigenphases with the unperturbed one. From now on, we refer the quasistate \( i \) to the series of perturbed states associated to \( |\phi_i(k_0)\rangle \) and the quantum number to the label \( i \) of the quasistate.

If we join lines through the eigenphases of each quasistate, we can establish where two of the quasistates have a crossing. In the vicinity of that intersection we find an AC of eigenstates that has the localized properties of the states at \( k = k_0 \). If the dimension \( N \) of the Hilbert space is small enough, the previous procedure can be done by visual inspection of the spectra as a function of the perturbation \( k \). The value of \( \delta k \) is crucial for the success of the procedure: if it is small and for an \( n, k = k = k_0 + n\delta k \) falls close to an AC, the quasistate loses the localization properties related to the unperturbed state and the method fails. On the contrary, if \( \delta k \) is very large the method also fails because the phase of the quasistate has an erratic development and hence it is not possible to find its crossing with other quasistates.

Once we have computed the quasistates for a series of unperturbed eigenstates \( |\phi_i(k_0)\rangle \), we obtain the position of the corresponding ACs looking at the intersection of the eigenphases \( i \) with \( j \). If we are considering a nonlinear resonance \( r:s \) with \( r \) the number of islands, we compute the series of ACs for quasistates with quantum numbers \( i \) and \( j \) such that

\[
\Delta n = |i - j| = lr
\]

with \( l \) an integer.

In ref. [15] the series of AC for two different nonlinear resonances of the Harper map was found for \( l = 1 \) using visual inspection of the spectra. This was feasible due to the small value of the dimension of the Hilbert space \( N \). In the following, we show that using the described method it is possible to find the series of ACs for greater \( l \) and \( N \).

**Results.** – The Harper map is a mixed system that has an usual regular to chaotic transition. As the perturbation strength \( k \) grows, nonlinear resonances get bigger as the surrounding chaotic layers and eventually disappear covered by the chaotic sea. The resonances 6:1 reach the largest size (see fig. 1(c), fig. 2(e), (f) and also refs. [14,15]). Other resonances as 8:1, 10:1 and 14:1 take up an appreciable region of phase space.

Our main goal is to disentangle the influence of nonlinear resonances on the eigenfunctions of a mixed system. We focus on the resonance 6:1 of the Harper map. Using the method described below, we have found the ACs associated to the intersections of the eigenphases of quasistates with a quantum number that differs in a multiple
of 6, the order of the resonance 6:1, that is, for \( \Delta n = 6l \), with \( l = 1, 2 \) and 3. The calculations are done for three sizes of the Hilbert space \( N = 80, 160 \) and 300. As an example, in figs. 1 and 2 we show the morphologies of the eigenstates in these ACs.

In fig. 1(a) and (b) the behavior of the wave functions at the center of an AC obtained from quasistates with quantum numbers that differ in 6 is exhibited. In fig. 1(d) we show the region of the spectra where the AC takes place. The eigenphases of the states that have the AC are plotted with red lines. The eigenfunctions before (A and B) and after (C and D) the AC are plotted at the bottom of fig. 1. As usual, the states exchange their distributions upon AC ((A) ↔ (D) and (B) ↔ (C)). But surprisingly, the distributions at the center of AC are highly localized. One state has the maximum of the probability of the Husimi distribution in the vicinity of the island chain and has 6 zeros near the corresponding unstable PO (see fig. 1(a)). The other state (fig. 1(b)), is localized in the vicinity of the island chain and has one zero in the center of each island. This is better displayed in fig. 1(c) where part of the classical phase space and the zeros of the states of fig. 1(a) and (b) are shown. The zeros of the states (a) are plotted with \( \times \) and with \( \circ \) for (b).

When the AC is between states with quantum numbers that differ in a multiple (greater than one) of the number of islands in the chain, the morphologies of the eigenstates are more impressive. As an example of this phenomenon, in fig. 2 we show the Husimi distributions at the center of AC between states with quantum numbers that differ in 12 (fig. 2(a), (c) and (e)) and 18 (fig. 2(b), (d) and (f)). As can be seen in fig. 1, one of the states is localized in the island chain, but in fig. 2(a) there is one zero inside each island and two zeros for fig. 2(b). This fact points out that these states are excited states of the island chain. The other states, fig. 2(c) and (d), are localized in the corresponding unstable PO and the zeros are accumulated inside the islands. This fact resemble the behavior of scar functions builded for chaotic system [20,21]. To see the location of the zeros in more detail, in fig. 2(e) and (f) we plot a part of the classical phase space and the zeros of the Husimi distributions of panels (a), (c) and (b), (d). We have seen that when \( \Delta n = 24 \) the structure of the wave functions at the AC has the same systematic with one more zero in each island of the chain. In summary, in the center of an AC with \( \Delta n = 6l \), one of the states is localized in the vicinity of the island chain and has \( l - 1 \) zeros in each island, whereas the other state has the maximum probability around the unstable PO of the resonance and has \( l \) zeros in each island. It is important to note that in figs. 1 and 2 only the zeros of the Husimi distribution that are inside or over the regions of maximum probability are plotted. The other zeros that lie outside these regions and have an exponentially small probability are not displayed.

The semiclassical theory of resonance assisted tunneling predicts a coupling strength between quasimodes located on opposite sides of a nonlinear resonance and therefore an eigenphase difference \( \Delta \phi \) for the ACs considered before. This theory was recently developed and applied in several situations [14,22–24]. The starting point is the classical secular perturbation theory which allows to construct an effective time-independent Hamiltonian that describes the local dynamics near a \( r:s \) resonance of the map,

\[
H_{r:s} \approx H_0(I_{r:s}) + \sum_{l=1}^{\infty} V_{r,l}(I_{r:s}) \cos(lr + \phi_l) \tag{5}
\]

with \( H_0(I_{r:s}) \) an integrable approximation of the Hamiltonian of the map [14]. This effective Hamiltonian entails a selection rule that an eigenstate of the unperturbed Hamiltonian of a quantum number \( n \) can be coupled to another state of a quantum number \( n + lr \) (1 an integer) with a strength proportional to \( V_{r,l} \):

\[
V_{r,l} e^{i\phi_l} = \frac{1}{i2\pi N} \int_0^{2\pi} \exp(-irl\theta) \delta I_{r,s}(\theta) d\theta, \tag{6}
\]

\[
\delta I_{r,s}(\theta) \text{ being given by}
\]

\[
\delta I_{r,s}(\theta) = I^{(-1)}(I_{r:s}, \theta) - I_{r,s}, \tag{7}
\]

where \( I^{(-1)}(I_{r:s}, \theta) \) is the action variable obtained by applying the inverse Poincaré map to \( (I, \theta) \). The interaction coupling strength (eq. (6)) is numerically computed following the next steps. First, the resonant periodic torus is found, and its action \( I_{r,s} \) calculated. Then, a large number of points \((q_i, p_i)\) and its corresponding angle variable \( \theta_i \) belonging to the resonant tours are computed. We applied a back-propagation for these points with the exact inverse map. The associated perturbed action of each point \( I^{(-1)}(I_{r:s}, \theta_i) \) is computed by numerical propagation in a complete cycle. Using these quantities the coupling interaction \( V_{r,l} \) is calculated with eq. (6). Finally, the semiclassical approximation of the eigenphases differences \( \Delta \phi \) produced by a resonance \( r:s \) for AC, that comes from the intersection of quasistates eigenphases with \( \Delta n = lr \), results in

\[
\Delta \phi \approx |V_{r,l}|/2h. \tag{8}
\]

We have computed the semiclassical approximation of the eigenphase difference for the resonance 6:1 with \( l = 1, 2 \) and 3 as a function of the strength \( k \). The integral was done using the 7-point Newton-Cotes formula and with an integrable approximation of the Harper Hamiltonian (eq. (2)) up to the 5th order that was obtained using the Baker-Campbell-Hausdorff formula in eq. (3) and the semiclassical relation between the quantum commutator and the Poisson brackets [25]. In fig. 3, the semiclassical approximation of the eigenphase difference \( \Delta \phi \) is plotted with lines (\( l = 1 \), solid; \( l = 2 \), dashed; and \( l = 3 \), dotted). The eigenphases differences \( \Delta \phi \) for the ACs between states with \( \Delta n = 6l \), with \( l = 1, 2 \) and 3 are plotted with symbols. These eigenphases differences were obtained from the quantum spectra using the method presented before.
for three values of the number of states of the Hilbert space $N = 80, 160$ and 300.

In fig. 3 we can see that, contrary to the expectations, the semiclassical approximation works very nice for all $l$ only in the case of $N = 80$, the minimum value of the considered number of states of the Hilbert space. This fact indicates that the semiclassical expression of $\Delta \phi$ (eq. (8)) works in the deep quantum regime and separates from quantum results as $N$ increases. The discrepancies for large $N$ become a strong evidence that the semiclassical theory of the interaction coupling needs an improvement [14]. We mention that in ref. [23] the action dependence to the interaction coupling strength (eq. (6)) was introduced. We have computed the semiclassical prediction including this correction but the agreement with the quantum eigenphase difference is clearly worse in all the cases that we have studied. We also note that a similar behavior to the size of the Hilbert space was observed in the tunneling-induced level splittings of a very simple one-dimensional model computed with the semiclassical theory of resonance assisted tunneling [24]. In fig. 4 we show an unexpected scaling of the $\Delta \phi$ for $l = 2$ and $l = 3$. The eigenphase difference scales with $h^{\frac{5}{2}}$ for $l = 2$ and with $h^3$ for $l = 3$. This could indicate the existence of an effective $h$ that depends on $l$ and could be a clue for the improvement of the semiclassical theory of the interaction coupling strength (eq. (6)).

**Final remarks.** – In this letter we have shown that a classical nonlinear resonance imprints a systematic influence on the quantum eigenvalues and eigenfunctions of a mixed system. We have found a universal structure embedded in the spectra: states localized in tori interact in AC if the quantum numbers differ in a multiple of the order of the resonance. These series of AC are observed when a parameter of the system is varied producing a development of the resonance characterized by a chain of islands. Surprisingly, eigenstates in the middle of the AC have a particular morphology. One state is localized in the island chain. The difference of the quantum numbers of the unperturbed states that are localized in tori and interact in the AC determines the distribution of the zeros of the Husimi function of the states. These findings, that are not predicted by the semiclassical theory of resonance assisted tunneling, could be of importance in the design of optical microcavities [26–28]. In those devices it is desirable to obtain a specific directional light emission that could be accomplished tuning a system parameter to reach an AC where the states have a desirable localization.

We have compared the eigenphases gaps of the AC with a semiclassical prediction based on the theory of resonance assisted tunneling [14]. We have shown that the semiclassical prediction deviates from the quantum results as we reach the semiclassical limit. This unexpected result indicates that an improvement of this theory is needed.

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