Classical invariants and the quantization of chaotic systems

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Long periodic orbits constitute a serious drawback in Gutzwiller’s theory of chaotic systems, and
then it would be desirable that other classical invariants, not suffering from the same problem,
could be used in the quantization of such systems. In this respect, we demonstrate how a suitable
dynamical analysis of chaotic quantum spectra unveils the fundamental role played by classical
invariant areas related to the stable and unstable manifolds of short periodic orbits.

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The correspondence between quantum and classical mechanics has been a topic of much interest since the
beginning of the quantum theory, and more recently in relation to quantum chaos [1, 2]. The question involves
eliciting the classical objects and properties on which to impose quantum restrictions, this being at the heart
of every semiclassical theory.

Very early, Ehrenfest noticed [3] the importance of classical adiabatic invariants, such as the action, in the
quantization of dynamical systems. Later, Einstein [4] realized that the proper arena to perform this quantiza-
tion for integrable motions are invariant tori [5]. He also remarked that this theory is not applicable to chaotic
motions, due to the lack of supporting invariant classical structures. After that, dynamical invariants are re-
garded as the geometrical objects upon which reason-
able semiclassical theories of quantum states should be constructed. Concerning the associated properties to be
used, those which are canonically invariant seem to be the natural choice, since they render descriptions inde-
pendent on the coordinate system.

Keeping within this scheme, Gutzwiller took in the 1970’s a new route, and chose periodic orbits (POs), and
their individual properties (actions, Maslov indices and stability matrices), leaving aside others (corresponding
manifolds), as the quantizable invariants [6]. In this way, he developed a semiclassical version of the quantum
mechanical Green function, that has become the cornerstone of the semiclassical quantization of chaotic systems.
The resulting density of states appears as the sum of contributions of all POs of the system, and their repetitions.
The phase of each contribution is the action (symplectic area) along the orbit (divided by ℏ), and the amplitude
is proportional to its stability. Unfortunately, this theory suffers from a serious computational problem in the
exponential growth of the number of contributing orbits with the Heisenberg time, \( t_H = 2\pi\hbar\rho(E) \), with \( \rho(E) \) the
energy density. This have precluded its use except in very special situations [7]. In this respect, it is worth empha-
sizing that Gutzwiller’s summation formula can be used in two opposite ways. In the direct route, it can be fed
with classical information to predict quantum eigenvalues. Or alternatively, it can be used in an inverse way to
extract classical magnitudes from the eigenvalues spectrum [8]. Curiously enough, these two operations are not
equivalent, in the following sense. When applied in the direct way, one needs to included longer and longer POs
(with periods of the order of \( t_H \)) to predict higher energy eigenvalues. However, when applied backwards, for ex-
ample, by Fourier transforming the eigenvalues spectrum of a chaotic billiard, the periods (or other properties) of
only short POs, with values up to the magnitude of the Ehrenfest time, \( t_E \), are obtained [10]. This asymmetry is not fully understood yet, and raises fundamental ques-
tions about our present understanding of the quantum mechanics of chaotic systems: are long POs (with peri-
ods of the order of \( t_H \)) relevant?, or its inclusion in the theory of Gutzwiller is only a drawback?, finally, respon-
sible for the unreasonable computational effort involved in the semiclassical computation of physical magnitudes.

In this Letter, we address this issue, by investigating the inverse route in a non–standard way. By explicitly
including the dynamics of short POs (the only relevant in this route) in the Fourier transform process, we de-
velop a method, relying only on purely quantum information, able to extract the pertinent associated informa-
tion from the actual full quantum dynamics of very chaotic systems. We have found conclusive evidence that
the corresponding quantum spectrum contains information about collective invariant objects associated to short
POs, namely, the homoclinic and heteroclinic areas enclosed by their stable and unstable manifolds. This im-
plies some sort of interaction between periodic structures, that can play a role equivalent to that of long POs in the
Gutzwiller formula.

To gauge the dynamical interaction between two POs, A and B, in a quantum sense, we propose the use of the
cross correlation function

\[ C(t) = |\langle \phi_B | \hat{U}(t) | \phi_A \rangle|^2 \]

where \( \hat{U}(t) \) is the time propagation operator, and \( \phi_{A,B} \) are suitable functions associated to the POs, whose nature will be discussed later. In our formula, the second part of the bracket follows the evolution of the nonstationary function associated to one of the POs, and the application of the bra extracts the information relative to the other PO contained in it, thus filtering out (at least to some extend) the rest. By choosing a correlation function as our indicator, we have the same information as in the corresponding spectra, but recast with a more dynamical perspective.

A natural choice for \( \phi_A \) and \( \phi_B \) are wavefunctions living in the vicinity of the corresponding POs. These functions are constructed very efficiently, either by dynamically averaging over the short time dynamics of the associated PO [11], or by minimizing the energy dispersion in a suitable basis of transversally excited resonances [12]. In this work, we use scar functions as defined in Ref. [12]. These functions are highly localized in energy around some mean values satisfying a Bohr–Sommerfeld type quantization rule

\[ \frac{S(E)}{\hbar} - \nu \frac{\pi}{2} = 2\pi n, \]  

where \( S(E) \) is the dynamical action at energy \( E \), \( \nu \) the Maslov index, and \( n \) an integer number.

In order to study the previous ideas, we choose a particle of mass \( 1/2 \) enclosed in a fully chaotic desymmetrized stadium billiard of radius \( r = 1 \) and area \( 1 + \pi/4 \), with Dirichlet conditions on the stadium boundary and Neumann conditions on the horizontal and vertical symmetry axis [see the inset in Fig. 1(a)]. For this system, the action takes a simple semiclassical relation in terms of the mean wavenumber, \( k \), and the length, \( L \), of the PO; namely, \( S(E)/\hbar = kL \).

In our numerical study, we consider the horizontal (A) and V–shaped (B) POs with lengths \( L_A = 4 \) and \( L_B = 2(1 + \sqrt{2}) \), respectively [see the inset in Fig. 1(a)]. Let \( \phi_A \) be the scar function for \( A \) with mean wave number \( k_A \) [obtained from Eq. (2)], and \( \phi_B \) the corresponding for \( B \), with the mean wave number \( k_B \) closest to \( k_A \). We focus in the cross correlation function as defined in Eq. (1), and accordingly, we present in Fig. 1(a) \( C(t) \) for \( k_A = 155.116 \). The most striking feature in the plot is the totally different behavior exhibited by the correlation, below and above times of the order of the Ehrenfest time, \( t_E \), (the actual value of which has been marked with an arrow in the figure). For short times, the correlation function increases monotonically from zero up to the first maximum. This maximum appears at approximately twice the value of \( t_E \), point at which interference starts to be relevant. After that, other maxima appear, and the behavior of the correlation gets very complex for times of the order of the Heisenberg time, \( t_H \), which is equal to one in the units system used by us.

To further characterize the interaction between POs, some representative dynamically meaningful magnitude along the spectra should be defined. For this purpose, we take the maximum of \( C(t) \) in the time interval \( [0, t_0] \)

\[ C_{\text{max}}(t_0, k_A) \equiv \max \{ C(t) : 0 < t < t_0 \}, \]

where the dependence on \( k_A \) has been explicitly included. [For instance, in the case of \( t_0 = t_H \), this maximum appears marked with an asterisk in Fig. 1(a)]. Obviously, other quantities, such as for example the integral of \( C(t) \) in the interval, can be used as the representative magnitude; our conclusions, however, are independent of this choice. In Fig. 1(b) we show \( C_{\text{max}}(t_0, k_A) \), as a function of \( k_A \), for two values of the maximum time \( t_0 \), that have been taken equal to \( t_E/4 \) (lower curve) and \( t_H \) (upper curve). As can be seen, both functions decay as \( k_A \) increases, while oscillating at the same time with a dominant frequency. To analyze the frequency dependence of

![Fig. 1: (a) Cross correlation function between the horizontal (A) and the V–shaped (B) periodic orbits shown in the inset, for a value of the wavenumber of \( k_A = 155.116 \). The time \( t \) is measure in units of the Heisenberg time. (b) Maximum value of the cross correlation function in the interval \( [0, t_0] \) as a function of the wavenumber, for \( t_0 = t_H/4 \) (lower curve) and \( t_0 = t_H \) (upper curve). The mean decreasing tendency is indicated in dotted line.](image-url)
these functions, we have Fourier transformed them, after the signal has been properly prepared by eliminating the decaying tendency (dotted line). The resulting spectra are shown in Fig. 2 (a) in full and dashed line, respectively. As can be seen, they both appears dominated by only one peak, at values of the action: $t_0 = t_E/4$, and $S = 0.828$ for $t_0 = t_H$. Notice that $S$ has units of length due to the fact that the total linear momentum of the particle has been set equal to one. From the discussion above, our aim is to correlate these two peaks with invariant classical structures related to the chosen POs. Taking into account the numerical values of their positions, the first peak (labelled HE in the figure) can be assigned to the heteroclinic area, $S_{AB}$, enclosed by the stable and unstable manifolds emanating from the fixed points associated to POs A and B. This region is shown, shaded with horizontal lines, in the phase space portrait of Fig. 3 which illustrates the classical structures relevant to our work. When calculated, the corresponding area is 0.22540, value that agrees extremely well with that numerically found for $S_{HE}$. Moreover, according to the results reported in Ref. 13 for a more abstract case, this heteroclinic area is related to the semiclassical Hamiltonian matrix element between scar functions through the relation

$$\langle \phi_B | \hat{H} | \phi_A \rangle^2 \propto \cos(S_{AB} k), \quad (3)$$

which presents the same oscillating frequency found by us. This fact can be taken as a further confirmation of our previous assignment.

Using the same kind of arguments as before, the peak on the dashed curve of Fig. 2 (a), corresponding to $t_0 = t_H$, can be assigned to the difference in length between POs A and B. This quantity amounts to 0.828426, again in excellent agreement with the value found numerically. The existence of this peak, which is associated to the difference in actions between orbits A and B [see Eq. (2)], reflects the strong dependence of the interaction $k_A - k_B$ (which can also be related with the energy separation between the resonant levels corresponding to $\phi_{A,B}$). This effect has been further confirmed by analyzing the oscillatory behaviour of this wavenumber difference, which turns out to be the same exhibited by $C_{AB}(t_0, k_A)$, although these two functions appear with opposite phases.

At this point it is worth to emphasize that the different origin of the two peaks reflects the existence of two regimes in the cross correlation function $\langle \phi_B | H | \phi_A \rangle$, with the corresponding transition taking place at $t \sim t_E$. These two regimes can be easily understood in terms of the Fermi golden rule, since $C_{AB}(t_0, k_A)$ is in fact a measure of the probability transition between the resonant states $\phi_A$ and $\phi_B$. Accordingly, the behavior of $C_{AB}$ is given by the competition between two factors: the square of the coupling matrix element and the separation in energy of the corresponding levels.

Let us now consider other components in the spectra of Fig. 2 (a). To observe them more clearly, we calculate the rescaled intensity that is obtained after the biggest peak has been removed. When this is done for the two plotted curves only the results corresponding to the dashed one are stable against local variations of $t_0$. They are
shown in the lower part of the figure. As can be seen, many different contributions appear, all with a comparable order of magnitude. Among them we have focussed in the highest one (labelled HO), as the most interesting. When the value of $S_{HO}$ is compared to the relevant classical invariants of our problem (see Fig. 3), we find that it matches remarkably well with the homoclinic area enclosed by the stable and unstable manifolds emanating from A; this region appears shadowed with vertical lines in Fig. 3. The assignment is also supported by the work by Ozorio de Almeida [14], which has shown how homoclinic motions can be quantized, using the corresponding invariant manifolds. We believe that all (or most) remaining peaks in the spectrum presented in the lower part of Fig. 2 can be interpreted in the same way, using different homoclinic and heteroclinic regions corresponding to the same POs. Actually, we have succeeded in assigning the two peaks located to the left of that at $S_{HO}$; however, a full description of the procedure is deferred to a future publication.

In summary, some aspects concerning the role of short POs in Gutzwiller’s summation formula, the cornerstone for the semiclassical quantization of chaotic systems, have been analyzed. For this purpose, only purely quantum information has been used, in order to obtain relevant classical invariants for a semiclassical theory of quantum chaos. We have found evidence that the short POs, and their associated heteroclinic and homoclinic intersecting areas, are relevant contributions to the spectra. Furthermore, our results provide a semiclassical interpretation on how structures localized along POs interact [15]. This interaction is found to be given as the competition of two effects: the energy separation between scar functions, and the squared coupling matrix element between them, following the celebrated Fermi golden rule. Also, we have shown how the values of the corresponding parameters can be theoretically evaluated a priori. Finally, our results point out to the possibility of constructing computationally tractable alternatives to Gutzwiller’s theory, in which the long POs are substituted by the interaction between short POs. In this respect, the steps given in Ref. 16 provide a suitable frame in this direction that, together with a deeper understanding of the interaction between POs, can be a bridge towards a fully satisfactory semiclassical theory of chaotic systems based on short POs. This theory would be interesting not only from a fundamental point of view, but also for its application, for example, to nanotechnology [2], where it has been recently shown useful, for example, in the study of electron transport in mesoscopic devices [17].

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