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Classical invariants and the quantization of chaotic systems

D. A. Wisniacki,[1,2] E. Vergini,[1,3] R. M. Benito,[4] and F. Borondo[1]
[1]*Departamento de Química C-IX, Universidad Autónoma de Madrid, Cantoblanco, 28049 Madrid, Spain*
[2]*Departamento de Física "J. J. Giambiagi," FCEN, UBA, Pabellón 1, Ciudad Universitaria, 1428 Buenos Aires, Argentina*
[3]*Departamento de Física, Comisión Nacional de Energía Atómica, Av. del Libertador 8250, 1429 Buenos Aires, Argentina*
[4]*Departamento de Física, E. T. S. I. Agrónomos, Universidad Politécnica de Madrid, 28040 Madrid, Spain*

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Due to their exponential proliferation, long periodic orbits constitute a serious drawback in Gutzwiller's theory of chaotic systems. Therefore, it would be desirable that other classical invariants, not suffering from the same problem, could be used in alternative semiclassical quantization schemes. In this Rapid Communication, we demonstrate how a suitable dynamical analysis of chaotic quantum spectra unveils the role played, in this respect, 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 elucidating 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 quantization 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 regarded as the geometrical objects upon which reasonable 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 independent on the coordinate system.

Keeping within this scheme, in the 1970's Gutzwiller took 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, which 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 $\hbar$), 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, $t_{\rm H}=2\pi\hbar\rho(E)$, with $\rho(E)$ the energy density. This has precluded its use except in very special situations [7]. In this respect, it is worth emphasizing 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 $t_{\rm H}$) to predict higher energy eigenvalues. However, when applied backwards, for example, 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, $t_{\rm E}$ [9], are obtained [10]. This asymmetry is not fully understood yet, and raises fundamental questions about our present understanding of the quantum mechanics of chaotic systems: are long POs (with periods of the order of $t_{\rm H}$) relevant, or is its inclusion in the theory of Gutzwiller only a drawback? Finally, what is responsible for the unreasonable computational effort involved in the semiclassical computation of physical magnitudes?

In this Rapid Communication, 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 information in this route) in the Fourier transform process, we develop a method, relying only on purely quantum information, able to extract the pertinent associated information 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 with short POs, namely, the homoclinic and heteroclinic areas enclosed by their stable and unstable manifolds. This implies 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

$$C(t) = |\langle \phi_{\rm B}|\hat{U}(t)|\phi_{\rm A}\rangle|^2, \qquad (1)$$

where $\hat{U}(t)$ is the time propagation operator, and $\phi_{\rm A,B}$ are suitable functions associated with the POs, whose nature will be discussed later. In our formula, the second part of the bracket follows the evolution of the non-stationary function associated with 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 extent) 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 $\phi_{\rm A}$ and $\phi_{\rm B}$ are wave functions 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

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

where $S(E)$ is the dynamical action at energy E, ν the Maslov index, and n an integer number. It should be emphasized that all classical information required for the constructions of scar functions of short POs can be obtained directly from pure quantum information, as explained in Refs. [8,10].

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 wave number, 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 $L_{\rm A}=4$ and $L_{\rm B}=2(1+\sqrt{2})$, respectively [see the inset in Fig. 1(a)]. Let $\phi_{\rm A}$ be the scar function for A with mean wave number $k_{\rm A}$ [obtained from Eq. (2)], and $\phi_{\rm B}$ the corresponding B, with the mean wave number $k_{\rm B}$ closest to $k_{\rm A}$. We focus on the cross correlation function as defined in Eq. (1), and accordingly, we present in Fig. 1(a) $C(t)$ for $k_{\rm A}=155.116$. 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, $t_{\rm E}$ (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 $t_{\rm E}$, the 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, $t_{\rm H}$, 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 $[0,t_0]$,

$$C_{\max}(t_0,k_{\rm A}) \equiv \max\{C(t); \quad \text{for} \quad 0 < t < t_0\},$$

where the dependence on $k_{\rm A}$ has been explicitly included. [For instance, in the case of $t_0=t_{\rm H}$, this maximum appears marked with an asterisk in Fig. 1(a)]. We have verified that the conclusions are the same if we use the integral of $C(t)$ in the interval, as the representative magnitude; this equivalence is justified below. In Fig. 1(b) we show $C_{\max}(t_0,k_{\rm A})$, as a function of $k_{\rm A}$, for two values of the maximum time t_0, that have been taken equal to $t_{\rm E}/4$ (lower curve) and $t_{\rm H}$ (upper curve). As can be seen, both functions decay as $k_{\rm A}$ increases, while oscillating at the same time with a dominant frequency. To analyze the frequency dependence of these functions, we have Fourier transformed them, after the signal has been properly prepared by eliminating the decaying tendency (dotted line). We emphasize that this Fourier approach is of great relevance for the classical-quantum correspondence analysis, because actions manifest directly in phase space as given symplectic areas. The resulting spectra are shown in Fig. 2(a) in full and dashed lines, respectively. As can be seen, they both appear dominated by only one peak, at values of the action: $S=0.227$ for $t_0=t_{\rm E}/4$, and $S=0.828$ for $t_0=t_{\rm H}$. 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 (labeled HE in the figure) can be assigned to the heteroclinic area, $S_{\rm AB}$, enclosed by the stable and unstable manifolds emanating from the fixed points associated

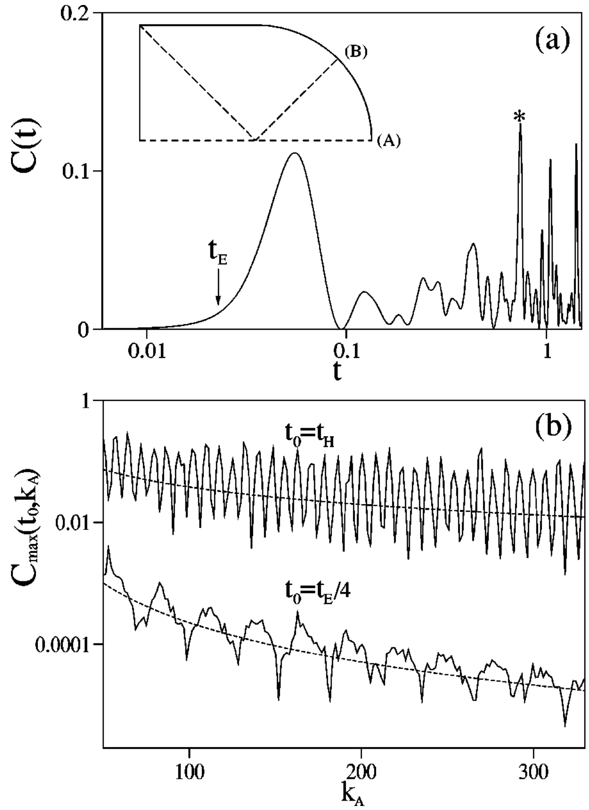

FIG. 1. (a) Cross-correlation function between the horizontal (A) and the V-shaped (B) periodic orbits shown in the inset, for a value of the wave number of $k_{\rm A}=155.116$. The time t is measured in units of the Heisenberg time. (b) Maximum value of the cross-correlation function in the interval $[0,t_0]$ as a function of the wave number, for $t_0=t_{\rm E}/4$ (lower curve) and $t_0=t_{\rm H}$ (upper curve). The mean decreasing tendency is indicated in dotted line.

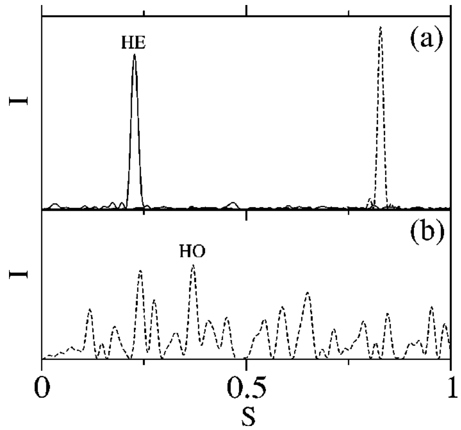

FIG. 2. (a) Fourier transform of the maximum cross-correlation functions in Fig. 1(b): $t_0 = t_E/4$ (full line), and $t_0 = t_H$ (dashed line). (b) Rescaled intensity of the Fourier transform for $t_0 = t_H$ in part (a) after the big peak has been removed.

with 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, a value that agrees extremely well with that numerically found for S_{HE}. Moreover, this heteroclinic area is related to the semiclassical Hamiltonian matrix element between scar functions through the relation

$$|\langle \phi_{\mathrm{B}}|\hat{H}|\phi_{\mathrm{A}}\rangle|^2 \propto \cos(S_{\mathrm{AB}}\, k),$$

which is an asymptotic estimate derived in Ref. [13], based on the knowledge of the semiclassical behavior of scar functions. This expression presents the same oscillating frequency found by us, and this fact can be taken as a further confirmation of our previous assignment, since $|\langle \phi_{\mathrm{B}}|\hat{H}|\phi_{\mathrm{A}}\rangle|^2$ controls the cross-correlation function, at least in the limit of $t_0 \to 0$.

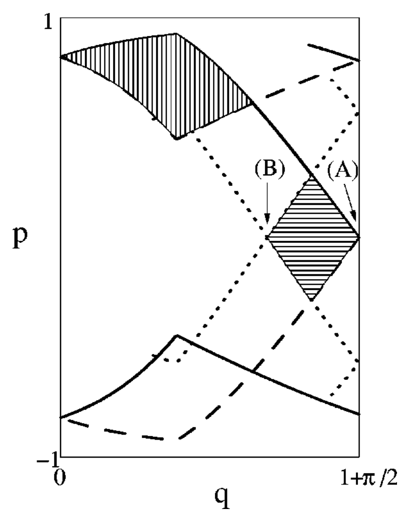

FIG. 3. Phase space portrait in Birkhoff coordinates of the classical structures relevant to our calculations. The fixed points marked with (A) and (B) correspond to the labeled turning points of periodic orbits A and B shown in the inset to Fig. 1(a). The unstable and stable manifolds of the horizontal PO are represented by full and dashed line, respectively, and those for the "V"-shaped PO by the dotted line. The shaded regions correspond to the heteroclinic (horizontal lines) and homoclinic (vertical lines) referenced in the text.

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 with the difference in actions between orbits A and B [see Eq. (2)], reflects the strong dependence of the interaction with $k_{\mathrm{A}} - k_{\mathrm{B}}$ (which can also be related with the energy separation between the resonant levels corresponding to $\phi_{\mathrm{A,B}}$). This effect has been further confirmed by analyzing the oscillatory behavior of this wave number difference, which turns out to be the same exhibited by $C_{\max}(t_{\mathrm{H}}, k_{\mathrm{A}})$, although these two functions appear with opposite phases.

At this point it is worth emphasizing that the different origin of the two peaks reflects the existence of two regimes in the cross-correlation function (1), with the corresponding transition taking place at $t \sim t_{\mathrm{E}}$. These two regimes can be easily understood in terms of the Fermi golden rule, since $C_{\max}(t_0, k_{\mathrm{A}})$ is in fact a measure of the probability transition between the resonant states ϕ_{A} and ϕ_{B}. Accordingly, the behavior of $C_{\max}$ 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 focused on the highest one (labeled HO), as the most interesting. When the value of $S_{\mathrm{HO}} = 0.370$ is compared to the relevant classical invariants of our problem (see Fig. 3), we find that it matches with the homoclinic area (=0.377) 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 Refs. [14,15], 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 succeded 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 [16]. 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 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. [17] provide a suitable frame in this direction that, together with a deeper understanding of the interaction between POs, can be a bridge toward 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 [18].

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