Classical Transport Effects on Chaotic Levels

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We show that the quantum spectra of simple systems whose classical counterpart is of a mixed nature, i.e., partly regular with widespread chaos, manifest the effects of classical transport through imperfect barriers. The partial barriers are characterized by the flux crossing them. We derive the relationship between this flux and quantum Hamiltonian matrix elements. This in turn predicts new statistical fluctuation properties for the spectrum and partial localization of the wave functions. The example of two coupled quartic oscillators is given in detail.

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The correspondence between quantum and classical mechanics is still not fully understood even when there are few degrees of freedom. This is especially true for nonintegrable Hamiltonian systems as there is no equivalent of Einstein-Brillouin-Keller quantization for the chaotic regions of phase space. This notwithstanding, we will show in this Letter that certain classical transport information is manifest in the quantum spectrum and ultimately in the eigenfunctions. To do so we derive a relationship between transport flux across partial barriers and matrix elements of the quantum Hamiltonian expressed in appropriate bases. This relationship has important consequences at finite energies. First of all, there will be significant effects on the spectral fluctuation properties of the system, and, second, the wave functions will be localized in that they will not uniformly explore the available chaotic phase space (in a semiclassical sense) but will tend to respect the partial barriers.

The first consequence arises in the following way: The fluctuation measures of chaotic systems are conjectured by Bohigas, Giannoni, and Schmit (BGS) to be given by the canonical random-matrix ensembles[1] which are characterized by level repulsion and long-range rigidity. We restrict our attention to systems having time-reversal invariance so the appropriate classical ensemble is the Gaussian orthogonal ensemble (GOE). In a generalization, Berry and Robnik[2] suggested each isolated chaotic region should be associated with an independent classical ensemble, to be superposed, whose relative importance, f_i, is given by its relative phase-space volume. In this picture the Hamiltonian is block diagonal, each block associated to a particular region. As a result of such a superposition, the spectrum is less rigid and exhibits less repulsion than if the regions are completely mixed.[3] With small or moderate transport between the chaotic regions one expects that the statistics will be intermediate between the two regimes (zero mixing or complete mixing). It is our purpose to investigate the transition from one to the other regime.

Generically, a classical Hamiltonian system will have a mixed phase space with regions of regular motion, i.e., Kolmogorov-Arnol'd-Moser (KAM) islands, embedded in widespread stochastic "seas." There will be a regular part of the spectrum[4] with which we must also deal.[5] This we can do either by superposing the statistics of the regular levels with the chaotic ones or by simply separating the regular spectrum from the total spectrum[6] allowing a finer look at the remaining spectrum. We shall do the latter.

For illustrative purposes, we study two coupled quartic oscillators[7] whose Hamiltonian is given by $H=\mathbf{p}^2/2+V(\mathbf{q})$, where

$$V(\mathbf{q})=a(\lambda)(q_1^4/b+bq_2^4+2\lambda q_1^2q_2^2)\,. \tag{1}$$

λ specifies the coupling of the two modes, b ($\neq 1$) lowers the symmetry from that of a square to a rectangle, and $a(\lambda)$ is an adjustable constant used in simplifying the quantum calculations. By varying λ we can select the desired degree of chaos since the system is integrable for $\lambda=0$ and thought to be completely chaotic for $\lambda=-1$. A simplifying feature of such a homogeneuos potential is that it is sufficient to make a classical study at one energy, say, $E=1$, and rescale the dynamics to understand all other energy surfaces.

For the results presented here we take $(\lambda,b)=(-0.35,\pi/4)$. There is a single chaotic sea and the KAM islands occupy 12% of the phase space. Among other reasons, this choice of the parameter is convenient because due to the reflection symmetries and to the dynamics of the problem, each torus has a duplicate elsewhere in phase space and we may then perform the separation of regular levels *via* the induced quasidegeneracies which originate from the quantization of two congruent tori[6] (see Ref. 8 for details).

In watching chaotic trajectories, they often seem to explore first one subregion of phase space, then another, etc. In two-degree-of-freedom systems there are two closely related possible mechanisms, cantori and/or is-

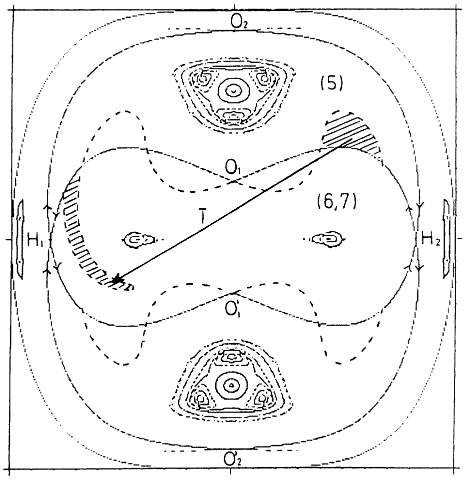

FIG. 1. Partial-barrier construction illustrated on the Poincaré section $q_2=0$. Starting from the hyperbolic fixed points H_1,H_2 one follows the stable and unstable manifolds to the primary homoclinic intersections O_1,O_1',O_2,O_2'. The shaded flux loop maps in one iteration to the new loop as indicated. See Fig. 2 caption and text for further explanation.

land chain partial barriers (broken separatrices).[9] In this case, $(-0.35,\pi/4)$, only the island chain barriers play a major role. We believe most simple systems should display this kind of behavior, although they may be missed if not searched for explicitly.

To see how the island chains form partial barriers, consider a short unstable periodic orbit created when an originally (small denominator) rational torus broke down. Associated with this orbit are a stable and unstable manifold which are tangent to the eigenvectors of the monodromy matrix. These manifolds are two dimensional and can be used to partition the three-dimensional energy surface. It should be clear that neither two stable nor two unstable manifolds ever cross, whereas a stable and an unstable manifold may cross an infinite number of times. Viewed from the surface of section the manifolds associated with a periodic orbit stretch smoothly away until they cross at the primary homoclinic intersection point where they start to oscillate more and more wildly (see Fig. 1). By following the smooth sections of the manifolds from the periodic orbit to the primary intersection, a region in phase space is isolated. The only exit from this region is to get caught in one of the loops (as viewed in the surface of section) formed by the manifold crossings. The smaller the flux the slower the transport or rate of escape. By way of canonical transformation to variables including energy and time, it can be shown that the rate of flux exiting per unit time is precisely the action (area) of the loop; quite often there is an additional integer factor depending on how many loops exit from the region in one iteration of the map [here 4, exiting region (6,7); see Fig. 1] depending on the island chain. For $(-0.35,\pi/4)$ there are eleven regions.

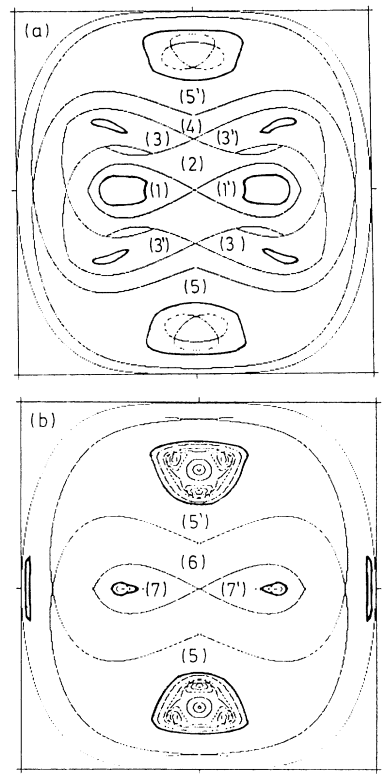

FIG. 2. Different regions in phase space separated by partial barriers; (a) $q_1=0$ Poincaré section and (b) $q_2=0$ Poincaré section. See text for further explanation.

Symmetry considerations reduce this to seven of which two had such large fluxes as to be essentially open, leaving five regions to be used in modeling the quantum oscillator. The results are summarized in Fig. 2 and Table I. (Note that only neighboring regions have connecting fluxes.)

The classical information can now be translated into

TABLE I. Relative volume of the chaotic phase space of the different regions as shown in Fig. 2 and their connecting fluxes. The fluxes are calculated for $E=1$ and must be scaled as $E^{3/4}$. Regions 1 and 2, and 6 and 7 could be grouped together because their connecting fluxes are such that their barriers could be ignored.

Region	Relative volume (%)	Total flux	
1+2	12		
		$(1+2)\leftrightarrow 3$	0.068
3	13		
		$3\leftrightarrow 4$	0.13
4	13		
		$4\leftrightarrow 5$	0.21
5	36		
		$5\leftrightarrow(6+7)$	0.28
6+7	26		

information on the quantum Hamiltonian. Assuming a basis exists such that each vector has its Wigner transform localized (in a semiclassical sense) in one subregion (note that only the existence of the basis is needed here, not its actual construction), the mean-square value $H^2_{\{i\},\{j\}}$ of the Hamiltonian matrix elements connecting a vector $|\alpha;i\rangle$, associated to region i, to $|\beta;j\rangle$, associated to region j, can be related to classical transport quantities. More precisely, if the chaotic subregions are large compared to $\hbar$, and connected through a Markovian-like process (i.e., each point of some subregion i can be considered to have equal probability to pass into some subregion j per unit time), it can be shown[8] that to leading order in $\hbar$, the dimensionless "mixing parameter" Λ_{ij} is given at energy E by

$$\Lambda_{ij} \equiv \frac{H^2_{\{i\}\{j\}}}{D^2} = \frac{\phi_{ij}(E)}{4\pi^2(2\pi\hbar)^{d-1} f_i f_j}, \qquad (2)$$

where D is the total mean spacing, d is the number of degrees of freedom, f_i is the relative phase-space volume of region i, and $\phi_{ij}(E)$ is the flux (i.e., the energy-surface volume per unit time) exchanged between regions i and j.[10] This result is at the root of all our conclusions concerning the quantum manifestations of limited classical transport.

In studying statistical fluctuations, as we discuss in what follows, our main tools are ensembles of random matrices adapted to the problem at hand. In this respect it is crucial to notice that the mixing parameter Λ_{ij}, namely, the mean-square matrix element in units of the total mean spacing, is also the transition parameter governing transitions in the fluctuation properties of ensembles of random matrices of various types [GOE $\to$ GUE (unitary), Poisson $\to$ GOE].[11] The Λ_{ij} are also the parameters governing the transition from several uncoupled GOE (zero mixing) to a simple GOE (complete mixing). The procedure is now fixed: From the classical dynamics compute the parameters f_i and ϕ_{ij}, which in their turn determine the Λ_{ij} that uniquely determine the fluctuations.[12]

Before comparing the above predictions to the spectral statistics of the quantum oscillators, some comments concerning the quantum calculation are in order. The spectral statistics describe the fluctuations about the mean density of states. To separate these two different phenomena, the spectrum $\{E_i\}$ is mapped into a new spectrum[1] $\{E_i'\}$ *via* $E_i' = \bar{N}_{ch}(E_i)$, where $\bar{N}_{ch}(E)$ is the locally smoothed integrated density of states for the chaotic levels. The regular levels removed represent a constant proportion f_R of the spectrum at all energies so $\bar{N}_{ch}(E) = (1-f_R)\bar{N}(E)$, where $\bar{N}(E)$ is the locally smoothed integrated density of states. For the quartic oscillator, we use an expansion of $\bar{N}(E)$ up to the third term in $\hbar$, i.e., $O(E^{-3/4})$. The proper symmetry decomposition has been used. We have put some effort into obtaining very long, highly accurate level sequences to insure accurate statistics. For the study given here, we have 22000 levels converged to an average error $\approx 10^{-5}D$ (mean spacing). We have several distinct, independent methods to determine the accuracies, one of which allows placing an error bound on each individual level.

Going back now to the spectral statistics of the chaotic levels, they will be of intermediate nature between that of a single GOE and five uncoupled GOE weighted by the relative volumes given in Table I. To measure quantitatively the fluctuations, we calculate the variance $\Sigma^2(r)$ of the number of levels in an interval of fixed length r. The r dependence is important here because therein lies the difference between independent superpositions of spectra and weakly coupled ones. For weak couplings at $r \ll \Lambda$, the statistics behave as though there is just one GOE and in the other extreme $r \gg \Lambda$ the statistics are more like the ones of five uncoupled GOE. This is confirmed in the example treated here. Indeed, Fig. 3 shows quite good agreement between the quartic oscillator and the theory presented here.

It is instructive now to reexamine the BGS conjecture[1] concerning the statistics of sufficiently chaotic systems. It is clear that even very chaotic systems could have partial barriers in phase space such as is trivially realized by placing two chaotic billiards side by side and poking a hole to connect them. The hole is essentially closed quantum mechanically when the natural wavelength is too long. As the wavelength decreases it becomes more and more apparent just as the classical flux would increase [for the quartic oscillator, $\phi_{ij}(E)$ scales the same as the actions, which is $(E/E_0)^{3/4}\phi_{ij}(E_0)$]. It is there-

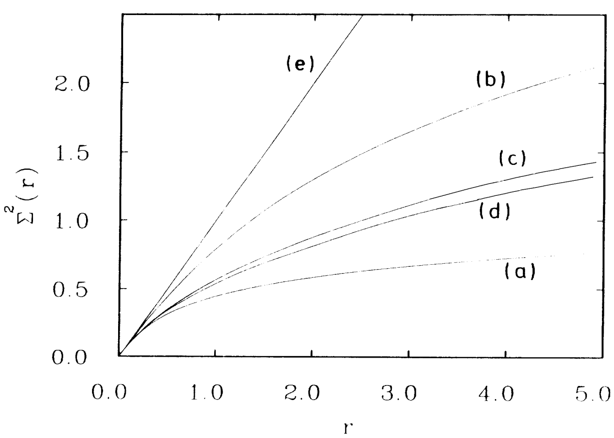

FIG. 3. Number variance $\Sigma^2(r)$: (a) one GOE; (b) five GOE blocks weighted according to the fraction of total phase-space volume (see Table I), the blocks are decoupled; (c) like (b), but with blocks coupled by the Λ_{ij} deduced from Table I by use of Eq. (2); (d) from the quantum spectrum (from the 16000th to the 22000th state)—the regular levels ($\sim 12\%$) have been subtracted; (e) from a Poissonian spectrum, for the sake of comparison. See text for further explanation.

fore very important to identify the time scales on which the complete phase space is explored before one can know if the system is sufficiently chaotic. For example, even the standard stadium billiard may show some deviations due to the bouncing-ball modes around which the phase space is diffusive. These considerations are even more likely to affect the Berry-Robnik surmise. Since these partial barriers are not exceptional in mixed systems, the modeling of each chaotic region by one GOE can be rather poor as is the case for the quartic oscillator; this accounts for the major deviations when looking at the complete spectrum. It has also been suggested[13] that weak connections between the regular and chaotic levels should change the statistics. In the quartic oscillator this was checked and seen for some special levels but was not statistically detectable.

The same ensemble theory also predicts localization of the eigenfunctions. Such nearly block-diagonal Hamiltonians would not completely mix upon diagonalization the various subspaces associated with each block. In fact, for Λ_{ij} small, a perturbed eigenvector $|E;i\rangle$ from space i has little projection in space j ($j\neq 1$). Using an ensemble-degenerate perturbation theory,[14] we find on average for weak coupling that the square of this projection is

$$\langle\langle E;i\,|\,\hat{P}_j\,|\,E;i\rangle\rangle_{\rm ls}=2f_j\left(\frac{2}{\pi}\Lambda_{ij}\right)^{1/2}=\left(\frac{2}{\pi^3}\frac{f_j\phi_{ij}(E)}{(2\pi\hbar)^{d-1}f_i}\right)^{1/2} \tag{3}$$

(with $\hat{P}_j$ the projector onto the jth subspace, and $\langle\ \rangle_{\rm ls}$ means local smoothing in E) valid for $\Lambda_{ij}\ll 1$. Equation (3) implies that the very-long-time phase-space exploration of a wave packet initially located in region i is not democratic over the entire chaotic region but remains mostly localized in region i, in sharp contrast to the classical dynamics. Clearly, transport barriers, depending on the flux, provide a very effective mechanism for "quantum dynamical suppression of classical chaos."

In conclusion, we have taken one more step closer to understanding how the correspondence principle applies for systems classically possessing KAM islands embedded in a chaotic sea. We have identified the influence of finite-time phase-space structures, such as partial barriers characterized by the flux crossing them, in the quantum spectrum. We have given a semiclassical theory for finite h which recovers as limiting cases (i) for chaotic systems, the BGS conjecture, and (ii) the Berry-Robnik surmise for the level statistics of mixed systems. For the wave functions, the partial barriers lead to localization. This should have important consequences for atomic and molecular systems currently under study.[10]

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