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 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 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. 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-Arnold-Moser (KAM) islands, embedded in widespread stochastic "seas." There will be a regular part of the spectrum which we must also deal. 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 allowing a finer look at the remaining spectrum. We shall do the latter.

For illustrative purposes, we study two coupled quartic oscillators whose Hamiltonian is given by

\[ H = p^2/2 + V(q), \]

where

\[ V(q) = a(\lambda) (q_1^4/b + bq_2^4 + 2\lambda q_1^2 q_2^2). \]

\( \lambda \) 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 \( \lambda \) 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 homogeneous 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 \((\lambda, b) = (0.5, \pi/4)\). 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 (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-
land chain partial barriers (broken separatrices). 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) stable 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.

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 1. (Note that only neighboring regions have connecting fluxes.)

The classical information can now be translated into

<table>
<thead>
<tr>
<th>Region</th>
<th>Relative volume (%)</th>
<th>Total flux</th>
</tr>
</thead>
<tbody>
<tr>
<td>1+2</td>
<td>12</td>
<td>((1+2) \rightarrow 3) 0.068</td>
</tr>
<tr>
<td>3</td>
<td>13</td>
<td>(3 \rightarrow 4) 0.13</td>
</tr>
<tr>
<td>4</td>
<td>13</td>
<td>(4 \rightarrow 5) 0.21</td>
</tr>
<tr>
<td>5</td>
<td>36</td>
<td>(5 \rightarrow (6+7)) 0.28</td>
</tr>
<tr>
<td>6+7</td>
<td>26</td>
<td></td>
</tr>
</tbody>
</table>
information on the quantum Hamiltonian. Assuming a
basis exists such that each vector has its Wigner trans-
form 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
$\langle H_{0j}^2 \rangle$ 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 con-
sidered to have equal probability to pass into some subre-
gion $j$ per unit time), it can be shown$^8$ that to leading or-
der in $\hbar$, the dimensionless "mixing parameter" $\Lambda_{ij}$ is
given at energy $E$ by

$$\Lambda_{ij} \equiv \frac{H_{0j}^2}{D^2} = \frac{\phi_{ij}(E)}{4\pi^2(2\pi\hbar)^k} \frac{1}{d_{ij}}, \quad (2)$$

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
$j$. This result is at the root of all our conclusions con-
cerning 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 $\Lambda_{ij}$,
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 en-
sambles of random matrices of various types [GOE
$\rightarrow$ GUE (unitary), Poisson $\rightarrow$ GOE].$^{11}$ The $\Lambda_{ij}$ are also
the parameters governing the transition from several un-
coupled GOE (zero mixing) to a simple GOE (complete
mixing). The procedure is now fixed: From the classical
dynamics compute the parameters $f_i$ and $\phi_{ij}$, which in
their turn determine the $\Lambda_{ij}$ 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., $O(\hbar^{3/4})$. The proper symmetry decom-
position has been used. We have put some effort into ob-
taining very long, highly accurate level sequences to in-
sure accurate statistics. For the study given here, we
have 22000 levels converged to an average error
$= 10^{-3} D$ (mean spacing). We have several distinct, in-
dependent 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 quanti-
titatively 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 super-
positions 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 in-
crease [for the quartic oscillator, $\phi_{ij}(E)$ scales the same
as the actions, which is $(E/E_0)^{1/4} \phi_{ij}(E_0)$]. 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 $\Lambda_{ij}$ deduced from Table I
by use of $\Sigma^2$; (d) from the quantum spectrum (from the
16000th to the 22000th state)—the regular levels (tor 12%) have
been subtracted; (e) from a Poissonian spectrum, for the
sake of comparison. See text for further explanation.](image-url)
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\(^\text{13}\) 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 \(\Lambda_{ij}\) small, a perturbed eigenvector \(E;i\) from space \(i\) has little projection in space \(j (j \neq 1)\). Using an ensemble-degenerate perturbation theory,\(^\text{14}\) we find on average for weak coupling that the square of this projection is

\[
\langle \langle E;i | \hat{P}_j | E;i \rangle \rangle_{\text{hs}} = 2\int \frac{2}{\pi} \left( \frac{2}{\varphi_{ij}(E)} \right)^{1/2} \left( \frac{f_j \varphi_{ij}(E)}{2\pi h} \right)^{1/2} \mathrm{d}t.
\]

(with \(\hat{P}_j\) the projector onto the \(j\)th subspace, and \(\langle \langle \rangle \rangle_{\text{hs}}\) 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 \(\hbar\) 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.\(^\text{10}\)

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\(^{\text{10}}\)Present address.


\(^{\text{18}}\)O. Bohigas, S. Tomsovic, and D. Ullmo (to be published).


\(^{\text{20}}\)In a different context, that the ratio of the classical flux compared to \(\hbar\) should be important has been conjectured in R. S. Mackay and J. D. Meiss, Phys. Rev. A 37, 4702 (1988).


\(^{\text{22}}\)Although the parameters governing the transition are known, the explicit results for the different correlation functions used to quantify the fluctuations are not. Therefore, one must resort to Monte Carlo calculations to compute the different statistics of these ensembles of random matrices.
