Non ergodic quantum behaviour in classically chaotic 3D billiards

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(March 23, 2022)

We study, analytically and numerically, the classical and quantum properties of a nearly spherical 3D billiard. In particular we show the appearance of quantum non ergodic behaviour and of the deviations from Random Matrix Theory predictions which are due to the quantum suppression of classically chaotic diffusion.

PACS number: 05.45.+b

In the ergodic theory of classical dynamical systems, billiards have played a fundamental role since they exhibit a clean and rich variety of dynamical properties, from completely integrable to true random motion. For this reason, since the early papers [1] in which level spacing distribution was numerically studied, they became of primary importance for the theoretical and experimental analysis of the various quantum properties which are connected to different features of classically chaotic motion. An important question is to understand under what conditions the predictions of Random Matrix Theory (RMT) can be applied to a generic conservative quantum system [2]. In this context the quite surprising phenomenon of localization inside the energy shell has been shown to play a fundamental role [3]. This phenomenon implies quantum non-ergodic behaviour and deviations from the predictions of Random Matrix theory. Moreover a very interesting asymmetry appears between the structure of exact and unperturbed eigenfunctions.

In a recent paper [4] quantum localization was shown to take place in a stadium billiard and this result was confirmed also in a similar model [5]. The important question is now what happens in more dimensions. In particular we would like to understand whether or not this interesting non ergodic quantum behaviour can take place in a 3D billiard. 3D billiards are certainly more complicated than plane billiards. However, in some cases, they can be more close to experimental investigations [6]-[9] and to physical applications; we refer for example to dielectric resonators which may find applications in microlasers and fibre-optic communications [10].

In this paper we consider a wiggly 3D spherical billiard, namely a particle of unit mass and velocity $\hat{v}$ moving freely inside a closed 3D domain and bouncing elastically off the boundary whose shape is given by a small, smooth but wiggly deformation of the unit sphere. The boundary of the billiard is described by the distance of the boundary point from the origin as a function of the unit direction vector $\hat{n}$, $r_B(\hat{n}) = 1 + \epsilon f(\hat{n})$ ($\hat{n}^2 = 1$). The small parameter $\epsilon$ controls the size of the wiggles of the boundary while $f(\hat{n})$ is an oscillatory function which is assumed to have unit average square modulus $\langle |f(\hat{n})|^2 \rangle = (1/4\pi) \int d^2\hat{n} f(\hat{n})^2 = 1$. The shape function $f(\hat{n})$ may be expanded in terms of spherical harmonics $Y_{\ell m}(\hat{n})$ with a given maximal order $L$, $f(\hat{n}) = \sum_{\ell\leq L} \sum_{m} c_{\ell m} Y_{\ell m}(\hat{n})$. The coefficients $c_{\ell m}$ have been specified by imposing three conditions: (i) $c_{\ell m}$ decrease with increasing order $\ell$ as $\sum_{m} c_{\ell m}^2 \propto 1/\ell^2$, (ii) the shape of the billiard is invariant under the cubic symmetry group $O_h$, $f(\hat{n}) = f(G\hat{n})$, $G \in O_h$, (iii) the shape function $f(\hat{n})$ is separable in cartesian coordinates, i.e. it can be written in a form $f(\hat{n}) = \sum_{\ell=0}^{L/2} a_{\ell} (n_x^2 + n_y^2 + n_z^2)$ with coefficients $a_{\ell}$.

By calculating the distribution of maximal Liapunov exponent, the classical dynamics of the billiard has been found to be almost completely chaotic for $\epsilon > \epsilon_c(L)$, where the critical chaos border $\epsilon_c(L)$ is a rapidly decreasing function of $L$. For the case $L = 14$ which will be taken in this paper, we found $\epsilon_c = 0.001$. For this value of the perturbation, most of phase space is covered by chaotic orbits. The billiard’s dynamics can be described in terms of the angular momentum $\hat{l} = \hat{r} \times \hat{v}$ and the unit direction vector $\hat{n} = \hat{r}/r$ of the forthcoming point of collision with the boundary. Labelling points of successive collisions by the discrete time variable $j$, one can write an approximate Poincare map for the dynamics in $(\hat{l}, \hat{n})$ variables:

\begin{align}
\hat{l}_{j+1} &= \hat{l}_j - 2\epsilon \left[(\hat{v}^2 - l_j^2)^{1/2} \hat{n}_j \times \nabla f(\hat{n}_j)\right] + O(\epsilon^2), \\
\hat{n}_{j+1} &= (2l_{j+1}^2 + \hat{v}^2 - 1)\hat{n}_j - 2(\hat{v}^2 - l_j^2)^{1/2} \hat{n}_j \times \hat{l}_{j+1}/v^2,
\end{align}

which is essentially four dimensional since we have two constraints, namely $\hat{l}_j \cdot \hat{n}_j = 0$ and $\hat{n}_j^2 = 1$. The components of $\hat{l}_j$ are the slow or adiabatic variables while $\hat{n}_j$ is the fast variable (only one of its components is independent due to constraints). By averaging over the fast variable one can calculate the average drift of the angular momentum vector $\Delta \hat{l}_j = \hat{l}_{j+1} - \hat{l}_j$,

$$
\langle \Delta \hat{l}_j \hat{l}_j \rangle = \hat{\Omega}(\hat{l}_j) \times \hat{l}_j,
$$

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\[ \bar{\Omega}(l) = 2\sqrt{\frac{1}{2^2 - p^2}} \sum_{p=1}^{l/2-1} \frac{(2p+1)!!}{(2p)!!} a_{p+1} \times \left( \frac{L_p^{2p}}{(L^2 - l^2)^p} - \frac{L_p^{2p}}{(L^2 - y^2)^p} + \frac{L_p^{2p}}{(L^2 - I^2)^p} \right) \]

From eq. (3) it is seen that the direction of angular momentum vector undergoes a precession with a frequency vector field \( \bar{\Omega}(l) = O(\epsilon L^{1/2}) \) which is an oscillatory function of angular momentum on a scale \( v/L \).

Let us first analyze the behaviour of the modulus \( l \) of angular momentum. From (3) we see that the average drift of \( l \) is zero \( \langle \Delta l_j \rangle = \langle l_{j+1} - l_j \rangle \approx (\bar{l}_l/l) \cdot \langle \Delta \bar{l}_l \rangle = 0 \). Then, above the chaos border \( \epsilon > \epsilon_c \), one typically expects the diffusive behaviour \( \langle (l_j - l_0)^2 \rangle \approx D(l_0)J \) where the diffusion coefficient can be estimated from (3) as \( D = O(\epsilon^2 v^2 L^2) \). However, our numerical analysis reveals that the above diffusive behaviour takes place only up to time \( J = J^* \), where \( J^* \approx L \). Instead, for \( J > J^* \), we find a slower, sublinear diffusion which obeys the empirical law \( \langle (l_j - l_0)^2 \rangle \approx \frac{\epsilon}{\alpha} \) with \( 0 < \alpha < 1 \).

For the variance of the component \( l_z \) of angular momentum, both, the drift and diffusion terms are important \( \langle (l_z - l_0)^2 \rangle \approx \langle (l_z - l_0)^2 \rangle + J \langle (\Delta l_z^2) - (\Delta l_0^2) \rangle \approx J^2 \langle \bar{l}_l \times l_0 \rangle^2 + JD(l_0) \). The first (drift) term is \( O(J^2 v^2 L) \) and the second (diffusive) term is \( O(J^2 v^2 L) \), so the drift may be neglected w.r.t. diffusion for \( J < J^* \), while for \( J > J^* \), the quadratic drift term prevails (2). It is not the purpose of the present paper to discuss the details of the classical diffusive mechanism. We would like only to stress that, as confirmed by our numerical analysis, the ‘diffusion’ of the direction of angular momentum is much faster than the diffusion of its modulus which is therefore the slowest variable in the system.

The classical steady state equilibrium distribution \( \rho_{eq}(l) \) of the angular momentum can be obtained analytically by substituting (provided \( \epsilon > \epsilon_c \)) time averages with phase averages:

\[ \rho_{eq}(l) = \lim_{J \to \infty} \frac{1}{J} \sum_{j=1}^{J} \Delta t_j \delta(l - l_j) = \frac{3l}{\nu^2} \sqrt{v^2 - l^2} \]

Here \( \Delta t_j = 2(v^2 - l_j^{1/2}/v)^2 \) are the time intervals between collisions. As a measure of the width of the classical distribution we introduce the quantity \( \sigma(l_0, t) = (1/v)\int_0^t f(t') \rho(l_0, t) dt' - (1/v)\int_0^t f(t') \rho(l_0, t) dt' \) with \( \rho(l, t = 0) = \delta(l - l_0) \). For the equilibrium steady state we find \( \sigma_{eq} = \sigma(l_0, \infty) = 0.2303 \). We have used expression (3) as an additional numerical test of ergodicity of our billiard for \( \epsilon > \epsilon_c \).

Let us now turn to the quantum dynamics. We have solved the Schrödinger equation \((\nabla^2 + k^2)\Psi_k(\vec{r}) = 0\) with Dirichlet boundary conditions \((\hbar = 1, E = k^2/2)\). Eigenvalues \( k^{(n)} \) and eigenfunctions \( \Psi_k^{(n)} \) have been computed very efficiently using the scaling method invented by Vergini and Saraceno and already implemented for smooth 3D billiards in Note that we have studied only the states belonging to 1-dim fully symmetric irrep of the 48-fold cubic group \( O_h \), so the Weyl formula which relates the wavenumber \( k \) with the sequential quantum number \( N \) in this symmetry class reads (for small \( \epsilon \)) \( N(k) \approx k^3/(216\pi) \). For sufficiently large \( k \) we expect that the statistical properties of eigenvalues and eigenfunctions of our billiard are well described by RMT. On the other hand, for sufficiently small \( k \) (or small \( \epsilon \) and fixed \( k \)) the perturbation theory is adequate and one can treat the problem as a small perturbation of a spherical billiard. We estimate the perturbative border \( \epsilon_p(k) \) as the critical value at which the change in the unperturbed levels, due to perturbation, is of the order of the spacing among levels, and therefore avoided crossings start to appear. Note that the unperturbed eigenvalues \( k_0^{(n|m)} \) of the sphere are \((2l + 1)\)-times degenerate with an average spacing \( \langle \Delta k_0 \rangle \approx 8/k \). The derivative with respect to \( \epsilon \) of a level \( k_0 \) of a spherical billiard with an eigenfunction \( \Psi_0(\vec{r}) \) can be expressed as an integral over the boundary of the billiard \( \partial_k k_0 = -1/(2k_0) \int d^2r \Psi_0(\vec{r}) \partial_n \Psi_0(\vec{r}) \) where \( \partial_n \) is a normal derivative w.r.t. boundary. Then, using the explicit form for \( f(\vec{r}) \) and \( \Psi_0(\vec{r}) \), we can estimate the level velocities \( \partial_k k_0 \approx k_0 g/(L + 1) \) where \( g = 48 \) is the symmetry factor. Therefore we obtain:

\[ \epsilon_p(k) \approx \frac{\langle \Delta k \rangle}{\partial_k k} \approx \frac{8(L + 1)}{\sqrt{g} k^2} \]

In fig. 1 we show the dependence of the eigenvalues on the perturbation parameter \( \epsilon \). It is clearly seen that avoided crossings appear above the perturbative border which, for the parameters of fig. 1 \((L = 14, k \approx 180.0)\), is \( \epsilon_p \approx 0.0005 \). Above the perturbative border, namely for \( \epsilon > \epsilon_p \), the quantum diffusion takes place according to the classical one. Our purpose is to try to understand if and under what conditions interference terms can suppress quantum diffusion, thus leading to localization and deviations from predictions of RMT. As it is known, quantum localization may take place after the Heisenberg time \( t_H = 2\pi dN/dE = k/36 \) at which the quantum motion resolves the discreteness of the energy spectrum. More precisely, eigenstates are expected to be localized in the angular momentum coordinates if the Heisenberg time \( t_H \) is less than the ergodic time \( t_E \), which is the time it takes for the classical distribution to reach the equilibrium state. Therefore, transition to ergodicity or delocalization takes place at \( t_H = t_E \). If we assume, for the time being, that the classical motion is diffusive with diffusion coefficient \( D \approx \epsilon^2 L^2 E \), then the ergodic time is given by \( t_E \approx \langle \Delta t \rangle_{\max}^2 / D \approx 8/(3\epsilon^2 L^2 k) \) where \( \langle \Delta t \rangle = 4/(3k) \) is the average time between collisions. The condition \( t_E = t_H \) leads to the estimate for the delocalization border \( \epsilon_l \):

\[ \epsilon_l = \frac{4\sqrt{6}}{Lk} \]
However, due to anomalous diffusion, the ergodic time will be longer than the one given by the above estimate and this will lead to a delocalization border even larger than (1). For example, for the data of figs. 1-4 \((L = 14, k \approx 180)\) the numerically estimated localization border is \(\epsilon_l = 0.010\).

Billiard’s eigenfunctions \(\Psi_k(\vec{r})\) can be expanded in terms of eigenfunctions of a perfectly spherical billiard \((\vec{r}nm\ell) = (\sqrt{2}/j_{l+1}(\xi_{n\ell}))j_l(\xi_{n\ell})Y_{\ell m}(\vec{r}), |\Psi_k\rangle = \sum_{nm\ell}(|nlm\ell\rangle|\Psi_k\rangle|nlm\rangle).\) We define the angular momentum distribution of an eigenstate \(\Psi_k\) with an eigenvalue \(k\) as \(h_k(l) = \frac{1}{\rho_{eq}(l)} \sum |(nlm\ell|\Psi_k\rangle|^2|l\rangle.\) Since we have divided by the classical stationary distribution \(\rho_{eq}(l)\) then, for completely delocalized, ergodic states, \(h_k(l)\) should approach a constant (apart from fluctuations). In fig. 2 we show the distributions \(h_k(l)\) for three typical eigenstates of the billiard at three different values of parameter \(\epsilon\). Eigenstates (a) and (b) are below the delocalization border and are exponentially localized while (c) is an ergodic extended eigenstate. However, eigenstates \(|nlm\ell\rangle\) are extended in the \(l = m\) variable as we expect as a consequence of the much faster classical diffusion of \(I_x\) w.r.t. \(l\).

For a comparison with theoretical predictions, in analogy with the classical case, we measure the size of eigenfunctions by the quantity \(\sigma_k = \frac{1}{k}((|\Psi_k|^2|\Psi_k\rangle - |\Psi_k(l)|^2)^{1/2}/2\). We expect that for ergodic (extended) eigenstates, \(\sigma_k\) should agree with the width of the classical steady state angular momentum distribution \(\sigma_{eq} = 0.2303\). Instead, for localized states, we expect that \(|\langle \sigma_k \rangle| = |\langle \sigma(l_0, \tau) \rangle|_{l_0}\) where \(\tau\) is of the order of Heisenberg time. In order to suppress fluctuations the quantum width is averaged over a sufficiently large number of consecutive eigenstates while the classical width is microcanonically averaged over the initial angular momentum \(l_0\). In order to take into account that, as empirically known, the width of eigenstates is approximately one half of the width of steady state we choose \(\tau = t_H/2 = k/T_2\). The comparison between \(\langle \sigma_k \rangle\) and \(|\sigma(l, t_H/2)\rangle\) is shown in fig. 3 for a fixed energy window. The agreement is surprisingly good. Moreover we have numerically checked that the above relation also holds for different energy windows with \(k\) ranging between \(k \approx 120\) and \(k \approx 260\) and for fixed \(\epsilon = 0.003\).

We have also calculated in the different regimes the most commonly studied statistical spectral properties, namely the nearest neighbour level spacings distribution \(P(S)\) and the number variance \(\Sigma^2(E)\). The distribution \(P(S)\) has been found to be characterized by the power-law level repulsion \(P(S) \propto S^2, S \ll 1\), where \(\beta\) smoothly increases from zero to one as a function of \(\epsilon\) or \(k\) moving from the perturbative to the ergodic regime. The functional relation \(\beta(\langle \sigma_k \rangle)\) is still to be systematically investigated. However, in the perturbative regime \(\epsilon < \epsilon_p(k), \beta \approx 0\) but the tails of \(P(S)\) decrease much slower than Poissonian \(\exp(-S)\) due to strong degeneracies at \(\epsilon = 0\). Moreover the convergence towards GOE distribution with increasing \(\epsilon\) or \(k\) is found to be very slow and in agreement with previous results on different models [3]. In this respect, the \(\Sigma^2(E)\) describing the long range correlations has been found to be more sensitive. In fig. 4 we plot \(\Sigma^2(E)\) computed in the window \(170 < k < 180\) and for \(\epsilon = 0.003, 0.010, 0.016\).

In this paper we have shown, on a model of classically chaotic 3D billiard, the appearance of the quantum dynamical localization phenomenon which results in the approach of the quantum distribution to a localized, non ergodic, steady state. This phenomenon, though in a different context, was discovered long ago [15] and it is related to the existence of different time scales of classical and quantum motion [16]. Finally we would like to remark that the 3D nearly spherical billiard studied here can be a realistic model for a new class of optical resonators [16]; in particular the localization in angular momentum can lead to an increase in the photons lifetime.

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FIGURE CAPTION

**FIG. 1.** Dependence of quantum eigenvalues on the perturbation parameter $\epsilon$ in the window $179.68 < k < 180.32$. This interval contains approximately 90 levels.

**FIG. 2.** Angular momentum probability distribution $h_k(l)$ of three eigenstates with $k \approx 180$ and different $\epsilon$: (a) strongly exponentially localized eigenstate for $\epsilon = 0.001$ with eigenvalue $k = 180.3009$, (b) localized eigenstate for $\epsilon = 0.003$ with eigenvalue $k = 179.8013$, and (c) extended (ergodic) eigenstate for $\epsilon = 0.016$ with eigenvalue $k = 179.8611$. Note that the probability distribution of the state (a) is divided by a factor $10^6$ and probability for the state (b) by a factor $10^3$ w.r.t. state (c).

**FIG. 3.** Comparison of the average width $\langle \sigma_k \rangle$ of angular momentum distribution of quantum eigenstates (bullets) and the corresponding widths $\langle \sigma(l_0, t_H/2) \rangle_{l_0}$ of classical distributions (diamonds) after half of Heisenberg time for different values of the perturbation parameter $\epsilon$ and fixed $L = 14$. The quantum distributions have been averaged over 90 consecutive states around $k \approx 180$.

**FIG. 4.** Number variance statistics $\Sigma^2(E)$ for three spectral stretches in the window $170 < k < 180$ corresponding to three different values of the perturbation parameter (a) $\epsilon = 0.003$, (b) $\epsilon = 0.010$, (c) $\epsilon = 0.016$. Each window contains about 1500 levels. The dashed curve is the logarithmic GOE number variance while the dotted curve is the linear (Poissonian) $\Sigma^2(E)$ statistics. The relevant energy scales for this plot are: mean level spacing $\Delta E = 72\pi/k \approx 1.26$; Thouless energy $E_T = 1/t_E \approx 3$ for curve (c); the bouncing energy $E_b = 2/\langle t \rangle \approx 270$ where $\langle t \rangle$ is the average bouncing time.