Deformations and dilations of chaotic billiards, dissipation rate, and quasi-orthogonality of the boundary wavefunctions

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We consider chaotic billiards in \(d\) dimensions, and study the matrix elements \(M_{nm}\) corresponding to general deformations of the boundary. We analyze the dependence of \(|M_{nm}|^2\) on \(\omega = (E_n - E_m)/\hbar\) using semiclassical considerations. This relates to an estimate of the energy dissipation rate when the deformation is periodic at frequency \(\omega\). We show that for dilations and translations of the boundary, \(|M_{nm}|^2\) vanishes like \(\omega^4\) as \(\omega \rightarrow 0\), for rotations like \(\omega^2\), whereas for generic deformations it goes to a constant. Such special cases lead to quasi-orthogonality of the eigenstates on the boundary.

Chaotic cavities (billiards) in \(d\) dimensions are prototype systems for the study of classical chaos and its fingerprints on the properties of the quantum-mechanical eigenstates. As the properties of static billiards are beginning to be understood, questions naturally arise about deformations and their time dependence. It is perhaps not widely appreciated that certain deformations are very special, and that there is a close connection between the quantum and classical mechanics of such deformations in the case of ergodic systems. In this paper, which takes beginning to be understood, questions naturally arise about deformations and their time dependence. It is perhaps not widely appreciated that certain deformations are very special, and that there is a close connection between the quantum and classical mechanics of such deformations in the case of ergodic systems. In this paper, which takes quantum and classical mechanics of such deformations in special, and that there is a close connection between the quantum and classical mechanics of such deformations in the case of ergodic systems. In this paper, which takes

We start with the one-particle Hamiltonian

\[ H_0(r, p) = p^2/2m + V(r), \]

where \(m\) is the particle mass, \(r\) is the position of the particle inside the cavity and \(p\) is the conjugate momentum. We will take the limit \(V(r) \rightarrow \infty\) outside the cavity, zero otherwise, corresponding to Dirichlet boundary conditions. In this limit, the Hamiltonian is completely defined by the boundary shape. The volume of the cavity we call \(V \equiv L^d\). Upon quantization a second length scale \(\lambda_n \equiv 2\pi/k\) appears, where \(k\) is the wavenumber. For simple geometries the typical time between collisions with the walls is \(\tau_{\text{col}} \sim L/v\), where \(v\) is the particle speed. The energy is \(E = \frac{1}{2}mv^2\). Upon quantization the eigenenergies are \(E_n = (\hbar\omega_n)^2/2m\).

![FIG. 1. The two-dimensional (2D) billiards under numerical study. Left: Bunimovich quarter-stadium \((a/R = 1)\). Right: Generalized Sinai billiard \((a/b = 2, \theta_1 = 0.2, \theta_2 = 0.5)\).](image)

A powerful tool for the classical analysis is known as the ‘Poincaré section’. Rather than following trajectories in the full \((r, p)\) phase-space, it is much more efficient to record only successive collisions with the boundary. This way we can deal with a canonical transformation (map) which is defined on a 2\((d-1)\) dimensional phase space. A similar idea is used in quantum-mechanics: By Green’s theorem is is clear that all the information about an eigenstate \(\psi(r)\) is contained in the boundary normal derivative function \(\varphi(s) \equiv n \nabla\psi\), where \(s\) is a \((d-1)\) dimensional coordinate on the boundary, and \(n(s)\) the outward unit normal vector.

However, unlike the classical case, the reduction to the boundary is not satisfactory. One cannot define an associated Hilbert space that consists of the boundary functions. In particular, the orthogonality relation \(\langle \psi_n | \psi_m \rangle = \delta_{nm}\) does not have an exact analog on the boundary. Still, the boundary functions ‘live’ in an effective Hilbert space of dimension \(\sim (L/\lambda_n)^{d-1}\), and it has been realized [1] that the following quasi-orthogonality relation holds. Define an inner product

\[ M_{nm} \equiv \frac{1}{2\hbar^2} \int \varphi_n(s)\varphi_m(s) (n \cdot D) ds \]  

(1)

where \(D(s) = r(s)\) is the displacement field corresponding to dilation (about an arbitrary origin), and \(k_n \approx k_m \approx k\). It is well known that the normalization condition \(\langle \psi_n | \psi_n \rangle = 1\) implies \(M_{nn} = 1\). We give a proof of this exact result in the Appendix. On the other hand the off-diagonal elements are only approximately zero [3].

The main purpose of this Letter is to study the band profile of the matrix \(M_{nm}\) for a general displacement field \(D(s)\). In particular we want to understand why for special choices of \(D(s)\), notably dilations, we have quasi-orthogonality. Later we will explain that \(M_{nm}\) can be interpreted as the matrix element of a perturbation \(\delta H\) associated with a deformation of the boundary, such that \((n \cdot D)\delta x\) is the normal displacement of a wall element, given a control parameter \(\delta x\). In the following two paragraphs we explain the main motivations for our study.

The matrix elements \(|M_{nm}|^2\) determine the rate of irreversible energy absorption by the particle (i.e. dissipation) due to external driving. Here ‘external driving’ means time-dependent deformation of the boundary. Having exceptionally small \(|M_{nm}|^2\) for special choices of
D(s), such as dilations, translations and rotations, implies exceptionally small dissipation rate (‘non-heating’ effect). This observation goes against the naive kinetic picture that the rate of heating should not depend on how we ‘shake’ the boundary. The special nature of translations and rotations for \( \omega = 0 \) has been recognized in the context of nuclear dissipation. Our present approach allows us to analyze the non-heating effect present for dilations as well, and provide the form of the low-frequency response of the system in all three cases (dilations, translations and rotations).

There is another good motivation to study this issue. Recently, a powerful technique for finding clusters of billiard eigenstates and eigenenergies has been found by Vergini and Saraceno [10], with a speed typically \( \sim 10^3 \) greater than previous methods. This efficiency relies on the above quasi-orthogonality relation, the associated numerical error being given by the deviation of \( M_{nm} \) from \( \delta_{nm} \). Those authors tried to establish quasi-orthogonality using the identity \( M_{nm} = \delta_{nm} + [ (k_n^2 - k_m^2) / 2k^2 ] B_{nm} \), with \( B_{nm} \equiv \langle \psi_n | r \nabla | \psi_m \rangle \), and by assuming [4] that \( |B_{nm}| \sim O(1) \). However, a naive random wave argument would predict \( |B_{nm}| \sim O( \lambda / \lambda_0 )^{(d-1)/2} \).

Fig. 2 displays the band profile \( |M_{nm}|^2 \) for three choices of the displacement field \( D(s) \). The band profile can be regarded as either a function of \( \kappa = k_n - k_m \), or equivalently of \( \omega = (E_n - E_m) / \hbar \), related via \( \omega = v \kappa \). The three band profiles differ in their peak structure, but \( \omega \to 0 \) limits: notably for dilations \( |M_{nm}|^2 \) vanishes in this limit. Our aim is to understand the overall \( \omega \) dependence, and the small \( \omega \) behavior in particular. For the calculation of band profile we used all 451 eigenstates of the 2D quarter-stadium (see Fig. 1) lying between \( 398 < k < 402 \), found using the method of Vergini and Saraceno [10]. For this particular chaotic shape a remarkably good basis set (size of order \( L / \lambda_0 \)) of real and evanescent plane waves has been devised [4], which allows the tension error (defined as the boundary integral of \( \psi^2 \)) to be typically \( 3 \times 10^{-11} \) in our calculation, (maximum \( 2 \times 10^{-10} \) for any state). The resulting errors in \( \varphi \) manifest themselves only when \( |M_{nm}|^2 \) reaches its lowest reliable value \( \sim 10^{-10} \), visible as bottoming-out in the leftmost point of the inset of Fig. 2.

In order to understand the quantum-mechanical band profile, we can first assume that the eigenstates look like uncorrelated random waves. A lengthy but straightforward calculation [2] leads to the result

\[
|M_{nm}|^2 \approx \frac{2\langle \cos(\theta) \rangle^3}{\Omega_d} \frac{\lambda_n^{d-1}}{\sqrt{2}} \int (n \cdot D)^2 ds, \tag{2}
\]

where the geometric factors for \( d = 2, 3, \cdots \) are \( \Omega_d = 2\pi, 4\pi \cdots \) and \( \langle \cos(\theta) \rangle^3 = 4/(3\pi), 1/4, \cdots \). If the displacement field is normalized such that \( |D| \sim L \), then we get \( |M_{nm}|^2 \sim (\lambda_n / L)^{d-1} \). Note that the above result implies that \( |M_{nm}|^2 \) is independent of \( \omega \).

![FIG. 2.](image)

To go beyond the random-wave estimate [4], we adopt a more physically appealing point of view. We include a parametric deformation of the billiard shape via the Hamiltonian \( H(r, p; x) = p^2 / 2m + V(r - xD(r)) \), where \( x \) controls the deformation. Note that the displacement field \( D \) is regarded as a function of \( r \). The normal displacement of a wall element is \((n \cdot D) r \). The position of a particle in the vicinity of a wall element is conveniently described by \( Q = (s, z) \), where \( s \) is a surface coordinate and \( z \) is a perpendicular ‘radial’ coordinate. We set \( V(r) = V_0 \) outside the undeformed billiard; later we take the limit \( V_0 \to \infty \). We have \( \partial H / \partial x = -[n(s) \cdot D(s)] V_0 \delta(z) \). The logarithmic derivative with respect to \( z \) of an eigenfunction on the boundary is \( \varphi(s) / \psi(s) \). For \( z > 0 \) the wavefunction \( \psi(r) \) is a decaying exponential. Hence the logarithmic derivative of the wavefunction on the boundary should be equal to \( -\sqrt{2mV_0 / \hbar} \). Consequently one obtains \( \partial H / \partial x_{nm} = \langle \psi_n | xD(r) \psi_m \rangle = \langle (\hbar k)^2 / \lambda_0 \rangle M_{nm} \). Thus the band profile of \( M_{nm} \) is equal (up to a factor) to the band profile of the perturbation \( \delta H \) due to a deformation of the boundary. See also [11,12].

We can now use semiclassical considerations [13]. The application to the cavity example has been introduced.
Here we summarize the recipe. First one should generate a very long (ergodic) classical trajectory, and define for it the fluctuating quantity $\mathcal{F}(t) = -\partial \mathcal{H}(\mathbf{r}, \mathbf{p}; x)/\partial x|_{x=0}$, where the time-dependence of $\mathcal{F}$ is due to the trajectory $(\mathbf{r}(t), \mathbf{p}(t))$. Hence

$$\mathcal{F}(t) = \sum_{\text{col}} 2mv \cos(\theta_{\text{col}}) D_{\text{col}} \delta(t-t_{\text{col}})$$  \hspace{1cm} (3)$$

where $t_{\text{col}}$ is the time of a collision, $D_{\text{col}}$ stands for $\mathbf{n} \cdot \mathbf{D}$ at the point of the collision, and $v \cos(\theta_{\text{col}})$ is the normal component of the particle’s collision velocity. If the deformation is volume-preserving then $\langle \mathcal{F}(t) \rangle = 0$, otherwise it is convenient to subtract the (constant) average value.

Now one can calculate the correlation function $C(\tau)$ of the fluctuating quantity $\mathcal{F}(t)$, and its Fourier transform $\tilde{C}(\omega) \equiv \int C(\tau) \exp(i\omega \tau) d\tau$. The semiclassical estimate for the matrix element is

$$\left\langle \left| \left( \frac{\partial H}{\partial x} \right)_{nm} \right|^2 \right\rangle \approx \frac{\Delta}{2\pi \hbar} \tilde{C} \left( \frac{E_n - E_m}{\hbar} \right)$$  \hspace{1cm} (4)$$

where $\Delta$ is the mean level spacing. In practice it is convenient, without loss of generality, to work with units such that in (3) the time $t$ is measured in units of length, and we make the replacements $m \mapsto 1$ and $v \mapsto 1$. Then (3) can be cast into the form $\langle |M_{nm}|^2 \rangle \approx (\Delta_k/2\pi) \tilde{C}(\kappa)$ where $\Delta_k$ is the mean level spacing in $k$.

Fig. 2 shows the excellent agreement between the actual band profile and that predicted by Eq. (3) for generic deformations and dilation. Note that there were no fitted parameters in this match. In all estimations of $\tilde{C}(\omega)$ we have used single trajectories of $\sim 10^8$ consecutive collisions.

Understanding the band profile of $|M_{nm}|^2$ has now been reduced to a matter of finding a classical theory for $\tilde{C}(\omega)$. If we assume that Eq. (3) is a train of uncorrelated impulses, then its power spectrum would be that of white noise, namely $\tilde{C}(\omega) \approx \text{const}$. A straightforward calculation [12] then leads to the random wave result [3] already presented. However, in reality there are correlations in this train, and therefore we should expect $\tilde{C}(\omega)$ to have some structure on the frequency scale $\omega \sim 1/\tau_{\text{col}}$. Looking at Fig. 2 we see that the white noise expectation is reasonably satisfied for one of the ‘generic’ deformations (G), but not in the other two cases (D, Gp). We also see non-universal peaks at $\omega \sim 1/\tau_{\text{col}} \sim 1$. We now explain that for $\omega \ll 1/\tau_{\text{col}}$ there is total failure of the white noise result for dilations, as well as for translations and rotations, and discuss further complications that may arise if the billiard system is not strongly chaotic.

In Fig. 3 we display $\tilde{C}(\omega)$ for a different billiard shape, a generalized Sinai billiard (Fig. 1), chosen because it does not suffer from the non-generic marginally stable orbits found in the quarter-stadium. Here we see very convincing evidence that for small frequencies we have $\tilde{C}(\omega) \approx \text{const}$ for generic deformation, while $\tilde{C}(\omega) \propto \omega^4$ for dilation and translation and $\tilde{C}(\omega) \propto \omega^2$ for rotation. Thus the white noise expectation is indeed satisfied in the $\omega \ll 1/\tau_{\text{col}}$ regime for generic deformations, but fails for dilations, translations and rotations, for which $\tilde{C}(\omega) \to 0$ as $\omega \to 0$. This property is known (in the context of eigenvalue spectra) as ‘rigidity’ [3]. It implies that the train of impulses is strongly correlated, a result which at first sight seems inconsistent with the assumption of chaotic motion. We will explain that there is no inconsistency here.

The quantity $\mathcal{F}(t) = -\partial \mathcal{H}/\partial x$ is related to $\dot{\mathbf{p}} = -\partial \mathcal{H}/\partial \mathbf{r} = -\nabla \mathcal{V}$, the instantaneous force on the particle, by $\mathcal{F}(t) = -\mathbf{D}(\mathbf{r}) \cdot \dot{\mathbf{p}}$. For translations we have $\mathbf{D} = \dot{\mathbf{e}}$, where $\dot{\mathbf{e}}$ is a constant vector that defines a direction in space. We can write $\mathcal{F}(t) = (d/dt)^2 G(t)$ where $G(t) = -\dot{\mathbf{e}} \cdot \mathbf{r}$. A similar relation holds for dilation $\mathbf{D} = \mathbf{r}$ with $G(t) = -\frac{1}{2} \dot{\mathbf{r}}^2$. It follows that $\tilde{C}(\omega) = \omega^4 \tilde{C}_G(\omega)$, where $\tilde{C}_G(\omega)$ is the power spectrum of $G(t)$. Assuming that $G(t)$, unlike $\mathcal{F}(t)$, is a generic fluctuating quantity that looks like white noise, it follows that $\tilde{C}(\omega)$ is generically characterized by $\omega^4$ behavior for either translations or dilations. For rotations we have $\mathbf{D} = \dot{\mathbf{e}} \times \mathbf{r}$, and we can write $\mathcal{F}(t) = (d/dt)^2 G(t)$, where $G(t) = -\dot{\mathbf{e}} \cdot (\mathbf{r} \times \mathbf{p})$, is a projection of the particle’s angular momentum vector. Consequently $\tilde{C}(\omega) = \omega^2 \tilde{C}_G(\omega)$, and we expect $\tilde{C}(\omega)$ to be generically characterized by $\omega^2$ behavior in the case of rotations.
In the previous paragraph we have assumed that generic fluctuating quantities such as $r^2$ and $\hat{e} \cdot r$ and $\hat{e} \cdot (r \times p)$, as well as $F(t)$ for any generic deformations, have a white noise power spectrum as $\omega \to 0$. Obviously, this ‘white noise assumption’ should be verified for any particular example. If the motion is not strongly chaotic, meaning that $C(\tau)$ decays like a power law (say $1/\tau^{1-\gamma}$ with $0 < \gamma < 1$) rather than an exponential, then the universal behavior is modified: we may have $\omega^{-\gamma}$ behavior for small frequencies. For a generic system, for instance the generalized Sinai billiard, we do not have this complication. The stadium example on the other hand is non-generic: the trajectory can remain in the marginally stable ‘bouncing ball’ orbit (between the top and bottom edges) for long times, with a probability scaling as a power law in time. Depending on the choice of $D(r)$ this may manifest itself in $C(\tau)$. For example, in Fig. 2 the deformation $G_p$ involves a parallel displacement of the upper edge, and the resulting sensitivity to the bouncing ball orbit leads to large enhancement of the fluctuations intensity $C(\omega=0)$, and is suggestive of singular $\omega^{-\gamma}$ behavior for small $\omega$.

Finally, consider the time-dependent problem which is described by the Hamiltonian $\mathcal{H}(r, p; x(t))$. It is well known that under quite general circumstances the dissipation is ohmic ($\propto \dot{x}^2$). See [11,12] and references therein. If $x(t) = A \sin(\omega t)$, linear response theory gives the long-time heating rate $d\langle \mathcal{H} \rangle / dt = \mu \cdot \frac{1}{2} (\omega A)^2$. The dissipation coefficient $\mu$ is determined by the matrix elements of $\mathcal{H}$, and therefore $\mu$ is proportional to $C(\omega)$. Our results imply that $\mu$ vanishes in the limit $\omega \to 0$ for translations. One should not be surprised since this follows from Galilean invariance: One can view the limit $\omega \to 0$ as corresponding to the special case of constant $\dot{x}$. For constant nonzero $\dot{x}$ the particle(s) in the cavity accommodate their motion to the reference frame of the cavity, and there is no dissipation. A similar argument holds for rotations. On the other hand it is somewhat surprising that the same conclusion holds for dilations (the only other shape-preserving deformation) as well. This observation, as far as we know, has not been introduced previously in the literature.

**Appendix:** There exist a couple of lengthy vector-identity proofs [11,12] of the normalization $M_{nn} = 1$ for the dilation case $D = \mathbf{r}$, for $d = 2$. Here we present a physically illuminating alternative that works for arbitrary $d$. We use a phase-space-preserving definition of dilation operator $U(\alpha) \equiv \exp(i\alpha G/h)$. It is generated by the hermitian operator $G = \frac{1}{2}(\mathbf{r} \cdot p + p \cdot \mathbf{r})$. Applying this dilation on wavefunctions gives the expansion:

$$U(\alpha)\psi(r) \approx \psi(r) + \alpha ((d/2)\psi + r \cdot \nabla \psi) + O(\alpha^2) \quad (5)$$

The operator also has the effect $U^\dagger U = e^{\alpha^2} r$ and $U^\dagger p U = e^{-\alpha^2} p$. Consider now any Hamiltonian $\mathcal{H}_0 = p^2/(2m) + V(r)$. Defining the parameter-dependent version $\mathcal{H}(\mathbf{r}, p; \alpha) = U(\alpha)\mathcal{H}_0(\mathbf{r}, p)U(\alpha)^\dagger$, it is straightforward to obtain

$$\left. \frac{\partial \mathcal{H}}{\partial \alpha} \right|_{\alpha=0} = \frac{\mathbf{p}^2}{m} - \mathbf{r} \cdot \nabla V, \quad (6)$$

whose matrix elements in the case of the billiard potential are $\langle \partial \mathcal{H}/\partial \alpha \rangle_{nm} = ((\hbar k)^2/m) [\delta_{nm} - M_{nm}]$. Thus the non-diagonal terms are the same as those of the deformation $D = \mathbf{r}$. The diagonal elements can be calculated directly by taking the limit $\alpha \to 0$ of the expression $\langle \langle \psi | \mathcal{H}_0 | \psi \rangle \rangle_{nm}$. Using (5) and the fact that $\langle \psi | \mathbf{r} \cdot \nabla | \psi \rangle = -d/2$ one can easily show that the result equals zero. From here it follows that $M_{nn} = 1$.

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[4] However, the behavior $B \sim |k_n - k_m|$ has since been observed numerically (E. Vergini, personal communication), in agreement with our results.
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