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Measuring billiard eigenfunctions with arbitrary trajectories

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We propose a method of measuring approximate quantum eigenfunctions in polygonalized billiard geometries, based on a quasiclassical evolution operator having a (smoothened) Perron-Frobenius kernel modulated by a phase arising from quantum considerations. Using a plane wave ansatz, we show that the condition under which this is an eigenfunction of the quasiclassical operator is identical to the condition for it to be an eigenfunction of the Schrödinger equation for polygonalized billiards. Finally, we demonstrate this technique by determining the quasiclassical eigenfunctions of the polygonalized stadium billiard using arbitrary trajectories and comparing this with the exact quantum stadium eigenfunctions.

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The quantum billiard problem consists of determining the eigenvalues and eigenfunctions of the Helmholtz equation $\nabla^2\psi(q)+k^2\psi(q)=0$ with $\psi(q)=0$ on the billiard boundary ∂B (Dirichlet boundary condition). This simple wave equation arises in various contexts and has been used extensively to test ideas of quantum chaos. It can describe acoustic waves, modes in microwave cavities and has relevance in studies on quantum dots, where the motion of electrons can be regarded as ''free'' inside an enclosure. The problem is analytically tractable only for the small subset of ''integrable'' boundaries for which the classical dynamics is regular. For other enclosures, the eigenstates must be computed numerically and a number of efficient ''boundary'' methods exist that allow us to study the eigenvalues and eigenfunctions.

Of particular interest is the determination of approximate quantum eigenstates using classical quantities. While the old quantum theory of Bohr and co-workers works only for regular or integrable systems, modern semiclassical theories have respondend to the challenge posed by chaotic classical dynamics and the successful quantization of the helium atom [1] points to its success. The aim, however, is not necessarily linked to the development of a cheap substitute for the computer intensive numerical methods that determine the exact quantum states. While this is a desirable consequence, semiclassical studies endeavor to provide an understanding of the quantum phenomenon in terms of classical objects that we are so familiar with. Modern semiclassical methods have indeed furthered our understanding of the quantum-classical correspondence. Thus, we are now aware of the duality of quantum eigenenergies and classical periodic orbits—a relationship that now forms the cornerstone of most semiclassical theories [2]. The study of ''scars'' has also revealed the structure of quantum eigenfunctions and classical trajectories have even been used to construct semiclassical eigenfunctions of chaotic systems [3]. Quantum states can, thus, be contemplated in classical terms as a first approximation with corrections providing its true quantum nature.

In this context, a question that may be asked is the following: *What is the degree of classical information that is required in order to extract a first approximation of a quantum state*? This is especially pertinent when the system in question is chaotic or mixed with islands of regularity interspersed in the chaotic sea. Since the quantum state (or the quasiprobability distributions constructed out of them) can essentially resolve phase space structures of the size of a Planck cell, is information finer than that redundant? For billiards, the de Broglie wavelength λ, provides a relevant length scale that can be used effectively to probe the boundary of the enclosure. If a smooth billiard boundary is polygonalized such that the short time classical dynamics is well approximated, the two billiards are semiclassically equivalent, provided, λ is larger than the average length of edges of the polygon [4]. Thus, instead of the full chaotic dynamics of the stadium billiard, one may as well consider the dynamics of its polygonal counterpart for a given de Broglie wavelength [5]. This idea has, however, not been used to determine *semiclassical* eigenvalues or eigenfunctions. Indeed, by most accounts, a polygonalized approach to semiclassics is bound to be even more difficult since periodic orbit quantization of polygons has proved largely unsuccessful [6] and it is generally believed that diffractive contributions must be included even for obtaining a first approximation of a polygonal quantum state [7,8].

The polygonalization approach is, however, aptly suited for a recently developed time domain technique [9,10] of determining quantum eigenvalues in marginally stable billiard geometries (which includes polygonalized ones). The algorithm involves shooting arbitrary trajectories in various directions from a point interior to the billiard (call it q') and at each time step, recording the fraction of trajectories that are in an ϵ neighborhood of a point q, weighted by a phase arising from quantum considerations. The peak positions in the power spectrum of this weighted fraction $F(t)$ are related to the quantum eigenvalues and as we shall show here, the heights of the peaks are a measure of the quantum eigenfunctions at the point q.

The arbitrary trajectory quantization method outlined above is based on a quasiclassical [11] propagator

$$\mathcal{L}^t_{qc}(\varphi)\circ\phi(q)=\int dq' \;\; \delta(q-q'^t(\varphi))e^{-i\nu(t)\pi/2} \;\; \phi(q'), \tag{1}$$

where $q'^t(\varphi)$ is the position at time t of a trajectory which starts at q' $(t=0)$ on an invariant surface labeled by φ and the energy E. The phase $\nu(t)=\nu(q'^t(\varphi))$ depends on the caustic structure of the trajectory and is identical to the phase in the semiclassical propagator [2]. For billiards, $\nu(t) = 2n(t)$, where $n(t)$ is the number of reflections suffered by the trajectory $q'^{t}(\varphi)$. When $\nu(t)$ is identically zero (as in case of Neumann boundary conditions), $\mathcal{L}^{t}_{qc}(\varphi)$ reduces to the (classical) Perron-Frobenius operator on the (E,φ) invariant surface.

Note that marginally stable billiards have an invariant surface labeled by two constants of motion one of which is the energy E [12]. We denote here the second constant by φ. For the circle billiard φ is a measure of the angular momentum, while for a rectangle billiard, φ is a measure of the linear momentum $(p\cos\varphi, p\sin\varphi)$ and can be taken as the angle that the unfolded trajectory makes with the X axis. In case of rational polygonal billiards too, φ can be taken to be a measure of the linear momentum even though, it is not directly a conserved quantity. However, in an unfolded picture where a family of trajectories can be denoted by a single straight band, φ is conserved and serves to label families of trajectories.

The full quasiclassical evolution operator is defined as

$$\begin{aligned}\mathcal{L}^{t}_{qc}\circ\phi(q) &= \int d\varphi\,\mathcal{L}^{t}_{qc}(\varphi)\\ &= \int dq'\left\{\int d\varphi\,\delta(q - q'^{t}(\varphi))\,e^{-i\nu(t)\pi/2}\right\}\phi(q')\\ &= \int dq'\,K_{qc}(q,q',t)\,\phi(q'),\end{aligned} \tag{2}$$

where K_{qc} is the quantity in $\{\}$. The operator $\mathcal{L}^{t}_{qc}$ takes into account the entire constant energy surface by summing (integrating) over all φ invariant surfaces.

The motivation in constructing the quasiclassical operator as in Eq. (1) is as follows. For polygonal billiards, the trace of the classical Perron-Frobenius operator is related to the trace of the semiclassical propagator when $\nu(t) = 0$. For Dirichlet boundary condition, this correspondence can be restored if the kernel contains the phase $e^{-i\nu(t)\pi/2}$ [9,10]. This gives rise to a quasiclassical propagator.

In the following, we shall first establish that the eigenfunctions of $\mathcal{L}^{t}_{qc}$ for polygonalized geometries are also eigenfunctions of the Schrödinger equation. We shall demonstrate this numerically for a polygonalized stadium billiard by constructing the quasiclassical kernel $K_{qc}(q,q,t)$ using arbitrary trajectories and use this to determine the eigenfunction intensities.

As an illustrative example, consider a particle in a one-dimensional box and consider the evolution of the quantum eigenfunction (Dirichlet boundary conditions) $\psi_n(q) = e^{ik_nq} - e^{-ik_nq}$, $k_n = n\pi/L$. Its time evolution in quantum mechanics is simply $e^{-iE_nt/\hbar}\psi(q)$, where $E_n = \hbar^2k_n^2/2m$. Its quasiclassical evolution for positive velocity, $\mathcal{L}^{t}_{qc}(+)\circ\psi_n(q)$, is given by

$$(e^{ik_nq^{-t}(+v)} - e^{-ik_nq^{-t}(+v)})\,e^{-i\pi n[q^{-t}(+v)]}, \tag{3}$$

where $n[q^{-t}(+v)]$ is the number of reflections suffered by a trajectory in time $-t$ with initial position q and initial velocity $+v$. Similarly, $\mathcal{L}^{t}_{qc}(-)\circ\psi_n(q)$ is

$$(e^{ik_n[q^{-t}(-v)]} - e^{-ik_n[q^{-t}(-v)]})\,e^{-i\pi n[q^{-t}(-v)]}, \tag{4}$$

with the $-$ sign in $\mathcal{L}^{t}_{qc}(-)$ denoting negative velocity. Note that the flow is such that the velocity changes sign at every reflection from the walls at $q = 0$ and $q = L$, while $n(t)$ increments by one at each of these instants. For the flow $q^{-t}(+v)$, the reflections occur at $t_n^{+} = (q + nL)/v$ so that for $t_0^{+} < t < t_1^{+}$, $q^{-t}(+v) = v(t - t_0^{+}) = vt - q$. Similarly, for the flow $q^{-t}(-v)$, the reflections occur at $t_n^{-} = (L - q + nL)/v$ and for $t_0^{+} < t < t_1^{+}$, $q^{-t}(-v) = L - v(t - t_0^{-}) = 2L - vt - q$. It follows, hence, that

$$\mathcal{L}^{t}_{qc}(\pm)\circ\psi_n(q) = e^{ik_n(q\,\mp\,vt)} - e^{-ik_n(q\,\mp\,vt)} \tag{5}$$

for all t. Finally, noting that there are only two possible values of φ (linear momentum) in this one-dimensional example, the full quasiclassical operator is expressed as $\mathcal{L}^{t}_{qc} = \mathcal{L}^{t}_{qc}(+) + \mathcal{L}^{t}_{qc}(-)$. It follows that

$$\mathcal{L}^{t}_{qc}\circ\psi_n(q) = 2\cos(k_nvt)\,\psi_n(q). \tag{6}$$

In other words, the quantum eigenfunction is also an eigenfunction of the full quasiclassical evolution operator $\mathcal{L}^{t}_{qc}$ [13].

This is true for general polygonalized billiards as well and we shall establish this by showing that the condition under which a plane wave superposition is a quantum (semiclassical) eigenfunction is identical to the condition for this plane wave superposition to be an eigenfunction of $\mathcal{L}^{t}_{qc}$.

For polygonalized billiards, the semiclassical wave function can be expressed as

$$\psi(q) = \sum_{j=1}^{M} A_j e^{ik\cos(\mu_j)x + ik\sin(\mu_j)y}, \tag{7}$$

where A_j are constants [14] and the number of terms M in the expansion is determined by closure of the wave vector $\vec{k} = (k\cos\mu_j, k\sin\mu_j)$ under reflection from the edges [15]. For this finite superposition of plane waves, the boundary condition $\psi(q) = 0$ on ∂B can be satisfied if the waves vanish in pairs with an incident wave giving rise to a reflected wave. Thus, on the lth segment $y = a_lx + b_l$, we must have

$$\begin{aligned}&A_j e^{i(k\cos\mu_j + a_lk\sin\mu_j)x + ib_lk\sin\mu_j}\\ &\qquad + A_{j'} e^{i(k\cos\mu_{j'} + a_lk\sin\mu_{j'})x + ib_lk\sin\mu_{j'}} = 0.\end{aligned} \tag{8}$$

Assuming that $\mu_{j'}$ is related to μ_j through the laws of reflection, it is easy to show that

$$\cos\mu_j + a_l\sin\mu_j = \cos\mu_{j'} + a_l\sin\mu_{j'} . \tag{9}$$

Thus, Eq. (8) reduces to

$$A_j e^{ib_lk\sin\mu_j} + A_{j'} e^{ib_lk\sin\mu_{j'}} = 0, \tag{10}$$

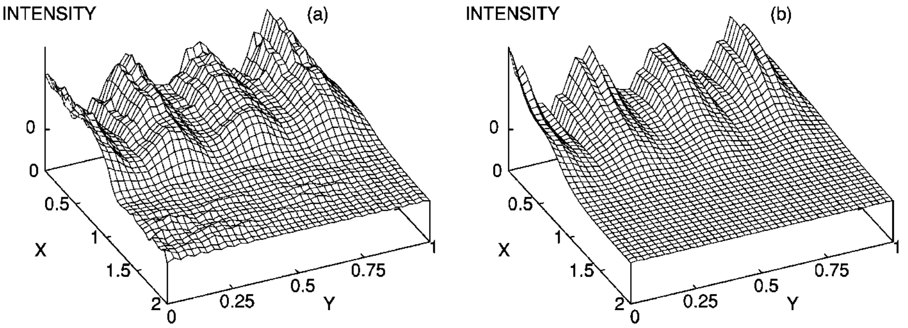

FIG. 1. (a) A quasiclassical bouncing ball eigenfunction of the polygonalized stadium and (b) its quantum counterpart in the smooth stadium.

where $\mu_{j'}=\pi-\mu_j+2\theta_l$ and θ_l is the angle between the positive X axis and the outward normal to the lth line segment.

Note that for each of the K segments on the boundary, the jth wave has, in general, a different reflected wave as a counterpart so that Eq. (10) gives K different expressions for A_j. In general (barring exceptions such as the rectangle billiard), these “boundary conditions” can be satisfied only approximately as we shall argue below. Recall that for the numerical determination of exact eigenvalues using a plane wave basis, the boundary is discretized (N points) and an appropriate measure (such as a determinant) is used to determine the eigenstates which satisfy the boundary condition at these points. Convergence can be achieved by increasing N so that as $N\to\infty$, the boundary condition is satisfied exactly. In contrast, the number of terms in Eq. 7 is fixed. Thus, if the exact eigenfunction contains additional plane waves, the boundary condition will be satisfied *approximately* and the plane wave expansion of Eq. (7) can only give an approximate quantum eigenfunction.

We shall now establish that the (finite) plane wave superposition [Eq. 7] is *also* an approximate eigenfunction of the quasiclassical evolution operator provided the set of “quantization” conditions given by Eq. (10) are satisfied.

Consider, therefore, the plane wave superposition of Eq. (7). Its quasiclassical evolution is given by

$$\mathcal{L}^{t}_{qc}(\varphi)\circ\psi_n(q)=\sum_{j=1}^{M} A_j e^{ik_x x^{-t}(\varphi)+ik_y y^{-t}(\varphi)}e^{-in(t)}, \quad (11)$$

where $k_x=k\cos(\mu_j)$, $k_y=k\sin(\mu_j)$, while $x^{-t}(\varphi)$ and $y^{-t}(\varphi)$ denote the flow at time $-t$ with initial position (x,y) and velocity $(v\cos\varphi, v\sin\varphi)$. For short times, this is given by

$$\mathcal{L}^{t}_{qc}(\varphi)\circ\psi_n=\sum_{j=1}^{M} A_j e^{ik_x(x-v\cos\varphi t)+ik_y(y-v\sin\varphi t)}, \quad (12)$$

since $n(t)=0$. We shall first determine the evolution of a single wave after reflection from one of the segments, $y=a_l x+b_l$. For the flow, $(x^{-t}(\varphi),y^{-t}(\varphi))$, reflection from the line segment takes place at $t_0=(x-x_0)/(v\cos\varphi)=(y-y_0)/(v\sin\varphi)$, where (x_0,y_0) is the point of impact. The flow at a time t after the reflection is given by

$$x^{-t}(\varphi)=x(t)=x_0+v\cos(\varphi-2\theta_l)(t-t_0),$$

$$y^{-t}(\varphi)=y(t)=y_0+v\sin(\varphi-2\theta_l)(t-t_0). \quad (13)$$

It is easy to verify that after one reflection from the segment $y=a_l x+b_l$, the wave $A_j e^{ik\cos\mu_j x+k\sin\mu_j y}$ evolves quasiclassically to

$$A_{j'}e^{k\cos\mu_{j'}(x-v\cos\varphi t)+k\sin\mu_{j'}(y-v\sin\varphi t)}, \quad (14)$$

where $\mu_{j'}=\pi-\mu_j+2\theta_l$ and

$$A_j e^{ikb_l\sin\mu_j}+A_{j'}e^{ikb_l\sin\mu_{j'}}=0. \quad (15)$$

Thus, after one reflection, the finite plane wave superposition assumes the form for small t provided the reflected waves are included in the superposition and the “quantization conditions” are (approximately) satisfied for a given value of k_n. It follows that $\psi_n(q)$ is an (approximate) eigenfunction of the full quasiclassical evolution operator:

$$\mathcal{L}^{t}_{qc}\circ\psi_n(q)=\int d\varphi\ \mathcal{L}_{qc}(\varphi)\psi_n(q) \quad (16)$$

$$=\int d\varphi\ e^{-ik_n vt\cos(\varphi-\mu_j)}\sum_j A_j e^{iS_j(k_n)} \quad (17)$$

$$=2\pi J_0(k_n vt)\ \psi_n(q), \quad (18)$$

where $S_j(k_n)=k_n\cos(\mu_j)x+k_n\sin(\mu_j)y$ and J_0 is the Bessel function. In summary then, *a finite plane wave superposition can be an approximate semiclassical and a quasiclassical eigenfunction under identical conditions*.

We shall now demonstrate our result for a stadium billiard consisting of two parallel straight segments of length 2 joined on either end by a semicircle of unit radius. For the evaluation of the quasiclassical eigenfunctions, we shall consider a polygonalized enclosure, where each semicircle is replaced by 12 straight edges of equal length. In order to determine the quasiclassical eigenfunctions, we shall first evaluate a smoothened quasiclassical kernel

$$K_{qc}(q,q',t)=\int d\varphi\ \delta_\epsilon(q-q'^{t}(\varphi))e^{-i\pi n[q'^{t}(\varphi)]}$$

$$=\sum_n \psi_n(q)\psi_n^{*}(q')\Lambda_n(t) \quad (19)$$

as a function of time (δ_ϵ is a smoothened δ function). This is achieved by shooting trajectories from a point q' at various angles and evaluating the fraction of trajectories in a cell of size ϵ [19] at q, weighted by the phase $e^{-i\pi n[q'^{t}(\varphi)]}$. Since

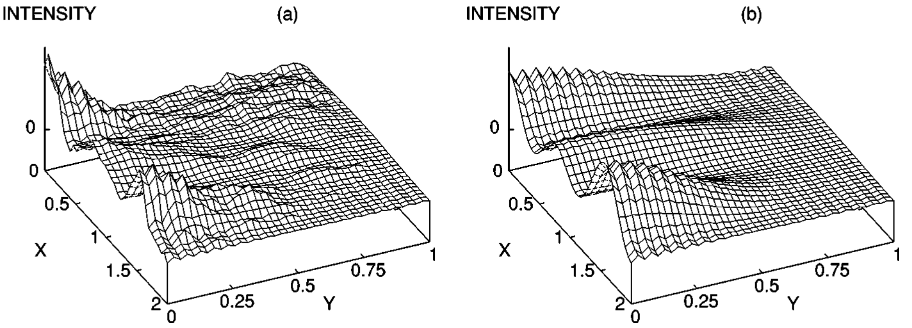

FIG. 2. (a) A quasiclassical eigenfunction peaked along the X axis and (b) its quantum counterpart.

$\Lambda_n = 2\pi J_0(k_n v t)$, for $v=1$, a Fourier transform of $K_{qc}(q,q',t)$ has peaks at $k=k_n$ and the heights are proportional to $\psi_n(q)$.

Note that the smoothening of the δ function kernel is essential for polygonalized billiards and shows up naturally in an alternate approach involving the trace of the quasiclassical and semiclassical propagators [20]. In the present formalism involving plane waves, smearing of the kernel leads to a modified quantization condition for the quasiclassical eigenfunctions. We shall however ignore these complications and merely remark that the parameter ϵ is $O(1/k)$ [10].

Figure 1(a) shows a "bouncing ball" quasiclassical eigenfunction intensity $|\psi_n(q)|^2$ at $k=10.97$ in the quarter stadium, while the corresponding quantum eigenfunction in the stadium at $k=11.05$ is shown in Fig. 1(b). An example of a quasiclassical eigenfunction at $k=4.02$ peaked along the X axis is shown in Fig. 2(a) along with its quantum conterpart at $k=4.38$. The quasiclassical eigenfunction clearly provides a first approximation of the quantum eigenfunction in both cases. Eigenfunctions of other billiards including triangles have also been obtained. Details of this work will be published elsewhere. In conclusion, we have demonstrated that the quasiclassical eigenfunctions determined using arbitrary trajectories in a polygonalized chaotic enclosure, approximate the quantum eigenfunctions of the smooth billiard. We have also shown that a finite plane wave expansion is an approximate eigenfunction of the quantum and quasiclassical evolution operators under identical conditions.

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[7] It has recently been shown [8] that closed almost-periodic (CAP) orbits also contribute in generic polygonal enclosures with weights that are comparable to periodic orbits. Also, they are more numerous and hence indispendable for quantization.

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[11] We reserve the term "semiclassical" for those studies which involve an approximation of the quantum propagator in the $\hbar \to 0$ limit and use the term "quasiclassical" for the modified classical propagator.

[12] Chaotic billiards have a single constant of motion, the energy E. Smooth integrable billiards such as the circle and the ellipse have two constants of motion but generic smooth billiards have only one global constant of motion. Polygonal billiards have two constants of motion, though generically, their invariant surface is not a torus.

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[19] Several other smoothened kernels can be used (see [10] for details).

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