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. We show that quasiclassical evolution differs from semiclassical (or quantum) evolution but the operators have the same set of eigenfunctions. We demonstrate this 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 $\partial B$ (Dirichlet boundary condition). This simple wave equation arises in various contexts and has been extensively used 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 responded 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 endeavour 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 quasi-probability distributions constructed out of them) can essentially resolve phase space structures of the size of a Plank cell, is information finer than that redundant? For billiards, the de Broglie wavelength $\lambda$, 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, $\lambda$ 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. The polygonalization concept is implicit even in the numerical computation of the “exact” eigenvalues using boundary methods in which the perimeter is discretized with the number of points $N \sim L/\lambda$ where $L$ is the perimeter of the enclosure. 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 $^5$. Also, it is generally believed that diffractive contributions must be included even for obtaining a first approximation of a polygonal quantum state. On the other hand, it has recently been shown $^6$ that closed almost-periodic (CAP) orbits also contribute in generic polygonal enclosures with weights that are comparable to periodic orbits. Besides, they are more numerous and hence indispensable for semiclassical quantization. Thus, the failure of periodic orbit quantization in polygons is not so much due to diffraction as due to the neglect of CAP orbits. The modified periodic orbit theory for polygons should in principle be able to provide approximate quantum eigenvalues although CAP contributions can be difficult to evaluate.

A recently developed time domain technique $^7$ of determining quantum eigenvalues in marginally stable
billiard geometries makes use of arbitrary classical trajectories. The algorithm involves shooting 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 \( \epsilon \) neighbourhood 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 in this letter, the heights of the peaks are a measure of the quantum eigenfunctions at the point \( q \). Thus, the arbitrary trajectory quantization method (ATQM) is aptly suited for polygonalized billiards and we shall demonstrate for the stadium billiard that the quasiclassical eigenfunctions of the polygonalized stadium do approximate the “exact” eigenfunctions of the full stadium.

The ATQM bypasses the need to evaluate periodic or CAP orbits but is nevertheless based on the modified periodic orbit theory for polygons. The parameter \( \epsilon \) \( (\mathcal{O}(1/k)) \) embodies the contribution of CAP orbits and must be nonzero for any calculation at finite \( k \). In the following, we shall first use a plane wave ansatz to show that the peak heights in the power spectrum are a measure of the approximate quantum eigenfunction and then demonstrate this for a polygonalized stadium.

We define the quasiclassical \( \frac{\partial}{\partial t} \) propagator \( \mathcal{L}^t_{qc}(\varphi) \) restricted to the \( \varphi \) invariant surface as

\[
\mathcal{L}^t_{qc}(\varphi) \circ \phi(q) = \int dq' \delta(q - q''(\varphi)) e^{-i\nu(t)\pi/2} \phi(q')
\]

where \( q''(\varphi) \) is the position at time \( t \) of a trajectory which starts at \( q' \) \( (t = 0) \) on an invariant surface labelled by \( \varphi \) and the energy \( E \). The phase \( \nu(t) = \nu(q''(\varphi)) \) depends on the caustic structure of the trajectory and is identical to the phase in the semiclassical propagator \( \frac{\partial}{\partial t} \). When \( \nu(t) \) is identically zero (as in case of Neumann boundary conditions), \( \mathcal{L}^t_{qc}(\varphi) \) reduces to the Perron-Frobenius operator on the \( \varphi \) invariant surface. Note that rational polygonal billiards have a second constant of motion due to which the invariant surface is 2-dimensional \( \frac{\partial}{\partial t} \). On successive reflections, the trajectory changes its momentum following the laws of reflection but continues to live on the same invariant surface labelled by \( E \) and \( \varphi \). Thus, \( \varphi \) also labels distinct trajectories that start from a given point \( q' \).

The full quasiclassical evolution operator is defined as

\[
\mathcal{L}^t_{qc} \circ \phi(q) = \int d\varphi \mathcal{L}^t_{qc}(\varphi) \circ \phi(q) = \int dq' \left\{ \int d\varphi \delta(q - q''(\varphi)) e^{-i\nu(t)\pi/2} \right\} \phi(q')
\]

Note that quasiclassical evolution differs from semiclassical evolution. To illustrate this, consider a particle in a one-dimensional box (Dirichlet boundary conditions) and consider the evolution of the quantum eigenfunction

\[
\psi_n(q) = e^{ik_n q} - e^{-ik_n q}, \quad k_n = n\pi/L.
\]

Its time evolution in quantum mechanics is simply \( e^{-iE_n t}\psi(q) \) where \( E_n = h^2 k_n^2 / 2m \). Its quasiclassical evolution, \( \mathcal{L}^t_{qc}(+) \circ \psi_n(q) \), is given by

\[
\left( e^{ik_n q - t(+) +} - e^{-ik_n q - t(+) +} \right) e^{-i\pi n(q - t(+) +)}
\]

where \( n(q^{-}(+) +) \) 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

\[
\left( e^{ik_n q - t(-) -} - e^{-ik_n q - t(-) -} \right) e^{-i\pi n(q - t(-) -)}
\]

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 \( q^{-}(+) + \), the reflections occur at \( t_n^+ = (q + nL)/v \) so that for \( t_n^+ < t < t_n^+ + q^{-}(+) + (v) = v(t - t_n^+) = vt - q \). Similarly, for the flow \( q^{-}(-) - \), the reflections occur at \( t_n^- = (L - q + nL)/v \) and for \( t_n^- < t < t_n^- + q^{-}(-) - (v) = L - v(t - t_n^-) = 2L - vt - q \). It follows hence that

\[
\mathcal{L}^t_{qc}(\pm) \circ \psi_n(q) = e^{ik_n q \mp vt} - e^{-ik_n q \mp vt}
\]

for all \( t \). Thus

\[
(\mathcal{L}^t_{qc}(+) + \mathcal{L}^t_{qc}(-)) \circ \psi_n(q) = 2\cos(k_n vt)\psi_n(q)
\]

In other words, \( \psi_n(q) \) is also an eigenfunction of the full quasiclassical evolution operator \( \mathcal{L}^t_{qc} = \mathcal{L}^t_{qc}(+) + \mathcal{L}^t_{qc}(-) \). Note that in the Neumann case, \( \psi_n(q) \) is not an eigenfunction; rather \( e^{ik_n q} + e^{-ik_n q} \) is an eigenfunction with \( n(t) = 0 \).

For a general 2-dimensional billiard, there is strong numerical evidence to suggest that a (real) plane wave superposition can be used to construct eigenfunctions \( \frac{\partial}{\partial t} \). We shall adopt here the view that a finite plane wave superposition does yield at least good approximate eigenfunctions. For polygonalized billiards, the semiclassical wavefunction can be expressed as

\[
\psi(q) = \sum_{j=1}^{M} A_j e^{ik \cos(\mu_j)x + ik \sin(\mu_j)y}.
\]

where \( A_j \) are constants \( \frac{\partial}{\partial t} \) and the number of terms \( M \) in the expansion is determined by closure of the wave vector \( \bar{k} = (k \cos \mu_j, k \sin \mu_j) \) under reflection from the edges.

For this finite superposition of plane waves, the boundary condition \( \psi(q) = 0 \) on \( \partial B \) can be satisfied if the waves vanish in pairs with an incident wave giving rise to a reflected wave. Thus on the \( l \)th segment \( y = a_lx + b_l \), we must have

\[
A_j e^{i(k \cos \mu_j + a_l k \sin \mu_j)x + ib_l k \sin \mu_j} + A_j e^{i(k \cos \mu_j' + a_l k \sin \mu_j')x + ib_l k \sin \mu_j'} = 0.
\]
Assuming that \( \mu' \) is related to \( \mu_j \) 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. (9) reduces to

\[
A_j e^{i \theta_l k \sin \mu_j} + A_j' e^{i \theta_l k \sin \mu_j'} = 0 \tag{10}
\]

where \( \mu_j' = \pi - \mu_j + 2 \theta_l \) and \( \theta_l \) is the angle between the positive \( X \)-axis and the outward normal to the \( l \)th line segment.

Note that for each of the \( K \) segments on the boundary, the \( j \)th 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. (10) 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. (10) can only give an approximate quantum eigenfunction.

We shall now establish that the (finite) plane wave superposition (eq. (10) 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. (10). Its quasiclassical evolution is given by

\[
L_{qc}^t(\psi) = \sum_{j=1}^{M} A_j e^{ik_x x - t(\psi) + ik_y y - t(\psi)} e^{-i n(t)} \tag{11}
\]

where \( k_x = k \cos(\mu_j) \), \( k_y = k \sin(\mu_j) \) while \( x^{-t}(\psi) \) and \( y^{-t}(\psi) \) 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

\[
L_{qc}^t(\psi) = \sum_{j=1}^{M} A_j e^{ik_x (x - v \cos \varphi t) + ik_y (y - v \sin \varphi t)} \tag{12}
\]

As before, 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

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

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

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

\[
A_{j'} e^{ik \cos \mu_{j'} (x - v \cos \varphi t) + k \sin \mu_{j'} (y - v \sin \varphi t)} \tag{14}
\]

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

\[
A_{j'} e^{ik \cos \mu_{j'} x + k \sin \mu_{j'} y} = 0 \tag{15}
\]

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 \( L_{qc} = \int d\varphi L_{qc}(\varphi) \)

\[
L_{qc}^t \circ \psi_n(q) = \int d\varphi L_{qc}(\varphi) \psi_n(q) = \int d\varphi e^{-ik_n vt \cos(\varphi - \mu_j)} \sum_j A_j e^{iS_j(k_n)} \tag{17}
\]

\[
= 2\pi J_0(k_n vt) \psi_n(q) \tag{18}
\]

where \( S_j(k_n) = k_n \cos(\mu_j x) + k_n \sin(\mu_j y) \). Thus, 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

\[
K_{qc}(q, q', t) = \int d\varphi \delta(q - q'^t(\varphi)) e^{-2\pi n(q'^t(\varphi))} \tag{19}
\]

as a function of time. Thus is achieved by shooting trajectories from a point \( q' \) at various angles and evaluating the fraction of trajectories in a cell of size \( \epsilon \) at \( q \), weighted by the phase \( e^{-2\pi n(q'^t(\varphi))} \). Since \( \Lambda_n = 2\pi J_0(k_n vt) \), 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 delta function kernel is essential in order to accommodate closed almost-periodic orbits and shows up naturally in an alternate proof (of the identity of the semiclassical and quasiclassical eigenvalues) involving the trace of the quasiclassical and semiclassical propagators. 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 reiterate that the parameter \( \epsilon \sim 1/k \).

Fig. 14 shows a “bouncing ball” quasiclassical eigenfunction intensity \( |\psi_n(q)|^2 \) at \( k = 10.97 \) in the quarter stadium.
FIG. 1. (a) A quasiclassical bouncing ball eigenfunction of the polygonalized stadium and (b) its quantum counterpart in the smooth stadium.

FIG. 2. (a) A quasiclassical eigenfunction peaked along the X axis and (b) its quantum counterpart while the corresponding quantum eigenfunction in the stadium at \( k = 11.05 \) is shown in fig. 1b. An example of a quasiclassical eigenfunction at \( k = 4.02 \) peaked along the X-axis is shown in fig. 2a, along with its quantum counterpart 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, approximates 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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[9] 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.
[10] For rational polygons, the angle \( \varphi \) measures the linear momentum \((p \cos \varphi, p \sin \varphi)\). It is not directly a conserved quantity but serves to label the invariant surface which consists of a finite number of copies of the polygon glued appropriately along the edges.
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