A Computational Study of the Quantization of Billiards with Mixed Dynamics

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ABSTRACT

We examine the relationship between the spectrum of quantum mushroom billiards and the structure of their classical counterparts, which have mixed integrable-chaotic dynamics. Accordingly, we study the eigenvalues corresponding to eigenfunctions of the stationary Schrödinger equation with homogeneous Dirichlet boundary conditions on half-mushroom-shaped geometries for very high energies/wavenumbers using the "scaling method," a technique for eigenvalue/boundary value problems. We compute several thousand consecutive eigenvalues to obtain a cumulative energy level spacing distribution that, according to a conjecture of Berry and Robnik, can also be determined from the relative volumes of the integrable components of the phase space of the classical billiard. Our results suggest that the Berry-Robnik conjecture for the quantization of systems with mixed dynamics holds for quantum mushroom billiards with circular caps.

This paper details a numerical study of the quantization of billiards with mixed dynamics. Such quantum billiards can be thought of as "particle in a box" models with corresponding classical Hamiltonian (energy-conserving) billiards that can exhibit either chaotic or integrable dynamics (depending upon initial conditions). Quantum billiards are more than just a theoretical curiosity, however, as they have been implemented experimentally using microwaves in reflective cavities [22], cold atoms [13], and quantum dots [22]. The particular problem in which we are interested is closely related to the question popularly known as "Can one hear the shape of a drum?" That is, can one uniquely describe the boundary of a planar region from its spectrum (i.e., its set of eigenvalues)? Here we investigate the relation of the classical billiard's dynamics to the cumulative nearest-neighbor spacing distribution (CNNSD) of the spectrum of its quantization. It is known that one type of statistical distribution (Poisson statistics) describes the CNNSD of systems displaying regular dynamics and another (Wigner statistics) describes the CNNSD of systems displaying chaotic dynamics. For intermediate cases (when the dynamics are mixed) in which the integrable and chaotic components of the classical dynamical system's phase space are well-separated, the Berry-Robnik conjecture states that the CNNSD of its quantization can be determined from the number and relative phase space volumes of its integrable components using a distribution that interpolates between Poisson and Wigner statistics.

INTRODUCTION

Billiards and Dynamical Systems

A dynamical system consists of an equation of motion $\dot{x}=f(x,t)$ on a phase space (representing the ambient space in which the variables take values). One class of dynamical systems are the Hamiltonian systems, which are derived from a real-valued function H (which is called the Hamiltonian and conserved along all trajectories) via *Hamilton's equations*,

$$\dot{p} = -\frac{\partial H}{\partial q}, \qquad \dot{q} = \frac{\partial H}{\partial p}, \tag{1}$$

where $p = p(t)$ and $q = q(t)$ are the momenta and coordinates, respectively. Each momentum/coordinate pair constitutes a degree-of-freedom of the system. For all chaotic systems, there are fewer constants of motion (quantities that take the same value along the trajectories of Equation (1)) than degrees-of-freedom. For integrable systems, the number of constants of motion and degrees-of-freedom are equal.

One class of Hamiltonian systems are planar billiards, which have two degrees-of-freedom and consist of a moving point particle confined to a closed container in the plane. The collisions of the particle against the boundary are elastic, so energy (the Hamiltonian) is conserved and the speed of the particle is constant. A billiard can exhibit either fully integrable (regular) dynamics, fully chaotic dynamics, or mixed integrable/chaotic dynamics. Loosely, chaotic dynamics imply that the trajectories of Equation (1) are sensitive to initial conditions and are thus unpredictable after some small time interval [15]. Two well-known chaotic billiards are the Sinai billiard (a square container with a circular boundary in the center) and the Bunimovich stadium (a rectangle capped on opposite ends by semi-circles) [21]. Chaos is one extreme form of dynamical behavior; the other is integrability, which (loosely) describes systems with low sensitivity to initial conditions and trajectories with long-term predictability. An example of a billiard with fully integrable dynamics is the circular billiard, in which both energy and angular momentum are constants of motion.

Mixed Dynamics

Most Hamiltonian dynamical systems are mixed; they are neither fully integrable nor fully chaotic but lie between these two extremes and have both integrable and chaotic trajectories. To better understand such systems, it is useful to study simple problems with well-separated regions of integrability and chaos. Examples include oval billiards [7], free particles interacting linearly with harmonic oscillators [12], and circular billiards with non-concentric circular barriers [20].

Perhaps the best candidate for a system with controllably mixed dynamics is the mushroom billiard [11], which lends itself to rigorous analytical study. Shaped like an idealization of its natural namesake, it exhibits either integrable or chaotic dynamics depending on the initial position and velocity of the confined particle. Bunimovich simultaneously introduced the mushroom billiard and proved several properties about its dynamics in the case of circular caps [11]. For example, if the particle begins in the mushroom's cap with a trajectory tangent to a caustic [23], then the particle remains in the cap and exhibits integrable dynamics. If the particle crosses the innermost foliating semicircular caustic, then its trajectory is chaotic. Described in terms of the mushroom's phase space, this means that there is one integrable "island" such that any set of initial conditions within it gives an (integrable) trajectory that remains within the island and any set of initial conditions outside the island yields a chaotic trajectory that remains outside. Hence, the relative volumes of the chaotic and integrable components in phase space can be easily controlled with simple adjustments of the mushroom's geometry (i.e., its stem length, stem width, etc.). Bunimovich also proved

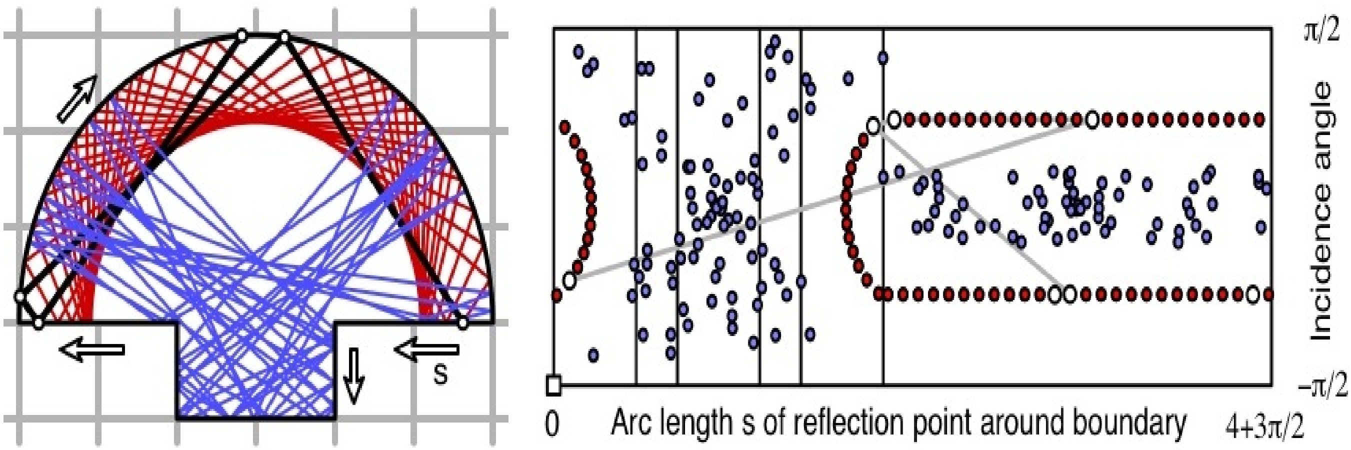

FIG. 1: An integrable (red) and a chaotic (blue) trajectory shown side by side in configuration space (left) and phase space (right). Vertical lines in phase space represent singular points (corners in configuration space). This plot originally appeared in [16].

that the phase space of billiards with elliptical caps contains one chaotic component and zero, one, or two integrable components, depending on stem placement and length [11]. For a sufficiently long stem (a) not intersecting the edge and (b) not containing the center of the cap, there are two integrable islands. If one of these conditions is violated, there is one integrable island. If both are violated, then there are no integrable islands. In addition to analytical work, classical mushroom billiards have also been the subject of several numerical investigations [19], [1].

Quantum Mushroom Billiards

In this paper, we examine the quantum half-mushroom billiard [24], which is a two-dimensional, half-mushroom-shaped region of zero potential (denoted by Ω) enclosed by a boundary ($\partial\Omega$) outside of which the potential is considered infinite, along with a function ψ defined on Ω that satisfies the Helmholtz equation (i.e., the stationary Schrödinger equation) with Dirichlet boundary conditions ($\|\psi\|_{\partial\Omega} = 0$). The system is a "particle in a box," with a nontrivial geometry resulting in interesting dynamics. This problem is closely related to the classic question in spectral theory

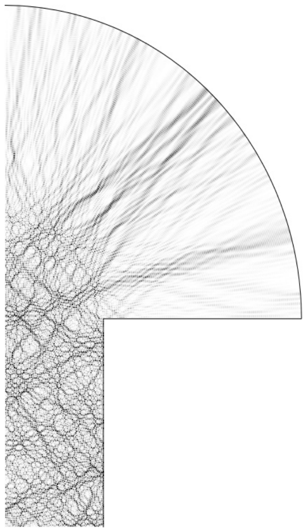

FIG. 2: High-energy wavefunction on a half-mushroom billiard with wavenumber $k_n = 499.856...$, $n \approx 45000$. (Image courtesy of A.H. Barnett and generated by Viewer [3].)

(first posed by M. Kac [17]) popularly known as "Can one hear the shape of a drum?" That is, can one exactly describe the boundary of a planar region from a list of the eigenvalues corresponding to eigenfunctions on that region satisfying Dirichlet boundary conditions? This question has recently been answered in the negative [14], although certain properties of the drum (such as area and perimeter) can be inferred from the spectrum.

One goal of this project was to test the "Berry-Robnik conjecture" for the quantization of mixed systems in the particular case of mushroom billiards. To paraphrase, this conjecture states that for the quantization of billiards with mixed dynamics, the contributions from integrable and chaotic regions to the *cumulative nearest-neighbor spacing distribution* (CNNSD) should superimpose in an uncorrelated fashion in the semiclassical limit [9]. That is, the CNNSD is conjectured to be a superposition of the Wigner and the Poisson distributions with their relative contributions determined by the numbers and relative phase space volumes of chaotic and regular regions. An integrable system such as a circle has no chaotic component in its classical phase space, so its CNNSD is a Poisson distribution. A chaotic system such as a Bunimovich stadium has no regular components in classical phase space, so its CNNSD is a Wigner distribution. The conjecture has an associated distribution formula (see Equation (10) below), so testing it for half-mushrooms entails checking the fit of computed data to this formula.

METHODS

Mathematical Underpinnings

We now discuss how to obtain and analyze the CNNSD of a particular quantum billiard. As a "particle-in-a-box," the eigenfunctions ψ of a quantum billiard have specific, discrete energies ("eigenvalues") $E = k^2$, where k is the wavenumber. The eigenfunctions satisfy the stationary Schrödinger equation

$$\hat{H}\psi = k^2 \cdot \psi. \tag{2}$$

Writing the quantum Hamiltonian operator $\hat{H}$ more explicitly yields

$$-\frac{\hbar}{2m}\Delta\psi = k^2\psi, \tag{3}$$

where $\hbar$ is Planck's constant, m is the mass of the confined particle and Δ is the Laplacian operator. We rescale Equation (3) with $\hbar = 2m = 1$ so that it is written

$$-\Delta\psi = k^2\psi. \tag{4}$$

Finding the eigenfunctions for successively higher eigenvalues yields a list of consecutive energy levels. We use an "unfolding" procedure [10] to transform the list of energies E_1, E_2,..., E_N so that the average spacing between consecutive energies is unity. Each energy ($E_n = k_n^2$) is mapped to a corresponding unfolded energy by the Weyl formula,

$$e_n = \frac{Ak_n^2}{4\pi} - \frac{Pk_n}{4\pi} + K, \tag{5}$$

where A and P are the area and perimeter of the billiard, respectively, and K is a constant determined by the billiard geometry (K is unimportant here, as later steps eliminate it). One then applies the formula

$$S_n = e_n - e_{n-1} \tag{6}$$

to obtain a list S_2, S_3,..., S_N, which is subsequently sorted from least to greatest. The CNNSD is given by

$$W(S) = \frac{1}{N}\sum_{n=1}^{N}\theta(S - S_n), \tag{7}$$

where θ represents the Heaviside unit step function, which is defined as $\theta(x) = 1$ for $x > 0$ and $\theta(x) = 0$ for $x < 0$. In the deep semiclassical regime (i.e., at very high k), the CNNSD is very close to a cumulative [25] Wigner distribution,

$$\tilde{W}(S) = 1 - e^{-\frac{\pi}{4}S^2}, \tag{8}$$

for chaotic systems and to a cumulative Poisson Distribution,

$$\tilde{W}(S) = 1 - e^{-S}, \tag{9}$$

for integrable ones. For the quantization of mixed systems with exactly one chaotic and exactly one integrable component (which are easily separated), such as mushroom billiards, the Berry-Robnik conjecture states that the CNNSD satisfies

$$\tilde{W}(S) = \int_0^S \left\{ q^2 erfc\left(\frac{1}{2}\sqrt{\pi}(1-q)x\right) + (2q(1-q) + \frac{1}{2}\pi(1-q)^3 x)e^{\frac{-\pi(1-q)^2x^2}{4}} \right\} e^{-qx}dx, \tag{10}$$

where q is the relative volume of the integrable component of phase space (on the interval [0,1]) and

$$erfc(x) = 1 - \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-t^2}dt \tag{11}$$

is the complementary error function.

Computation

Given a mushroom billiard, the first step is to solve the stationary Schrödinger equation to obtain a list of consecutive eigenvalues in the deep semiclassical regime. To perform this step, one can use Vergini, a partial differential equation solver written by A. H. Barnett [2] that uses the so-called "scaling method." Vergini cannot solve Equation (4) in general but requires that a specific type of function be defined to limit the choice of eigenfunctions ψ. This general function, referred to as a "basis function," must be picked with the particular billiard in mind in order to ensure the reliability of the calculated eigenvalues. The selection is based on approximation theory and certain physical heuristics involving particular features of the billiard geometry [5]. Any basis must allow Ω to contract or dilate slightly about the origin while still remaining a basis. As an example of the physical heuristic, the basis function for the quarter stadium is a combination of symmetrized plane-waves and evanescent waves [8], the latter of which handles the curvature discontinuity where the arc meets the straight line. The mushroom, on the other hand, has a reentrant corner where the cap meets the stem, so the basis function must have the right singularity at that point. The Fourier-Bessel basis, which is built into Vergini, meets this requirement [6].

Vergini takes as inputs the billiard dimensions, a basis function, and a range of wavenumbers k over which to find eigenvalues. It then returns the (approximate) sequence of eigenvalues within that range as well as values of the "tension" and "perinorm." For a particular eigenenergy k^2 (with eigenfunction ψ), the tension is defined as

$$t(\psi) = \frac{\|\psi\|_{\partial\Omega}}{\|\psi\|_{\Omega}}, \tag{12}$$

where $\|\psi\|_{\partial\Omega}$ and $\|\psi\|_{\Omega}$ are the L^2-norms of the function ψ on the boundary and the interior of the billiard region, respectively. Tension indicates how well the eigenfunction obeys Dirichlet boundary conditions; an eigenvalue is considered unreliable if the tension is greater than some threshold (say, 10^{-4}). The perinorm is the ratio between the normalization computed by the scaling method and that computed with a Rellich formula [4]. If the perinorm of an eigenvalue differs from unity by more than some threshold amount (say, .1), the eigenvalue is considered unreliable. We selected a Fourier-Bessel function for the basis, limited wavenumber ranges to .2, and used only eigenvalues below 600 to avoid aberrant ones resulting from shortcomings of the scaling method. We also used error-checking algorithms to verify that no unreliable eigenvalues appeared in the data.

To obtain a sufficiently wide range of nearest-neighbor spacings to plot a meaningful distribution, it is necessary to find eigenvalues over a wavenumber range of about 30. We achieve this by patching together a series of the smaller sequences by calling Vergini from Matlab repeatedly and collating the individual program outputs into a matrix. To prevent the omission of eigenvalues at the edges of search windows, the search intervals overlapped slightly. To prevent eigenvalue duplication, we used an ad hoc method to identify likely duplications due to overlap. An eigenvalue E_D was judged to be a duplication and removed if and only if it (a) was the first eigenvalue in its search radius and (b) S_D was smaller than both S_{D-1} and S_{D+1} by an order of magnitude or more. The CNNSD of the billiard is then obtained by applying the unfolding procedure described earlier, taking the nearest-neighbor spacings of the unfolded list, and using Equation (7).

The remainder of the computation consists of fitting the cumulative Berry-Robnik formula to the data. To do this, we need to estimate the relative volume of the mushroom's phase space that is integrable and use this number to compute an approximate Berry-Robnik distribution. We estimate relative volume using S. Lansel's classical billiard simulator [18]. In classical mushroom phase portraits, the integrable island appears as in Figure 3. We can use

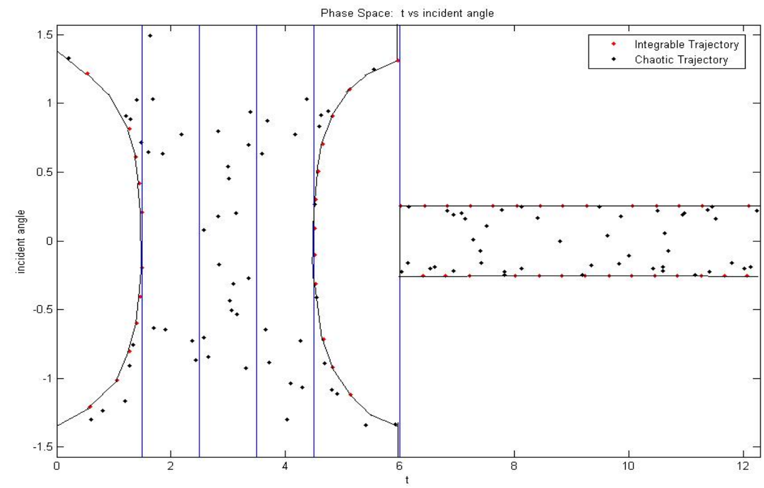

FIG. 3: The chaotic region appears as an hourglass-shaped figure on the left and a rectangle on the right. The rest of the figure constitutes the integrable island.

such phase portraits to calculate the relative volumes of the integrable components in the phase space of a particular billiard and hence determine the expected distribution.

RESULTS AND CONCLUSIONS

We generated reliable data for two mushroom geometries, a quarter-circle (which is provably integrable), and a quarter Bunimovich stadium (which is provably chaotic). As expected, their CNNSDs fit very closely with cumulative Poisson and Wigner distributions, respectively. This gives us confidence in the reliability of our computational methods.

Though we have not yet completed the exact fitting to test the Berry-Robnik conjecture, our results nevertheless suggest the expected behavior for the half-mushrooms. A narrow-stemmed mushroom (with cap radius 1.4, stem width 0.4, and stem height 0.8), whose integrable component has a large relative volume, has a CNNSD very close

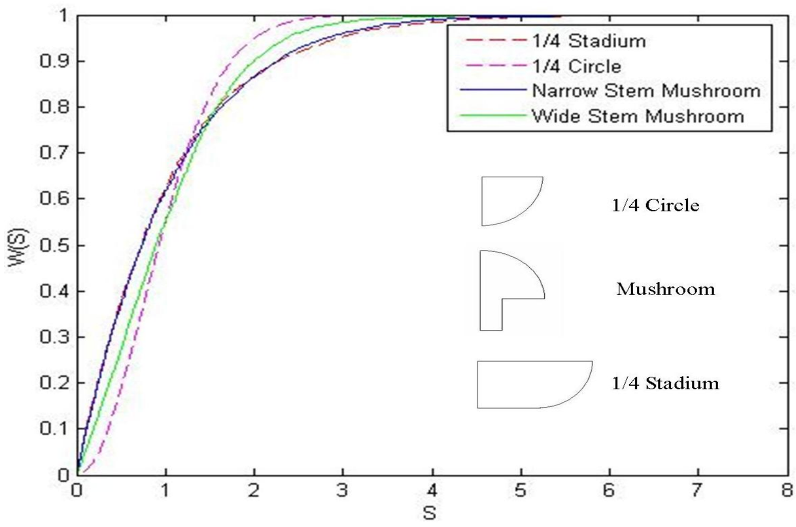

FIG. 4: CNNSDs of a quarter circle (integrable), quarter stadium (chaotic), and two half-mushroom (mixed) geometries. The narrow-stem mushroom has dimensions of (cap radius:stem width:stem height) 1.4:0.4:0.8 and the wide-stem mushroom has dimensions of 3:2:1.333.

to the cumulative Poisson distribution (see Figure 4). A wide-stem mushroom (with cap radius 3, stem width 2, and stem height 1.333), on the other hand, has a CNNSD closer to the cumulative Wigner distribution.

Future work includes gathering data for more circular-cap mushrooms and completing the curve-fitting to check the Berry-Robnik conjecture more reliably. We will also modify Vergini so that it can be used to study elliptical half-mushrooms and a wider range of circular mushrooms and extend the current investigation to include them. Additionally, it would be useful to refine existing software tools by creating Matlab implementations of Vergini and Viewer (with graphical user interfaces).

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[24] It is necessary to remove symmetry from the system to avoid degenerate (repeated) eigenvalues, which could corrupt the data.
[25] Cumulative distributions $\tilde{W}(S)$ are defined in terms of probability distributions $\tilde{P}(S)$ as $\tilde{W}(S) = \int_0^S \tilde{P}(x)dx$