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A model for the computation of quantum billiards with arbitrary shapes

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Abstract

An expansion method for the stationary Schrödinger equation of a three-dimensional quantum billiard system whose boundary is defined by an arbitrary analytic function is introduced. The method is based on a coordinate transformation and an expansion in spherical harmonics. The effectiveness is verified and confirmed by a numerical example, which is a billiard system depending on a parameter.

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1. Introduction

Investigation of quantum mechanical systems whose classical analogs are chaotic has received considerable interest recently. In 1981 Bohigas, Giannoni and Schmit [3] conjectured that the statistical spectral properties of quantum systems with regular and chaotic classical counterparts are quite different. Although not rigorously proved, this conjecture has later been reinforced by a number of numerical results [5,13,15]. Significant progress was achieved by studying lower-dimensional systems, including one-dimensional time-dependent and two-dimensional conservative systems. Due to their simplicity,

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the two-dimensional billiard systems were investigated thoroughly [2,8,16,21]. Of particular interest are billiard families depending on a parameter, the shape of which changes as the parameter varies in some given range [7,14].

The quantum billiard problem is modeled by the stationary Schrödinger equation for a particle with zero potential, where the wavefunction disappears on the boundary of the billiard. Such a problem is known to be exactly solvable only in very few cases in which boundaries are constant in some coordinate system. However, chaotic motion usually occurs in billiards with *odd* shapes whose boundary is not constant. As a result, the mathematical model describing the corresponding quantum billiard system does not admit an exact analytical solution. On the other hand, in order to perform a reliable statistical spectral analysis one needs long energy sequences. Unfortunately, finding approximate solutions of the problem within a reasonable degree of accuracy still remains a very difficult task. Moreover, despite the plentiful literature about the numerical treatment of the quantum billiard problem in two dimensions, results on the three-dimensional case are quite few [9–12].

The aim of this study is to propose a quite general three-dimensional quantum billiard model and to develop a method for its numerical implementation. Thus, the paper is organized as follows: in Section 2 the quantum billiard model and its mapping into the unit ball are introduced. An eigenfunction expansion which reduces the transformed Schrödinger equation to a system of ordinary differential equations (ODEs) is presented in Section 3. In Section 4, the resulting system of ODEs is analyzed and converted to a generalized matrix eigenvalue problem. The method is then applied to a specimen example in Section 5, where the statistical analysis of the calculated spectra is also performed. The last section is devoted to concluding remarks.

2. The quantum billiard model

We introduce a three-dimensional axisymmetric quantum billiard model whose boundary is defined by an analytic function. To be specific, the billiard is described by

$$\mathcal{D} = \{(r, \theta, \phi) \mid 0 \leq r \leq f(\theta), 0 \leq \theta \leq \pi, 0 \leq \phi \leq 2\pi\}, \quad \mathcal{D} \subset \mathbb{R}^3, \quad (2.1)$$

where (r, θ, ϕ) are the spherical coordinates. The function $f(\theta)$ can be identified as a *shape function* since it determines the shape of the billiard under consideration. We assume that it is an arbitrary analytic function of θ . A similar shape function has been previously used to determine the Stokes flow past an arbitrary body [18,19]. Note that, the billiard \mathcal{D} in (2.1) may be obtained by rotating a two-dimensional region

$$\mathcal{B} = \{(r, \theta) \mid 0 \leq r \leq f(\theta), 0 \leq \theta \leq \pi\} \quad (2.2)$$

in the yz -plane about the z -axis (see Fig. 1).

In the spherical coordinates, the Schrödinger equation for a particle moving freely inside such a billiard \mathcal{D} can be written as

$$\left\{ \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + \frac{\cot \theta}{r^2} \frac{\partial}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + E \right\} \Psi(r, \theta, \phi) = 0, \quad (2.3)$$

where the wavefunction Ψ disappears on the boundary, i.e.

$$\Psi(r, \theta, \phi) = 0 \quad \text{on } \partial \mathcal{D} \quad (2.4)$$

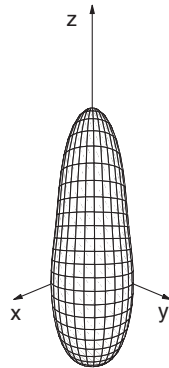


Fig. 1. Three-dimensional axisymmetric billiard.

and, in addition, satisfies the square integrability condition

$$\int \int \int_{\mathcal{D}} |\Psi|^2 dV < \infty \tag{2.5}$$

arising from the fact that Ψ should belong to the Hilbert space of square integrable functions on $\mathcal{D} \subset \mathbb{R}^3$.

The mathematical and computational treatment of the problem requires an explicit specification of the boundary of the billiard. It is worth mentioning that the analyticity of $f(\theta)$ suggests proposing a shape function of the form

$$f(\theta) = 1 + \sum_{k=1}^{\infty} \alpha_k \cos^k \theta, \quad \alpha_k \in \mathbb{R}, \tag{2.6}$$

where α_k may be regarded as the shape parameters. It is shown that the condition

$$1 \leq f(\theta) < \infty \tag{2.7}$$

must hold for all $\theta \in [0, \pi]$ in order to have a bounded geometrical region, and that the particular case, in which $\alpha_k = 0$ for all $k \in \mathbb{Z}^+$, corresponds to the well-known exactly solvable spherical billiard. By means of the flexible parameters α_k in (2.6), it is possible to construct various billiards. In fact, even very simple choices of $f(\theta)$ like finite sums containing a few terms can generate several shapes.

In practice, we deal with a truncated series representation of the shape function, say $F(\eta)$,

$$F(\eta) = 1 + \sum_{k=1}^K \alpha_k \eta^k, \tag{2.8}$$

which is a polynomial of degree K in the new variable η ,

$$\eta = \cos \theta, \quad \eta \in [-1, 1] \tag{2.9}$$

provided that K is large enough. Furthermore, if we make use of the unusual substitution

$$\xi = \frac{r}{F(\eta)}, \quad \xi \in [0, 1] \tag{2.10}$$

billiard (2.1) with an arbitrary shape is reduced to a unit ball

$$\mathcal{D}_u = \{(\xi, \eta, \phi) \mid 0 \leq \xi \leq 1, -1 \leq \eta \leq 1, 0 \leq \phi \leq 2\pi\} \quad (2.11)$$

in the (ξ, η, ϕ) coordinate system.

Unfortunately, this standardization has been accomplished at the cost of transforming the Schrödinger equation (2.3) into a quite complicated form

$$\left\{ G_1(\eta) \frac{\partial^2}{\partial \xi^2} + [2G_1(\eta) + G_2(\eta) - G_3(\eta)] \frac{1}{\xi} \frac{\partial}{\partial \xi} - \frac{1}{\xi \eta} (1 - \eta^2) G_2(\eta) \frac{\partial^2}{\partial \xi \partial \eta} + G_0(\eta) \left[\frac{1}{\xi^2} \mathcal{T} + E G_0(\eta) \right] \right\} \Psi(\xi, \eta, \phi) = 0, \quad (2.12)$$

where \mathcal{T} stands for the second-order differential operator

$$\mathcal{T} = (1 - \eta^2) \frac{\partial^2}{\partial \eta^2} - 2\eta \frac{\partial}{\partial \eta} - \frac{1}{1 - \eta^2} \frac{\partial^2}{\partial \phi^2} \quad (2.13)$$

and $G_i(\eta)$ denote the following polynomials of degree $2K$ in η :

$$\begin{aligned} G_0(\eta) &:= [F(\eta)]^2, & G_1(\eta) &:= [F(\eta)]^2 + (1 - \eta^2)[F'(\eta)]^2, & G_2(\eta) &:= 2\eta F'(\eta)F(\eta), \\ G_3(\eta) &:= (1 - \eta^2)F''(\eta)F(\eta) \end{aligned} \quad (2.14)$$

introduced for the sake of brevity. As shown, the shape effects are now characterized completely by the partial differential equation (PDE) in (2.12), which cannot be treated by the method of separation of variables.

3. Eigenfunction expansion

In the new coordinates, the square integrability condition (2.5) takes the form

$$\int_0^{2\pi} \int_{-1}^1 \int_0^1 |\Psi(\xi, \eta, \phi)|^2 [F(\eta)]^3 \xi^2 d\xi d\eta d\phi < \infty, \quad (3.1)$$

where the shape function appears as a weight. However, on using (2.7) we have

$$\int_0^{2\pi} \int_{-1}^1 \int_0^1 |\Psi(\xi, \eta, \phi)|^2 \xi^2 d\xi d\eta d\phi < \infty \quad (3.2)$$

implying the boundedness of the integral

$$\int_0^{2\pi} \int_{-1}^1 |\Psi(\xi, \eta, \phi)|^2 d\eta d\phi < \infty \quad (3.3)$$

as well, for all fixed $\xi \in (0, 1]$. In what follows, (3.3) suggests that $\Psi(\xi, \eta, \phi)$ can also be regarded as a square integrable function over the region $[-1, 1] \times [0, 2\pi]$ with the unit weight for a fixed ξ . In fact, such a region is nothing but a sphere of radius ξ .

Consider now the differential operator \mathcal{T} in (2.13). The eigenvalue problem associated with this operator generates the orthogonal sequence of the spherical harmonics

$$Y_m^n(\eta, \phi) = P_m^{|n|}(\eta)e^{in\phi}, \quad 0 \leq m \leq \infty, \quad -m \leq n \leq m \tag{3.4}$$

corresponding to the eigenvalues $-m(m+1)$, in which P_m^n stands for the associated Legendre functions. It is well known that the spherical harmonics form an orthogonal basis for the space of the square integrable functions over a sphere [17]. Therefore, we may propose an expansion in spherical harmonics for the transformed wavefunction $\Psi(\xi, \eta, \phi)$ in the form

$$\Psi(\xi, \eta, \phi) = \sum_{m=0}^{\infty} \sum_{n=0}^m [\Phi_m^n(\xi) \cos n\phi + \psi_m^n(\xi) \sin n\phi] P_m^n(\eta), \tag{3.5}$$

where Φ_m^n and ψ_m^n are the Fourier coefficients, for which the superscript n is used merely as a notation in accordance with that of P_m^n so that it does not mean the power. In fact, n may be regarded as an azimuthal quantum number. It is important to note that the axial symmetry of the region allows the separation of (3.5) into two parts containing even and odd eigenfunctions in ϕ . Without loss of generality, we then consider only the even eigenfunctions. More precisely, we deal with the expansion

$$\Psi_e(\xi, \eta, \phi) = \sum_{m=0}^{\infty} \sum_{n=0}^m \Phi_m^n(\xi) P_m^n(\eta) \cos n\phi \tag{3.6}$$

which converges to the function $\Psi_e(\xi, \eta, \phi)$ in the mean, for every fixed $\xi \in (0, 1]$. Substituting Ψ_e into (2.12), reordering the double sums as $\sum_{n=0}^{\infty} \sum_{m=n}^{\infty}$ and using the orthogonality of the cosine functions over $\phi \in (0, 2\pi)$, we obtain

$$\sum_{m=n}^{\infty} \left\{ G_1 P_m^n \xi^2 \frac{d^2}{d\xi^2} + \left[(2G_1 - mG_2 - G_3) P_m^n + (m - n + 1) \frac{G_2}{\eta} P_{m+1}^n \right] \xi \frac{d}{d\xi} - m(m + 1) G_0 P_m^n + E^n \xi^2 G_0^2 P_m^n \right\} \Phi_m^n(\xi) = 0 \tag{3.7}$$

for $n \geq 0$, where we have dropped the η -dependence of the G_i and P_j^n for simplicity. Observe that the differential–difference relation of the associated Legendre functions [1]

$$(1 - \eta^2) \frac{d}{d\eta} P_m^n(\eta) = (m + 1)\eta P_m^n(\eta) - (m - n + 1) P_{m+1}^n(\eta) \tag{3.8}$$

has been used to eliminate of the terms proportional to the first derivative of $P_m^n(\eta)$.

An eigenfunction expansion of type (3.6) makes it possible to reduce the PDE to a system of ODEs in the Fourier coefficients $\Phi_m^n(\xi)$ [6,20]. To this end, first note that the polynomials $G_i(\eta)$ in (3.7) may be written as

$$G_i(\eta) = \sum_{k=0}^{2K} g_{i,k} \eta^k, \quad i = 0, 1, 2, 3, \tag{3.9}$$

where the coefficients $g_{i,k}$ can easily be calculated in terms of the shape parameters α_k . Likewise, $[G_0(\eta)]^2$ is of the form

$$[G_0(\eta)]^2 = \sum_{k=0}^{4K} g_{4,k} \eta^k, \quad (3.10)$$

where $g_{4,k}$ are certain combinations of the $g_{0,k}$. Thus, it is shown that the η -dependency of Eq. (3.7) solely comprises the products $\eta^k P_j^n(\eta)$ with $j = m$ and $m + 1$. Then we expand the $\eta^k P_j^n(\eta)$ into a series of associated Legendre functions

$$\eta^k P_j^n(\eta) = \sum_{l=n}^{\infty} \gamma_{ljk}^n P_l^n(\eta) \quad (3.11)$$

in which the coefficients γ_{ljk}^n ,

$$\gamma_{ljk}^n = \int_{-1}^1 \eta^k P_l^n(\eta) P_j^n(\eta) d\eta, \quad \gamma_{ljk}^n = \gamma_{jlk}^n \quad (3.12)$$

can be evaluated recursively by means of the functional equation [1]

$$\eta P_m^n(\eta) = \frac{m-n+1}{2m+1} P_{m+1}^n + \frac{m+n}{2m+1} P_{m-1}^n. \quad (3.13)$$

Therefore, it suffices to compute only the γ_{lj0}^n from the orthogonality relation of the associated Legendre functions, i.e.

$$\gamma_{lj0}^n = \int_{-1}^1 P_j^n(\eta) P_l^n(\eta) d\eta = \frac{2}{2j+1} \frac{(j+n)!}{(j-n)!} \delta_{lj}, \quad (3.14)$$

where δ_{lj} is the Kronecker delta.

Next we define the matrices $\mathbf{A}^n := [a_{lm}^n]$, $\mathbf{B}^n := [b_{lm}^n]$, $\mathbf{C}^n := [c_{lm}^n]$ and $\mathbf{D}^n := [d_{lm}^n]$ having the general elements

$$a_{lm}^n = \sum_{k=0}^{2K} g_{1,k} \gamma_{lmk}^n, \quad (3.15a)$$

$$b_{lm}^n = \sum_{k=0}^{2K} (2g_{1,k} - mg_{2,k} - g_{3,k}) \gamma_{lmk}^n + (m-n+1) \sum_{k=0}^{2K-1} g_{2,k+1} \gamma_{l(m+1)k}^n, \quad (3.15b)$$

$$c_{lm}^n = \sum_{k=0}^{2K} g_{0,k} \gamma_{lmk}^n \quad (3.15c)$$

and

$$d_{lm}^n = \sum_{k=0}^{4K} g_{4,k} \gamma_{lmk}^n, \quad (3.15d)$$

respectively. Once again, note that in the definition of the matrices, γ , and the eigenvalue parameter E , the superscript n is just a notational convenience. Now substituting (3.9) and (3.10) into (3.7) and making use of (3.11) and (3.15), it follows that

$$\sum_{l=n}^{\infty} \sum_{m=n}^{\infty} \left[a_{lm}^n \xi^2 \frac{d^2}{d\xi^2} + b_{lm}^n \xi \frac{d}{d\xi} - m(m+1)c_{lm}^n + E^n \xi^2 d_{lm}^n \right] \Phi_m^n(\xi) P_l^n(\eta) = 0 \tag{3.16}$$

implying that

$$\sum_{m=n}^{\infty} \left[a_{lm}^n \xi^2 \frac{d^2}{d\xi^2} + b_{lm}^n \xi \frac{d}{d\xi} - m(m+1)c_{lm}^n + E^n \xi^2 d_{lm}^n \right] \Phi_m^n(\xi) = 0 \tag{3.17}$$

for $l = n, n + 1, \dots$, since the set $\{P_n^n(\eta), P_{n+1}^n(\eta), P_{n+2}^n(\eta), \dots\}$ is linearly independent for each fixed n . Hence we arrive at an infinite system of coupled ODEs for the determination of the Fourier coefficients $\Phi_m^n(\xi)$. In matrix-vector form, system (3.17) is given by

$$\left(\mathbf{A}^n \xi^2 \frac{d^2}{d\xi^2} + \mathbf{B}^n \xi \frac{d}{d\xi} + \mathbf{\Lambda} \mathbf{C}^n + E^n \xi^2 \mathbf{D}^n \right) \mathbf{\Phi}^n = \mathbf{0}, \tag{3.18}$$

where $\mathbf{\Lambda} := \text{diag}\{-m(m+1)\}$ is a diagonal matrix containing the eigenvalues of the operator \mathcal{T} . Clearly, $\mathbf{\Phi}^n$ stands for the unknown vector-valued function

$$\mathbf{\Phi}^n = [\Phi_n^n(\xi), \Phi_{n+1}^n(\xi), \Phi_{n+2}^n(\xi), \dots]^T \tag{3.19}$$

whose entries are the Fourier coefficients.

For a complete reformulation of the problem, we need to redefine the boundary and square integrability conditions in accordance with the vector differential equation just obtained. With expansion (3.6) the boundary condition (2.4) is altered to

$$\mathbf{\Phi}^n(1) = \mathbf{0}, \quad n = 0, 1, \dots \tag{3.20}$$

by the orthogonality of the spherical harmonics. Similarly, the square integrability condition (3.3) reads as

$$\int_0^1 \sum_{n=0}^{\infty} \sum_{m=n}^{\infty} [\Phi_m^n(\xi)]^2 \xi^2 d\xi < \infty \tag{3.21}$$

which becomes

$$\sum_{n=0}^{\infty} \int_0^1 \xi^2 [\mathbf{\Phi}^n(\xi) \cdot \mathbf{\Phi}^n(\xi)] d\xi < \infty \tag{3.22}$$

on formally interchanging the first summation and integration, where the *dot* denotes the usual scalar product of two vectors. So we may impose the boundedness of the integral

$$\int_0^1 \xi^2 \|\mathbf{\Phi}^n(\xi)\|^2 d\xi < \infty \tag{3.23}$$

for each $n = 0, 1, \dots$ as a necessary condition for (3.22) to hold.

Amongst the axisymmetric billiards defined by the general shape function $F(\eta)$, the sphere is the only exactly solvable model. Therefore, in practice, we seek approximate solutions of the system in (3.17) over finite-dimensional subspaces, for $l = n, n + 1, \dots, N$ and $n = 0, 1, \dots, N$, where N is a sufficiently large positive integer. An important point to bear in mind is that the dimension of the N -truncated system is not the same for each n . Indeed, it decreases as n increases from 0 to N , i.e. we have $N + 1$ equations when $n = 0$, N equations when $n = 1$, and finally a single equation when $n = N$.

4. Analysis of the ODE system and reduction to a matrix eigenvalue problem

A careful inspection of the coefficient matrices defined by (3.15) shows that they possess special structures. These structures become apparent when the integral forms of the general entries of the matrices in (3.15) are introduced. Actually, the matrices may be written as

$$a_{lm}^n = \int_{-1}^1 G_1(\eta) P_l^n(\eta) P_m^n(\eta) d\eta, \quad (4.1)$$

$$b_{lm}^n = 2a_{lm}^n + \int_{-1}^1 \left\{ [G_2(\eta) - G_3(\eta)] P_m^n(\eta) - \frac{1}{\eta} (1 - \eta^2) G_2(\eta) [P_m^n(\eta)]' \right\} P_l^n(\eta) d\eta, \quad (4.2)$$

$$c_{lm}^n = \int_{-1}^1 G_0(\eta) P_l^n(\eta) P_m^n(\eta) d\eta \quad (4.3)$$

and

$$d_{lm}^n = \int_{-1}^1 [G_0(\eta)]^2 P_l^n(\eta) P_m^n(\eta) d\eta \quad (4.4)$$

with $l, m = n, n + 1, \dots$ for a fixed n . Now we can prove the statements below.

Proposition 1. *The matrices \mathbf{A}^n , \mathbf{C}^n and \mathbf{D}^n are symmetric positive definite.*

Proof. The symmetry of the matrices follows from their definitions. Let $\mathbf{u} = [u_n, u_{n+1}, \dots]^T$ be a nonzero vector and consider the quadratic forms Q_A , Q_C and Q_D

$$Q_A = \mathbf{u}^T \mathbf{A}^n \mathbf{u}, \quad Q_C = \mathbf{u}^T \mathbf{C}^n \mathbf{u}, \quad Q_D = \mathbf{u}^T \mathbf{D}^n \mathbf{u} \quad (4.5)$$

associated with the matrices \mathbf{A}^n , \mathbf{C}^n and \mathbf{D}^n , respectively. Using the integral representations of the matrix elements in (4.1), (4.3) and (4.4) we find that

$$Q_A = \int_{-1}^1 h(\eta) G_1(\eta) d\eta, \quad Q_C = \int_{-1}^1 h(\eta) G_0(\eta) d\eta, \quad Q_D = \int_{-1}^1 h(\eta) [G_0(\eta)]^2 d\eta, \quad (4.6)$$

where we have defined the function $h(\eta)$ as

$$h(\eta) = \left[\sum_{m=n}^{\infty} u_m P_m^n(\eta) \right]^2, \quad (4.7)$$

which is evidently positive valued. Moreover, recalling that $G_0(\eta)$ and $G_1(\eta)$ take on positive values for $\eta \in (-1, 1)$, we conclude that the quadratic forms in (4.6) are all positive implying the positive definiteness of the matrices \mathbf{A}^n , \mathbf{C}^n and \mathbf{D}^n and, hence, the proof is complete. \square

Proposition 2. *The matrix \mathbf{B}^n can be written as the sum of matrices*

$$\mathbf{B}^n = 2\mathbf{A}^n + \mathbf{B}^{n,1} + \mathbf{B}^{n,2} \tag{4.8}$$

such that $\mathbf{B}^{n,1}$ and $\mathbf{B}^{n,2}$ are symmetric positive semidefinite and skew symmetric, respectively.

Proof. First we perceive the identity

$$\frac{d}{d\eta} \left[\frac{1}{2\eta} (1 - \eta^2) G_2(\eta) \right] = G_3(\eta) - G_2(\eta) + G_1(\eta) - G_0(\eta) \tag{4.9}$$

valid between the polynomials $G_i(\eta)$ in (2.14). Then using this identity and adding and subtracting the integral $\int_{-1}^1 [G_1(\eta) - G_0(\eta)] P_l^n(\eta) P_m^n(\eta) d\eta$ on the right-hand side of (4.2), we have

$$b_{lm}^n = 2a_{lm}^n + b_{lm}^{n,1} + b_{lm}^{n,2}, \tag{4.10}$$

where $b_{lm}^{n,1}$ and $b_{lm}^{n,2}$ stand for

$$b_{lm}^{n,1} = \int_{-1}^1 [G_1(\eta) - G_0(\eta)] P_l^n(\eta) P_m^n(\eta) d\eta \tag{4.11}$$

and

$$b_{lm}^{n,2} = - \int_{-1}^1 \left\{ \left[\frac{1}{2\eta} (1 - \eta^2) G_2(\eta) \right]' P_m^n(\eta) + \frac{1}{\eta} (1 - \eta^2) G_2(\eta) [P_m^n(\eta)]' \right\} P_l^n(\eta) d\eta \tag{4.12}$$

which can be regarded, respectively, as the general entries of the matrices $\mathbf{B}^{n,1}$ and $\mathbf{B}^{n,2}$. It is clear that the term $2a_{lm}^n$ in (4.10) generates the matrix $2\mathbf{A}^n$. On the other hand, the positive semidefiniteness of $\mathbf{B}^{n,1}$ can be shown easily by the method of the proof of Proposition 1. Indeed

$$\mathbf{u}^T \mathbf{B}^{n,1} \mathbf{u} \geq 0, \tag{4.13}$$

where the equality holds only when $F(\eta) = 1$, corresponding to the exactly solvable case of a spherical billiard for which $G_0(\eta) = G_1(\eta)$ and $G_2(\eta) = 0$ for all η .

Now setting $U = P_l^n(\eta) P_m^n(\eta)$ and $dV = [(1 - \eta^2) G_2(\eta) / (2\eta)]' d\eta$ and applying integration by parts to evaluate the first term of integral (4.12), we see that the entries $b_{lm}^{n,2}$ are expressible as

$$b_{lm}^{n,2} = \int_{-1}^1 \frac{1}{2\eta} (1 - \eta^2) G_2(\eta) W(P_m^n, P_l^n)(\eta) d\eta, \tag{4.14}$$

where $W(f, g)(x) = f(x)g'(x) - f'(x)g(x)$ is the Wronsky determinant of the functions f and g . Since $W(f, g) = -W(g, f)$ the matrix $\mathbf{B}^{n,2}$ is skew symmetric, which completes the proof. \square

The positive definiteness of \mathbf{A}^n suggests the Cholesky decomposition $\mathbf{A}^n = \mathbf{L}\mathbf{L}^T$, where \mathbf{L} is a lower triangular matrix with positive diagonal entries. Hence, we may introduce a new vector-valued function $\mathbf{Z}^n(\xi) = [Z_n^n(\xi), Z_{n+1}^n(\xi), \dots]^T$ of the form

$$\mathbf{Z}^n(\xi) = \mathbf{L}^T \Phi^n(\xi) \tag{4.15}$$

and transform (3.18) to

$$\mathcal{L}^n \mathbf{Z}^n(\xi) = E^n \xi^2 \mathbf{T}^n \mathbf{Z}^n(\xi), \quad \mathcal{L}^n := -\mathbf{I} \xi^2 \frac{d^2}{d\xi^2} - \mathbf{Q}^n \xi \frac{d}{d\xi} + \mathbf{R}^n, \tag{4.16}$$

where the matrix coefficients $\mathbf{Q}^n := [q_{lm}^n]$, $\mathbf{R}^n := [r_{lm}^n]$ and $\mathbf{T}^n := [t_{lm}^n]$ in the differential operator $\mathcal{L}^n := [\mathcal{L}_{lm}^n]$ are defined by

$$\mathbf{Q}^n = \mathbf{L}^{-1} \mathbf{B}^n \mathbf{L}^{-T}, \quad \mathbf{R}^n = -\mathbf{L}^{-1} \mathbf{A} \mathbf{C}^n \mathbf{L}^{-T}, \quad \mathbf{T}^n = \mathbf{L}^{-1} \mathbf{D}^n \mathbf{L}^{-T}. \tag{4.17}$$

Note that the coefficient of the highest derivative term in \mathcal{L}^n has been reduced to the identity matrix \mathbf{I} . In other words, now the second-order derivatives appear only on the main diagonal of \mathcal{L}^n . Clearly, the transformed variable $\mathbf{Z}^n(\xi)$ satisfies the same conditions as $\Phi^n(\xi)$, i.e.

$$\mathbf{Z}^n(1) = \mathbf{0} \tag{4.18}$$

and

$$\int_0^1 \xi^2 \|\mathbf{Z}^n(\xi)\|^2 d\xi < \infty \tag{4.19}$$

for $n = 0, 1, \dots, N$. The following propositions are necessary for further analysis.

Proposition 3. *The diagonal entries of the matrix \mathbf{Q}^n satisfy $2 \leq q_{ll}^n < 3$ for all $l = n, n + 1, \dots, N$.*

Proof. By Proposition 2, the matrix \mathbf{Q}^n may be written as

$$\mathbf{Q}^n = 2\mathbf{I} + \mathbf{Q}^{n,1} + \mathbf{Q}^{n,2}, \tag{4.20}$$

where $\mathbf{Q}^{n,1} = \mathbf{L}^{-1} \mathbf{B}^{n,1} \mathbf{L}^{-T}$ and $\mathbf{Q}^{n,2} = \mathbf{L}^{-1} \mathbf{B}^{n,2} \mathbf{L}^{-T}$ stand for symmetric positive semidefinite and skew-symmetric matrices, respectively. Because $q_{ll}^{n,1} \geq 0$ the q_{ll}^n satisfy

$$q_{ll}^n = 2 + q_{ll}^{n,1} \geq 2. \tag{4.21}$$

On the other hand, it is easy to see from (4.11), (4.1) and (4.3) that $\mathbf{A}^n = \mathbf{B}^{n,1} + \mathbf{C}^n$ and that

$$\mathbf{I} = \mathbf{Q}^{n,1} + \mathbf{L}^{-1} \mathbf{C}^n \mathbf{L}^{-T}. \tag{4.22}$$

Since the matrix $\mathbf{L}^{-1} \mathbf{C}^n \mathbf{L}^{-T}$ is also positive definite by Proposition 1, we must have $0 \leq q_{ll}^{n,1} < 1$. Therefore, the two-sided bounds for q_{ll}^n

$$2 \leq q_{ll}^n < 3, \quad l = n, n + 1, \dots, N \tag{4.23}$$

are proved. \square

Proposition 4. *The diagonal entries r_{ll}^n of the matrix \mathbf{R}^n are nonnegative.*

Proof. Recalling the definition of the diagonal matrix $\mathbf{\Lambda}$ in (3.18), $\mathbf{\Lambda} := [-m(m + 1)\delta_{lm}]$, we find from (4.17) that the r_{ll}^n are expressible as

$$r_{ll}^n = l(l + 1)r_{ll}^{n,1}, \tag{4.24}$$

where the $r_{ll}^{n,1}$ denote the diagonal entries of the matrix $\mathbf{R}^{n,1} = \mathbf{L}^{-1}\mathbf{C}^n\mathbf{L}^{-T}$. The positive definiteness of this matrix implies $r_{ll}^{n,1} > 0$, so that $r_{ll}^n \geq 0$. If we take into account that the *fixed* parameter n changes from 0 to N , the equality $r_{ll}^n = 0$ holds only when $l = n = 0$. \square

The dominant second-order differential operators \mathcal{L}_{ll}^n on the main diagonal of the coefficient matrix of system (4.16) are closely related to the operator provided by the Bessel differential equation. Actually, transforming the entries of $\mathbf{Z}^n(\xi)$ from $Z_l^n(\xi)$ to $X_l^n(\xi)$, where

$$Z_l^n(\xi) = \xi^{\mu_l^n} X_l^n(\xi) \tag{4.25}$$

with

$$\mu_l^n = \frac{1}{2}(1 - q_l^n), \quad l = n, n + 1, \dots, N \tag{4.26}$$

we see that the highest order term $\mathcal{L}_{ll}^n Z_l^n(\xi)$ on the left-hand side of each equation of the system (4.16) takes the form

$$\mathcal{L}_{ll}^n Z_l^n(\xi) = -\xi^{\mu_l^n} \left[\xi^2 \frac{d^2}{d\xi^2} + \xi \frac{d}{d\xi} - (\mu_l^n)^2 - r_{ll}^n \right] X_l^n(\xi). \tag{4.27}$$

If v_l^n denotes a positive parameter defined by

$$v_l^n = \sqrt{(\mu_l^n)^2 + r_{ll}^n} \tag{4.28}$$

then (4.27) suggests the consideration of the eigenvalue problem which consists of the Bessel equation

$$-\left[\xi^2 \frac{d^2}{d\xi^2} + \xi \frac{d}{d\xi} - (v_l^n)^2 \right] y = \lambda^2 \xi^2 y \tag{4.29}$$

with accompanying appropriate conditions. Specifically, the sequence $\{J_{v_l^n}(\lambda_{l,j}\xi)\}_{j=1,2,\dots}$ of the Bessel functions of the first kind is available as the square integrable eigensolutions of (4.29) over $(0, 1)$ relative to the weight ξ , where the $\lambda_{l,j}$ stand for the positive zeros of $J_{v_l^n}(z) = 0$. In what follows, we infer from the square integrability condition in (4.19) that the functions $X_l^n(\xi)$ should behave similarly. Indeed we must have

$$\int_0^1 \xi |X_l^n(\xi)|^2 d\xi \leq \int_0^1 \xi^{2+2\mu_l^n} |\overline{X}_l^n(\xi)|^2 d\xi < \infty, \tag{4.30}$$

where the first inequality follows from Proposition 3, which implies that the exponents $2 + 2\mu_l^n = 3 - q_{ll}^n$ satisfy $0 < 2 + 2\mu_l^n \leq 1$. Furthermore, if we expand each function $X_l^n(\xi)$ into a Fourier–Bessel series

$$X_l^n(\xi) = \lim_{M \rightarrow \infty} \sum_{j=1}^M x_{l,j}^n J_{v_l^n}(\lambda_{l,j}\xi), \quad l = n, n + 1, \dots, N \tag{4.31}$$

the boundary condition (4.18), equivalent to $X_l^n(1) = 0$, is also satisfied immediately as $J_{\nu_l^n}(\lambda_{l,j}) = 0$. It is a well-known fact that the Fourier–Bessel series converges to $X_l^n(\xi)$ in the mean as $M \rightarrow \infty$; however, by truncating the series we suppose a finite M for computational purposes. Therefore, the only thing which remains is the determination of the Fourier–Bessel coefficients $x_{l,j}^n$.

To this end, first note that the dominant second-order terms in (4.27) are replaced by the algebraic terms proportional to the eigenvalues of (4.29). Second, the first derivative terms in system (4.16)

$$\mathcal{L}_{lm}^n Z_m^n(\xi) = -\xi^{\mu_m^n} \left(q_{lm}^n \xi \frac{d}{d\xi} + \mu_m^n q_{lm}^n - r_{lm}^n \right) X_m^n(\xi) \tag{4.32}$$

generated by the off-diagonal entries of the matrix operator \mathcal{L}^n may also be written as algebraic expressions on using expansion (4.31) and the differential–difference identity

$$\frac{d}{dz} J_\nu(\lambda z) = \frac{\nu}{z} J_\nu(\lambda z) - \lambda J_{\nu+1}(\lambda z) \tag{4.33}$$

for the Bessel functions [1].

We then find, after some manipulation, that the representative l th equation of our system of ODEs becomes

$$\sum_{m=n}^N \sum_{j=1}^M \xi^{\mu_m^n} \{ [q_{lm}^n \lambda_{m,j} \xi J_{\nu_m^n+1}(\lambda_{m,j} \xi) - \kappa_{lm}^n J_{\nu_m^n}(\lambda_{m,j} \xi)] (1 - \delta_{lm}) + \lambda_{m,j}^2 J_{\nu_m^n}(\lambda_{m,j} \xi) \delta_{lm} - E^n t_{lm}^n \xi^2 J_{\nu_m^n}(\lambda_{m,j} \xi) \} x_{m,j}^n = 0 \tag{4.34}$$

containing no derivatives anymore, where κ_{lm}^n denotes a new parameter

$$\kappa_{lm}^n = q_{lm}^n (\mu_m^n + \nu_m^n) - r_{lm}^n \tag{4.35}$$

for brevity. Finally, multiplying (4.34) by $\xi^{-\mu_l^n - 1} J_{\nu_l^n}(\lambda_{l,i} \xi)$ and integrating with respect to ξ from 0 to 1 we arrive at algebraic equations of the form

$$\sum_{m=n}^N (\mathbf{H}_{lm}^n - E^n \mathbf{W}_{lm}^n) \mathbf{x}_m^n = \mathbf{0}, \quad l = n, n + 1, \dots, N, \tag{4.36}$$

where we have used the orthogonality of the Bessel functions

$$\int_0^1 \xi J_\nu(\lambda_n \xi) J_\nu(\lambda_m \xi) d\xi = \frac{1}{2} [J_{\nu+1}(\lambda_m)]^2 \delta_{mn}. \tag{4.37}$$

Note that the system in (4.36) is a generalized matrix eigenvalue problem

$$\mathcal{H}^n \mathcal{X}^n = E^n \mathcal{W}^n \mathcal{X}^n \tag{4.38}$$

with the block matrices \mathcal{H}^n and \mathcal{W}^n of order $M(N - n + 1) \times M(N - n + 1)$

$$\mathcal{H}^n = \begin{bmatrix} \mathbf{H}_{nn}^n & \cdots & \mathbf{H}_{nN}^n \\ \vdots & \ddots & \vdots \\ \mathbf{H}_{Nn}^n & \cdots & \mathbf{H}_{NN}^n \end{bmatrix}, \quad \mathcal{W}^n = \begin{bmatrix} \mathbf{W}_{nn}^n & \cdots & \mathbf{W}_{nN}^n \\ \vdots & \ddots & \vdots \\ \mathbf{W}_{Nn}^n & \cdots & \mathbf{W}_{NN}^n \end{bmatrix}, \tag{4.39}$$

and with the block vector \mathcal{X}^n of order $M(N - n + 1) \times 1$

$$\mathcal{X}^n = \begin{bmatrix} \mathbf{x}_n^n \\ \mathbf{x}_{n+1}^n \\ \vdots \\ \mathbf{x}_N^n \end{bmatrix}, \quad \mathbf{x}_m^n = \begin{bmatrix} x_{m,1}^n \\ x_{m,2}^n \\ \vdots \\ x_{m,M}^n \end{bmatrix} \tag{4.40}$$

including the unknown Fourier–Bessel coefficients in (4.31). Here the entries h_{lm}^n and w_{lm}^n of matrices $\mathbf{H}_{lm}^n := [h_{lm}^n]$ and $\mathbf{W}_{lm}^n := [w_{lm}^n]$ are given in neat forms as

$$h_{lm}^n = \frac{1}{2} \lambda_{l,i}^2 [J_{\nu_l^n+1}(\lambda_{l,i})]^2 \delta_{ij} \delta_{lm} - [\kappa_{lm}^n \mathcal{I}_{\nu_l^n, \nu_m^n}(\mu_m^n - \mu_l^n - 1, \lambda_{l,i}, \lambda_{m,j}) - q_{lm}^n \lambda_{m,j} \mathcal{I}_{\nu_l^n, \nu_m^n+1}(\mu_m^n - \mu_l^n, \lambda_{l,i}, \lambda_{m,j})](1 - \delta_{lm}) \tag{4.41}$$

and

$$w_{lm}^n = \frac{1}{2} t_{ll}^n [J_{\nu_l^n+1}(\lambda_{l,i})]^2 \delta_{ij} \delta_{lm} + t_{lm}^n \mathcal{I}_{\nu_l^n, \nu_m^n}(\mu_m^n - \mu_l^n + 1, \lambda_{l,i}, \lambda_{m,j})(1 - \delta_{lm}), \tag{4.42}$$

respectively, where the function $\mathcal{I}_{\nu, \sigma}(\rho, \alpha, \beta)$ stands for an integral of the type

$$\mathcal{I}_{\nu, \sigma}(\rho, \alpha, \beta) = \int_0^1 \xi^\rho J_\nu(\alpha \xi) J_\sigma(\beta \xi) d\xi \tag{4.43}$$

whose integrand contains the product of two Bessel functions.

Thus, in summary, we have established a two-dimensional array of approximations, say $[N, M]$, to deal with the computational problem. Unfortunately, integrals (4.43) appearing in the definitions of the elements of the matrices \mathbf{H}_{lm}^n and \mathbf{W}_{lm}^n cannot be evaluated analytically by using recurrence relations of the Bessel functions, or otherwise. Theoretically, the integral $\mathcal{I}_{\nu, \sigma}$ may be proved to be proper and finite for the ranges of parameters encountered in this work. However, its numerical evaluation is not an easy task.

5. A numerical example

As a benchmark application, we deal with a one-parameter family of billiards defined by

$$f(\theta) = 1 + \delta \cos^2 \theta, \quad 0 \leq \delta < 1 \tag{5.1}$$

which is a special case of the general shape function in (2.6). That is, our billiard is described by the region

$$\mathcal{D} = \{(r, \theta, \phi) \mid 0 \leq r \leq 1 + \delta \cos^2 \theta, 0 \leq \theta \leq \pi, 0 \leq \phi \leq 2\pi\}. \tag{5.2}$$

Despite its simplicity, $f(\theta)$ reflects various shapes becoming nonconvex for $0.5 < \delta < 1$ and reducing to the unit ball when $\delta = 0$. To our knowledge, it has not been studied earlier either classically or as a quantum system. Nevertheless, it seems to provide a good testing ground for the present method. Note that billiard (5.2) is symmetric about the xy -plane and characterized by the transformed shape function $F(\eta)$ in (2.8) with $K = 2, \alpha_1 = 0$ and $\alpha_2 = \delta$, i.e.

$$F(\eta) = 1 + \delta \eta^2, \tag{5.3}$$

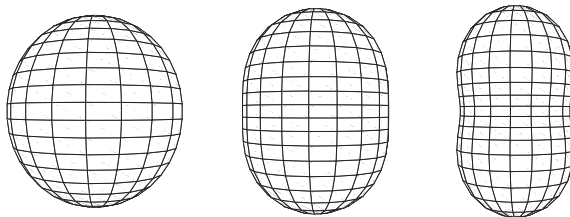


Fig. 2. The billiards for $\delta = 0.1, 0.5$ and 0.9 .

representing an even function of η . Therefore, the symmetric (even) and antisymmetric (odd) state eigenvalues E_{2i}^n and E_{2i+1}^n corresponding, respectively, to even and odd eigenfunctions of η may be calculated separately.

We determine six particular spectra numerically, namely, the sets of symmetric and antisymmetric eigenvalues for three different billiards with $\delta = 0.1, 0.5$ and 0.9 (see Fig. 2). Each spectral set contains about 120 consecutive eigenvalues accurate at least to four digits. We employ Mathematica packages to determine the zeros of the Bessel functions to a satisfactory accuracy. The most costly part of the numerical implementation is the computation of the integrals $\mathcal{J}_{\nu,\sigma}(\rho, \alpha, \beta)$. Moreover, the non-integral orders of the Bessel functions appearing in these integrals cause additional problems. In any case, however, the use of an eigenfunction expansion of Fourier–Bessel type usually increases the cost of the computations, especially when applied to billiard problems [14]. Hence in the numerical evaluation of integrals (4.43) and in the solution of the resulting generalized eigenvalue problem (4.38), we make use of the usual Fortran routines.

In all calculations, we observe that the best converged results are reached on the specific subsequent of the two-dimensional array $[N, M]$ of approximations for which $M = N - n + 1$. Hence, in Table 1, the convergence rates of a few typical symmetric state eigenvalues E_{2i}^n are displayed as a function of the approximation orders $[N, N - n + 1]$ for each δ , for illustration. As shown, the tabulated eigenvalues stabilize to at least four significant digits. Note that E_0^0, E_2^0 and E_0^1 stand for the smallest three eigenvalues for each δ . On the other hand, for instance at $\delta = 0.1$, the results E_0^5, E_{18}^1 and E_{20}^3 correspond, respectively, to the 20th, 50th and 100th eigenvalues ordered in magnitude.

Typical for such approximations is that only a fraction of the eigenvalues of the truncated $[N, M]$ system is a “good” approximation to those of the infinite system. These fractions depend mainly on the parameter δ . Specifically, when we require a four-digit accuracy, we deduce by numerical experiments that the fractions lie between 0.29 and 0.32, 0.20 and 0.24 and 0.14 and 0.18 for $\delta = 0.1, 0.5$ and 0.9 , respectively.

In the studies concerning statistical properties of quantal spectra, the most common statistics is the nearest-neighbor spacing (NNS) distribution. It has been observed, in a number of numerical results [3,5,13], that the NNS distribution of the energy levels of quantum systems with regular classical analogs resembles the Poissonian distribution

$$p(s) = e^{-s}, \quad (5.4)$$

while the spectra of quantum systems with chaotic classical counterparts behave like eigenvalues of a matrix of the Gaussian orthogonal ensemble (GOE) type

$$p(s) = \frac{1}{2} \pi s e^{-\pi s^2/4}. \quad (5.5)$$

Table 1

Convergence rates of a few symmetric state eigenvalues $E_{2i}^n(\delta)$ as a function of the billiard parameter δ , for ascending truncation orders $[N, N - n + 1]$

n	i	N	$E_{2i}^n(0.1)$	$E_{2i}^n(0.5)$	$E_{2i}^n(0.9)$
0	0	3	9.2649242	7.635913	6.591853
		4	9.2648530	7.635772	6.591447
		5	9.2648641	7.635691	6.591330
		7	9.2648682	7.635689	6.591303
		9	9.2648682	7.635688	6.591271
0	1	3	29.679738	19.90062	15.12841
		4	26.679537	19.90051	15.12828
		5	26.679478	19.90028	15.12774
		7	26.679451	19.90016	15.12725
		9	26.679451	19.90016	15.12724
1	0	4	30.569266	22.88507	17.74454
		5	30.569096	22.88401	17.74416
		6	30.569045	22.88367	17.74361
		8	30.569020	22.88367	17.74346
		10	30.569018	22.88367	17.74346
5	0	8	106.20292	90.53120	75.74572
		9	106.20270	90.52818	75.74476
		10	106.20262	90.52749	75.74456
		12	106.20262	90.52730	75.74453
1	9	6	204.74939	149.5363	—
		8	204.73433	149.5331	105.5378
		10	204.73392	149.5330	105.5364
3	10	8	320.44071	—	—
		10	320.43716	231.4346	179.8509
		12	320.43715	231.4345	179.8447

Finally, for systems in which both types of motion co-exist, the Brody distribution [4]

$$p(s) = (v + 1)a_v s^v e^{-a_v s^{v+1}}, \tag{5.6}$$

where

$$a_v = \left[\Gamma \left(\frac{v + 2}{v + 1} \right) \right]^{v+1} \tag{5.7}$$

is one of the mostly used models. Clearly, the Brody distribution becomes Poissonian for $v = 0$ and GOE for $v = 1$. By taking the normalized spacings

$$s_i = \frac{E_{i+1} - E_i}{\langle E_{i+1} - E_i \rangle}, \tag{5.8}$$

where $\langle c_i \rangle$ denotes the mean of a sequence $\{c_i\}$, we thus plot the nearest-neighbor spacing histograms (NNSH) for each eigenvalue set. The best v parameters in the Brody distribution have been obtained by

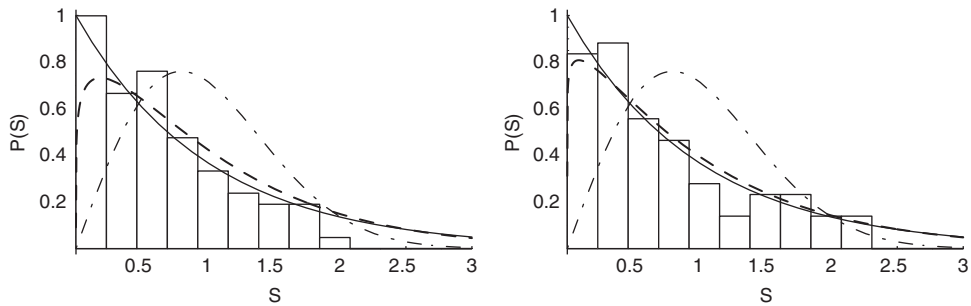


Fig. 3. NNSH for the even- and odd-state eigenvalues of a billiard with $\delta = 0.1$ (solid line: Poisson distribution, dashed line: Brody distribution, dotted–dashed line: GOE distribution).

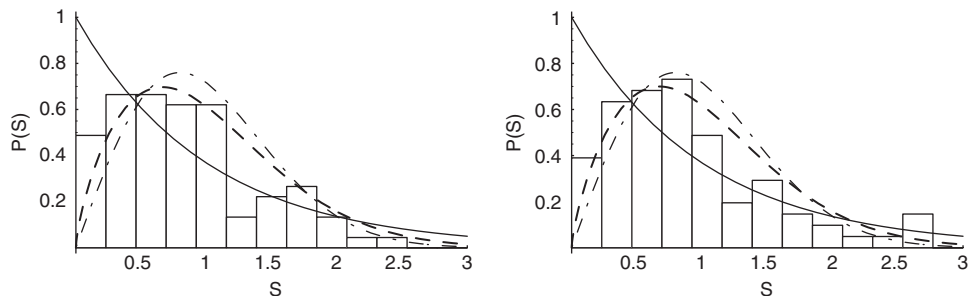


Fig. 4. NNSH for the even- and odd-state eigenvalues of a billiard with $\delta = 0.5$ (solid line: Poisson distribution, dashed line: Brody distribution, dotted–dashed line: GOE distribution).

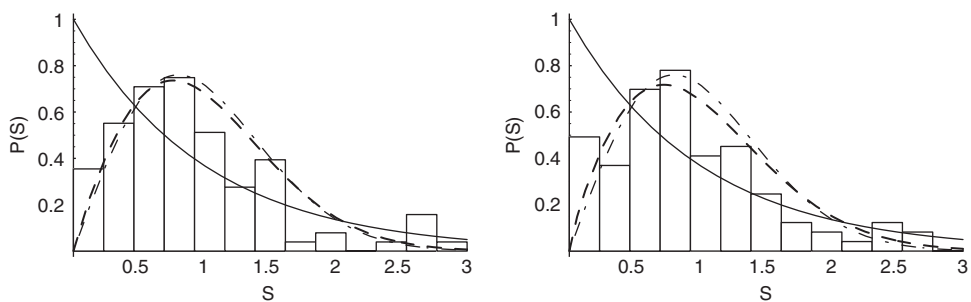


Fig. 5. NNSH for the even- and odd-state eigenvalues of a billiard with $\delta = 0.9$ (solid line: Poisson distribution, dashed line: Brody distribution, dotted–dashed line: GOE distribution).

a fitting procedure. For comparison we have also plotted the Poissonian and GOE distributions. Despite the relatively small number of eigenvalues included in our analysis, we observe a good agreement with the Brody model (see Figs. 3–5).

6. Conclusion

In this paper, the three-dimensional axisymmetric quantum billiards are dealt with using a decomposition in the spherical harmonics. Obviously, the restriction to the axially symmetric cases leads to an important simplification. Nevertheless, the existing methods in three dimensions also assume certain cubic symmetries for the shape of the billiard [10–12].

Although the method presented here seems to be a standard expansion technique, it has two very significant properties. First, it employs an unusual coordinate transformation which standardizes the billiard. Second, it deals with an expansion in the Bessel functions with real orders which is interesting from a mathematical point of view. On the other hand, the general form of the shape function allows us to reproduce several billiard shapes yielding an important tool for a researcher who wishes to study the quantum chaos.

The efficiency of our approach depends strongly on the choice of the billiard. In order to obtain a faster algorithm one must consider a shape function whose power series representation is rapidly convergent. Otherwise, the method requires the use of a great number of coefficients γ_{lmk}^n decelerating the rate of convergence. Furthermore, since the billiard defined by the shape function $f(\theta)$ may be regarded as a perturbation of the unit ball, it is necessary to have

$$f(\theta) = 1 + \sum_{k=1}^{\infty} \alpha_k \cos^k \theta < 2 \quad (6.1)$$

so that the perturbation is regular. However, these additional conditions imposed on the shape function do not considerably restrict the variety of billiards generated by (2.8) in this way.

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