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An Expansion Method for Schrödinger Equation of Quantum Billiards with Arbitrary Shapes

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Abstract — A numerical method for solving the time-independent Schrödinger equation of a particle moving freely in a three-dimensional axisymmetric region is developed. The boundary of the region is defined by an arbitrary analytic function. The method uses a coordinate transformation and an expansion in eigenfunctions. The effectiveness is checked and confirmed by applying the method to a particular example, which is a prolate spheroid.

Keywords — Bessel functions, Eigenfunction expansion, Quantum billiard, Schrödinger equation, Spherical harmonics.

I. INTRODUCTION

THE most frequently occurring equation in quantum mechanics is the stationary Schrödinger equation, which is an ordinary differential equation(ODE) in the case of a one dimensional problem and a partial differential equation(PDE) if the corresponding physical system is higher dimensional. Unfortunately, the analytical solvability of this equation, even in one dimension is restricted to a few classes of potentials. Therefore, the use of numerical methods for the relevant problem gains a lot of significance. The stationary Schrödinger equation for a particle moving freely inside a closed region, the so called "Quantum billiard problem" has received considerable interest recently [1],[2]. Despite its simplicity, such a problem is known to be exactly solvable only in few cases in which the boundary of the closed region, the billiard, is constant in some coordinate system. From quantum mechanical point of view, the billiards with non-constant boundaries are much more interesting. However, to find approximate solutions 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 [3]-[5], results on three dimensional case are only few [6],[7].

The aim of this work is to propose a quite general three dimensional quantum billiard model and to develop a method for its numerical implementation, more precisely, to compute the energy spectra of the system. Thus the paper is organized as follows: In section II the mathematical model of the quantum billiard and a coordinate transformation is introduced. An eigenfunction expansion which reduces the transformed Schrödinger equation to a system of ODEs and its convertion to a generalized matrix eigenvalue problem are given in section III. The method is then applied to a particular example, namely, a prolate spheroid in section IV, where the numerical results are presented. The last section is devoted to the concluding remarks.

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II. MATHEMATICAL MODEL OF THE PROBLEM

We introduce a closed three dimensional axisymmetric region (the billiard), whose boundary is defined by an analytic function. To be specific, the billiard is described by

$$\mathcal{D} = \{(r,\theta,\phi) \mid 0 \le r \le f(\theta),\ 0 \le \theta \le \pi,\ 0 \le \phi \le 2\pi\} \tag{1}$$

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. Note that, the billiard $\mathcal{D}$ in (1) is a solid of revolution obtained by rotating a two-dimensional region in the yz-plane about the z-axis (see Fig. 1). In spherical coordinates, the Schrödinger equation for a

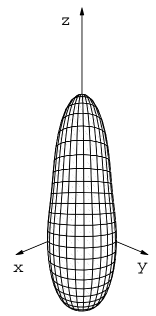

Fig. 1. Three dimensional axisymmetric billiard

particle moving freely inside the region $\mathcal{D}$ can be written as

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

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

$$\Psi(r,\theta,\phi) = 0 \qquad \text{on} \qquad \partial\mathcal{D} \tag{3}$$

and, in addition, satisfies the square integrability condition

$$\int\int_{\mathcal{D}}\int \mid \Psi \mid^2 dV < \infty \tag{4}$$

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

We propose the following form for the analytic shape function $f(\theta)$

$$f(\theta) = 1 + \sum_{k=1}^{\infty} \alpha_k \cos^k \theta, \qquad \alpha_k \in \mathbb{R} \tag{5}$$

where the α_k may be regarded as the shape parameters. By means of these flexible parameters it is possible to construct various shapes. Observe that,

$$1 \leq f(\theta) \leq \infty \tag{6}$$

should be satisfied in order to have a bounded geometric region.

For computational purposes, we deal with a truncated power series representation of the shape function, say $F(\eta)$,

$$F(\eta) = 1 + \sum_{k=1}^{K} \alpha_k \eta^k, \tag{7}$$

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

$$\eta = \cos\theta, \qquad \eta \in [-1, 1] \tag{8}$$

where K is large enough. Furthermore, if we apply the unusual substitution

$$\xi = \frac{r}{F(\eta)}, \qquad \xi \in [0, 1] \tag{9}$$

the billiard in (1) with an arbitrary shape reduces to a unit ball

$$\mathcal{D}_u = \{(\xi, \eta, \phi) \mid 0 \leq \xi \leq 1,\ -1 \leq \eta \leq 1,\ 0 \leq \phi \leq 2\pi\} \tag{10}$$

in the (ξ, η, ϕ) coordinate system.

Unfortunately, this standardization has been accomplished at the cost of transforming the Schrödinger equation (2) into a quite complicated form

$$\begin{aligned}\Big\{ & G_1 \frac{\partial^2}{\partial \xi^2} + [2G_1 + G_2 - G_3] \frac{1}{\xi} \frac{\partial}{\partial \xi} + \frac{1}{\xi^2} G_0 \mathcal{T} \\ & - \frac{1}{\xi\eta}(1 - \eta^2) G_2 \frac{\partial^2}{\partial \xi \partial \eta} + E G_0^2 \Big\} \Psi(\xi, \eta, \phi) = 0\end{aligned} \tag{11}$$

where $\mathcal{T}$ is the second order differential operator in η

$$\mathcal{T} = (1 - \eta^2) \frac{\partial^2}{\partial \eta^2} - 2\eta \frac{\partial}{\partial \eta} - \frac{1}{1 - \eta^2} \frac{\partial^2}{\partial \phi^2}, \tag{12}$$

and the G_i denote the polynomials of degree $2K$ in η

$$\begin{aligned} G_0 &:= [F(\eta)]^2 & G_1 &:= [F(\eta)]^2 + (1 - \eta^2) [F'(\eta)]^2 \\ G_2 &:= 2\eta F'(\eta) F(\eta) & G_3 &:= (1 - \eta^2) F''(\eta) F(\eta) \end{aligned} \tag{13}$$

introduced for the sake of brevity.

III. Expansion in Eigenfunctions and Transformation to a Matrix Eigenvalue Problem

The transformed square integrability condition which now reads

$$\int_0^{2\pi} \int_{-1}^{1} \int_0^{1} \mid \Psi(\xi, \eta, \phi) \mid^2 \xi^2 [F(\eta)]^3 \mathrm{d}\xi \mathrm{d}\eta \mathrm{d}\phi < \infty \tag{14}$$

suggests that the integral

$$\int_0^{2\pi} \int_{-1}^{1} \mid \Psi(\xi, \eta, \phi) \mid^2 \mathrm{d}\eta \mathrm{d}\phi < \infty \tag{15}$$

is also bounded for all fixed $\xi \in (0, 1]$. In what follows, the wavefunction $\Psi(\xi, \eta, \phi)$ 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 simply a sphere of radius ξ.

On the other hand, observe that the eigenfunctions of the operator $\mathcal{T}$ in (12) are the spherical harmonics

$$Y_m^n(\eta, \phi) = P_m^{|n|}(\eta) \mathrm{e}^{in\phi}, \quad 0 \leq m \leq \infty, \quad -m \leq n \leq m \tag{16}$$

corresponding to the eigenvalues $-m(m+1)$, in which the 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 [8]. Therefore, we may propose an expansion in spherical harmonics for the transformed wavefunction $\Psi(\xi, \eta, \phi)$ in the form

$$\Psi(\xi, \eta, \phi) = \sum_{m=0}^{\infty} \sum_{n=0}^{m} [\Phi_m^n(\xi) \cos n\phi + \psi_m^n(\xi) \sin n\phi] P_m^n(\eta) \tag{17}$$

where the 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. Note that the axial symmetry of the region allows a separation of (17) into two parts containing even and odd eigenfunctions in ϕ. Hereafter, we consider only the even eigenfunctions, that is, we deal with the expansion

$$\Psi_e(\xi, \eta, \phi) = \sum_{m=0}^{\infty} \sum_{n=0}^{m} \Phi_m^n(\xi) P_m^n(\eta) \cos n\phi. \tag{18}$$

Substituting Ψ_e into (11), and using the orthogonality of the cosine functions over $\phi \in (0, 2\pi)$, we obtain

$$\begin{aligned}\sum_{m=n}^{\infty} \Big\{ & G_1 P_m^n \frac{\mathrm{d}^2}{\mathrm{d}\xi^2} \\ & + \left[(2G_1 - mG_2 - G_3) P_m^n + \frac{1}{\eta}(m - n + 1) G_2 P_{m+1}^n \right] \frac{1}{\xi} \frac{\mathrm{d}}{\mathrm{d}\xi} \\ & - m(m+1) G_0 P_m^n \frac{1}{\xi^2} + E G_0^2 P_m^n \Big\} \Phi_m^n(\xi) = 0\end{aligned} \tag{19}$$

for $n \geq 0$.

An eigenfunction expansion of type (18) makes it possible to reduce the PDE to a system of ODEs in the Fourier coefficients $\Phi_m^n(\xi)$ [9]. To this end, first note that the polynomials G_i in (19) may be written as

$$G_i = \sum_{k=0}^{2K} g_{i,k}\eta^k, \qquad i = 0, 1, 2, 3 \tag{20}$$

where the coefficients $g_{i,k}$ can easily be calculated in terms of the shape parameters α_k. On the other hand,

$$[G_0]^2 = \sum_{k=0}^{4K} g_{4,k}\eta^k, \tag{21}$$

where the $g_{4,k}$ are certain combinations of $g_{0,k}$.

Thus, it is shown that the η-dependency of equation (19) comprises solely the products $\eta^k P_j^n(\eta)$ with $j = m$ and $j = m + 1$. Then we expand the $\eta^k P_j^n(\eta)$ into a series of the associated Legendre functions

$$\eta^k P_j^n(\eta) = \sum_{l=n}^{\infty} \gamma_{ljk}^n P_l^n(\eta) \tag{22}$$

in which the coefficients γ_{ljk}^n

$$\gamma_{ljk}^n = \int_{-1}^{1} \eta^k P_l^n(\eta) P_j^n(\eta)\mathrm{d}\eta, \qquad \gamma_{ljk}^n = \gamma_{jlk}^n \tag{23}$$

can be evaluated exactly using the truly nice identities of the associated Legendre functions [10].

Next we define the matrices $\mathbf{A}^n$, $\mathbf{B}^n$, $\mathbf{C}^n$ and $\mathbf{D}^n$ whose entries are

$$a_{lm}^n = \sum_{k=0}^{2K} g_{1,k}\gamma_{lmk}^n \tag{24}$$

$$\begin{aligned} b_{lm}^n = &\sum_{k=0}^{2K} (2g_{1,k} - m g_{2,k} - g_{3,k})\gamma_{lmk}^n \\ &+(m - n + 1)\sum_{k=0}^{2K-1} g_{2,k+1}\gamma_{l(m+1)k}^n \end{aligned} \tag{25}$$

and

$$c_{lm}^n = \sum_{k=0}^{2K} g_{0,k}\gamma_{lmk}^n, \quad d_{lm}^n = \sum_{k=0}^{4K} g_{4,k}\gamma_{lmk}^n \tag{26}$$

respectively. Using these definitions and the orthogonality of the associated Legendre functions, we end up with the infinite system of coupled ODEs for the determination of the Fourier coefficients $\Phi_m^n(\xi)$. In matrix-vector form, this system is written as

$$\left(\mathbf{A}^n\xi^2\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} + \mathbf{B}^n\xi\frac{\mathrm{d}}{\mathrm{d}\xi} + \mathbf{\Lambda}\mathbf{C}^n + E\xi^2\mathbf{D}^n\right)\mathbf{\Phi}^n = \mathbf{0} \tag{27}$$

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

$$\mathbf{\Phi}^n = \left[\Phi_n^n(\xi), \Phi_{n+1}^n(\xi), \Phi_{n+2}^n(\xi), \ldots\right]^{\mathrm{T}} \tag{28}$$

whose entries are the Fourier coefficients.

For a complete reformulation of the problem, the boundary and square integrability conditions should be reconsidered in accordance with the vector differential equation just obtained. With the expansion (18) the boundary condition (3) is altered to

$$\mathbf{\Phi}^n(1) = \mathbf{0}, \qquad n = 0, 1, \ldots. \tag{29}$$

Similarly, the square integrability condition requires the boundedness of the integral

$$\int_0^1 \xi^2 \parallel \mathbf{\Phi}^n(\xi) \parallel^2 \mathrm{d}\xi < \infty. \tag{30}$$

In practice, we seek approximate solutions of the system in (27) over finite-dimensional subspaces, for $l = n, n+1, \ldots, N$ and $n = 0, 1, \ldots, N$, where N is a sufficiently large positive integer.

It can be shown that the coefficient matrices $\mathbf{A}^n$ and $\mathbf{D}^n$ are positive definite. In addition, the matrix $\mathbf{B}^n$ has a special structure. The positive definiteness of $\mathbf{A}^n$ suggests the Cholesky decomposition $\mathbf{A}^n = \mathbf{L}\mathbf{L}^{\mathrm{T}}$, where $\mathbf{L}$ is a lower triangular matrix with positive diagonal entries. Hence, we may introduce a new vector-valued function $\mathbf{Z}^n(\xi) = [Z_n^n(\xi), Z_{n+1}^n(\xi), \ldots]^{\mathrm{T}}$ of the form

$$\mathbf{Z}^n(\xi) = \mathbf{L}^{\mathrm{T}}\mathbf{\Phi}^n(\xi) \tag{31}$$

and transform (27) to

$$\boldsymbol{\mathcal{L}}^n\mathbf{Z}^n(\xi) = E\xi^2\mathbf{T}^n\mathbf{Z}^n(\xi) \tag{32}$$

where

$$\boldsymbol{\mathcal{L}}^n := -\mathbf{I}\xi^2\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} - \mathbf{Q}^n\xi\frac{\mathrm{d}}{\mathrm{d}\xi} + \mathbf{R}^n \tag{33}$$

where the matrices $\mathbf{Q}^n$, $\mathbf{R}^n$ and $\mathbf{T}^n$ are defined by

$$\begin{gathered} \mathbf{Q}^n = \mathbf{L}^{-1}\mathbf{B}^n\mathbf{L}^{-\mathrm{T}}, \quad \mathbf{R}^n = -\mathbf{L}^{-1}\mathbf{\Lambda}\mathbf{C}^n\mathbf{L}^{-\mathrm{T}}, \\ \mathbf{T}^n = \mathbf{L}^{-1}\mathbf{D}^n\mathbf{L}^{-\mathrm{T}}. \end{gathered} \tag{34}$$

Clearly, the transformed variable $\mathbf{Z}^n(\xi)$ satisfies the same conditions as $\mathbf{\Phi}^n(\xi)$. Next we transform the entries of $\mathbf{Z}^n(\xi)$ from $Z_l^n(\xi)$ to $X_l^n(\xi)$, where

$$Z_l^n(\xi) = \xi^{\mu_l^n} X_l^n(\xi) \tag{35}$$

and

$$\mu_l^n = \frac{1}{2}\left(1 - q_{ll}^n\right), \qquad l = n, n+1, \ldots, N. \tag{36}$$

Then the highest order term $\mathcal{L}_{ll}^n Z_l^n(\xi)$ on the left hand side of each equation of the system (33) takes the form

$$\mathcal{L}_{ll}^n Z_l^n(\xi) = -\xi^{\mu_l^n}\left[\xi^2\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} + \xi\frac{\mathrm{d}}{\mathrm{d}\xi} - (\mu_l^n)^2 - r_{ll}^n\right] X_l^n(\xi). \tag{37}$$

If ν_l^n denotes a positive parameter defined by

$$\nu_l^n = \sqrt{(\mu_l^n)^2 + r_{ll}^n} \tag{38}$$

the (37) suggests the consideration of the eigenvalue problem which consists of the Bessel equation

$$-\left[\xi^2\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} + \xi\frac{\mathrm{d}}{\mathrm{d}\xi} - (\nu_l^n)^2\right] y = \lambda^2\xi^2 y \tag{39}$$

with accompanying appropriate conditions. To be more specific, the sequence $\{J_{\nu_l^n}(\lambda_{l,j}\xi)\}_{j=1}^{\infty}$ of the Bessel functions of the first kind is available as the square integrable eigensolutions of (39) over $(0,1)$ relative to the weight ξ, where the $\lambda_{l,j}$ stand for the positive zeros of $J_{\nu_l^n}(z)=0$. In what follows, we expand each function $X_l^n(\xi)$ into a Fourier-Bessel series

$$X_l^n(\xi)=\lim_{M\to\infty}\sum_{j=1}^{M}x_{l,j}^n J_{\nu_l^n}(\lambda_{l,j}\xi), \qquad l=n,n+1,\ldots,N. \tag{40}$$

Substituting these expansions into the system, after a long but straightforward computation we end up with a generalized matrix eigenvalue problem

$$\boldsymbol{\mathcal{H}}^n\boldsymbol{\mathcal{X}}^n=E\boldsymbol{\mathcal{W}}^n\boldsymbol{\mathcal{X}}^n \tag{41}$$

where $\boldsymbol{\mathcal{H}}^n$ and $\boldsymbol{\mathcal{W}}^n$ are block matrices of order $M(N-n+1)\times M(N-n+1)$ and $\boldsymbol{\mathcal{X}}^n$ is a block vector of order $M(N-n+1)\times 1$. Here the entries of the matrices $\boldsymbol{\mathcal{H}}^n$ and $\boldsymbol{\mathcal{W}}^n$ contain integrals of the type

$$\mathcal{I}_{\nu,\sigma}(\rho,\alpha,\beta)=\int_0^1\xi^\rho J_\nu(\alpha\xi)J_\sigma(\beta\xi)\mathrm{d}\xi \tag{42}$$

the computation of which is the most difficult and expensive part of the method.

Thus, in summary, we have transformed the eigenvalue problem (2)-(4) into a matrix eigenvalue problem.

IV. An Example: Prolate Spheroid

As an application of the method, we consider the so-called prolate spheroid which in Cartesian coordinates can be written as

$$\mathcal{D}=\left\{(x,y,z)\mid \frac{x^2+y^2}{a^2}+\frac{z^2}{b^2}\le 1\right\} \tag{43}$$

where $b^2>a^2$. For this particular example the function $F(\eta)$ is obtained as

$$F(\eta)=a+2a\sum_{k=1}^{K}\frac{\beta^k}{4^k}\frac{\Gamma(2k)}{\Gamma(k)\Gamma(k-1)}\eta^{2k} \tag{44}$$

where $\beta=1-\frac{a^2}{b^2}$.

The numerical implementation of the problem has been performed by using two types of software, MATHEMATICA for finding zeros of Bessel functions and FORTRAN for the rest of computations. It must be pointed out that, the generalized eigenvalue problem (41) has been solved for all values of n from 0 to N. We treated the cases of a prolate spheroid with $a=1$ and $b=1.01$ and $a=1$ and $b=1.5$. The first case is obviously a slight perturbation of the sphere. The calculated eigenvalues are given in Tables I and II respectively. For comparison, we have obtained approximate eigenvalues of the same problem using an alternative method proposed by Moszkowski[11]. In both tables $E^{(1)}$ denotes eigenvalues obtained using our method, and $E^{(2)}$ denotes eigenvalues obtained by the method of Moszkowski.

TABLE I
FIRST 10 EIGENVALUES FOR A PROLATE SPHEROID WITH $a=1$ AND $b=1.01$

n	$E_n^{(1)}$	$E_n^{(2)}$
1	9.8047447	9.8047447
2	32.867762	32.867761
3	32.936688	32.936688
4	33.123826	33.123826
5	39.225609	39.225609
6	66.278007	66.278005
7	66.313557	66.313555
8	66.419504	66.419503
9	66.593947	66.593946
10	66.834143	66.834142

TABLE II
FIRST 10 EIGENVALUES FOR A PROLATE SPHEROID WITH $a=1$ AND $b=1.5$

n	$E_n^{(1)}$	$E_n^{(2)}$
1	7.9953	7.9953
2	20.394	20.393
3	24.986	24.986
4	30.410	30.410
5	34.893	34.893
6	39.909	39.905
7	44.098	44.097
8	49.663	49.662
9	55.982	55.980
10	56.121	56.121

V. Conclusion

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 region. Second, it deals with an expansion in the Bessel functions with real orders which is interesting from a mathematical point of view.

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