

# Eigenvalue statistics for some quantum billiard systems

Jonathan Bober

May 4, 2004

## Abstract

In this paper I give some description of what happens to the eigenvalues of the Laplacian in the as the shape for a quantum billiard system is deformed from the non-chaotic circle to the chaotic stadium. Included is a description of the method used and some error analysis thereof. Also, there are some cool pictures, and would be cool animations if printed paper could support it.

## Contents

<b>1</b>	<b>Introduction</b>	<b>2</b>
1.1	Mathematical description of the problem . . . . .	2
1.2	Physical description of the problem . . . . .	2
1.2.1	Non Chaotic systems . . . . .	3
1.2.2	Chaotic systems . . . . .	5
1.3	About the rest of the paper . . . . .	5
<b>2</b>	<b>The deformation of the circle into the stadium</b>	<b>5</b>
<b>3</b>	<b>The numerical method</b>	<b>5</b>
3.1	High level overview . . . . .	5
3.2	More detail . . . . .	15
3.3	Even more detail: sweep range and basis size . . . . .	21
3.4	Even more detail: truncating the generalized eigenvalue problem . . . . .	21
3.5	Better numerical methods . . . . .	21

<b>4</b>	<b>Error analysis of the method</b>	<b>21</b>
<b>5</b>	<b>More tables and pictures</b>	<b>21</b>
<b>6</b>	<b>A note of thanks</b>	<b>21</b>
<b>7</b>	<b>References</b>	<b>21</b>

# 1 Introduction

## 1.1 Mathematical description of the problem

Mathematically, our problem statement is rather simple. We wish to find nontrivial eigenvalues  $\lambda$  and eigenfunctions  $\psi(\vec{r})$  that satisfy the two-dimensional Helmholtz equation

$$\nabla^2 \psi(\vec{r}) = \lambda \psi(\vec{r}), \quad (1)$$

subject to the condition that

$$\psi(\vec{r}) = 0, \forall \vec{r} \in \Gamma \quad (2)$$

where  $\Gamma$  is some simple closed curve in the  $x, y$  plane. For future ease of use, we define  $k$  with

$$k^2 = \lambda, k > 0$$

Here  $\nabla^2$  signifies the Laplacian operator. In two dimensions, this is defined as:

$$\nabla^2 u(\vec{r}) = \left( \frac{\delta^2 u}{\delta r_1^2} + \frac{\delta^2 u}{\delta r_2^2} \right) (\vec{r}).$$

## 1.2 Physical description of the problem

A classical billiard system is just what one would expect from the name - a particle (the cue ball) bouncing around a walled system (the billiard table.) The quantum analogue is a wave packet moving around a 2D cavity - for example, the cue ball might now be an electron, and it is thus small enough that quantum effects are noticed.

This system is governed by the two dimensional time independent Schrodinger equation:

$$\nabla^2 \psi(\vec{r}) = E_n \psi_n(\vec{r}).$$

For a hard walled cavity, we have Dirichlet boundary conditions:

$$\psi(\vec{r}) = 0, \forall \vec{r} \in \Gamma,$$

where  $\Gamma$  is the wall of the cavity.

Due to the restriction imposed by the Dirichlet boundary conditions, the energy spectrum  $\{E_n\}$  is discrete, and the physical problem is to find the energy levels and their associated eigenstates.

Also, it should be noted that the very same conditions govern the vibrations of a tightly stretched drum head. For this we have an equation using yet different notation:

$$\nabla^2 u(\vec{r}) = k^2 u(\vec{r}).$$

Here  $k$  is proportional to a principle frequency of vibration.

Kac's problem is phrased as "Can one hear the shape of a drum?" [Kac], and asks if two different drums can have the same frequency spectrum. This is discussed in [TD].

In this paper I focus on quantum billiards, but past section 1 everything is really just plain mathematics.

### 1.2.1 Non Chaotic systems

One example of a regular system is a circle (figure 1.2.1). The plotted eigenstates for the circle show a regular tendency of having small values in the middle. This corresponds to the classical analogue - a particle bouncing around inside the circle will tend to have a trajectory that keeps it away from the center. The same is true for a wave packet inside a circular quantum cavity.

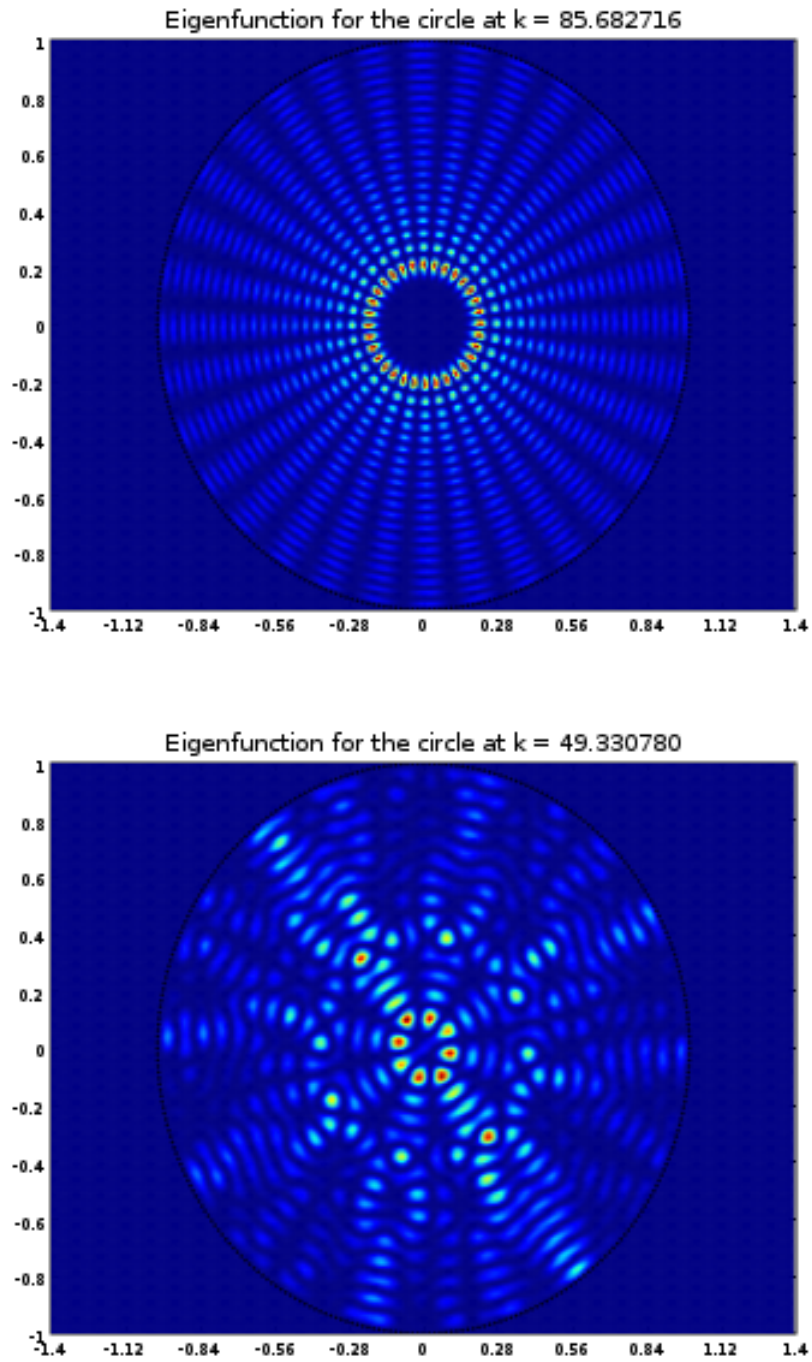


Figure 1: Plots of  $\psi^2$  for the circle. Noticable in the top figure is that many orbits for a classical particle stay away from the center, and the quantum system shares the same property.

### **1.2.2 Chaotic systems**

A chaotic billiard system, classically, is one in which the typical motion of a particle does not have any regularity to it. Two particles launched with the same velocity but slightly different positions in a chaotic system will tend to have very different positions and velocities in a short time. Also, the orbit of a particle typically takes it across the whole system, rather than just a subset, as we see in the circle. Figure 1.2.2 shows two typical eigenstates for the stadium. One of the states shows quite clearly the "scarring" that occurs due to the back and forth bouncing motion that the horizontal walls cause. The other state shows clearly the chaotic nature of the stadium. It is spread out over the whole system, the way a particle would bounce over the whole system.

### **1.3 About the rest of the paper**

Section 2 describes bits of what happens to the eigenvalues and eigenstates of the circle as it is deformed into a stadium. Section 3 describes the method that was used to find this data. Section 4 analyzes the error of the numerical method used by comparing the found values for the circle to their analytically known actual values. Section 5 is used for some nice pictures and tables which are better left out of the main text.

## **2 The deformation of the circle into the stadium**

The section is currently presented as figures with captions.

## **3 The numerical method**

### **3.1 High level overview**

The method used is discussed in full generality in [AB] chapter 5. Here I discuss specifically the methods that were used for this paper, and perhaps give a gentler introduction to the general method.

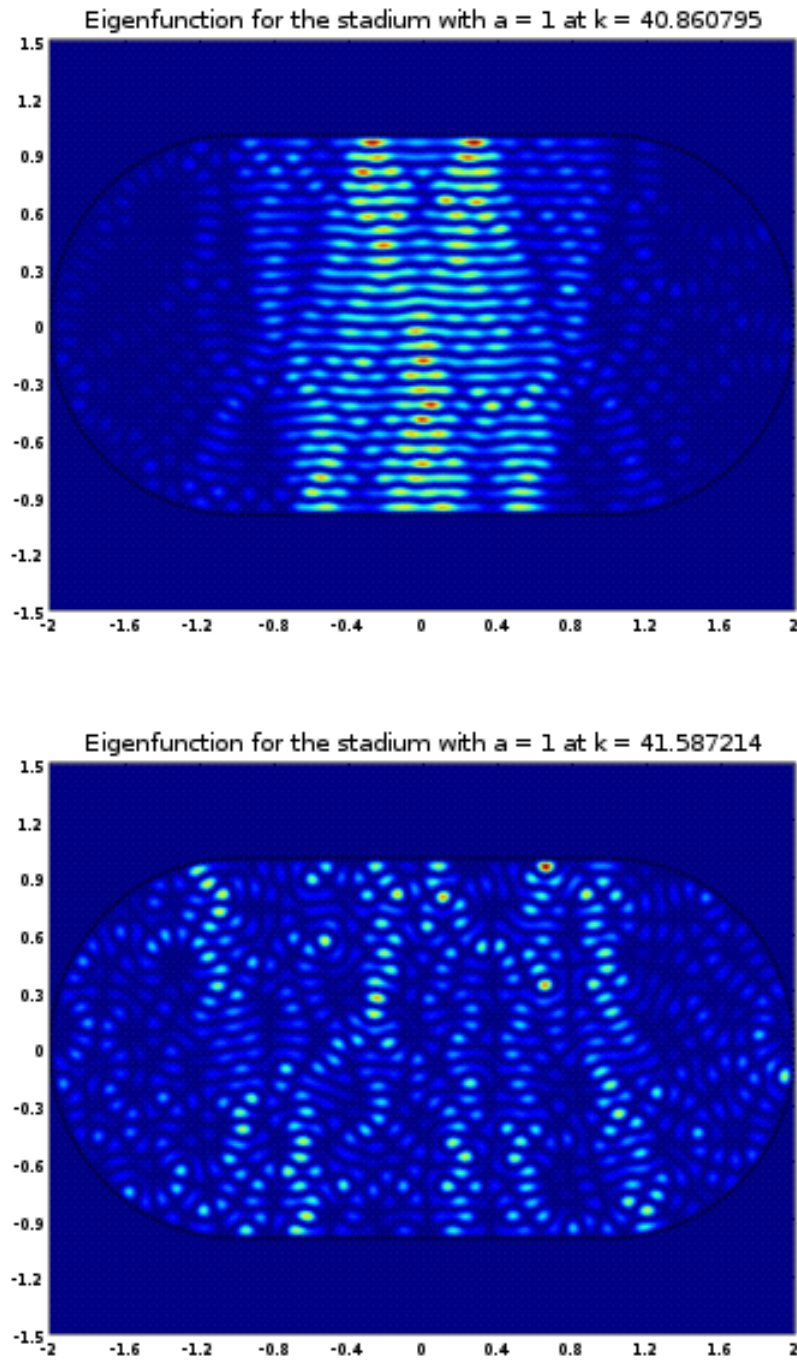
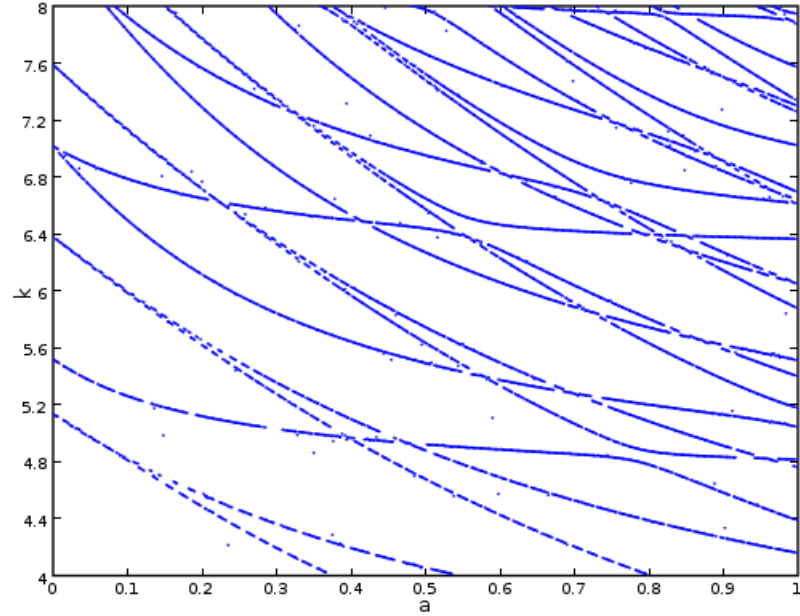


Figure 2: Plots of  $\psi^2$  for the stadium. The top shows the "scarring" that occurs due to the likelihood of a particle spending time bouncing from the top to the bottom of the stadium. The bottom plot, however, looks more like a random superposition of plane waves. As the energy level increases, we see more eigenstates like this, which we will never find in the circle.

Eigenvalues for the stadium as a (1/2 width of rectangular section) changes.



Eigenvalues for the stadium as a (1/2 width of rectangular section) changes.

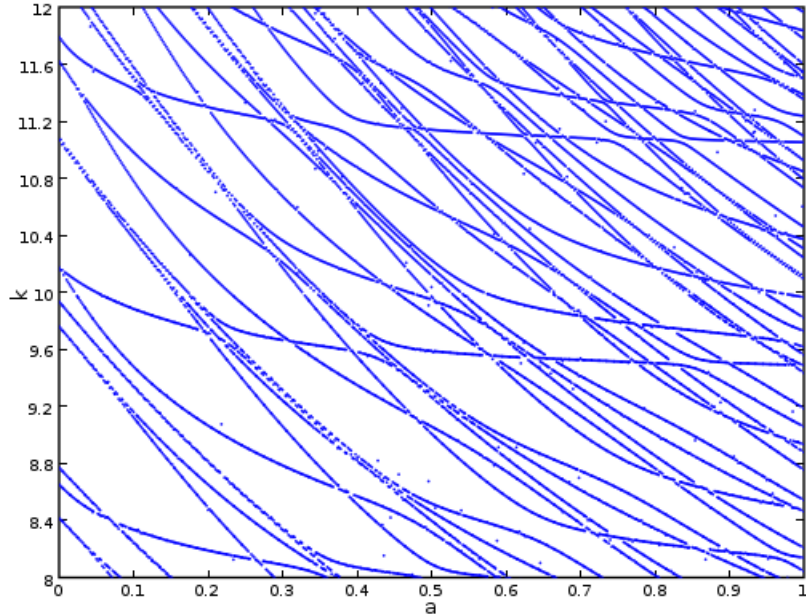


Figure 3: Change in eigenvalues as the circle is deformed into the stadium. Many crossings and avoided crossings are apparent. Some eigenvalues decrease together, evenly spaced, while others interfere with each other, resulting in a change of the overall distribution of the eigenvalues. The random dots which are outside of any curve occur from errors in the search, and are not actual eigenvalues.

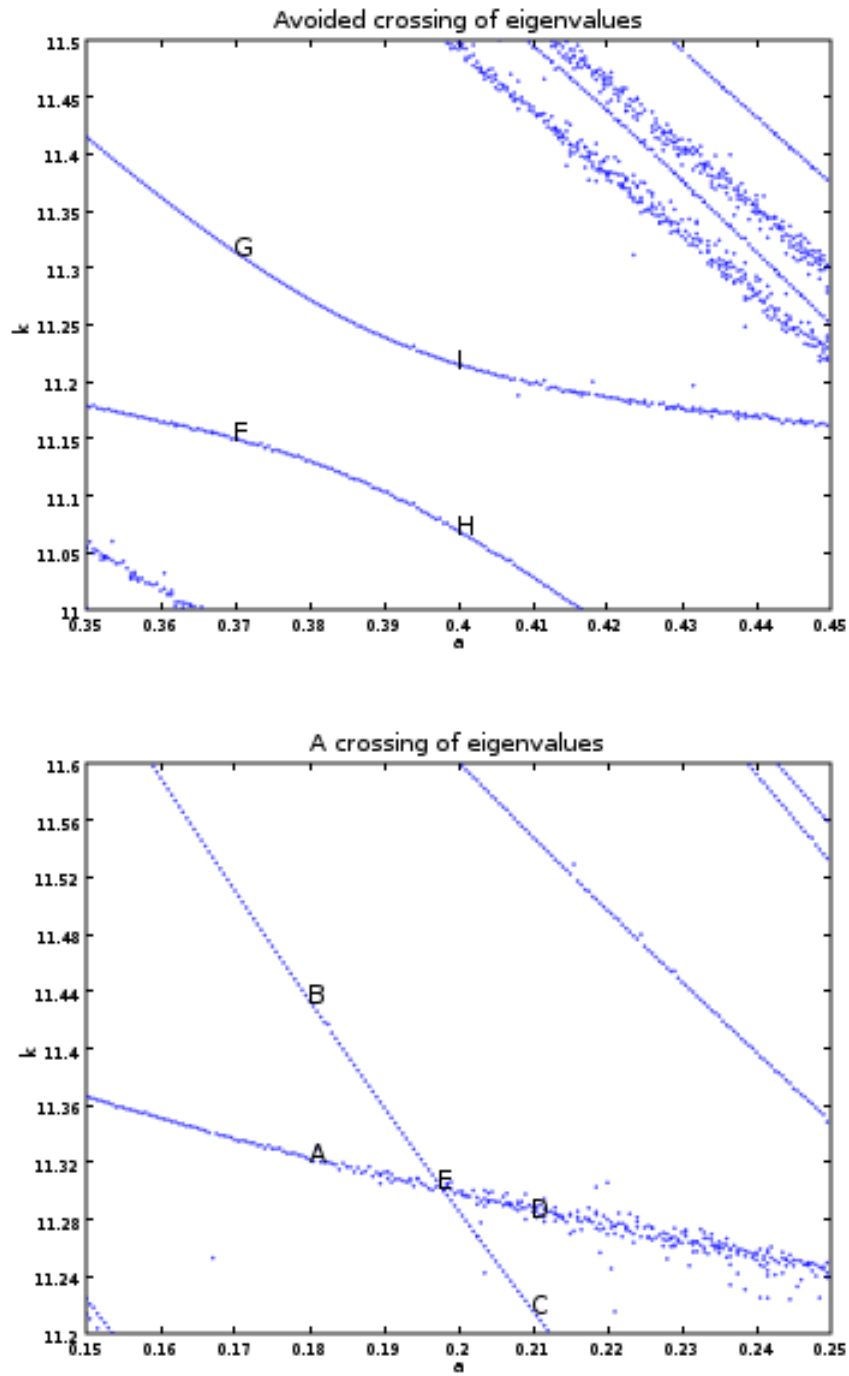


Figure 4: A crossing and an avoided crossing. Associated eigenstates for lettered points are shown in other plots. The scattered plots are most likely a result of errors in the code that searches for eigenvalues.



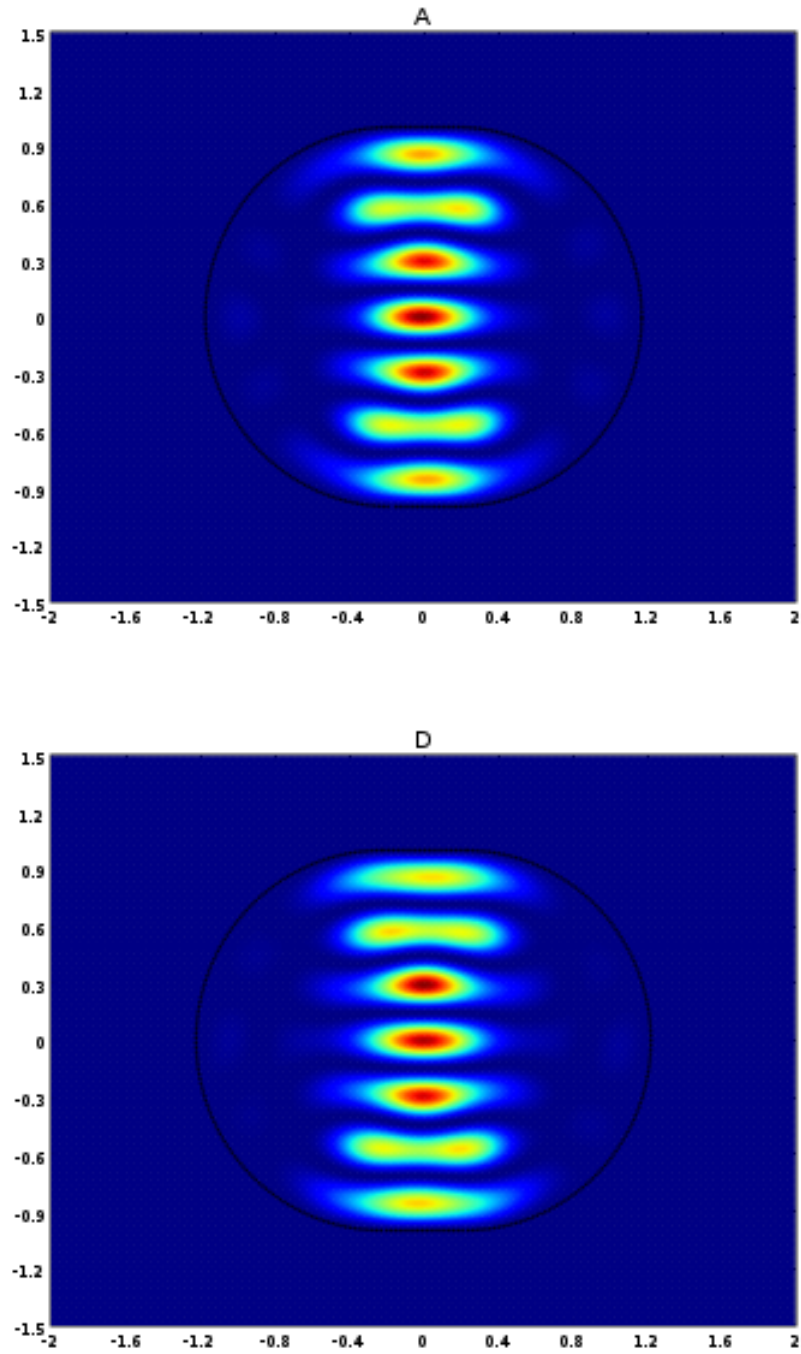


Figure 5: Eigenstates A and D before and after the crossing of eigenvalues. There is little change.

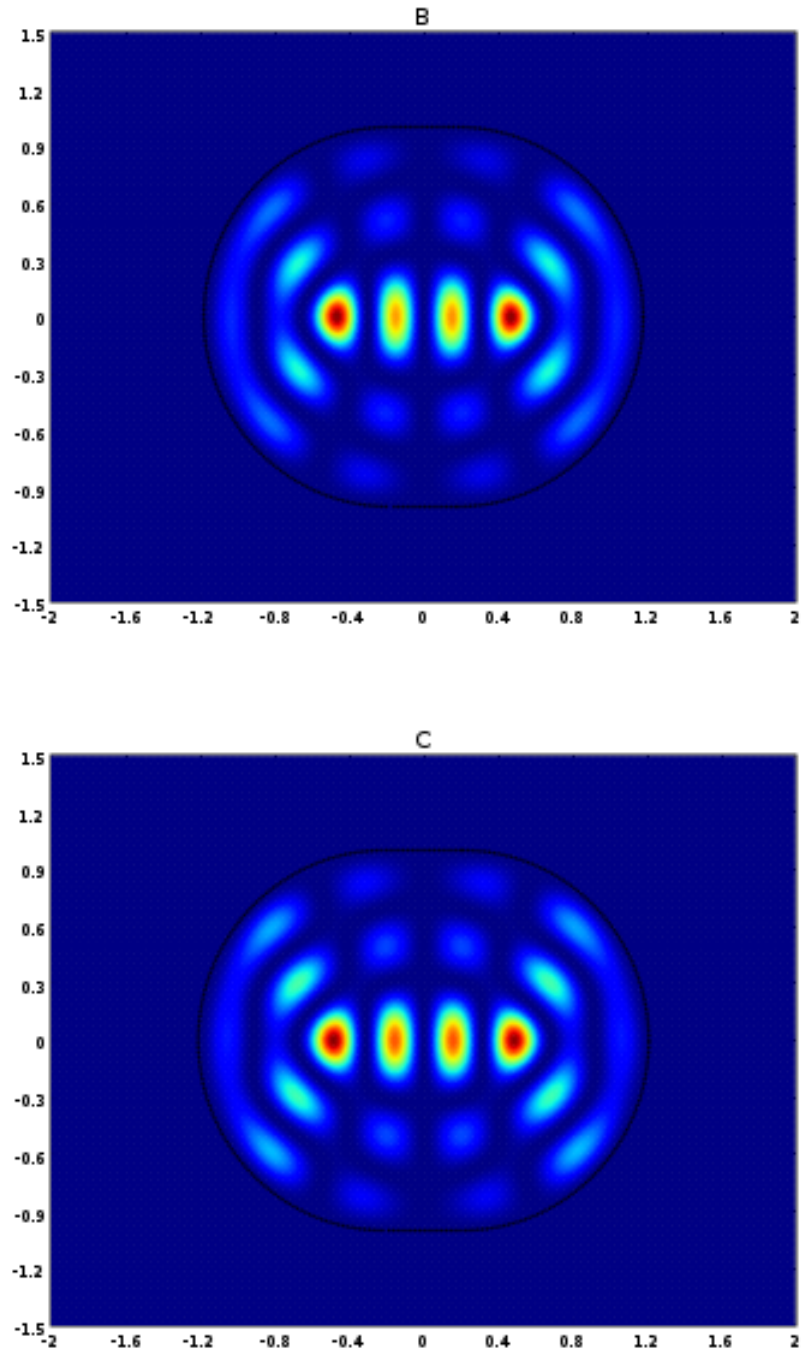


Figure 6: Eigenstates B and C before and after the crossing of eigenvalues. There is little change.

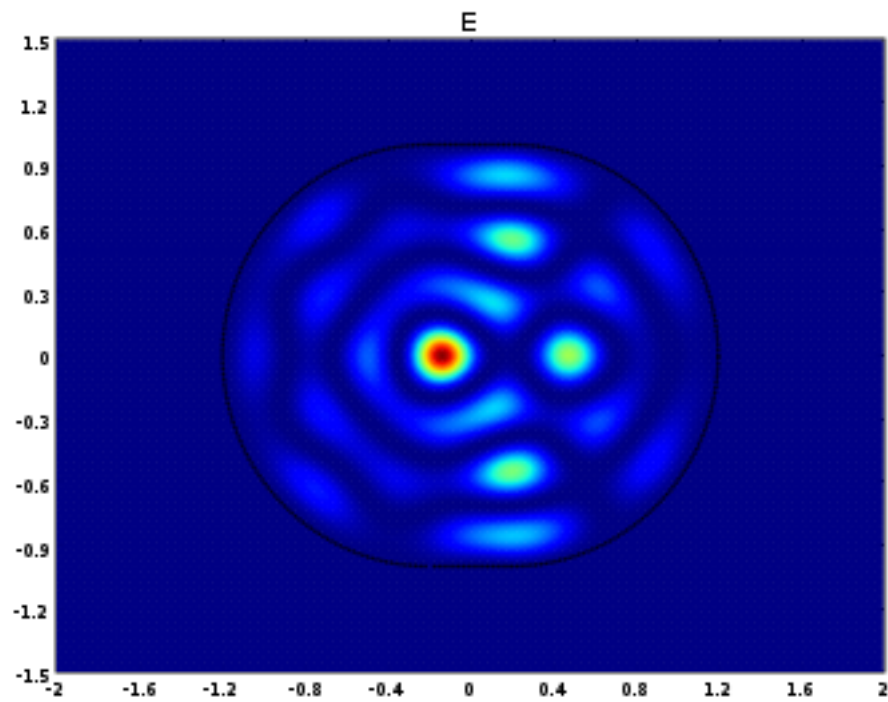


Figure 7: Eigenstate E, in the middle of the crossing. This state seems to be a superposition of the crossing states.

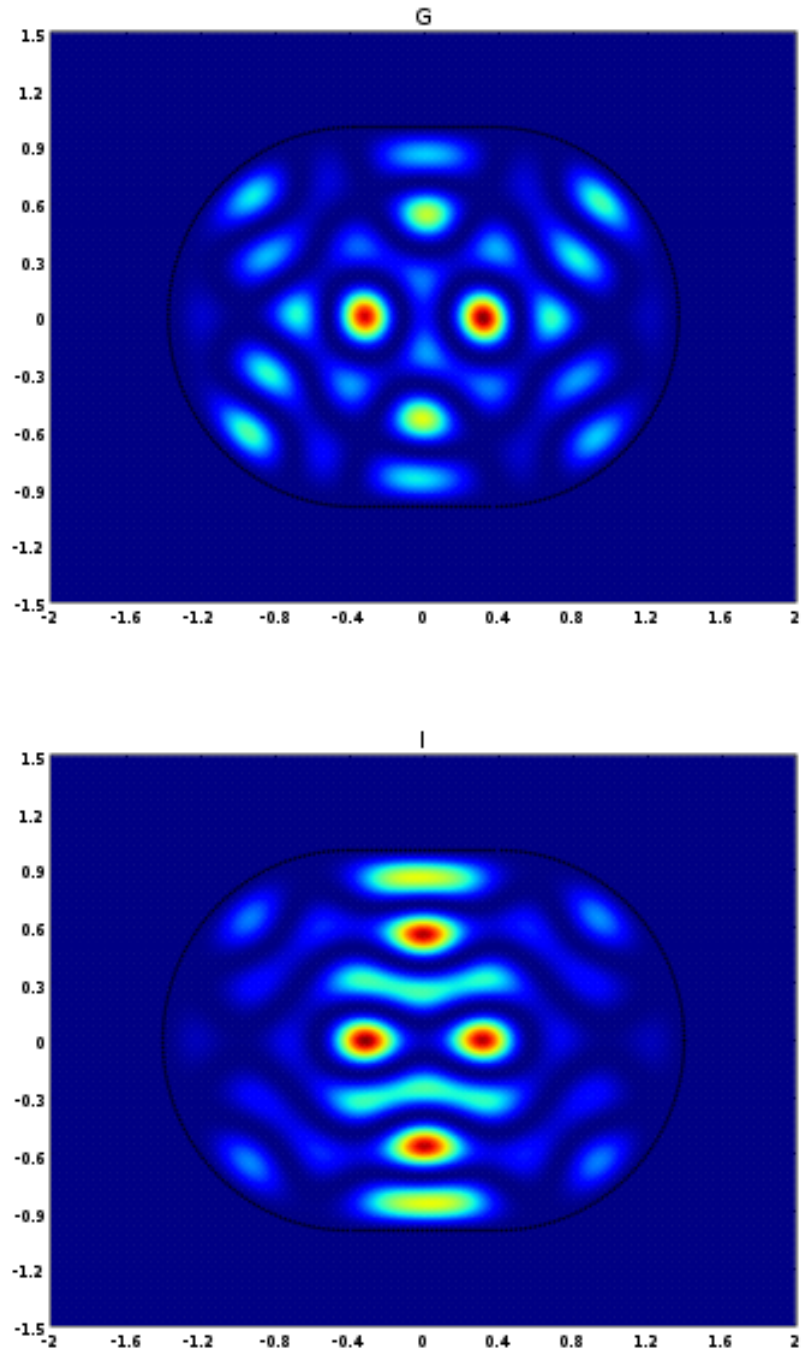


Figure 8: Eigenstates G and I before and after the avoided crossing of eigenvalues. The states spread out during the interference, and somehow becoming more chaotic.

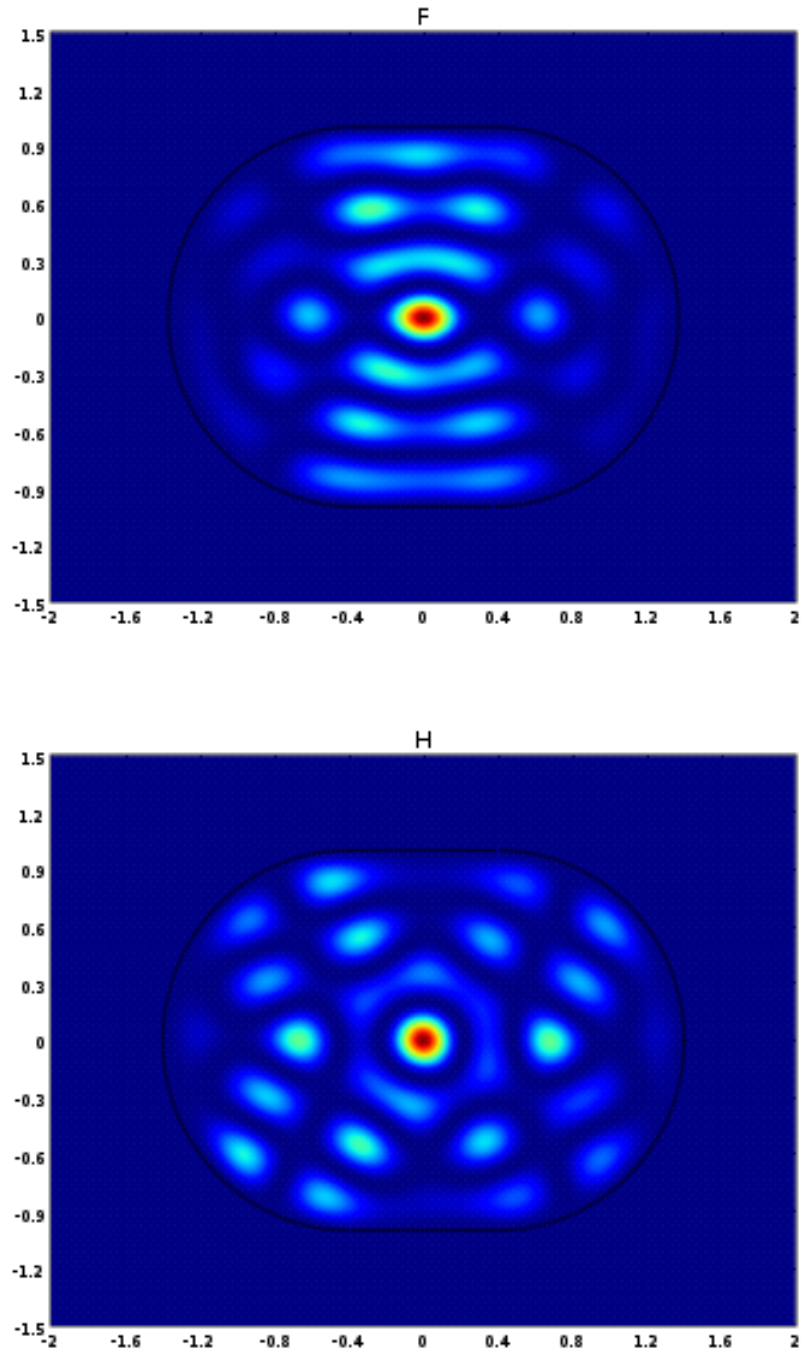


Figure 9: Eigenstates F and H before and after the avoided crossing of eigenvalues. The states spread out during the interference, and somehow becoming more chaotic.

Real plane waves (mathematically, sine and cosine functions) satisfy the Helmholtz equation. That is,

$$\nabla^2 \sin(k\vec{r} \cdot \vec{u}) = -k^2 \sin(k\vec{r} \cdot \vec{u})$$

and

$$\nabla^2 \cos(k\vec{r} \cdot \vec{u}) = -k^2 \cos(k\vec{r} \cdot \vec{u})$$

where  $|\vec{u}| = 1$ .

Also, the Laplacian operator is linear, so for functions  $\psi_1, \psi_2$ , and scalar  $c$ ,

$$\nabla^2 \psi_1 + \nabla^2 \psi_2 = \nabla^2 (\psi_1 + \psi_2)$$

and

$$\nabla^2 c\psi_1 = c\nabla^2 \psi_1$$

and thus if  $\psi_1$  and  $\psi_2$  satisfy the Helmholtz equation for the same  $k^2$ , then so does  $c\psi_1 + d\psi_2$ , for scalars  $c$  and  $d$ . This suggests a method for searching for a solution to the Helmholtz equation for a given  $k$ . We choose a basis consisting of sine and cosine functions for evenly spaced  $n$  in the range  $[0, 2\pi)$ , and then choose coefficients for them which minimize their sum on the boundary. Specifically, for fixed  $N, k$ , we choose coefficients  $x_n$  to create a function

$$\psi(\vec{r}) = \sum_{n=0}^{2N-1} x_n \phi_n(\vec{r})$$

where the basis functions  $\phi_n$  are defined by

$$\phi_n = \begin{cases} \cos(k\vec{r} \cdot \vec{u}_n) & \text{if } n < N \\ \sin(k\vec{r} \cdot \vec{u}_{n-N}) & \text{if } n \geq N \end{cases}$$

and the  $u_n$  are unit vectors with even angular spacing in  $[0, \pi)$ , so

$$u_n = \left( \cos\left(\frac{\pi n}{N}\right), \sin\left(\frac{\pi n}{N}\right) \right).$$

The coefficients  $x_n$  are chosen so that the integral

$$\int_{\Gamma} \psi(\vec{r})^2 d\vec{r} \tag{3}$$

is minimized nontrivially. The idea is that if we have enough basis functions, then whenever  $k^2$  is close to an eigenvalue, we can choose coefficients so that the

integral is near zero, and we can get very good approximations for the eigenvalues and functions.

This is a high level overview of the method used, so the details on how to actually do anything are left to section 3.2. Also, some pointers to other methods are given in section 3.5.

### 3.2 More detail

A discretized numerical approximation for 3 is given by

$$\frac{1}{M} \sum_{m=0}^{M-1} \psi(\vec{r}_m)^2$$

where the  $r_m$  are  $M$  evenly spaced points on the boundary  $\Gamma$ . If we write this out in terms of the basis components, we have

$$\frac{1}{M} \sum_{m=0}^{M-1} (x_1^2 \phi_1 \phi_1 + x_1 x_2 \phi_1 \phi_2 + \dots + x_{2N}^2 \phi_{2N} \phi_{2N}).$$

The sum is the quadratic form

$$x^T F x$$

where

$$F_{2N \times 2N} = \begin{bmatrix} \sum_{m=1}^M \phi_1 \phi_1(\vec{r}_m) & \sum_{m=1}^M \phi_1 \phi_2(\vec{r}_m) & \dots & \sum_{m=1}^M \phi_1 \phi_{2N}(\vec{r}_m) \\ \sum_{m=1}^M \phi_2 \phi_1(\vec{r}_m) & \sum_{m=1}^M \phi_2 \phi_2(\vec{r}_m) & \dots & \sum_{m=1}^M \phi_2 \phi_{2N}(\vec{r}_m) \\ \sum_{m=1}^M \phi_3 \phi_1(\vec{r}_m) & \sum_{m=1}^M \phi_3 \phi_2(\vec{r}_m) & \dots & \sum_{m=1}^M \phi_3 \phi_{2N}(\vec{r}_m) \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \sum_{m=1}^M \phi_{2N} \phi_1(\vec{r}_m) & \sum_{m=1}^M \phi_{2N} \phi_2(\vec{r}_m) & \dots & \sum_{m=1}^M \phi_{2N} \phi_{2N}(\vec{r}_m) \end{bmatrix}.$$

and  $F$  itself is equal to the product  $A^T A$ , where

$$A_{M \times 2N} = \begin{bmatrix} \phi_1(\vec{r}_1) & \phi_2(\vec{r}_1) & \dots & \dots & \phi_{2N}(\vec{r}_1) \\ \phi_1(\vec{r}_2) & \phi_2(\vec{r}_2) & \dots & \dots & \phi_{2N}(\vec{r}_2) \\ \phi_1(\vec{r}_3) & \phi_2(\vec{r}_3) & \dots & \dots & \phi_{2N}(\vec{r}_3) \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \phi_1(\vec{r}_m) & \phi_2(\vec{r}_m) & \dots & \dots & \phi_{2N}(\vec{r}_m) \end{bmatrix}$$

A basic method, then, is to fill  $A$  and find its singular values (which are the same as the eigenvalues of  $F$ .) The smallest singular value is the minimum of the quadratic form, and the corresponding singular vector will be the coefficients which minimize it.

If we do this for a range of  $k$ , we will find minima, which occur when  $k$  leads to a solution that satisfies our constraints.

Unfortunately, the matrix gives bad results when too many basis functions are added. Because the basis functions are so close together in our closed system,  $F$  becomes numerically singular when there are too many basis functions.

The solution is to introduce a normalization factor. Basically, we wish to minimize the boundary integral while keeping the interior integral constant. That is we add a new constraint of

$$\int_{\Omega} \psi^2(\vec{r}) d\vec{r} = 1.$$

where  $\Omega$  is the interior of  $\Gamma$ . As above, this leads to a quadratic form,

$$x^T G x = 1$$



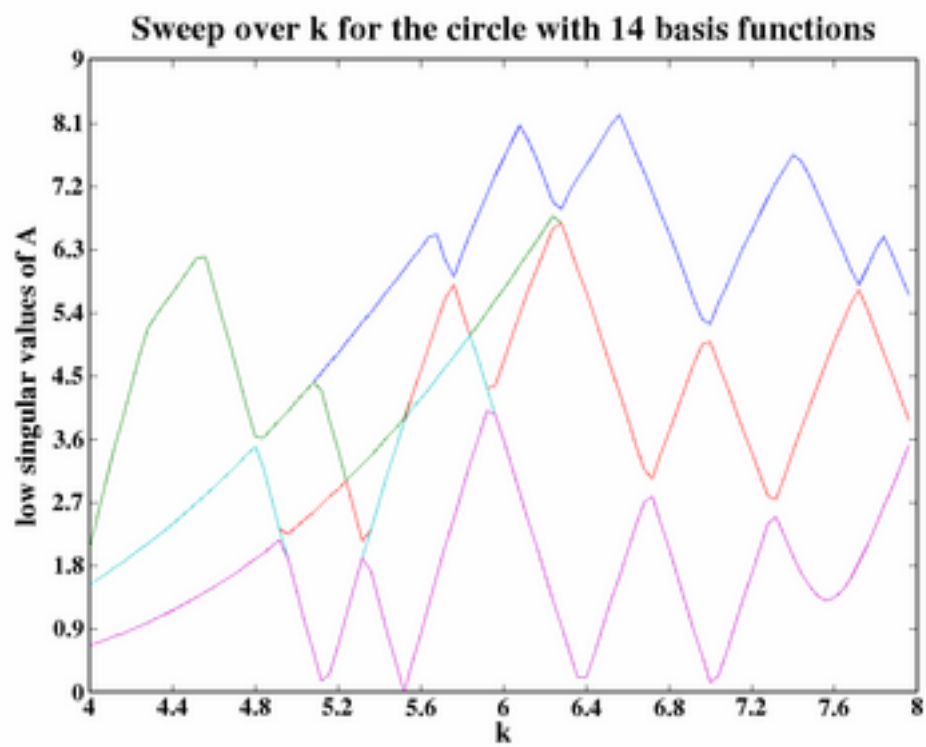


Figure 10: Sweep over  $k$  for the circle. Lower singular values are plotted, and the eigenvalues occur when the singular values are minimized.

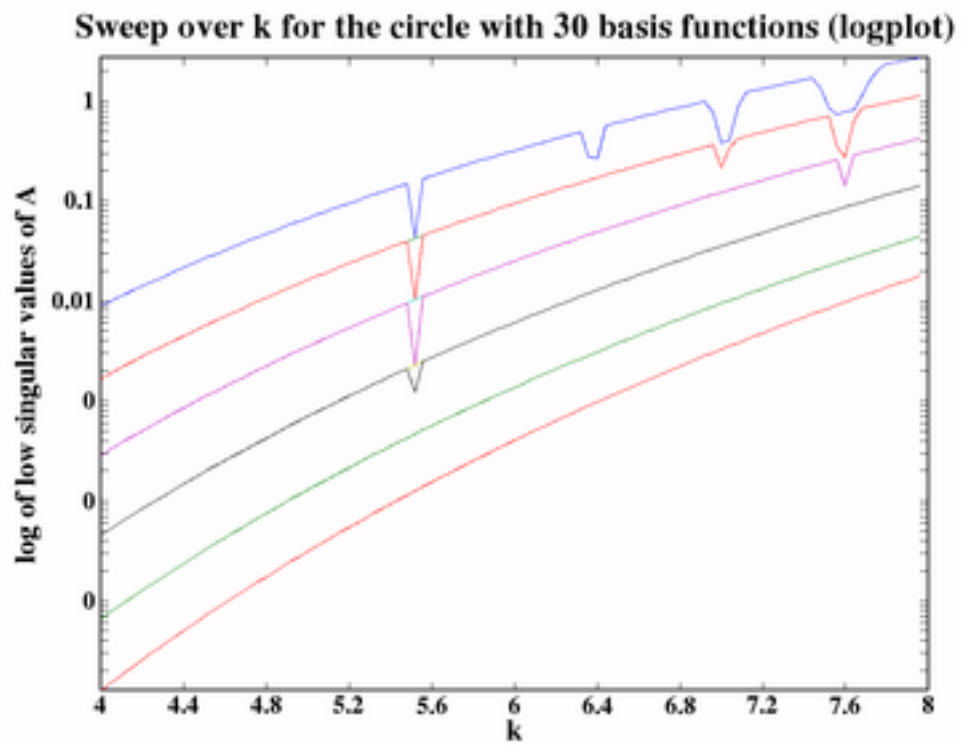


Figure 11: Sweep over the same  $k$  as in 3.2. Here more basis functions are added, however, so the matrix  $F$  is singular.

where  $G = B^T B$  and

$$B_{M_I \times 2N} = \begin{bmatrix} \phi_1(\vec{s}_1) & \phi_2(\vec{s}_1) & \dots & \dots & \phi_{2N}(\vec{s}_1) \\ \phi_1(\vec{s}_2) & \phi_2(\vec{s}_2) & \dots & \dots & \phi_{2N}(\vec{s}_2) \\ \phi_1(\vec{s}_3) & \phi_2(\vec{s}_3) & \dots & \dots & \phi_{2N}(\vec{s}_3) \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \phi_1(\vec{s}_{M_I}) & \phi_2(\vec{s}_{M_I}) & \dots & \dots & \phi_{2N}(\vec{s}_{M_I}) \end{bmatrix}$$

where the  $s_m$  are  $M_I$  points chosen uniformly at random from the interior of our system. Satisfying these constraints together leads to the generalized eigenvalue problem

$$G\vec{x} = \lambda F\vec{x} \quad (4)$$

where the minima is now given by the inverse maximum eigenvalue of (4)

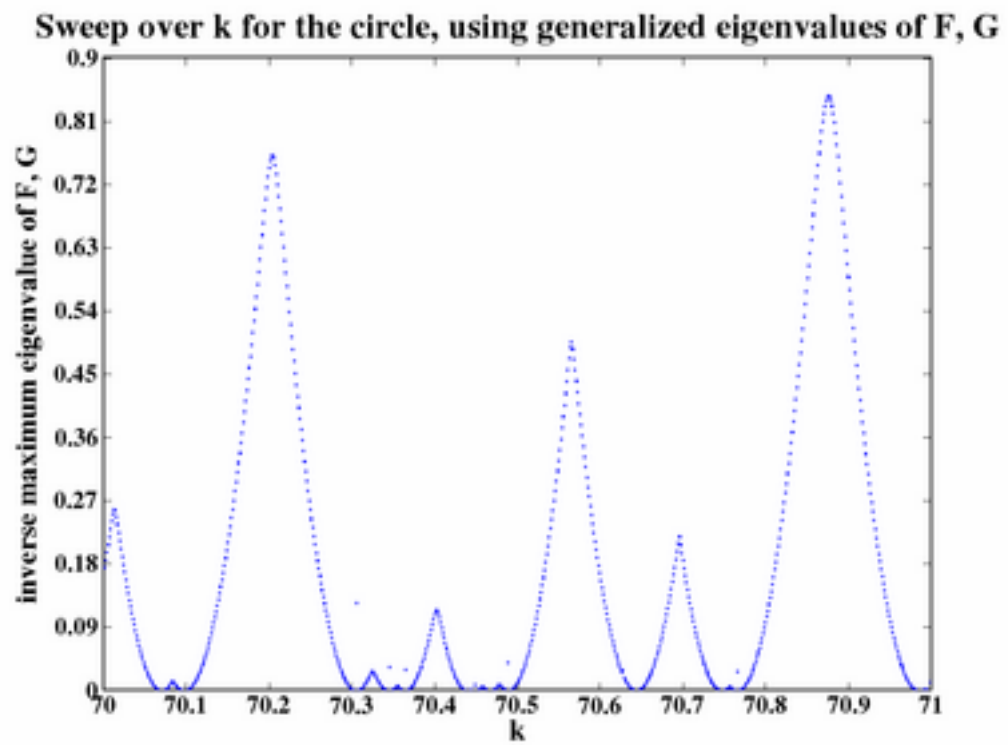


Figure 12: Using the generalized eigenvalue solution, we get much better results and can go to higher values of  $k$

- 3.3 Even more detail: sweep range and basis size**
- 3.4 Even more detail: truncating the generalized eigenvalue problem**
- 3.5 Better numerical methods**
- 4 Error analysis of the method**
- 5 More tables and pictures**
- 6 A note of thanks**
- 7 References**

## **References**

- [AB] A. Barnett, *Dissipation in Deforming Chaotic Billiards*, Doctoral Thesis.  
Available at <http://cims.nyu.edu/~barnett/>
- [TD] T. Driscoll, *Eigenmodes of Isopectral Drums*, Siam Rev. Vol 39, No. 1, pp. 1-17, March 1997
- [Kac] M. Kac, *Can one hear the shape of a drum?*, Amer. Math. Monthly, 73 Part II(1966) pp. 1 - 23