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Eigenfrequency Determination for Arbitrary Cross-Section Waveguides

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Abstract—In this paper, we outline the construction of Maple routines for the solution of the Helmholtz equation $\nabla^2\psi + k^2\psi = 0$ with Dirichlet boundary conditions in two-dimensional domains. By means of the symbolic manipulator, we are able to perform a numerical study of the eigenvalues for quantum billiards. © 2001 Elsevier Science Ltd. All rights reserved.

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1. INTRODUCTION

With the more widespread availability of PCs for the general public, in the very recent past many high-level languages have been developed, with the ultimate aim of sparing the unsophisticated end-user the burden of programming, in the opinion of some computer scientists. New environments like the world wide web have stimulated this development, to make full use of its resources. Consider, for instance, search engines and browsers, as well as tools for graphics and animations. On the other hand, heavy scientific computation has relied on the use of Fortran since its invention in the 1950s. Contrary to expectations, the use of this language does not die, in spite of the wider attention received in recent years by other more modern languages, e.g., C. This might very well be due to the heavy investment in computer codes, the result of decades of efforts by the early developers, through all the various releases of the language that appeared in the past decades. It is indeed probably easier to "update" a code to a new version of the very same basic language than to rewrite it completely from scratch. Moreover, until a few years ago at least, the lack of reliable numerical libraries of C routines was hindering the use of the latter language in scientific milieus. An example of this situation is given by Linpack and Eispack, the classic free on-line basic set of codes for linear algebra problems. It is only in recent years that the C version of these routines has become available, together with their newer version Lapack, which not only merges the two libraries, but also optimizes them both for vector and parallel supercomputers. Nowadays, reliable and sophisticated symbolic manipulators

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have also become available, whose power goes far beyond the pure ability of manipulating strings of characters. From the numerical point of view, they are able to perform computations with a variable wordlength, thus, allowing in a sense, arbitrarily high precision in the course of the calculations. Although computationally intensive, this is certainly a great benefit when one has to deal with ill-posed or badly conditioned problems, so that the accuracy of the result can be tailored to the needs of the scientist performing the calculation.

Among these evolved symbolic languages, Maple plays an important role, due both to the quality of the institution releasing it, and to its computational power and friendly user interface. In particular, it provides a huge set of special libraries for specific mathematical subdomains, which can be loaded at the user's request [1]. In linear algebra, these allow the use of basic codes for purposes ranging, e.g., from the symbolic evaluation of the determinant to the computation of Sylvester's matrix from two polynomials. Evidently, the power of such a tool can only be beneficial if used in computationally intensive environments. With the aid of these resources, it is possible to write very powerful programs by means of extremely short codes.

In this paper, we discuss an instance of an application of this symbolic manipulator to an advanced physics current research problem. Namely, we consider an eigenvalue problem arising in quantum physics and tackle it using a well-known technique, the boundary collocation method. The domain in which the governing equation is formulated is in a certain sense arbitrary, however. It does not allow separation of variables, which is the usual textbook example. By using an eigenfunction expansion with unknown coefficients for the solution and then imposing the boundary condition, we obtain a homogeneous system, the nontrivial solution of which gives the sought eigenvalues of the problem.

In this note, we analyze the method and implement the corresponding algorithm in Maple. In view of the versatility of Maple, and of the fact that it can work with arbitrary precision, we are able to keep under control numerical errors in a better way than by using a Fortran code.

The paper is organized as follows. In the next section, we present the physical problem, while the mathematical method is expounded in Section 3. The interpretation of the numerical results is discussed in Section 4. Section 5 is devoted to a detailed analysis of the strategy used for implementing the computations and to some more specific comments on the Maple programs. Finally, the last section contains an application to an important problem in electromagnetics, concerning the determination of the eigenfrequencies in waveguides.

2. THE PROBLEM

Various kinds of physical problems involve the solution of the 2D Helmholtz equation:

$$\nabla^2\psi + k^2\psi = 0, \tag{1}$$

plus boundary conditions, from the classical problem of the vibrating membrane, to electromagnetic propagation in waveguides. An important example in electromagnetic applications is treated in the last section. In recent years, however, the need for good and powerful numerical methods for solving (1) has increased because of new developments in quantum mechanics. From the mathematical point of view, the Helmholtz equation is identical to the Schroedinger equation of quantum mechanics. In this context, the eigenvalues ($E = k^2$) represent the allowed energies of a quantum particle, i.e., of an electron, confined to a two-dimensional region, usually called a *quantum billiard*, while the norms of the eigenfunctions give the probability density function of finding the particle, with a given energy, in a certain region of space. Usually, all textbook examples or problems deal with the very few cases in which one can separate the variables in (1). However, physicists have now recognized that, in quantum mechanics, the problem of separation of variables, or of integrability, is very subtle [2] and that the solutions of (1) present particular features if the variables cannot be separated. In addition, it should be self evident that most of

the *real* physical problems connected with (1) do not admit exact, i.e., analytical, solution, so that one has to use numerical methods.

Direct discretization of (1) requires a great computational effort. On the other hand, boundary methods eliminate one degree of freedom, since all information on the shape is given with the boundary, allowing a large reduction of CPU time. The most common method in the recent physical works is probably the boundary integral method (BIM) [3], which leads to an integral eigenvalue equation associated with (1). However, in order to avoid singularities due to the Green function, the authors are forced to introduce spurious eigenvalues.

3. THE METHOD

As in [4], our starting point is the fact that the solution in $\mathbf{R}^2$ of (1) is known. Only regular eigenfunctions at the origin are considered, the regularity condition being needed to ensure boundedness of the physical quantities in the problem. In polar coordinates, in particular, the former eigenfunctions are

$$\Psi(r,\theta) = J_m(kr)e^{im\theta},$$

where $J_m(x)$ denotes the integer Bessel function. Let us stress the fact that the energy eigenvalue ($E = k^2$) does not depend on m, so that the general eigenfunction with associated eigenvalue E is

$$\Psi(r,\theta) = \sum_m C_m J_m(kr)e^{im\theta}. \tag{2}$$

Let us now consider our two-dimensional region of boundary γ, and impose the Dirichlet boundary condition

$$\Psi(r,\theta) = 0, \qquad (r,\theta) \in \gamma. \tag{3}$$

This condition can be satisfied only for some discrete values of k which are the eigenvalues of (1). To carry out the discretization procedure, we select N points along the boundary. Replacing then the series by a finite sum and satisfying the boundary condition (3) at the nodes, we obtain

$$\Psi(r_j,\theta_j) = \sum_{m=1}^{M} J_m(kr_j)\left[C_m \cos m\theta + D_m \sin m\theta\right] + C_0 J_0(kr_j). \tag{4}$$

The choice $2M + 1 = N$ leads to a homogeneous system possessing nontrivial solutions if

$$\det M(k) = 0, \tag{5}$$

where the matrix $M(k)$ has the structure

$$\begin{pmatrix} J_0(kr_1) & J_1(kr_1)\cos\theta_1 & J_1(kr_1)\sin\theta_1 & \dots & J_M(kr_1)\cos M\theta_1 \\ \dots & \dots & \dots & \dots & \dots \\ J_0(kr_N) & J_1(kr_N)\cos\theta_N & J_1(kr_N)\sin\theta_N & \dots & J_M(kr_N)\cos M\theta_N \end{pmatrix}.$$

In our calculations, we have chosen the following domain:

$$r = r_0(1 + \alpha\cos 2\theta). \tag{6}$$

For $\alpha = 0$, this is the parametric equation of a circle of radius r_0 and area πr_0^2. If we give α a small value, we weakly deform the shape of the circle, but this suffices to lose separability (i.e., integrability) of the problem. In view of the symmetry of the domain, the eigenfunction and the spectrum can be partitioned into classes. For instance, in order to get the even-even eigenfunctions, we have to impose the $(+,+)$ symmetry conditions:

$$\Psi(r,\theta) = \Psi(r,-\theta) = \Psi(r,\theta-\pi). \tag{7}$$

This requirement selects the even value of m and only the cosine terms in the sum (4). It also avoids eigenvalue degeneracies due to the symmetry of the domain. The other symmetries used are the following ones:

$$
\begin{aligned}
(+,-): &\quad \Psi(r,\theta) = \Psi(r,-\theta) = -\Psi(r,\theta-\pi);\\
(-,+): &\quad \Psi(r,\theta) = -\Psi(r,-\theta) = \Psi(r,\theta-\pi);\\
(-,-): &\quad \Psi(r,\theta) = -\Psi(r,-\theta) = -\Psi(r,\theta-\pi).
\end{aligned}
$$

As an example, let us choose $\alpha = .2$ and $r_0 = 1$, fix a value for N, and define $f \equiv \det(M(k))$ as a Maple procedure. This can be easily done since Bessel functions are built in standard Maple libraries. We then decide the resolution for the sought eigenvalues, i.e., the stepsize with which the sweeps through a given interval are taken. Then f is evaluated at points of the interval whose distance is given by the chosen stepsize. Once a sign difference between two consecutive values of f is encountered, the so found abscissae are recorded, as starting values for the bisection method. We then start the bisection method in each marked subinterval, until a zero of $f(k)$ is found to within a given tolerance.

In order to validate our method, we have calculated a few eigenvalues of the rectangular billiard of dimensions a and b. The former are known exactly because the problem is separable. The exact eigenvalues are analytically evaluated by means of the formula $\pi\sqrt{(m/a)^2 + (n/b)^2}$, while the numerical eigenvalues are calculated using the proposed method with a matrix of dimension $N = 12$, resolution 0.1, and tolerance 0.01. In these calculations, the dimensions chosen for the rectangle are $a = 2$, $b = 1$. In Tables 1–4, we show the good agreement between the exact and the approximated eigenvalues related to each symmetry class. The results are quite satisfactory in spite of the small dimension of the matrix and in spite of the fact that, in our method, we use Bessel functions. The latter are indeed supposed to give the best results for domains not too much different from circles, but perform well enough even in the rectangular case.

Notice that in Tables 1–4, one eigenvalue is evaluated twice analytically, but it is not found numerically. This happens because the symmetry implies degeneracy, and the proposed method cannot find degenerate eigenvalues. Indeed, in such a case, the determinant changes sign twice, i.e., does not change sign for the degenerate eigenvalue. It is thus necessary to solve for all four symmetries in order to find all the required eigenvalues. Analytically, of course, there is no need to account for the symmetries, since the formula gives all the eigenvalues. However, we have listed the analytical values separately in each table to facilitate the comparison with the numerical values. The double values appearing among the analytical values are caused by the fact that they are degenerate. For example, 9.93 is a degenerate eigenvalue since it can be obtain-

Table 1. Eigenvalues from the $(-,-)$ symmetry of the rectangle, with $a = 2$, $b = 1$, $N = 12$.

k	Numerical	Analytical $= \pi\sqrt{\frac{m^2}{4} + n^2}$	m	n
1	6.478125000	6.476559175	1	2
2	7.853125000	7.853981635	3	2
3	10.05937500	10.05800404	5	2
		12.66416486	1	4
		12.66416486	7	2
4	13.42187500	13.42088970	3	4
5	14.82187500	14.81886291	5	4

Table 2. Eigenvalues from the $(-,+)$ symmetry of the rectangle, with $a = 2$, $b = 1$, $N = 12$.

k	Numerical	Analytical $= \pi\sqrt{\frac{m^2}{4} + n^2}$	m	n
1	7.021875000	7.024814734	2	2
2	8.884375000	8.885765876	4	2
3	11.32812500	11.32717340	6	2
4	12.95312500	12.95311835	2	4
		14.04962947	4	4
		14.04962947	8	2

Table 3. Eigenvalues from the $(+,-)$ symmetry of the rectangle, with $a = 2$, $b = 1$, $N = 12$.

k	Numerical	Analytical $= \pi\sqrt{\frac{m^2}{4} + n^2}$	m	n
1	4.440625000	4.442882938	2	1
2	7.021875000	7.024814734	4	1
		9.934588267	2	3
		9.934588267	6	1
3	11.32812500	11.32717340	4	3
4	12.95312500	12.95311835	8	1
5	13.32812500	13.32864881	6	3

Table 4. Eigenvalues from the $(+,+)$ symmetry of the rectangle, with $a = 2$, $b = 1$, $N = 12$.

k	Numerical	Analytical $= \pi\sqrt{\frac{m^2}{4} + n^2}$	m	n
1	3.509375000	3.512407367	1	1
2	5.665625000	5.663586700	3	1
3	8.459375000	8.458997100	5	1
4	9.553125000	9.554781040	1	3
5	10.53437500	10.53722210	3	3
6	11.43437500	11.43556988	7	1
7	12.26562500	12.26831151	5	3
		14.48202657	7	3
		14.48202657	9	1

ed from the formula for the pairs $(m,n) = (2,3)$, or alternatively, $(m,n) = (6,1)$, see Table 3. This degeneracy is not due to symmetries, so that on this particular eigenvalue, the method is not working correctly.

After this necessary check for consistency, we turned to our original problem over the domain given by (6). In this case, we applied the proposed method, searching for eigenvalues in the

interval $[0, 10]$ with a resolution of 0.1 and a tolerance of 0.01. In order to check the stability of our method for small values of k, we have calculated the zero of $f(k)$ fixing $N = 10, 15$. The results are shown in Tables 5–8.

Table 5. Numerically found eigenvalues for the $(-,-)$ symmetry in $(0, 10)$ for the billiard (6) with $\alpha = 0.2$, $r_0 = 1$.

k	$N = 10$	$N = 15$
1	4.305566407	4.305566865
2	6.204199220	6.204199083
3	8.141503907	8.141503685
4	8.385839844	9.385839859

Table 6. Numerically found eigenvalues for the $(-,+)$ symmetry in $(0, 10)$ for the billiard (6) with $\alpha = 0.2$, $r_0 = 1$.

k	$N = 10$	$N = 15$
1	5.177050782	5.177050978
2	7.275292970	7.275287740
3	8.886425722	8.886425782

Table 7. Numerically found eigenvalues for the $(+,-)$ symmetry in $(0, 10)$ for the billiard (6) with $\alpha = 0.2$, $r_0 = 1$.

k	$N = 10$	$N = 15$
1	3.440798728	3.440728332
2	6.344484829	6.344487879
3	7.040726372	7.040738294
4	7.352473738	7.352483683

Table 8. Numerically found eigenvalues for the $(+,+)$ symmetry in $(0, 10)$ for the billiard (6) with $\alpha = 0.2$, $r_0 = 1$.

k	$N = 10$	$N = 15$
1	2.472184737	2.482737373
2	4.643838377	4.646362688
3	6.218938383	6.212983747
4	7.270527272	7.283838661

4. DISCUSSION

In this note, we have presented a simple method based on a Maple program, to calculate the first eigenvalues of (1) over arbitrary domains, here given by (6). Two main features stand out from our analysis, one on the positive side, the other one somewhat negative.

The major advantage of this method is that it is widely independent of the shape of the domain chosen (as we have tested). An additional advantage of using Maple is that we can decide the precision of our calculation. This is indeed another major help for the calculations, since the values of f become very small as the dimension of the matrix increases. Of course, an increase in the precision of the calculation will entail a corresponding increase of CPU time.

On the other hand, we also noticed that the stability found in analyzing the low part of the spectrum, which can be observed by looking at Tables 5–8, is lost if we increase the dimension of the matrix. This fact could be related to the values of f approaching zero as mentioned above. This will indeed cause some problems, should one want to explore a larger part of the spectrum or determine eigenvalues far away from the origin.

5. COMMENTS ON THE IMPLEMENTATION

Here we present some more specific comments on the routines used for the above computations. We have used the symbolic manipulator Maple in its version Maple V.3, in a Windows NT environment, on a Pentium PC running at 300 MHz.

An immediate example of the power of Maple is given by the fact that the eigenfunction expansions have been implemented by using a call to the appropriate library for Bessel functions. The following strategy was used for tackling the problem. First, we wrote a routine for the calculation of the value of the determinant. It has been recursively used to determine the sign of the determinant function, saving in a file the intervals in which the determinant changed sign. Starting from the value .1, we increased the value of the independent variable by a .1 stepsize up to a value of about 15, iteratively recording the intervals containing the determinant sign changes. To check the work, we used different "approximation degrees", i.e., we first run the program with 15 terms in the eigenfunction expansion, then repeated the computations using 20 terms, to make sure no appreciable changes occurred in the intervals thus found.

We then constructed a routine for implementing the rootfinding bisection method. It is well known that this is a slow method, but it has the advantage of being reliable and in this situation robustness is the key issue. We sacrificed speed for the sake of accuracy. The output file of the first program has been used as input for the calls to the bisection method, giving the starting intervals in which to search for the zeros of the determinant function. The final tolerance used to terminate the iterations of bisection has been fixed to 10^{-5}, thus guaranteeing at least 4 digit accuracy. To check that we did not miss any eigenvalue, we then repeated the eigenvalues calculation, by determining once more the starting intervals for the bisection with the very same criteria exposed above, starting now from the value .05, still with increments of .1. Let us remark indeed that the procedure followed does not guarantee that all eigenvalues will be found. Actually, no such strategy exists, since in an arbitrarily small interval with no sign change, there could, in principle, always be an even number of zeros for the function under scrutiny. Since decreasing the stepsize would entail too many computations even in a fast environment, we chose to use a different starting point to double-check that the initial intervals for the bisection method were indeed the same, so that no other zeros were present at least in the interval $[0, 10]$. The occurrence of this fact would have indeed denoted that we missed some eigenvalues in the previous code runs. At this point, we were confident that the interval $[0, 10]$ had been thoroughly investigated. At times, we experienced some problems in the implementation, originating from the use of a student version of Maple, these being mainly due to lack of memory. But we were able to overcome them by splitting the runs of the code over smaller subtasks. Indeed, by saving the partial results to a file, we were able to suitably restart the code every time it crashed. Omitting the work already done, whose results were already saved, by restarting the program from the point where it crashed before, we have finally been able to complete the task.

6. APPLICATIONS

In this section, we outline the possible application of our calculation to the problem of electromagnetic propagation in waveguides. The interested reader can find further details in any standard book of electromagnetism. In the following, we will introduce physical constants and dimensions. In particular, notice the following change of notation. According to physics notation,

the symbol k which we are going to introduce is the wave number and should therefore not be confused with the adimensional parameter appearing in equation (1).

In a waveguide of constant cross-section, the transverse electric and magnetic fields are related according to

$$H_t = \pm\frac{1}{Z} e_3 \times E_t.$$

This relation is valid both for TM waves and TE waves. As it is well known, transverse fields are determined by the longitudinal ones according to

$$E_t = \pm\frac{ik}{\gamma^2}\nabla_t\psi, \quad \psi e^{\pm ikz} = E_z; \qquad \text{TM waves},$$

$$H_t = \pm\frac{ik}{\gamma^2}\nabla_t\psi, \quad \psi e^{\pm ikz} = H_z; \qquad \text{TE waves},$$

where $\gamma^2 = \mu\epsilon(\omega^2/c^2) - k^2$ and $\nabla_t = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$. The scalar function $\psi(x, y)$ satisfies the 2D equation

$$\nabla_t^2\psi + \gamma^2\psi = 0.$$

The boundary condition for the TM case is that $\psi = 0$ on ∂S, where S represents the cross-section of the waveguide. The last equation is an eigenvalue problem, i.e., there exists a spectrum of eigenvalues γ_n^2 and of associated eigenfunctions ψ_n. For each frequency ω, the wave number k is determined, for each value of n by $k_n^2 = \mu\epsilon(\omega^2/c^2) - \gamma_n^2$. If we define the cut-off frequency $\omega_n = c(\gamma_n/\sqrt{\mu\epsilon})$, the wave number k_n can be written as $(1/c)\sqrt{\mu\epsilon}\sqrt{\omega^2 - \omega_n^2}$. Let us notice that, for $\omega > \omega_n$, the wave number is real, while below the cut-off frequency, it is imaginary, giving rise to the so called evanescent waves. Thus, for each prescribed frequency, there is only a finite number of modes that can propagate. In this context then, the method presented in this work becomes useful to determine the eigenfrequencies of the waves propagating in the waveguide.

The application to the analysis of waveguides outlined in this section has to be regarded as a conceivable application of the method proposed in this paper. Technical generalizations can be developed towards the analysis of the eigenvalue problem related to the Schrödinger equation [5] (possibly related to control problems); to the analysis of hte linear wave equation [6]; and so on. The interested reader should hopefully find sufficient information to exploit the computational procedure proposed in this paper.

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