Doubly diabolical points in the spectra of pentagons

By Szymon Wojczyszyn and Lloyd N. Trefethen

U. of Michigan and Oxford U. Computing Laboratory

Eigenvalues of self-adjoint systems tend to avoid one another: double eigenvalues appear with codimension 2 and triple eigenvalues with codimension 5. Thus generically, it takes two real parameters for a double eigenvalue and five for a triple. By numerical computations based on newly developed algorithms, pentagonal planar "drums" are found with triple eigenvalues (to 8 digit accuracy) for the Laplace operator. This extends work of Berry and Wilkinson (1984) in which triangular drums were constructed with double eigenvalues. The new algorithms are applied to the Berry-Wilkinson problem too, verifying all their examples and finding many more.

Keywords: eigenvalue avoidance, level repulsion

1. Introduction

The phenomenon of eigenvalue avoidance has been known since von Neumann and Wigner (1929) and is illustrated on the cover of Peter Lax's book *Linear Algebra* (1996). In a family of real self-adjoint operators, one might expect eigenvalues to cross each other as a parameter is adjusted, but generically, eigenvalues avoid each other and it takes two parameters to achieve a crossing. The essential reason can be seen by considering the set of 2×2 real symmetric matrices. Matrices in this class are determined by three parameters, whereas the subset of matrices whose two eigenvalues are equal has dimension only one, since such a matrix must be a multiple of the identity. Thus the codimension of the set of degenerate matrices is 2. Similarly, in the 3×3 case, 6 parameters determine a real symmetric matrix while only one determines a matrix with $\lambda_1 = \lambda_2 = \lambda_3$. Thus the codimension is 5 and generically, one needs five real parameters to get a triple eigenvalue, or as we will also say, "double degeneracy". For the rigorous extension of these ideas from matrices to operators, see Teytel (1999).

Degenerate and nearly-degenerate eigenvalues have long been of interest to physicists, since the energy levels of atomic and molecular systems are governed by eigenvalues of Schrödinger operators. They are also of interest to number theorists, in view of the longstanding conjecture associated with Hilbert and Pólya that the Riemann Hypothesis may hold because, in some sense, the zeros of the zeta function are eigenvalues of a hermitian operator (rotated by 90°). The Hilbert–Pólya conjecture suggests that the higher zeros of the zeta function might be spaced with a probability distribution close to that of the eigenvalues of high-dimensional random hermitian matrices (Montgomery 1977, Katz & Sarnak 1999, Keating & Snaith 2000), and this idea has received powerful support from the numerical computation of hundreds of millions of these zeros by Odlyzko (2001), who found close quantitative agreement with predictions from random matrices. In these Schrödinger and zeta function applications, the operators are complex hermitian, and the eigenvalue avoidance effect is even stronger than in the real self-adjoint case (codimensions 3 and 8 for double and triple eigenvalues, respectively).

After matrices, perhaps the simplest example of a real self-adjoint eigenvalue problem is the Dirichlet Laplace problem for a connected region Ω in the x-y plane (Kuttler & Sigillito 1972, Trefethen & Betcke 2006),

$$-\Delta u = \lambda u, \qquad u = 0 \text{ on } \partial\Omega. \tag{1.1}$$

The eigenvalues are positive and infinite in number and can be labelled $\lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots$. Physically, this can be interpreted as an idealized "drum" involving a thin membrane, or the cross-section of a microwave cavity, or a 2D quantum mechanical well—"quantum billiards". Here our concern is not with physical implications but with the mathematical problem, can drums be found with degenerate eigenvalues? Certainly they can if Ω has geometric symmetries. For example, as one varies the aspect ratio of a rectangle there are many eigenvalue crossings, and likewise as one varies the aspect ratio of an isoceles triangle. Degeneracies in the absence of such symmetries, however, are rare. It is these *accidental degeneracies* that we seek.

Apart from the orientation and overall scale, which do not matter for the problem of degeneracies, a triangle is determined by two real parameters, a quadrilateral by four, a pentagon by six, and so on. Thus one may expect to find accidental degeneracies in certain symmetry-free triangles, and this is the task that Berry and Wilkinson addressed in a beautiful article published in 1984. Using a numerical method different from our own, they identified twelve nonsymmetric triangles with degenerate eigenvalues, which they calculated to about three digits of accuracy and also verified by a topological argument that we shall discuss leter. They comment,

> Finally we remark that degeneracies involving more than two levels can be made to occur by varying more parameters. . . . The simplest case is degeneracies of three levels, and typically requires five parameters. . . , so that numerical exploration of higher degeneracies is daunting.

What was dauting in 1984 has proved challenging but possible in 2007. In this paper we first sketch a numerical method for solving such problems accurately. Returning to the triangles of Berry and Wilkinson, we confirm all of their degeneracies, which we calculate to about 8 digit of accuracy, and find quite a few more. Then we look for triple eigenvalues in pentagons. This is an optimization problem on top of a highly nontrivial eigenvalue calculation. The search is successful and we present six examples of the form $\lambda_3 = \lambda_4 = \lambda_5$, $\lambda_6 = \lambda_7 = \lambda_8$ (three times), and $\lambda_7 = \lambda_8 = \lambda_9$ (twice). We do not have a proof that these degeneracies are genuine, but we discuss our reasons for confidence in these examples.

2. Numerical methods

There are two main numerical issues for these computations: determining the Laplace eigenvalues of a specified polygon; and performing optimization in the family of polygons to find examples where the eigenvalues are degenerate.

Given a polygon P, we find its lower eigenvalues by a variant of the *method of particular solutions*. The original method of this kind, capable of treating simple

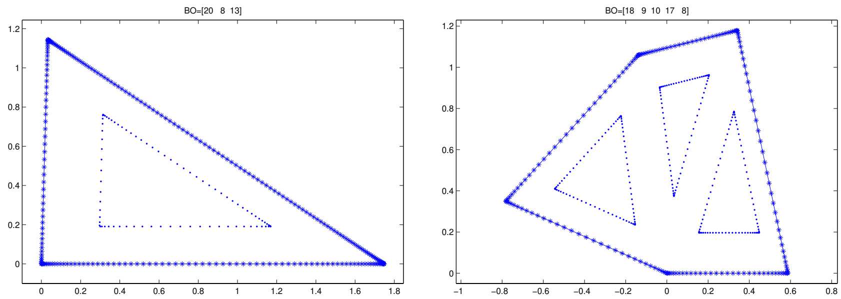

Figure 1. Illustration of boundary and interior points used to discretize a triangle and a pentagon. The numerical method permits these points to be more or less arbitrary so long as there are plenty of them. [Need to change color to black, and delete labels.]

polygons, was introduced by Fox, Henrici & Moler (1967). More accurate and robust variations have been introduced in the past few years (Barnett 2000, Betcke and Trefethen 2005, Betcke 2005, Betcke 2007), and it is these that we follow. We only sketch the method here; full details are given in (Wojczyszyn 2007).

The method is based on the fact that for any $\lambda > 0$ and positive integer k, the Fourier–Bessel function

$$u(r,\theta) = J_{\alpha k}(\sqrt{\lambda}\, r)\sin(\alpha k\theta)$$

is an eigenfunction of (1.1) in the region Ω consisting of an infinite wedge of angle π/α. The fact that λ is arbitrary reflects the fact that Ω is unbounded, with a continuous spectrum. For a polygon Ω with d vertices, we now approximate eigenfunctions by sums of the form

$$u(r,\theta) = \sum_{j=1}^{d}\sum_{k=1}^{N_j} c_{j,k} J_{\alpha_j k}(\sqrt{\lambda}\, r)\sin(\alpha_j k\theta).$$

The unknowns are λ and the expansion coefficients $\{c_{j,k}\}$, which must be found so that u is nearly zero on the boundary but nonzero in the interior. For this calculation the boundary of the polygon is discretized by a few hundred points, and a similar number of points in the interior is selected in an arbitrary fashion so long as it depends smoothly on the vertices of the polygon as they are varied (Figure 1). For a given value of λ, the functions $J_{\alpha_j k}(\sqrt{\lambda}\, r)\sin(\alpha_j k\theta)$ are then sampled at all of these points an a set of coefficients $\{c_{j,k}\}$ to minimize the ratio of a boundary norm divided by an interior norm are determined by a solving an appropriate generalized singular value decomposition (GSVD) problem. Then λ is varied to find values where this ratio is zero.

[Give a pseudocode summary of the method, analogous to SW's pp. 21–22.]

3. Triangles

We now present our results for triangles, in extension of Berry and Wilkinson (1984).

We parameterize a triangle by an angle α and a side length ratio (without loss of generality) $d > 1$, as shown in Figure 2. The overall scale factor s is then

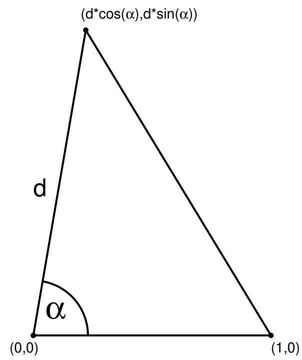

Figure 2. Parameterization of a triangle by the angle α and the length d. The scalar s is adjusted to make the area $(4\pi)^{-1/2}$. [Need to change labels to put s on one side and ds on the other, and delete labels on vertices.]

adjusted so that the area is $(4\pi)^{-1/2}$. We are looking for a double eigenvalue, so the optimization problem takes the form

$$\min_{\alpha,d} \min_{a\le\lambda\le b} \sigma_2(\lambda;\alpha,d)$$

with $[a,b]$ representing the interval in which eigenvalues are sought. Berry and Wilkinson took $[a,b]=[0,72\pi]$. Since there do not appear to be any degeneracies with $\lambda<100$, we took $[a,b]=[100,400]$.

All together, we found 145 accidental degeneracies. These are listed in the Appendix with parameters reported both in α,d form an also in the different X,Y form used by Berry and Wilkinson (which we do not describe). We believe this represents most if not all of the degeneracies in the range of λ investigated. [Is this right?] Berry and Wilkinson found 12 accidental degeneracies in $[0,72\pi]$. In this interval we found all of their degeneracies, and eight more besides, giving 20 in total, which we also find to many more digits of accuracy. We confirm the result of Berry and Wilkinson that the lowest degenerate eigenvalue in this normalization appears to be one with $\lambda_6=\lambda_7\approx 123.056919$, one of two examples we have found with $\lambda_6=\lambda_7$. There is also a single example with $\lambda_5=\lambda_6$, but the value of λ in question is slightly higher. There do not appear to be any triangle degeneracies with $\lambda_2=\lambda_3$, $\lambda_3=\lambda_4$, or $\lambda_4=\lambda_5$.

4. Pentagons

Apart from scale and orientation, a pentagon is determined by six parameters. Our choice is three angles $\alpha_1,\alpha_2,\alpha_3$ and three side length ratios d_1,d_2,d_3, as indicated in Figure 7. As with the triangles, once these parameters are set, the pentagon is scaled uniformly so that its area is $(4\pi)^{-1/2}$. We have made no attempt to search this six-dimensional space exhaustively, but have contented ourselves with finding some examples of pentagons with triple eigenvalues.

In this article we report six such examples, which are, so far as we know, the first examples of systems of this kind with accidental double degeneracies. The

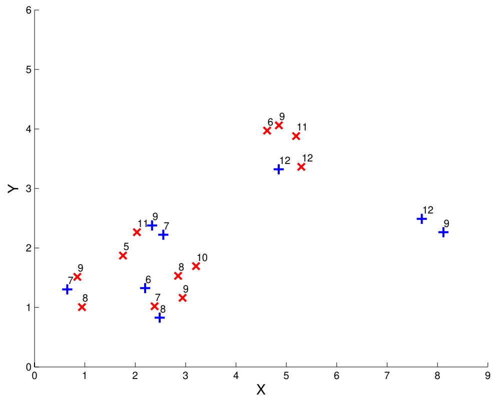

Figure 3. Locations in parameter space of the lowest 20 triangle degeneracies we have found, all lying in the range $[0, 72\pi]$. The 12 original degeneracies found by Berry and Wilkinson are marked by crosses, and the 8 new ones by plus signs. The number next to each mark shows which levels are crossing. [Need to redraw this in α, d parameters.]

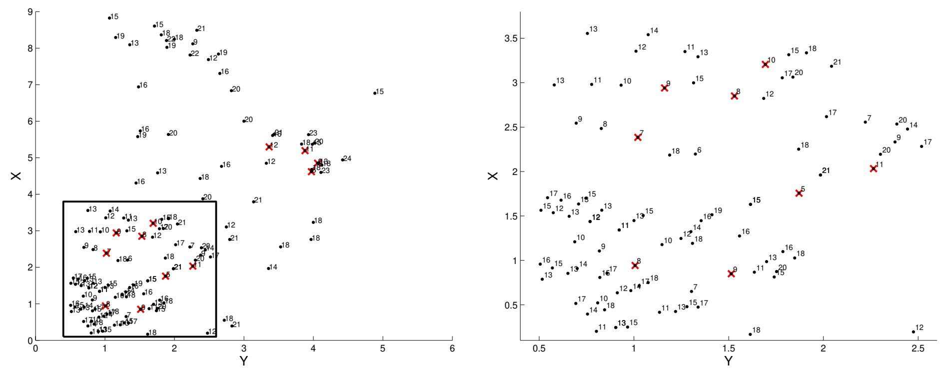

Figure 4. A larger plot showing all 145 triangle degeneracies we have found. On the right, a zoom of the portion of the figure on the left marked by a rectangle. [Need to redraw this in α, d parameters.]

calculation involved the following minimization:

$$\min_{\alpha_1,\alpha_2,\alpha_3,d_1,d_2,d_3} \min_{a\leq\lambda\leq b} \sigma_3(\lambda; \{\alpha_j\}, \{d_j\})$$

Figure 8 shows the first of our examples. Here the double degeneracy is of the form $\lambda_3 = \lambda_4 = \lambda_5$. Figure 9 shows one of the examples we have found with $\lambda_6 = \lambda_7 = \lambda_8$. Figures 10 and 11 show two examples with $\lambda_7 = \lambda_8 = \lambda_9$, one convex and the other nonconvex.

Since pentagons are determined by six parameters, while only five are needed for a double degeneracy, these examples are presumably just samples from a one-dimensional manifold of doubly degenerate pentagons. It would be interesting to explore this set in detail, but we defer that project to the future as the computations are already quite challenging.

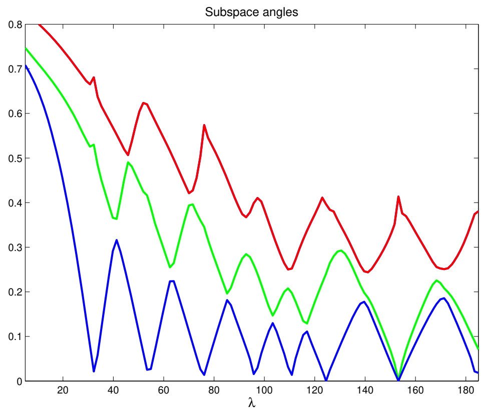

Figure 5. Subspace angles for the third triangle in Table xx, showing that the 7th eigenvalue is degenerate.

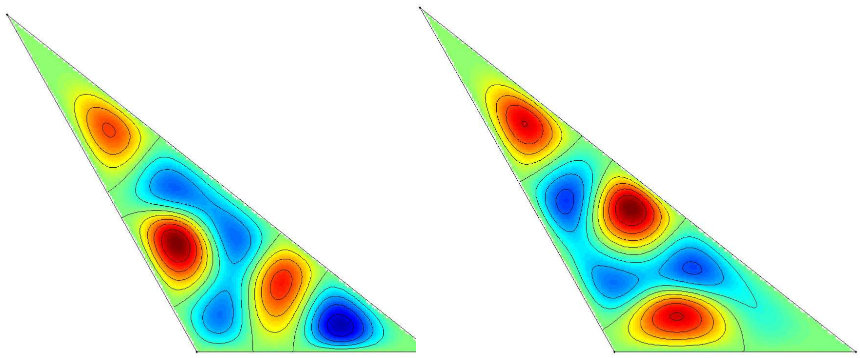

Figure 6. The degenerate eigenmodes of this triangle, with $\lambda_7 \approx \lambda_8 \approx 153.22399$.

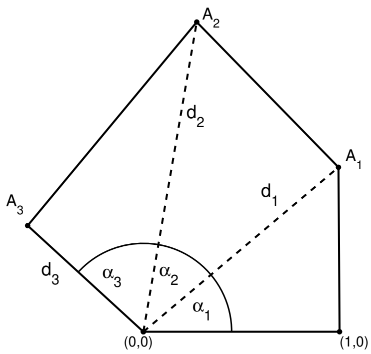

Figure 7. Parameters for a pentagon.

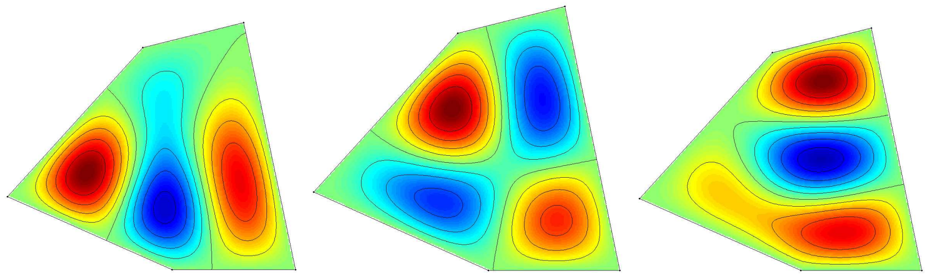

Figure 8. Doubly degenerate pentagon with $\lambda_3 = \lambda_4 = \lambda_5$.

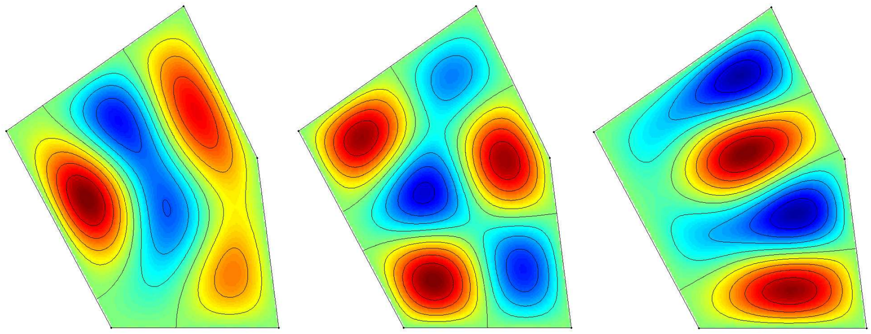

Figure 9. Doubly degenerate pentagon with $\lambda_6 = \lambda_7 = \lambda_8$.

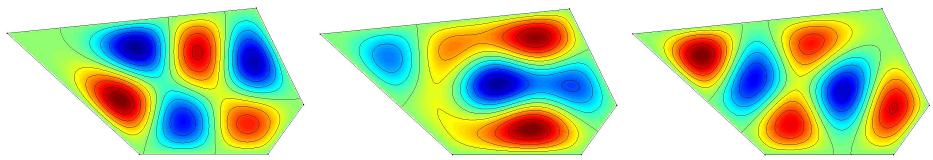

Figure 10. Doubly degenerate pentagon with $\lambda_7 = \lambda_8 = \lambda_9$.

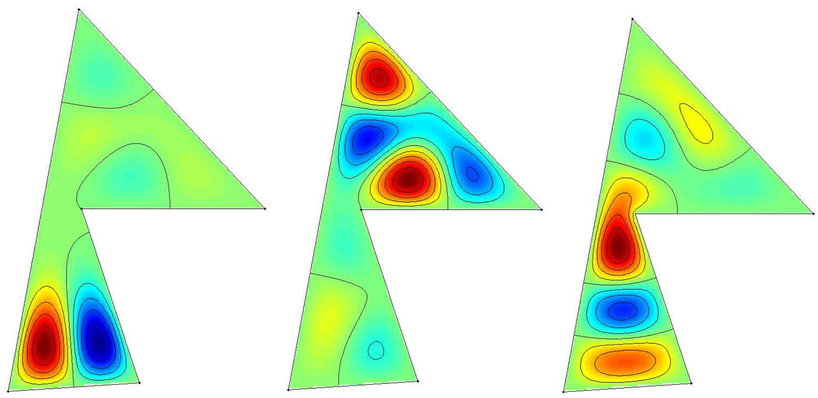

Figure 11. Another doubly degenerate pentagon with $\lambda_7 = \lambda_8 = \lambda_9$.

5. Verification of the degeneracies

?

6. Conclusion

We have presented what may be the first examples of generic self-adjoint systems with triple eigenvalues, or *accidental double degeneracies*. Along the way we have also confirmed and extended earlier results of Berry and Wilkinson (1984) on triangles with double eigenvalues.

We offer these results not because of any direct physical application, but because the underlying principles are important and we believe it is worthwhile to investigate them in this most concrete of contexts.

Appendix. Triangles with accidental degeneracies

References

A. H. Barnett 2000 *Dissipation in Deforming Chaotic Billiards.* PhD thesis, Dept. of Physics, Harvard University.

M. V. Berry and M. Wilkinson 1984 Diabolical points in the spectra of triangles. *Proc. Roy. Soc. Lond. A* **392**, 15–43.

T. Betcke 2005 *Numerical Computation of Eigenfunctions of Planar Regions.* D.Phil. thesis, Oxford University Computing Laboratory.

T. Betcke 2007 A GSVD formulation of a domain decomposition method for planar eigenvalue problems, *IMA J. Numer. Anal.* **27** 451–478.

T. Betcke and L. N. Trefethen 2005 Reviving the method of particular solutions. *SIAM Rev.* **47** 469–491.

L. Fox, P. Henrici, and C. B. Moler 1967 Approximations and bounds for eigenvalues of elliptic operators. *SIAM J. Numer. Anal.* **4** 89–102.

N. M. Katz and P. Sarnak 1999 *Random Matrices, Frobenius Eigenvalues, and Monodromy.* Amer. Math. Soc., Providence, RI.

J. P. Keating and N. C. Snaith 2000 Random matrix theory and $\zeta(1/2+it)$. *Comm. Math. Phys.* **214** 57–89.

J. R. Kuttler and V. G. Sigillito 1984 Eigenvalues of the Laplacian in two dimensions. *SIAM Rev.* **26**, 163–193.

P. Lax 1996 *Linear Algebra*, Wiley.

H. C. Longuet-Higgins 1975 The intersection of potential energy surfaces in polyatomic molecules. *Proc. Roy. Soc. Lond. A* **344**, 147–156.

H. L. Montgomery 1977 The pair correlation of zeros of the zeta function. Proc. Symp. Pure Math. **24** 181–193.

A. M. Odlyzko 2001 The 10^{22}-nd zero of the Riemann zeta function. Contemp. Math. **290** 139–144.

M. Teytel 1999 How rare are multiple eigenvalues? *Comm. Pure Appl. Math.* **52** 917–934.

L. N. Trefethen and T. Betcke 2006 Computed eigenmodes of planar regions. *Contemp. Math.* **412** (2006) 297–314.

K. Uhlenbeck 1976 Generic properties of eigenfunctions. *Amer. J. Math.* **98** 1059–1078.

J. von Neumann and E. Wigner 1929 Über das Verhalten von Eigenwerten bei adiabatischen Prozessen, *Z. Phys. A* **30** 467–470.

S. Wojczyszyn 2007 Eigenvalues of Pentagonal Drums. MSc thesis, Computing Laboratory, Oxford University. (Available from first author.)