Computation of Eigenfunctions on Various Domains

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Overview

Quantum Mechanics

- In classical mechanics, determining an object's location can be precise.
- In quantum mechanics, we can only know the probability that a particle can be located somewhere.
- We describe this probability density with a wave function.

$$P(r \in A) = \int_{r \in A} \Psi(r)\Psi^*(r)dr$$

- This wave function is similar to that of a violin string or drum membrane – the amplitude must be zero along the boundary of the domain.
- This property restricts the possible energy values to discrete values.[1]

() [1] Casey Blood. *A Primer on Quantum Mechanics and Its Interpretations*. Tech. rep. Rutgers University. URL: https://arxiv.org/ftp/arxiv/papers/1001/1001.3080.pdf.

Shrödinger Equation

For stationary particles, these wave functions have to obey certain rules by satisfying the time-independent Shrödinger Equation:

$$\hat{H}\Psi_n(r) = \Big[-\frac{\hbar^2}{2M}\Delta + \mathcal{V}(r) \Big]\Psi_n(r) = E_n\Psi_n(r)$$

Where $\mathcal{V}(r)$ is the potential energy. For a free stationary particle in some open domain $\mathscr{D}$, we have:

$$\mathcal{V}(r) = \begin{cases} 0 & r \in \mathscr{D} \\ \infty & r \notin \mathscr{D} \end{cases}$$

Shrödinger Equation

The time-independent Shrödinger Equation:

$$\hat{H}\Psi_n(r) = \Big[- \frac{\hbar^2}{2M}\Delta + \mathcal{V}(r)\Big]\Psi_n(r) = E_n\Psi_n(r)$$

is equivalent to the familiar Helmholtz equation with Dirichlet boundary conditions:

$$(\Delta + k^2)\Psi_n(r) = 0, \quad r \in \mathscr{D}$$

$$\Psi_n(r) = 0, \;\; r \in \partial\mathscr{D}$$

Obtaining the Helmholtz Equation from the Shrödinger Equation

$$\hat{H}\Psi_n(r) = \Big[-\frac{\hbar^2}{2M}\Delta + \mathcal{V}(r)\Big]\Psi_n(r) = E_n\Psi_n(r)$$

We set $\mathcal{V}(r) = 0$ in the domain. Giving us:

$$\hat{H}\Psi_n(r) = \Big[-\frac{\hbar^2}{2M}\Delta\Big]\Psi_n(r) = E_n\Psi_n(r) \implies$$

$$\frac{\hbar^2}{2M}\Delta\Psi_n(r) + E_n\Psi_n(r) = 0 \implies$$

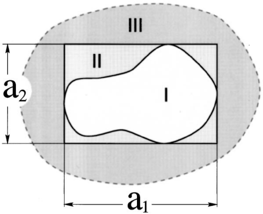
$$(\Delta + \frac{2ME_n}{\hbar^2})\Psi_n(r) = 0, \quad r \in \mathscr{D}$$

And we set $\frac{2ME_n}{\hbar^2} = k_n^2$

$$\implies (\Delta + k^2)\Psi_n(r) = 0, \quad r \in \mathscr{D}$$

Expansion Method for Solving the Helmholtz Equation[2]

- This method approximates Ψ_n by fitting the domain $\mathscr{D}$ in a rectangle.
- $\Psi_n(r) \approx 0$ outside of the domain $\mathscr{D}$.
- We do this by properly picking a large constant $\mathcal{V}_0$ which simulates setting $\mathcal{V}(r) = \infty$ in region II.



$$\widetilde{V}(r) = \begin{cases} 0 & r \in \mathrm{I} = \mathscr{D} \\ \mathcal{V}_0 & r \in \mathrm{II} \\ \infty & r \in \mathrm{III} \end{cases}$$

( ) [2] Ioan Kosztin David L. Kaufman and Klaus Schulten. *Expansion method for stationary states of quantum billiards*. American Journal of Physics 6. American Association of Physics Teachers, 1999. URL: https://aapt.scitation.org/doi/pdf/10.1119/1.19208?class=pdf9.

Expansion Method

The solutions for the Helmholtz equation in the rectangular domain:

$$(\Delta + k^2)\Psi_n(r) = 0, \quad r \in \mathscr{D}$$

are of the form:

$$\phi_m(r) = \phi_{m1,m2}(x_1, x_2) = \sqrt{\frac{2}{a_1}} \sin\left(\frac{\pi}{a_1} m_1 x_1\right) \sqrt{\frac{2}{a_2}} \sin\left(\frac{\pi}{a_2} m_2 x_2\right)$$

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And the solution should be a linear combination of these functions:

$$\Psi_n(r) = \sum_m c_m \phi_m(r)$$

With coefficients c_m.

Expansion Method

We determine the coefficients c_m by solving the eigenvalue equation:

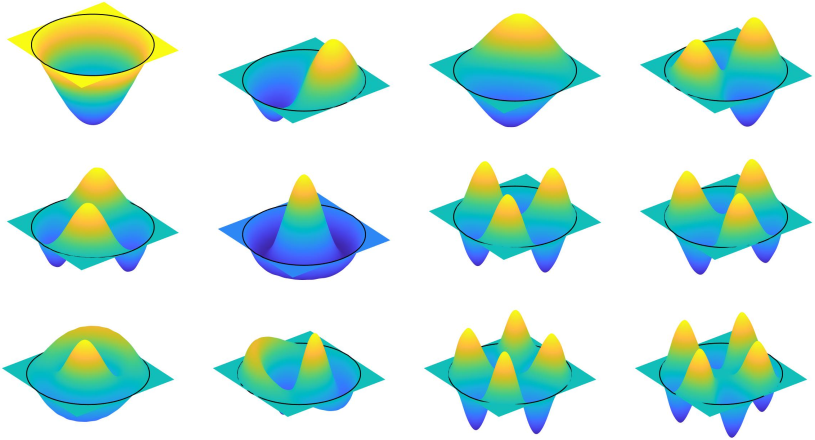
$$\sum_m (H_{nm} - E\delta_{nm})c_m = 0$$

and from the the Shrödinger Equation, we evaluate the Laplacian on our basis functions and obtain H:

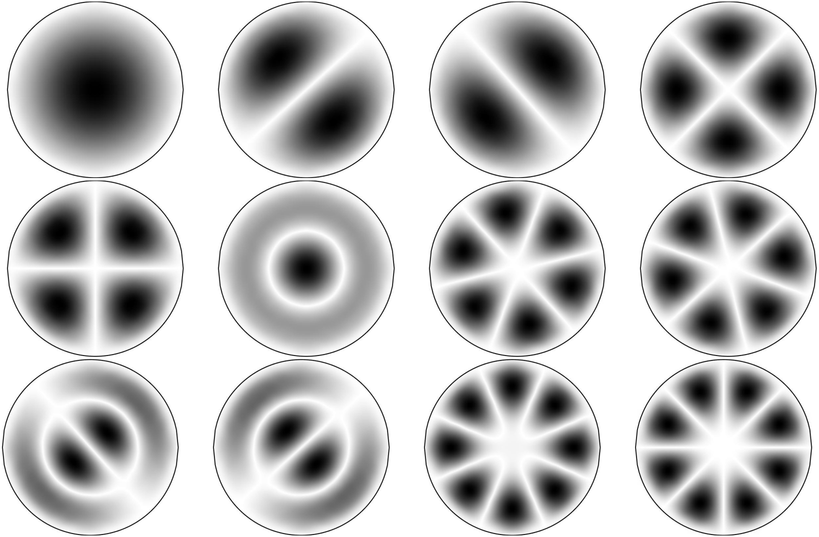
$$H_{nm} = \frac{\pi^2\hbar^2}{2M}\left[(\frac{m_1}{a_1})^2 + (\frac{m_2}{a_2})^2\right]\delta_{nm} + \mathcal{V}_0 \int_{\mathrm{II}} \phi_n(r)\phi_m(r)d^2r$$

We then obtain the eigenvectors and associated eigenvalues of H.

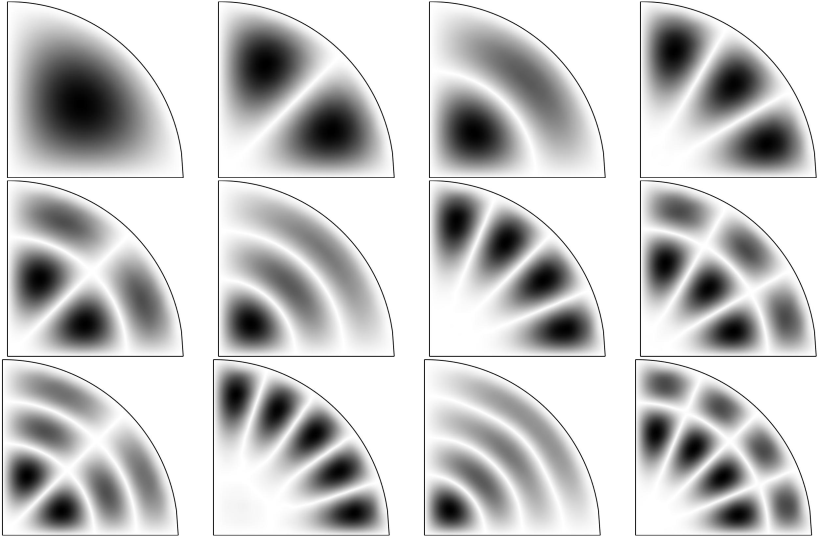
3D Plots for Circle Domain - First 12 Energy States



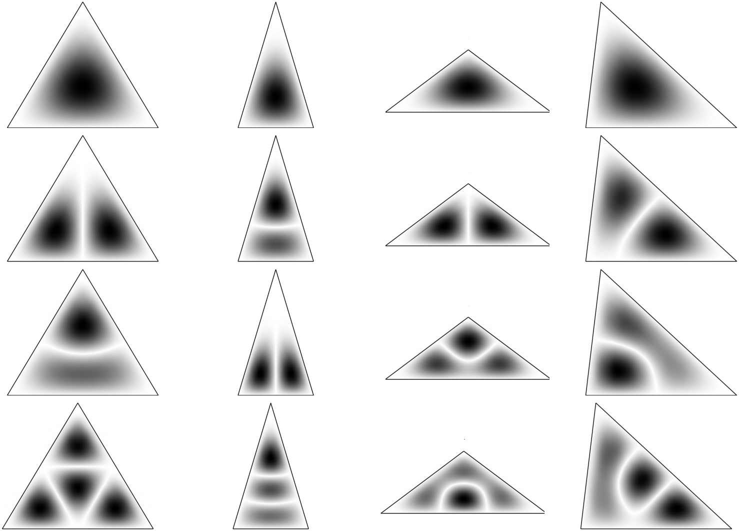
2D Density Plot for Circle Domain - First 12 Energy States



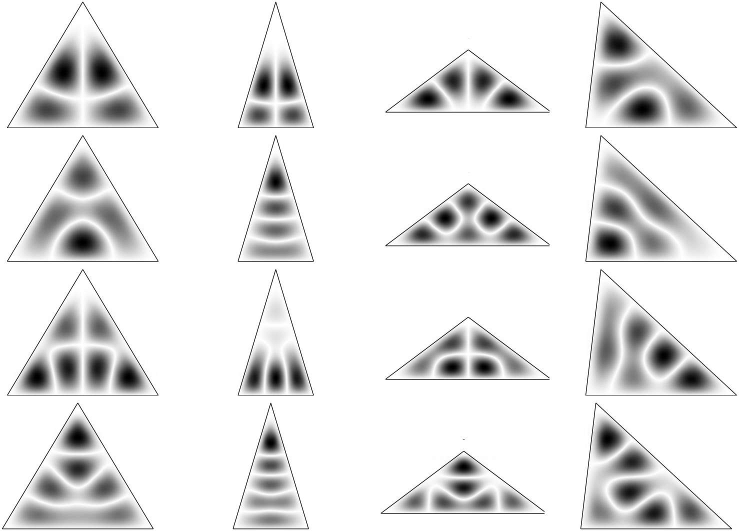
First 12 Energy States for Quarter-Circle Domain



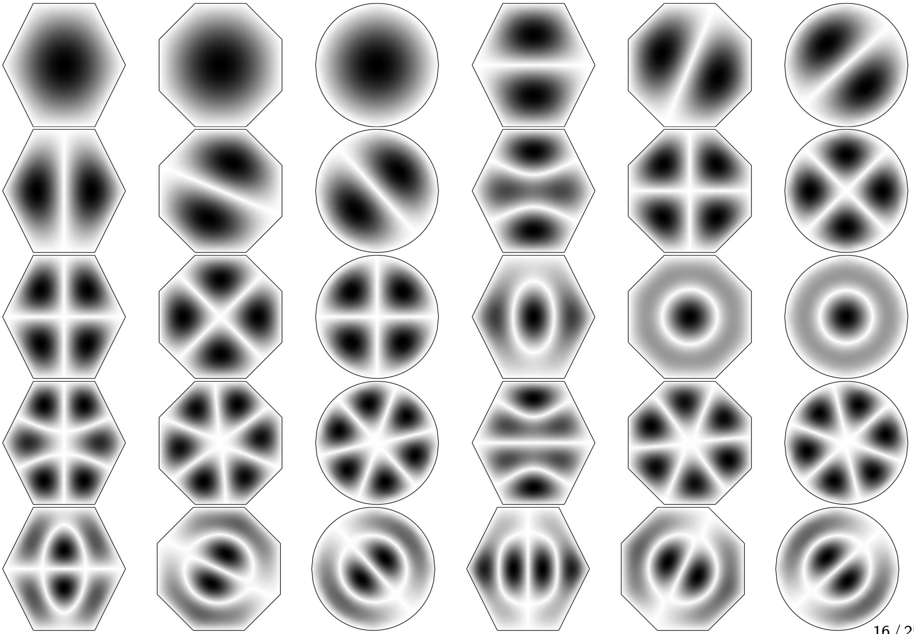
First 4 Energy States of Various Triangle Domains



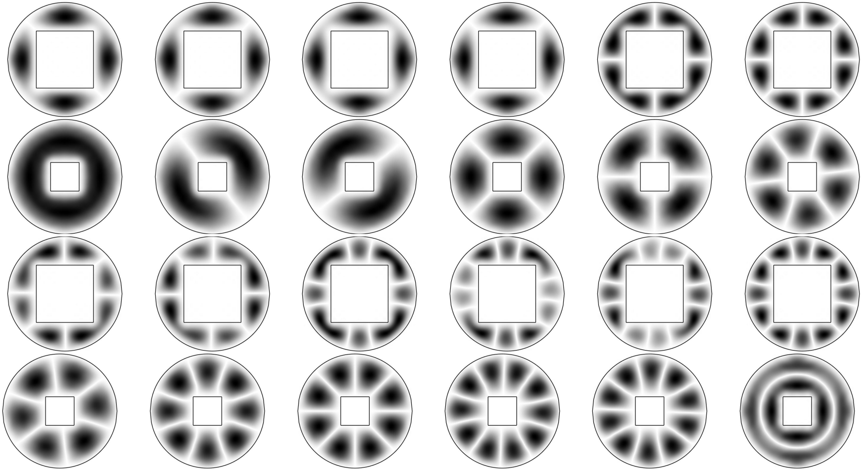
5th - 8th Energy States of Various Triangle Domains



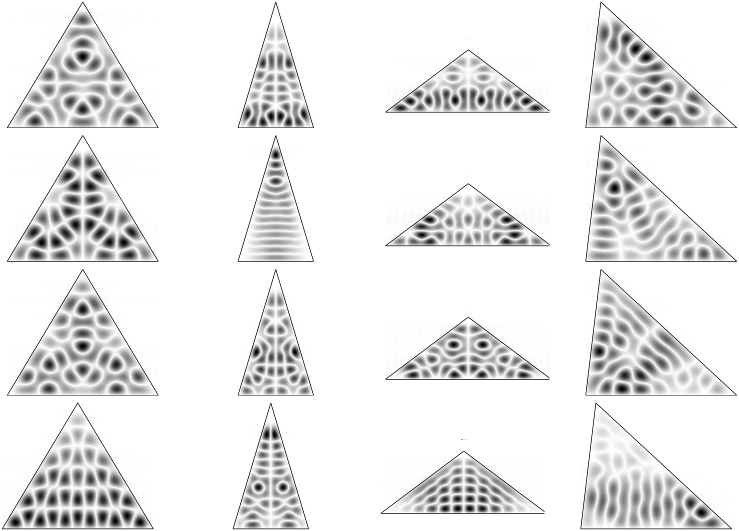
First 10 Energy States of Hex, Oct, and Circle Domains



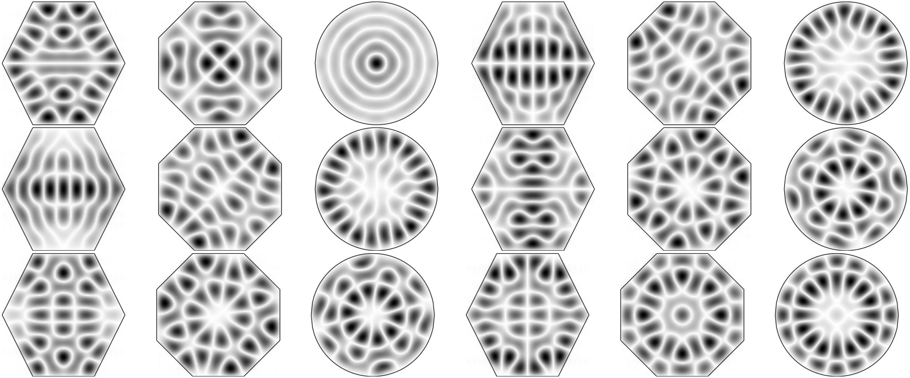
First 12 Energy States in Wide and Thin Ring Domains



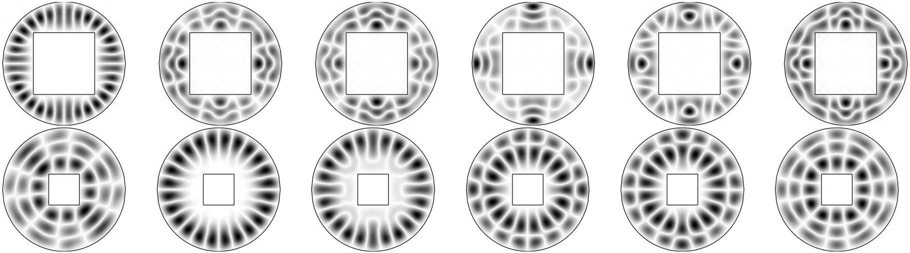
51st - 54th Energy States of Triangle Domains



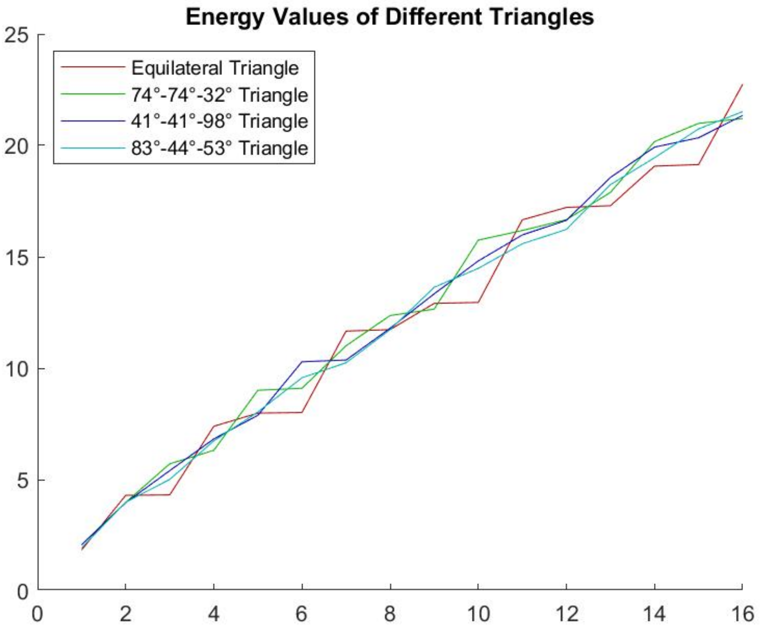
51st - 56th Energy States of Hexagon, Octagon, and Circle Domains



51st - 56th Energy States of Ring Domains



Energy Values



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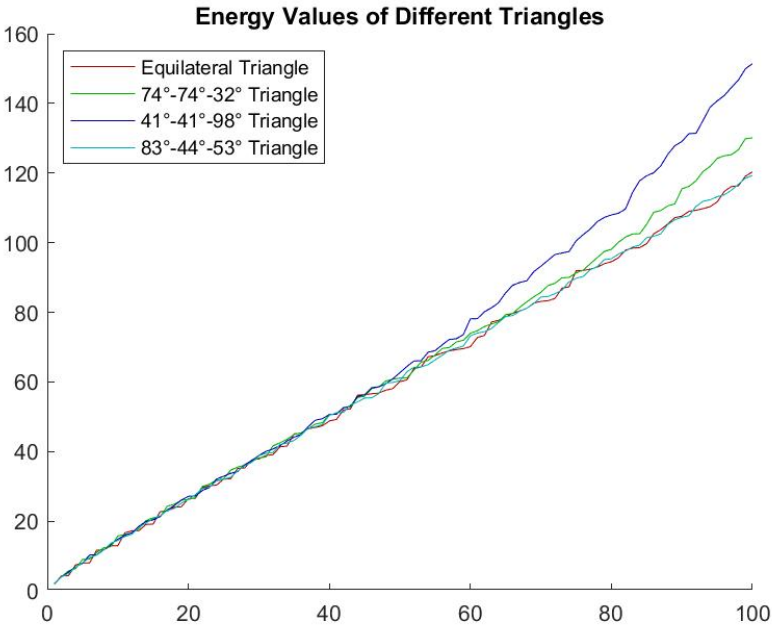

Further Research Possibilities

- Analyze bifurcation of eigenfunctions and phase transitions of different domains.[3]
- More spectral analysis of eigenstates through random matrix theory and possible correlation to the distribution of the zeroes of the Riemann Zeta function.[4][5]
- Possible inverse problems, such as determining the shape of the domain from the eigenvalues.[6]

() [3] Jonathan P. Keating Paul Bourgade. *Quantum chaos, random matrix theory, and the Riemann $\zeta-$ function*. Tech. rep. University of Bristol, 2010. URL: http://www.bourbaphy.fr/keating.pdf.

() [4] David L. Kaufman and Schulten, *Expansion method for stationary states of quantum billiards*.

() [5] Paul Bourgade, *Quantum chaos, random matrix theory, and the Riemann $\zeta-$ function*.

() [6] Mark Kac. *Can One Hear the Shape of a Drum?* The American Mathematical Monthly, Vol. 73, No. 4, Part 2: Papers in Analysis (Apr., 1966), pp. 1-23. Mathematical Association of America, 1966. URL: https://www.math.ucdavis.edu/~hunter/m207b/kac.pdf.

Citations

Blood, Casey. *A Primer on Quantum Mechanics and Its Interpretations*. Tech. rep. Rutgers University. URL: https://arxiv.org/ftp/arxiv/papers/1001/1001.3080.pdf.

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