From the 1D Schrödinger Infinite Well to Dirac-Weyl Graphene Flakes

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- The initial objective of this thesis was to study the spectrum of finite regions of twisted bilayer graphene (TBLG).
- In TBLG, a periodic structure emerges for commensurate angles, with the period growing as $\frac{1}{\sin\theta/2}$.
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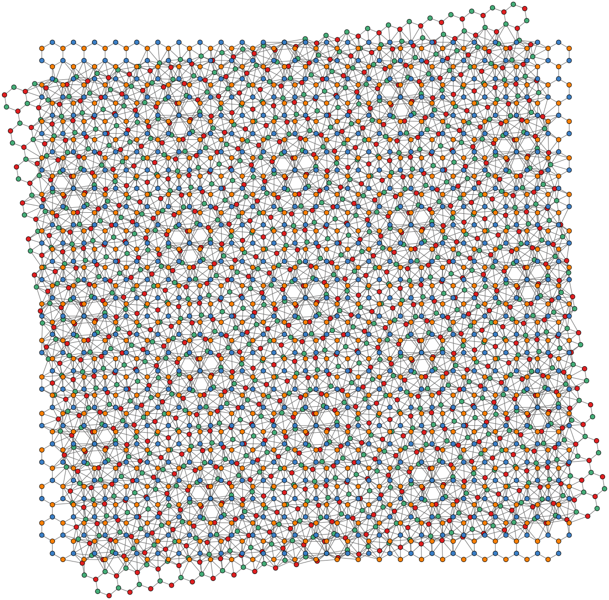
Motivation – TBLG



Separation of Variables

To solve partial differential equations, one usually assumes separation of variables. In the Schrödinger equation, this translates to

$$-\frac{\hbar^2}{2m}\nabla^2\Psi = E\Psi$$

$$\Psi\left(x,y\right) = f\left(x\right)g\left(y\right)$$

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Imposing Boundary Conditions

The polynomial method consists of creating a function that obeys boundary conditions,

$$\psi_0(x,y) = N_0 \prod_{s=1}^{n} \varphi_s\left(x,y\right),$$

where the different φ_s are the equations of the edges of the polygon:

$$y - mx - b = 0$$

The Hamiltonian matrix entries will the given by the following integral

$$H_{ij} = -\frac{\hbar^2}{2m}\iint_\Omega dA\ \psi_i^*\left(x,y\right)\nabla^2\psi_j\left(x,y\right)$$

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Defining the Complete Basis

The complete basis is defined by Gram-Schmidt orthogonalization

$$\psi_i(x,y) = N_i \left[f_i(x,y)\,\psi_0(x,y) - \sum_{j=0}^{i-1} \langle f_i(x,y)\,\psi_0(x,y)\,|\psi_j(x,y)\rangle \psi_j(x,y) \right],$$

defining generically

$$\langle g(x,y)\,|h(x,y)\rangle := \iint_\Omega dA\; g^\dagger(x,y)\,h(x,y)$$

Where $f_m(x,y)$ is a sorting of the $x^i y^j$-monomials as a list [Liew (1991)]

$$f_m(x,y) = \left\{1, x, y, xy, x^2, y^2, x^2y, xy^2, x^2y^2, x^3, y^3, x^3y, xy^3, (...)\right\}.$$

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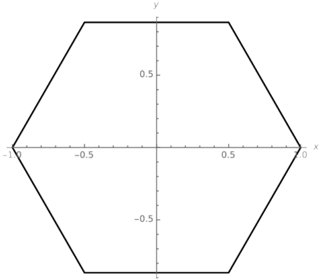
Hexagonal Infinite Potential Well

The fundamental function will now be a sixth order polynomial, defined in the same way as before

$$\Psi_0(x,y) = N_0 \prod_{s=1}^{6} (y - m_s x - b_s)$$

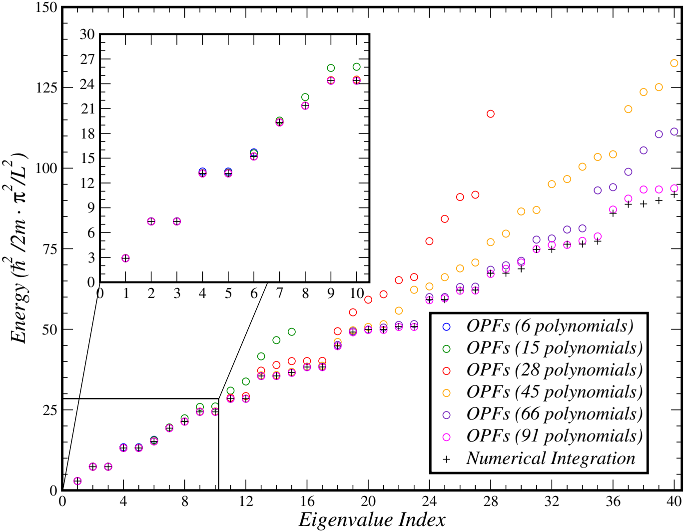
The integration region is defined as

$$\iint_A dxdy \rightarrow \int_{-\frac{\sqrt{3}}{2}}^{\frac{\sqrt{3}}{2}} dy \int_{-1+\frac{|y|}{\sqrt{3}}}^{1-\frac{|y|}{\sqrt{3}}} dx$$



Hexagonal Infinite Potential Well

The obtained eigenvalues for different basis sizes are as follows



Creating Spinors by Imposing Boundary Conditions

The Dirac-Weyl Hamiltonian is given by

$$\mathcal{H} = \hbar v_F \vec{\sigma} \cdot \vec{p}$$

The necessary condition to finding confined states of this equation is imposing zero normal probability current

$$\vec{j}_{\text{normal}} = v_F \Psi^\dagger \vec{\sigma}_{\text{normal}} \Psi = 0$$

Imposing this, we obtain the boundary condition for an edge at an α angle with the x-axis

$$\frac{\psi_B}{\psi_A} = t e^{i\alpha}, \;\; t \in \mathbb{R}$$

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1-Dimensional Toy-Model

Setting $t = 1$ is the equivalent [Berry and Mondragan (1987)] of changing the Hamiltonian as

$$\mathcal{H}_{\mathcal{K}} \to \mathcal{H}_{\mathcal{K}} + m\left(\vec{r}\right)\sigma_z, \qquad m\left(\vec{r}\right) = \begin{cases} 0 & \text{inside} \\ +\infty & \text{outside} \end{cases}$$

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A function that respects these boundary conditions in $y = \pm\frac{L}{2}$ is

$$\Psi_0\left(y\right) = N_0 \left[\begin{array}{c} 1 \\ -\frac{y}{L/2} \end{array} \right]$$

The valence-band initial function for $t = 1$ will be given by

$$\Phi_0 = \sigma_x \cdot \Psi_0^*$$

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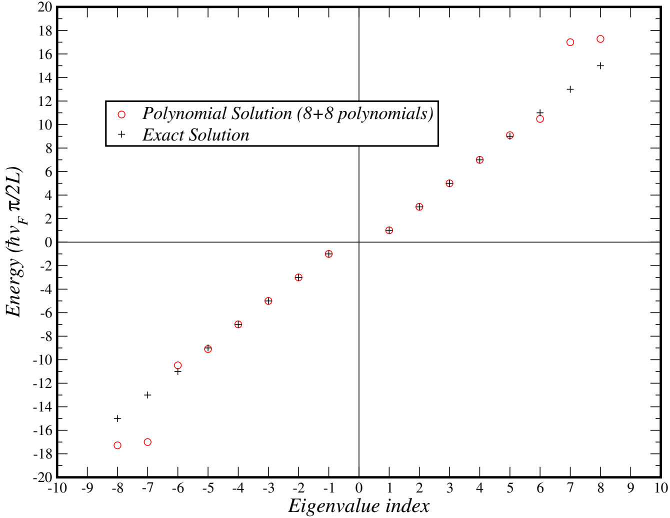
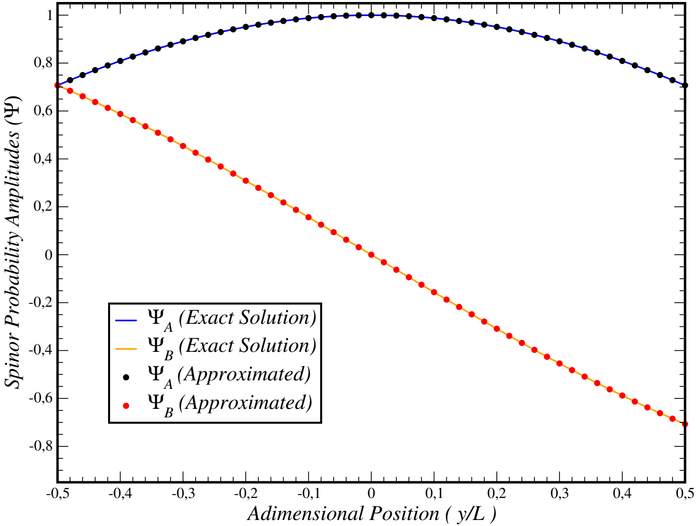
Choosing a basis size, the eigenvalues of the Hamiltonian are



1-Dimensional Toy-Model

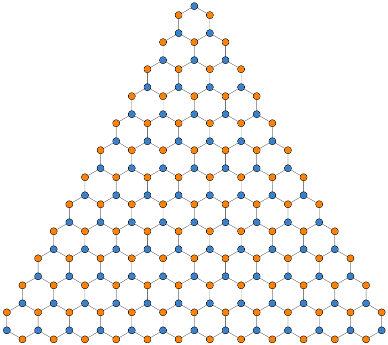
The first eigenfunction also matches perfectly:



Exact Solution by Gaddah

Gaddah considers the problem of the triangular graphene dot with φ_A terminations on all three edges [Gaddah (2018)].

Considering the system's innate C_{3v} symmetries, the author is able to find analytical expressions for both the eigenfunctions and the eigenvalues of the Dirac-Weyl Hamiltonian squared.



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The Hamiltonian for graphene near the Dirac point $\mathcal{K}$ is given by

$$\mathcal{H}_{\mathcal{K}} = \hbar v_F \vec{\sigma} \cdot \vec{p}$$

with boundary conditions $t = \infty$, or simply

$$\psi_A = 0, \qquad \left(\partial_x - i\partial_y\right) \psi_B = 0$$

The only state of exactly-zero energy one can write that obeys the necessary conditions is

$$\Psi\left(x, y\right) = \begin{bmatrix} 0 \\ \frac{2}{\sqrt[4]{3}L} \end{bmatrix}$$

This solution is not present in neither treatment, as it is the trivial solution in the sublattice that is being considered $\left(\psi_A\right)$.

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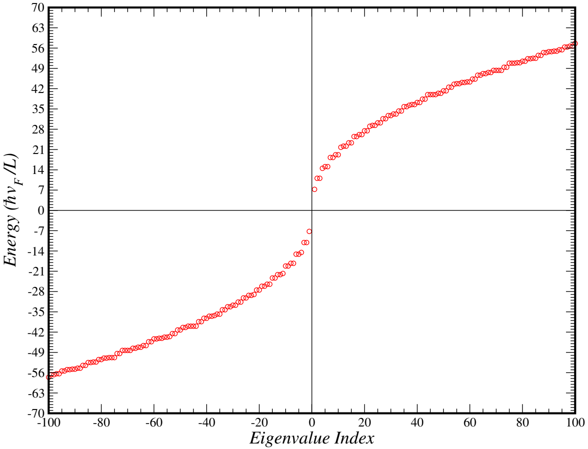
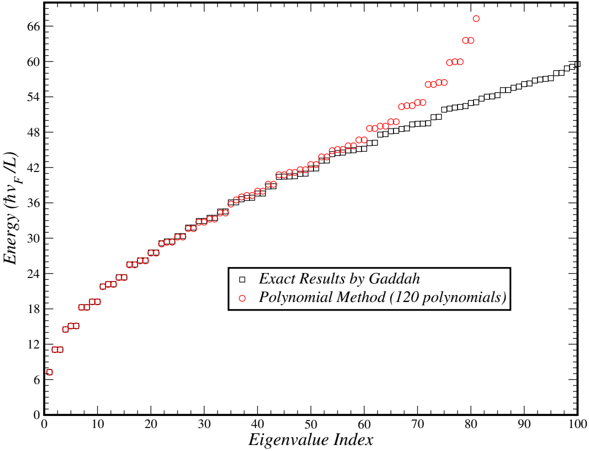
Transforming this problem into two identical Helmholtz problems, Gaddah obtains the spectrum with a gap of $2\sqrt{3}\frac{4\pi}{3L}\hbar v_F$:



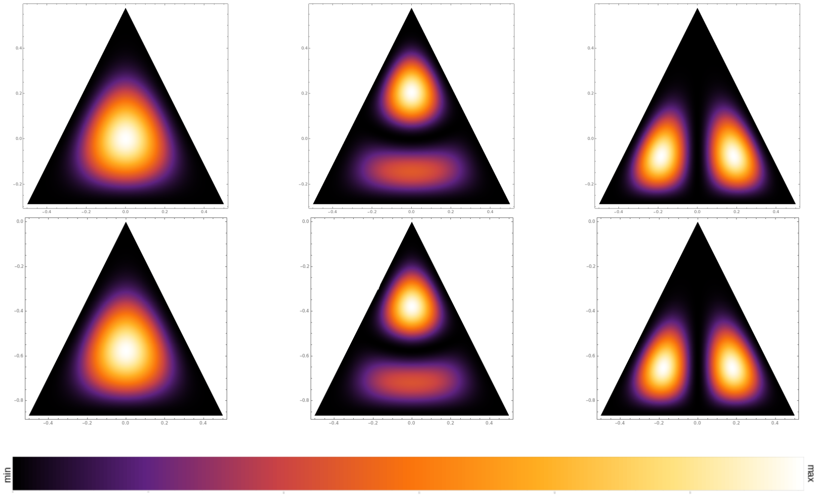
Polynomial Method

Due to the specific boundary conditions, the polynomial method can be applied in the same way as in the Schrödinger problem.



Polynomial Method

With this, we compare $|\psi_A|^2$ for the first three eigenfunctions.



2-Dimensional Results: Uniform Square

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To preserve the ratio between the two sublattices at the boundaries, the initial spinor is constructed by adding a term for each opposing pair of edges.

$$\Psi_0(x,y) = N_0\left[\left(\frac{L^2}{4} - x^2\right)\begin{pmatrix} 1 \\ -\frac{2y}{L} \end{pmatrix} + \left(\frac{L^2}{4} - y^2\right)\begin{pmatrix} 1 \\ \frac{2ix}{L} \end{pmatrix}\right]$$

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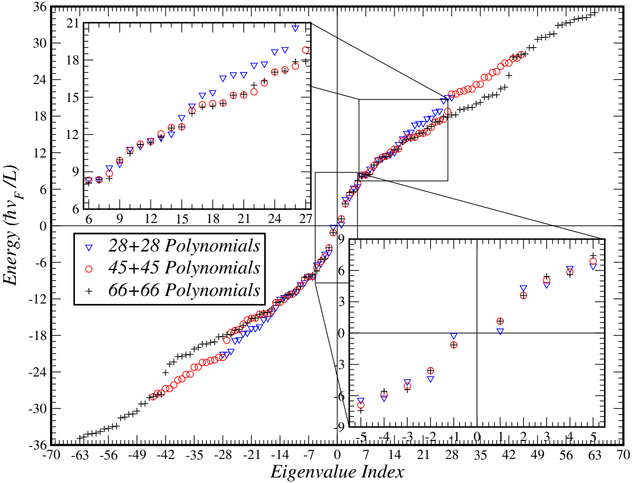
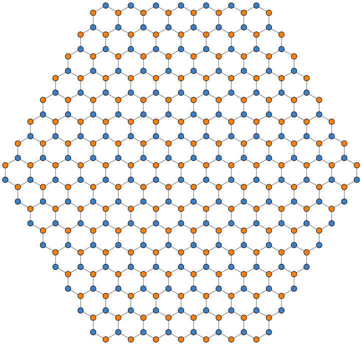
The obtained spectrum, after orthogonalization, is



2-Dimensional Results: Zigzag Hexagon

In this system, the boundary conditions will switch $t \leftrightarrow t^{-1}$ when one changes edges:

- ψ_A-terminated, $t = \infty$;
- ψ_B-terminated, $t = 0$.



2-Dimensional Results: Zigzag Hexagon

As t is no longer finite, adding the BCs in the extra sides will not disturb the ψ_B/ψ_A ratio. As such, each spinor component will be a product of three factors of the form

$$\varphi_i\,(x,y) \sim y - mx - b$$

Due to the non-equivalence of the two components, the valence-band initial function will be

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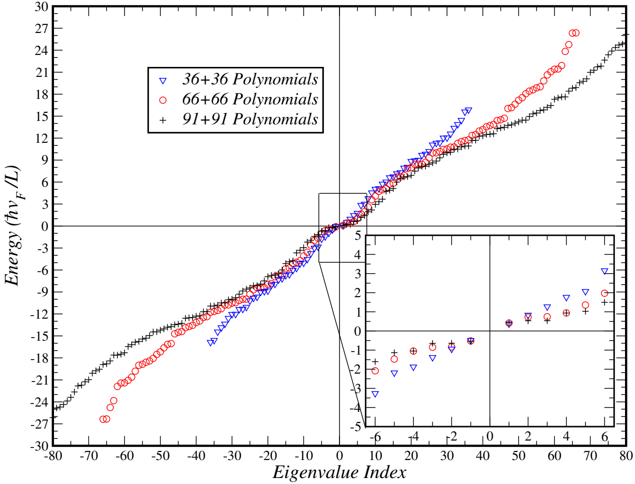
After G-S orthogonalization, the obtained spectrum is



Squaring the Hamiltonian

We can simplify this problem by squaring the Hamiltonian:

$$\begin{aligned} H^{\dagger} H \Psi &= -\hbar^2 v_F^2 \left(\vec{\sigma} \cdot \vec{p}\right)^{\dagger} \cdot \left(\vec{\sigma} \cdot \vec{p}\right) \Psi \\ &= -\hbar^2 v_F^2 \begin{pmatrix} \partial_x^2 + \partial_y^2 & 0 \\ 0 & \partial_x^2 + \partial_y^2 \end{pmatrix} \Psi \end{aligned}$$

This turns our problem into a one-band problem, which halves the necessary number of polynomials, significantly accelerating the calculations.

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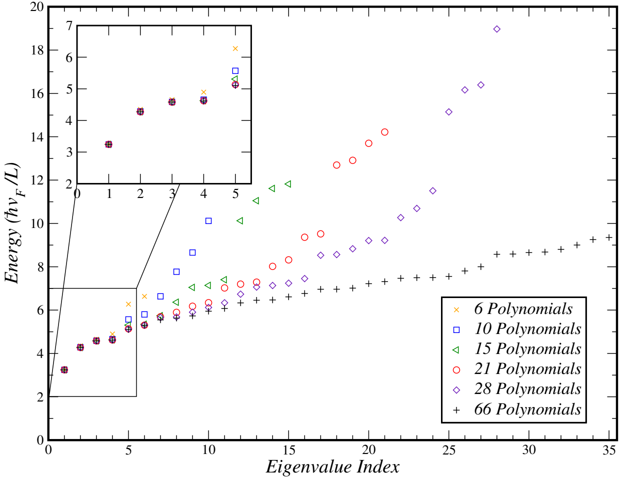
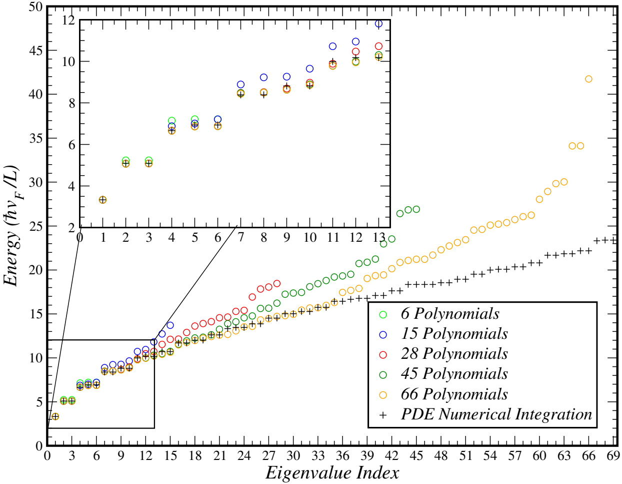
Uniform-Boundary Square

With this method, the obtained spectrum is



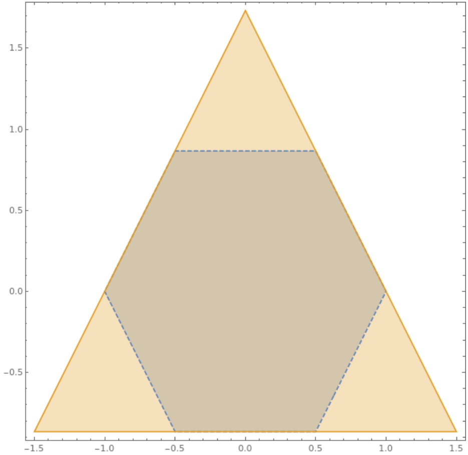
Zigzag Hexagon

Finally, for the zigzag-like hexagon, we obtain



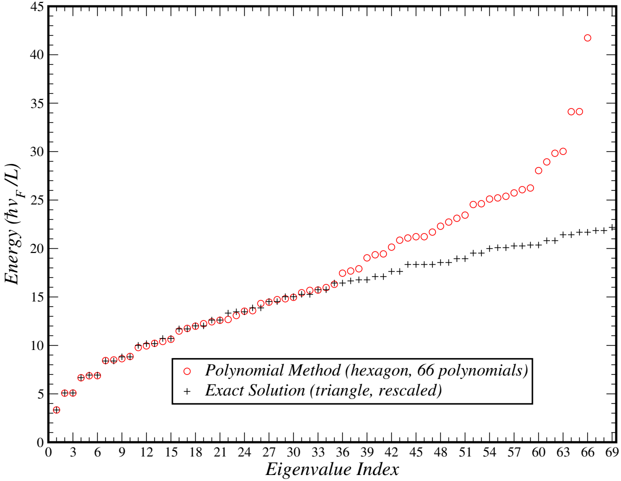
Hexagon – Triangle Equivalence

Due to the equivalence of boundary conditions, one can imagine a symmetry between the results for the triangle and the hexagon:



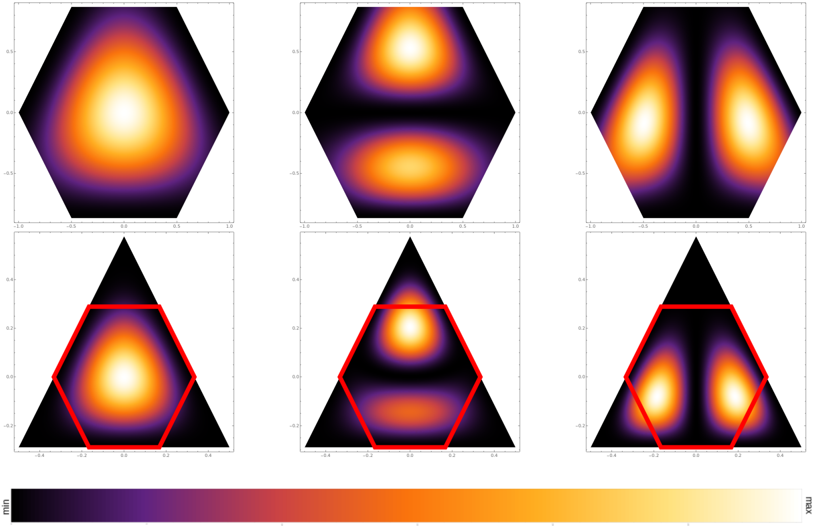
Comparison with the Results for the Triangle

Comparing against the spectrum obtained for the zigzag triangle:



Comparison with the Results for the Triangle

Comparing the three lowest-energy eigenfunctions for $|\psi_A|^2$:



Conclusions

- This method allows us to replicate the existing exact solutions of both the Schrödinger and the Dirac-Weyl equation in polygonal enclosures.

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Future Work

In the future, we hope to apply this method in the study of the AA-stacking regions of twisted bilayer.

Main References

- G. Tarnopolsky, A. J. Kruchkov, and A. Vishwanath. Origin of Magic Angles in Twisted Bilayer Graphene. Physical Review Letters, 122(10):106405, March 2019.
- K. M. Liew and K. Y. Lam. A Set of Orthogonal Plate Functions for Flexural Vibration of Regular Polygonal Plates. Journal of Vibration and Acoustics, 113(2):182–186, April 1991.
- W. A. Gaddah. Exact solutions to the Dirac equation for equilateral triangular billiard systems. Journal of Physics A: Mathematical and Theoretical, 51(38):385304, September 2018.
- M. V. Berry and R. J. Mondragon Neutrino billiards: time-reversal symmetry-breaking without magnetic fields. Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences, 412(1842):53–74, July 1987.
- L. Brey and H. A. Fertig. Electronic States of Graphene Nanoribbons. Physical Review B, 73(23):235411, June 2006.

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Thank you!