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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- These regions are hexagons whose boundaries that are approximately zigzag in one of the layers.
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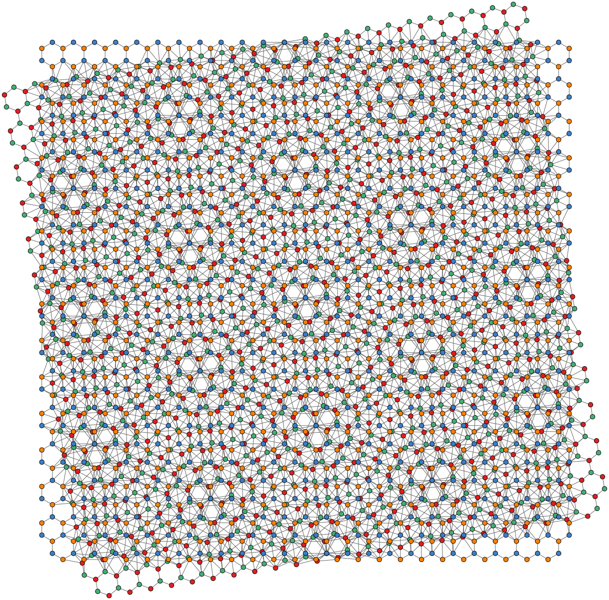
Motivation – TBLG



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,

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

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

$$H_{ij} = -\frac{\hbar^2}{2m} \iint_A dA \psi_i (x, y) \nabla^2 \psi_j (x, y)$$

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Defining the Complete Basis

The complete basis is defined by Gram-Schmidt orthogonalization

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

defining

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

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

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

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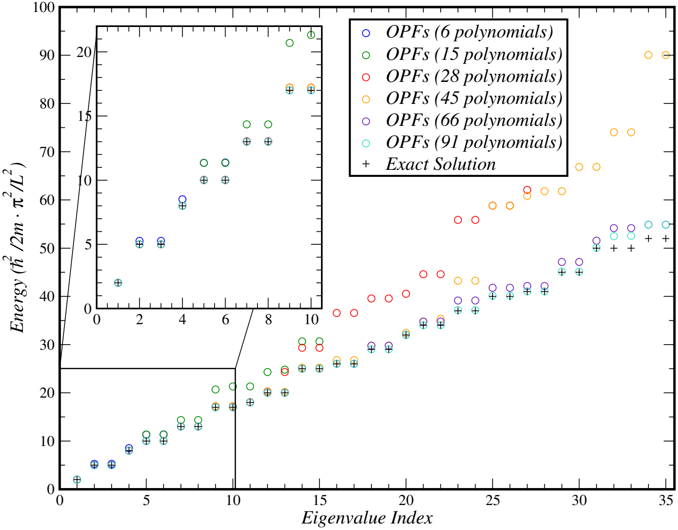
Square Infinite Potential Well

The obtained spectrum converges gradually to the exact results



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This $f_m(x, y)$ list can also be built from polynomials that belong to the irreducible representations of the symmetry group of the enclosure in question.

This will accelerate the calculation of the Hamiltonian matrix, but will be require a more involved approach when generating the higher order polynomials.

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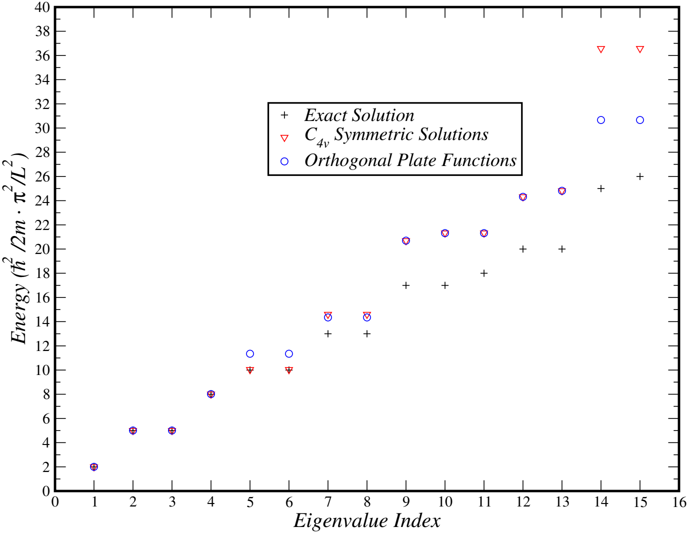
Square Infinite Potential Well

For this specific enclosure, the point-group in question is C_{4v}.



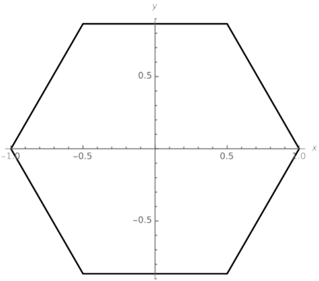
Hexagonal Infinite Potential Well

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

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

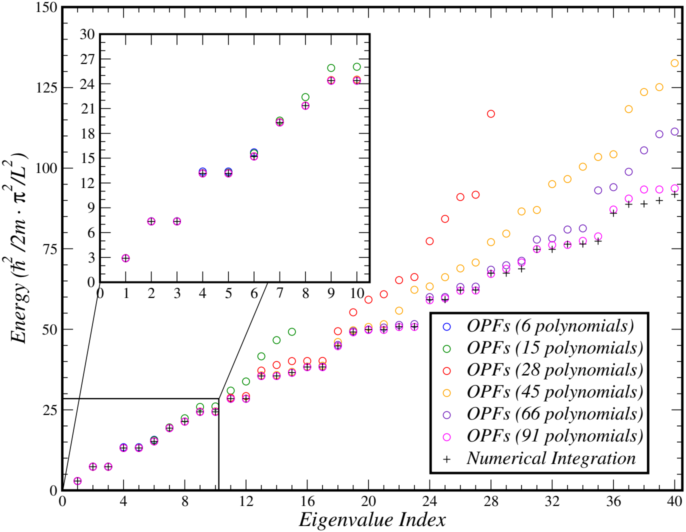
We must define the integration region carefully

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



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

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

This problem is solvable exactly in 1D, where we obtain the spectrum

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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 average energy of this function is

$$\langle\epsilon\rangle = -i\int_{-L/2}^{L/2} dy \Psi_0^\dagger \sigma^y \partial_y \Psi_0 = \frac{3}{2L}$$

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

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

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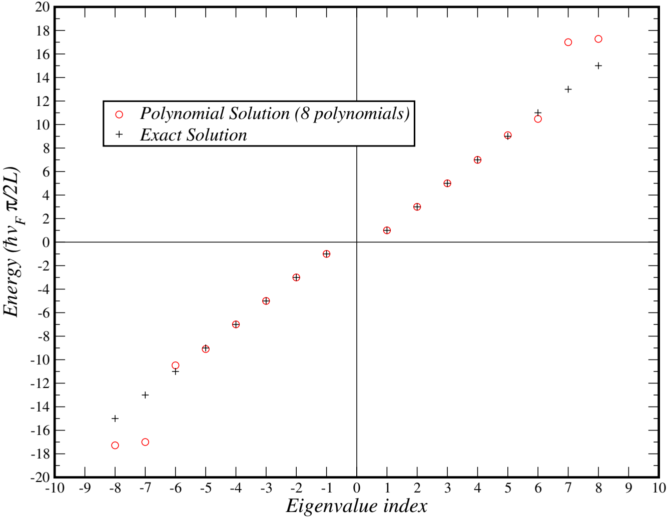
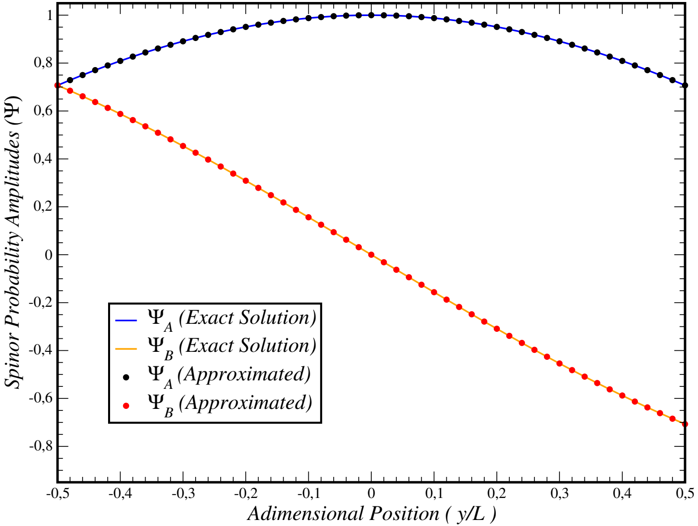
Choosing a basis size, the eigenvalues of the Hamiltonian are



1-Dimensional Toy-Model

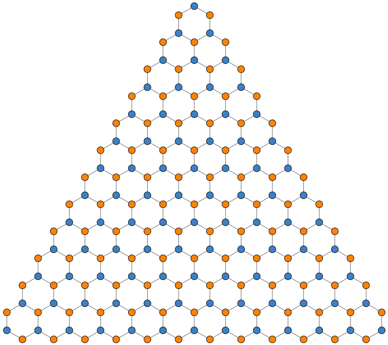
The first eigenfunction also matches perfectly:



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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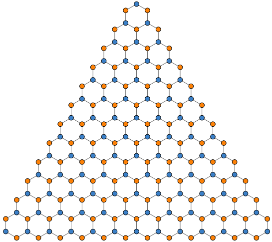
If we were to calculate the spectrum of this region with a tight-binding model, there would be many states of exactly zero-energy. How many and why?



As the Hamiltonian is a linear operator that transforms $\psi_A \leftrightarrow \psi_B$, the dimension of its kernel will be the same as the difference between the dimensions (i.e., number of sites) of each subspace.

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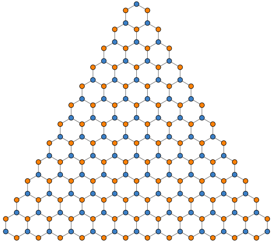

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The Hamiltonian for graphene near the Dirac point $\mathcal{K}$ is given by

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

Regarding the boundary conditions, we have that

$$\psi_A = 0$$
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where A, B are the sublattice indices.

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The only state of exactly-zero energy one can write that obeys both the boundary conditions and the Dirac-Weyl equation for this system is

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

This solution is not present in neither Gaddah's treatment nor in our polynomial method, as it is the trivial solution in the sublattice that is being considered (ψ_A).

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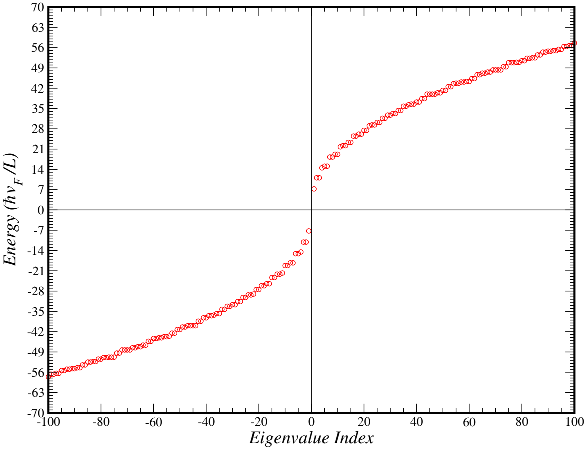
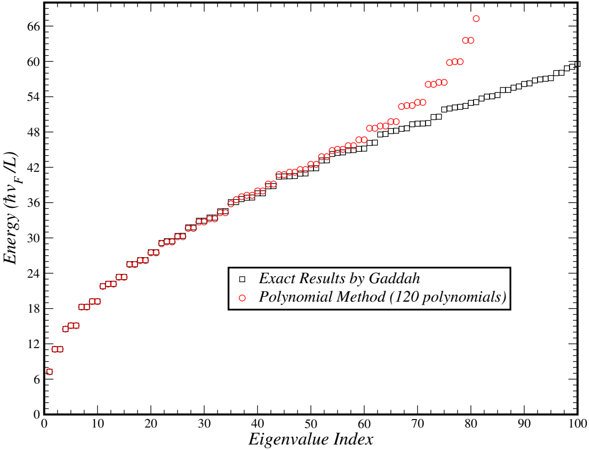
Transforming this problem into two identical Helmholtz problems, Gaddah obtains the spectrum with a gap of $2\sqrt{3}\frac{4\pi}{3L}\hbar v_F$:



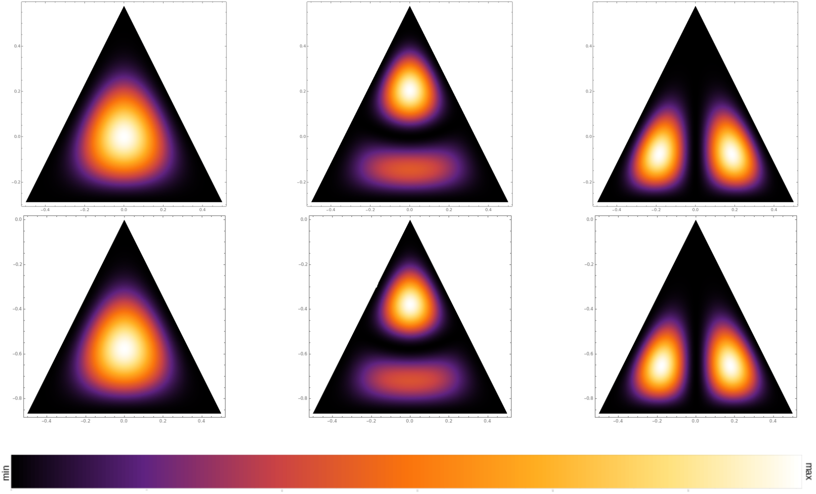
Polynomial Method

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.

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

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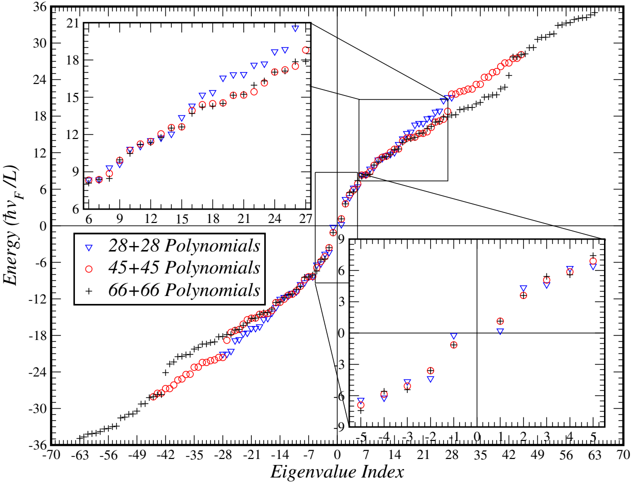
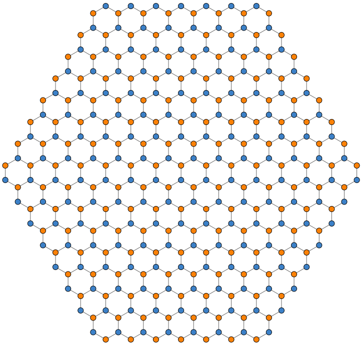
The obtained spectrum, after orthogonalization, is



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, $t = 0$.



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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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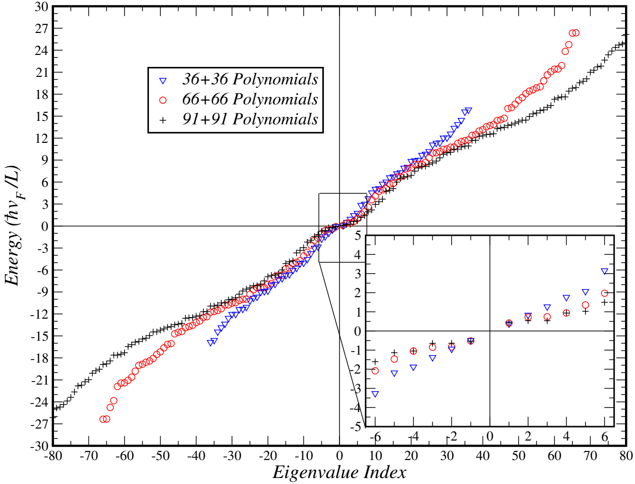
After G-S orthogonalization, the obtained spectrum is



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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The new matrix elements will be

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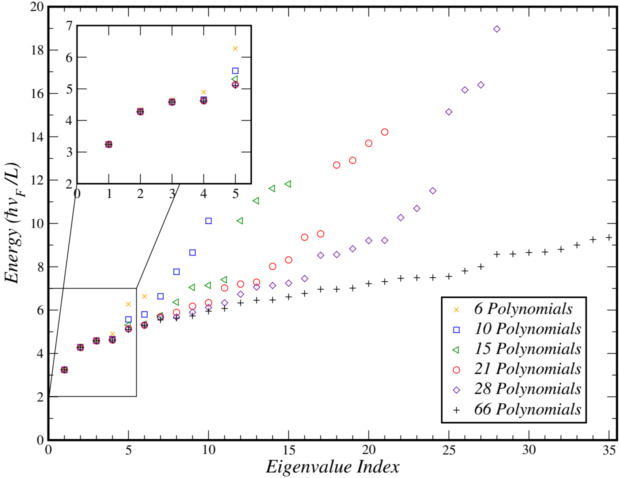
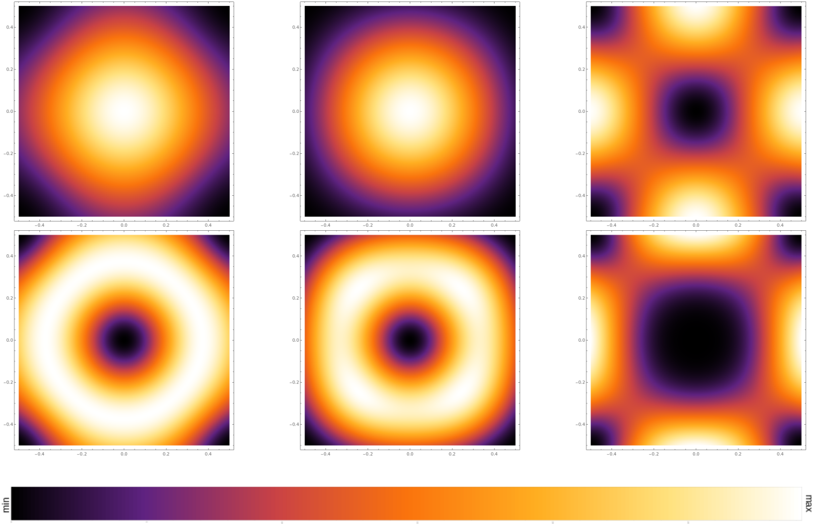
Uniform-Boundary Square

With this method, the obtained spectrum is



Uniform-Boundary Square

$|\psi_A|^2 + |\psi_B|^2$ $\quad$ $|\psi_A|^2$ $\quad$ $|\psi_B|^2$



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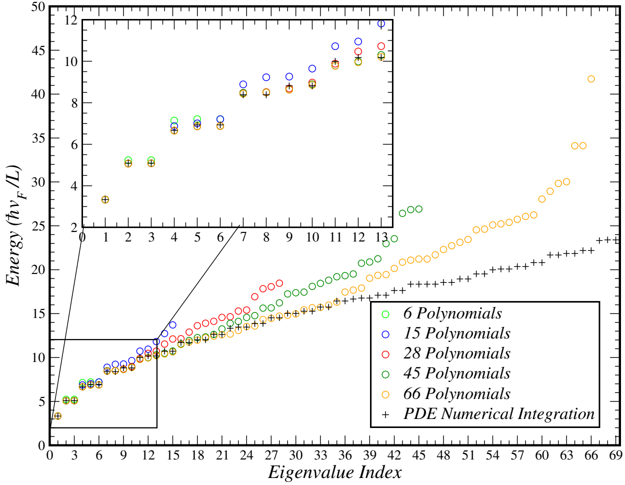
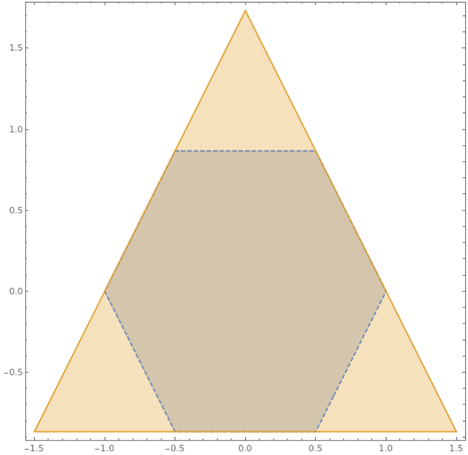


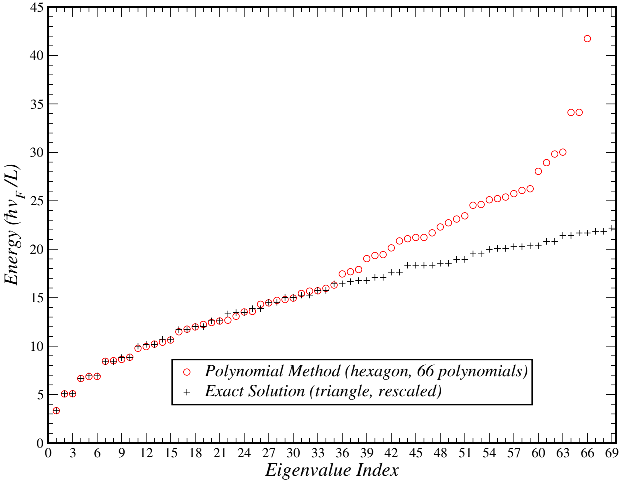
Hexagon – Triangle Equivalence

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



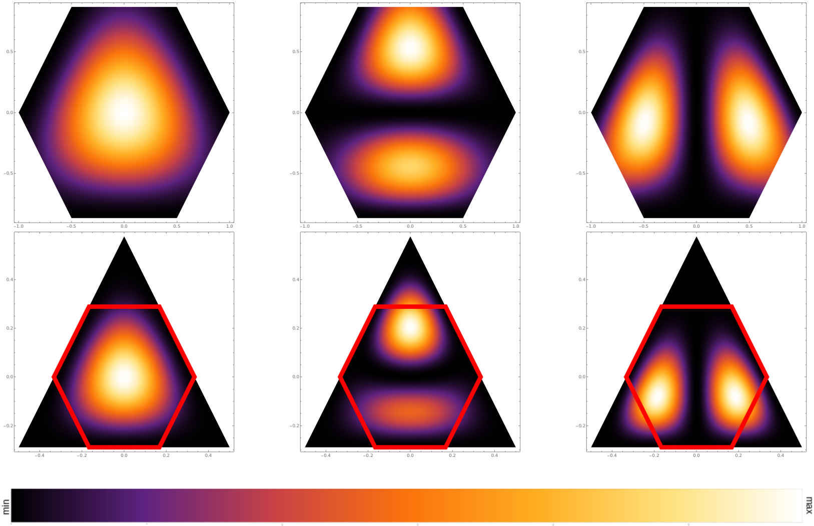
Comparison with the Results for the Triangle

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 and Future Work

- This method allows us to replicate the existing exact solutions of both the Schrödinger and the Dirac-Weyl equation in polygonal enclosures.
- When applying directly to the Dirac-Weyl equation, the Gram-Schmidt process has to be performed more carefully to generate the functions of both bands.

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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.
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