A Polynomial Approach to the Spectrum of Dirac-Weyl Graphene Flakes

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1 Introduction to the Polynomial Method

In general polygonal enclosures, separation of variables cannot be used to determine the spectrum.

Problem: How to solve Schrödinger or Dirac-Weyl equations in general polygonal enclosures?

Solution: The polynomial method[1].

1.1 Defining the Polynomial Method

1. Start with lowest (non-zero) order polynomial that satisfies boundary conditions. For a triangle with Dirichlet BC,

$$\phi_0(x,y) = N_0 xy(1-x-y);$$

2. Generate a basis with increasing order polynomials

$$\mathcal{P}_n(x,y)\,\phi_0(x,y),$$

where $\mathcal{P}_n$ is a sorting of ascending-order monomials (for example, as defined by Liew *et al*[1])

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

3. Orthogonalize using the Gram-Schmidt process, and normalize them;
4. Diagonalize the Hamiltonian in this truncated basis.

2 Boundary Conditions for the Dirac-Weyl Equation

We will now review possible types of BCs[2, 3], and generalize the polynomial method for two-component spinors.

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

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

Confinement to enclosure: use a mass term outside to open a gap in energies close to zero

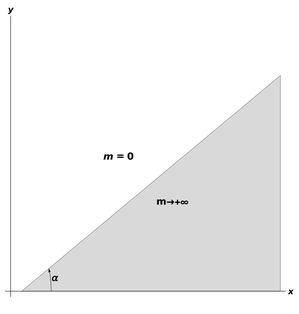
$$\mathcal{H}_\mathcal{K} = \hbar v_F \vec{\sigma}\cdot\vec{p} + m(\vec{r})(\sigma_z - \cos\theta).$$

The necessary condition is imposing zero normal probability current

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

Hard boundary: let $m(\vec{r}) \to \infty$ outside the enclosure $\Longrightarrow$ BC for an edge at an angle α with the x-axis

$$\frac{\psi_B}{\psi_A} = te^{i\alpha}, \quad t \in Reals.$$



2.1 One-Dimensional Toy-Model

For the case where $t = 1$, the Hamiltonian is[2]

$$\mathcal{H}_\mathcal{K} \to \mathcal{H}_\mathcal{K} + \mathrm{m}(\tilde{\mathrm{r}})\,\sigma_\mathrm{z}, \quad m(\vec{r}) = \begin{cases} 0 & \text{inside} \\ +\infty & \text{outside} \end{cases},$$

and the problem is exactly solvable in 1D, with spectrum

$$E_{n,\pm} = \pm\hbar v_F (2n+1)\frac{\pi}{2L}.$$

Defining an initial spinor polynomial (Ψ_0) that respects the necessary BCs,

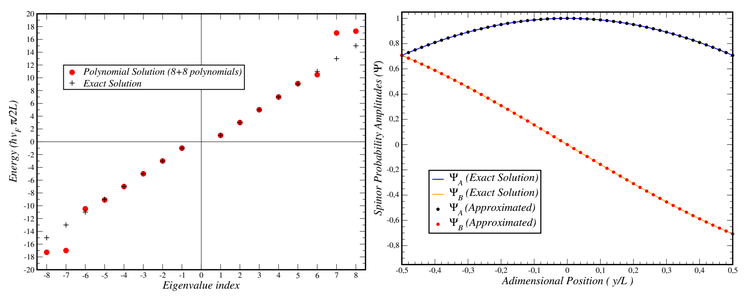
$$\Psi_0(y) = N_0 \begin{bmatrix} 1 \\ -\frac{2y}{L} \end{bmatrix},$$

the valence-band will be

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

The G-S process for higher order functions is the same, with the only caveat being the necessity of orthogonalizing the polynomials of the two bands.

Integrating the Hamiltonian matrix, we obtain the eigenvalues (left) and eigenfunctions (right, first conduction-band eigenfunction) for the basis size in question.



2.2 Infinite-Mass Confined Square

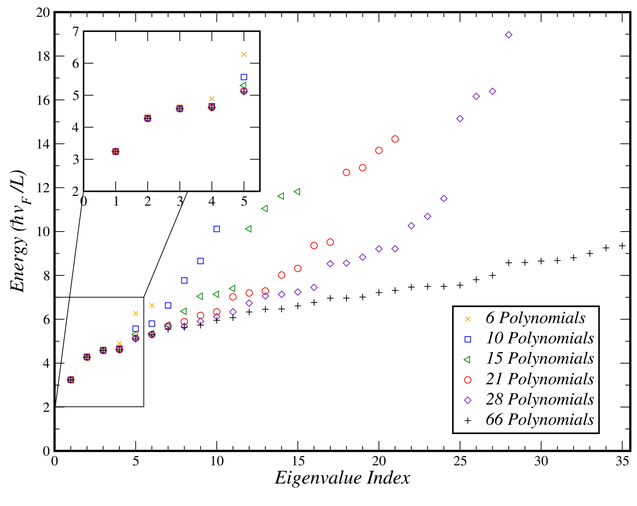
To apply this method to $t = 1$ square, the initial spinor is defined as

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

Applying again the G-S process, we square the Dirac Hamiltonian to eliminate the valence band,

$$\langle\Psi_i|\, H^\dagger H\, |\Psi_j\rangle = -\hbar^2 v_F^2 \left\langle \begin{pmatrix}\psi_{i,A}\\ \psi_{i,B}\end{pmatrix} \middle| \begin{pmatrix}\nabla^2 & 0\\ 0 & \nabla^2\end{pmatrix} \middle| \begin{pmatrix}\psi_{j,A}\\ \psi_{j,B}\end{pmatrix} \right\rangle$$

obtaining the convergent approximate spectrum.



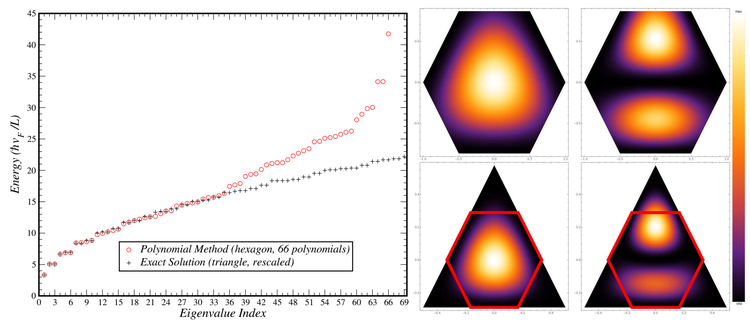
2.3 Zigzag-like Hexagon

The BCs for this system are $\psi_B = 0$ or $\psi_A = 0$ ($t = 0$ or $t = \infty$), alternating. The initial function is

$$\Psi_0(x,y) = N_0\begin{pmatrix}\left[\frac{\sqrt{3}L}{2} + y\right]\left[L + x - \frac{y}{\sqrt{3}}\right]\left[L - x - \frac{y}{\sqrt{3}}\right] \\ \left[\frac{\sqrt{3}L}{2} - y\right]\left[L + x + \frac{y}{\sqrt{3}}\right]\left[L - x + \frac{y}{\sqrt{3}}\right]\end{pmatrix}$$

These BCs define a larger equilateral triangle, similar to the one used by Gaddah [4].

As such, we compare the polynomial spectrum with the exact solution by Gaddah (left side), as well as the probability density for $|\psi_A|^2$ of the first two eigenfunctions (on the right, highlighting the corresponding region).



3 Conclusions and Future Work

We were able to develop a polynomial method of approximating the solutions to the Dirac-Weyl equation in polynomial enclosures. We observed an equivalence between the zigzag-like hexagon and the exact solution for the zigzag-like triangle.

In the future, we hope to apply this method in the study of the AA-stacking regions of twisted bilayer graphene[5].

4 Acknowledgements

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5 References

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