Spectral Touching Points in 2 Dimensional Materials

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Introduction

What is a 2D material?

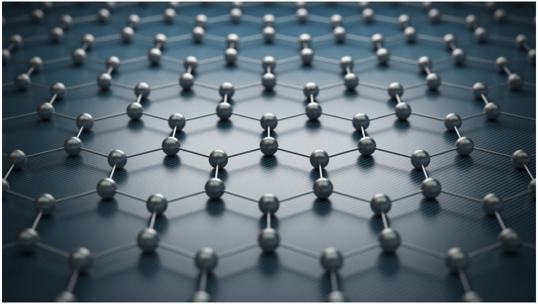

Image source: [1]

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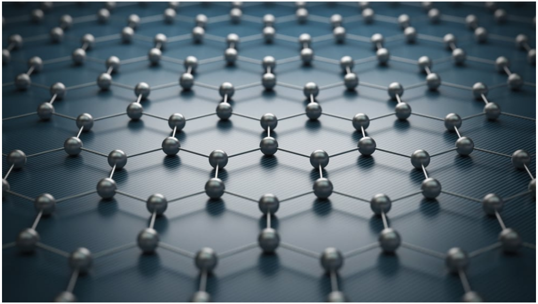

Image source: [1]

2D Material: crystalline materials consisting of a single layer of atoms with applications such as photovoltaics, semiconductors, electrodes and water purification

Definitions

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Infinite Periodic Graph: infinite graph containing a finite subgraph that can be tessellated to produce the full infinite graph

Fundamental Domain: a smallest subgraph of the infinite graph that can be used to generate the complete infinite graph

Background & Motivation for Research

- Graphene has many unique properties as a building material & energy storage medium

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- Conjectured relationship between Dirac conical points & Graphene properties
- Previously, only graphene's structure had been studied in relation to Dirac conical points
- Goal: Search for other 2D materials with Dirac conical points, potentially indicating properties similar to graphene

Graphene 2D Structure

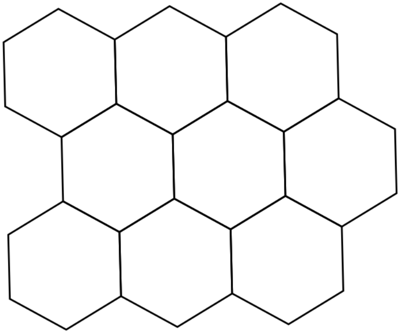

Figure: A section of the infinite periodic graph representing graphene's 2D structure.

Graphene Fundamental Domain

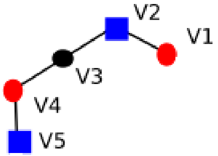

Figure: The chosen fundamental domain for graphene as seen in previous research. [3], [2]

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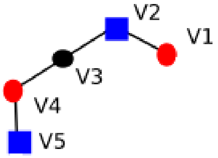

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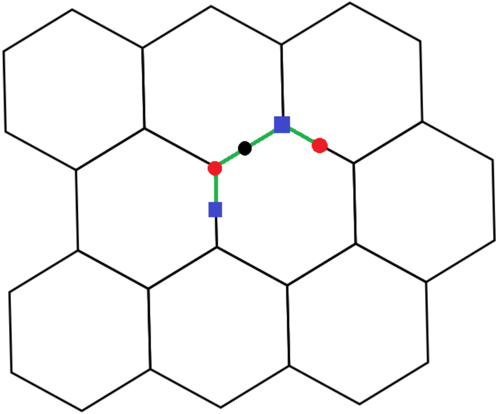
Paired Quasi-Connected Vertices: vertices of a fundamental domain of a graph which arise from breaking an edge on the infinite periodic graph and defining two new vertices at the break

Tiling Animation



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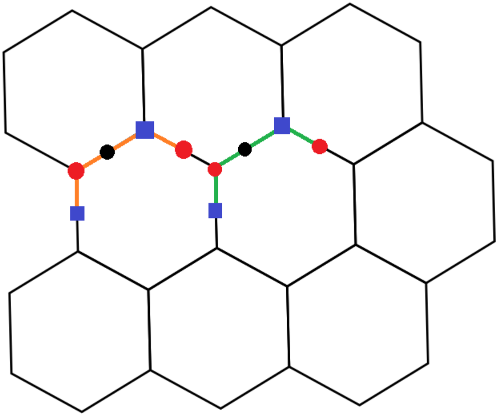

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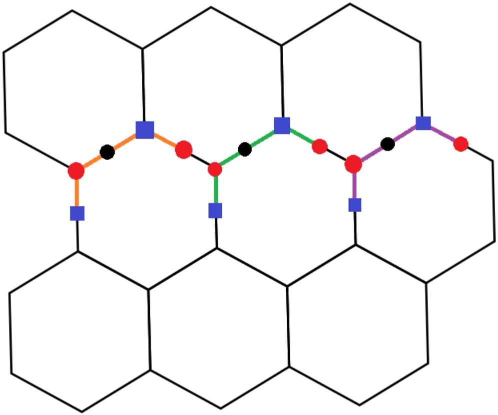

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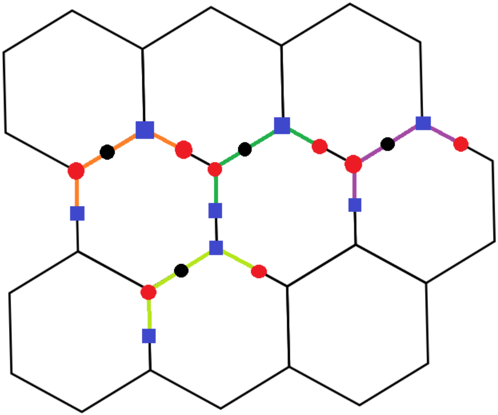

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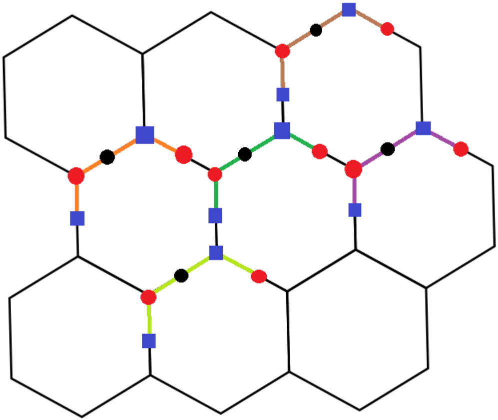

Finding Magnetic Flux Schrodinger Operator

1. Find the fundamental domain, and label all vertices. Define the set of vertices $V = \{1, 2, ..., n\}$ where n is the total number of vertices in the fundamental domain.

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3. For each vertex i define $\lambda f_i = q_i f_i - \sum_{k \in V} f_k$ where $k \neq i$, k is adjacent to i and $f_1, f_2, ..., f_n$ represent the function values on the vertices of the discrete graph. If k is from another copy of the fundamental domain, add the coefficient e^{ic} where c is a linear combination of α_1 and α_2 representing the direction in which the new copy of the fundamental domain was shifted.

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4. Write this system of equations as a matrix equation to find the eigenvalues.

Finding Magnetic Flux Schrodinger Operator for Graphene

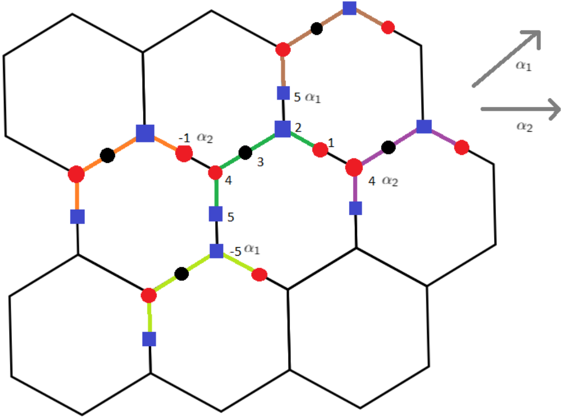

Figure: The graph representing the 2D structure of graphene, with labeled vertices and α_1, α_2.

Finding Magnetic Flux Schrodinger Operator for Graphene

$$\begin{pmatrix} q_1 & -1 & 0 & -e^{i\alpha_1} & 0 \\ -1 & q_2 & -1 & 0 & -e^{i\alpha_2} \\ 0 & -1 & q_3 & -1 & 0 \\ -e^{-i\alpha_1} & 0 & -1 & q_4 & -1 \\ 0 & -e^{-i\alpha_2} & 0 & -1 & q_5 \end{pmatrix}$$

Additional Definitions

Spectral Touching Point: occurs when the spectral surfaces between two eigenvalues touch

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Dirac Conical Point: a spectral touching point where the spectral surfaces of the two eigenvalues form cone-like projections

Graphene Plotted Spectrum

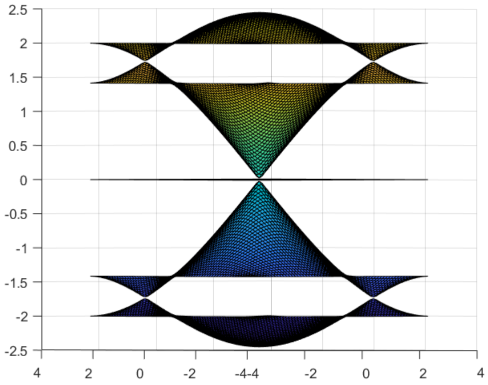

Figure: The plot of the spectrum of graphene.

Graphene Spectral Graph

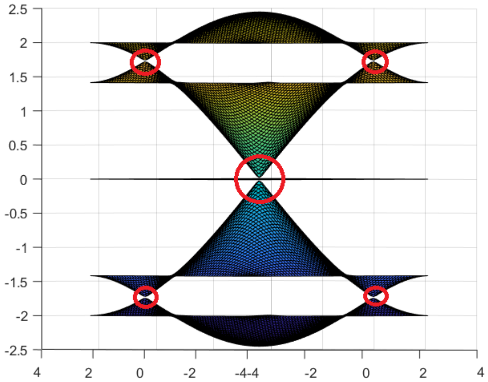

Figure: The plot of the spectrum of graphene. Dirac conical touching points highlighted in red.

Other Materials with Graphene's Structure

- Bismuthene
- Germanene
- Silicene
- Phosphorene

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Assumptions:

- Must be represented as 2-dimensional structure
- Edge lengths irrelevant

Muscovite 2D Structure

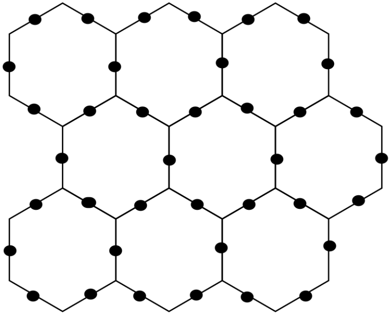


Figure: A section of the infinite periodic graph representing muscovite's 2D structure.

Muscovite Fundamental Domain

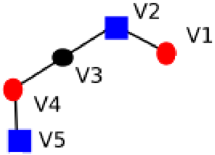


Figure: The chosen fundamental domain for muscovite as seen in previous research [2] [3]. Note: Identical to chosen fundamental domain for graphene.

Muscovite Fundamental Domain

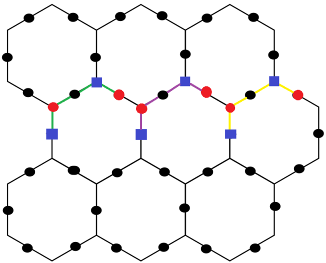


Figure: 3 instances of muscovite's fundamental domain highlighted on its infinite periodic graph.

Note on Addition of Vertices

- Discrete graph only defined on vertices
- Discrete graph is approximation of continuous graph
- Adding or removing degree-2 vertices gives a better or worse approximation, but does not change structure of graph
- Adding vertices on edges gives more information about the 2D structure without changing system of atoms themselves

Having the same fundamental domain implies also having the same magnetic flux Schrodinger operator, so muscovite's 2D structure is mathematically identical to graphene.

Initial Investigation of Different Structures

Examples:

- Sodium Chloride
- Quartz
- Transition Metal Oxides

Sodium Chloride Infinite Periodic Graph

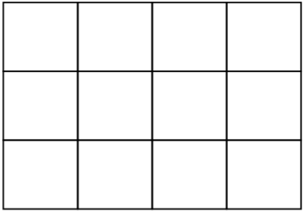


Figure: Sodium chloride infinite periodic graph. All points of intersection are vertices where atoms are present.

Sodium Chloride Fundamental Domain

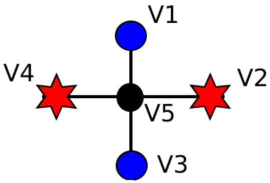


Figure: Chosen sodium chloride fundamental domain. Same color & shape indicates quasi-connected vertex pairs.

Sodium Chloride Plotted Spectrum

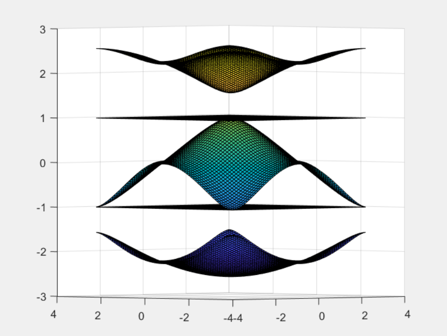


Figure: Plot of spectrum of chosen fundamental domain for Sodium Chloride.

Sodium Chloride Plotted Spectrum

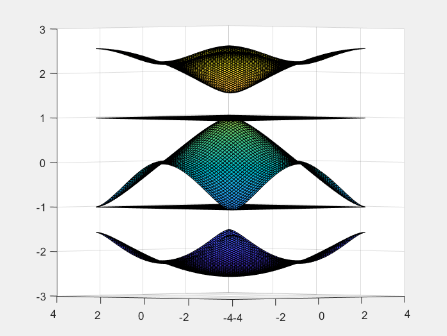


Figure: Plot of spectrum of chosen fundamental domain for Sodium Chloride.

Flat Sheet Touching Point: a spectral touching point where the spectral surface of one of the eigenvalues forms a flat sheet

Process for Proving Touching Point

1. Substitute all electric potential (q) values, as well as α_1 and α_2 values, in the magnetic flux Schrodinger operator H^α.
2. Prove that it has a repeated eigenvalue with two linearly independent eigenvectors.

Quartz Infinite Periodic Graph

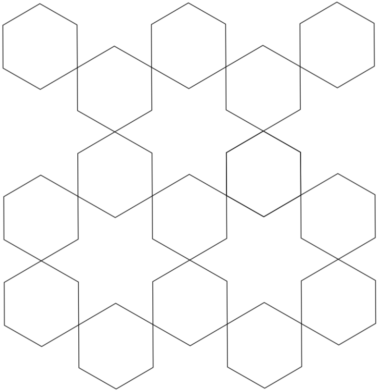


Figure: A portion of the infinite periodic graph representing the 2D structure of quartz. Each of the vertices represents an atom in the physical structure.

Quartz Simplified Infinite Periodic Graph

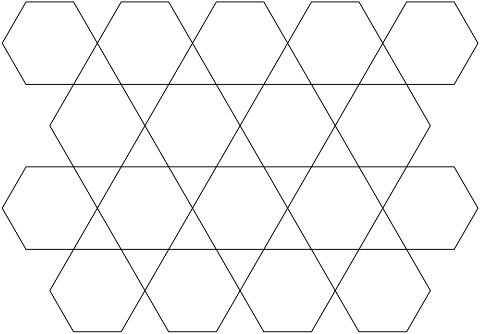
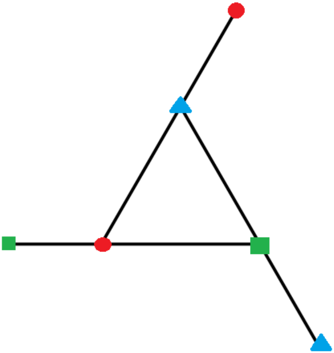


Figure: A portion of the infinite periodic graph representing the 2D structure of quartz (with one of the vertices corresponding to an atom in the 2D structure removed).

Quartz Simplified Fundamental Domain



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Quartz Spectrum Plot

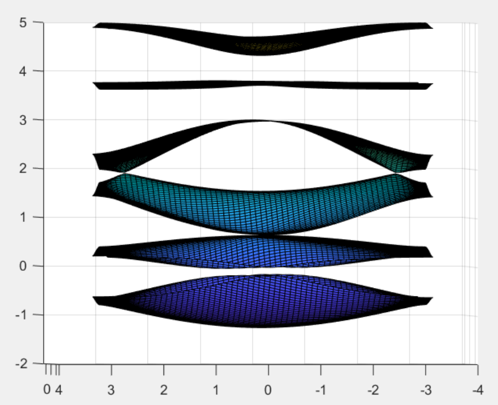

Figure: Plot of the spectrum of Quartz, using the chosen fundamental domain.

Conclusion

Some 2D materials, other than graphene, have spectral touching points. This would be a good starting point for further investigation into the physical properties of these materials.

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Future Research:

- Study different types of touching points
- Vary conditions on electric potential
- Study other materials with Dirac conical points for special properties
- Investigate effects of different symmetry conditions on spectral touching points

References

[1] Graphene battery feature image.

[2] Reese A. Martin. *Necessary Conditions on Electric Potential for the Formation of Spectral Touching Points*. Baylor University, 2017.

[3] Tracy Kathleen Weyand. *Zeros of Eigenfunctions of the Schrodinger Operator on Graphs and Their Relation to the Spectrum of the Magnetic Schrodinger Operator*. Texas A & M University, 2014.