Spectral Touching Points in 2 Dimensional Materials

Andrea Wynn

Rose-Hulman Institute of Technology
Terre Haute, IN

Advised by Dr. Tracy Weyand (Rose-Hulman)

NCUWM Conference - Jan 2021
What is a 2D material?

Image source: [1]
Introduction

What is a 2D material?

Image source: [1]

2D Material: crystalline materials consisting of a single layer of atoms with applications such as photovoltaics, semiconductors, electrodes and water purification
Discrete Graph: a graph that is completely defined by a finite set of vertices $V$ and a finite set of edges $E$; functions on discrete graphs are defined only on the vertices, not the edges.
Discrete Graph: a graph that is completely defined by a finite set of vertices $V$ and a finite set of edges $E$; functions on discrete graphs are defined only on the vertices, not the edges.

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

**Discrete Graph**: a graph that is completely defined by a finite set of vertices $V$ and a finite set of edges $E$; functions on discrete graphs are defined only on the vertices, not the edges.

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

Conjectured relationship between Dirac conical points & Graphene properties.
Background & Motivation for Research

- Graphene has many unique properties as a building material & energy storage medium
- Conjectured relationship between Dirac conical points & Graphene properties
- Previously, only graphene’s structure had been studied in relation to Dirac conical points
Graphene has many unique properties as a building material & energy storage medium

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
Figure: A section of the infinite periodic graph representing graphene’s 2D structure.
**Figure:** The chosen fundamental domain for graphene as seen in previous research. [3], [2]
**Graphene Fundamental Domain**

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

**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
Tiling Animation
Tiling Animation
Tiling Animation
Finding Magnetic Flux Schrödinger Operator

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

2. Define two linearly independent vectors, \( \alpha_1 \) and \( \alpha_2 \), pointing in the directions in which the fundamental domain is shifted to tile the infinite graph.

For each vertex \( i \) define 
\[
\lambda_f i = q_i f_i - \sum_{k \in V, k \neq i} f_k
\]
where \( k \) 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 \( \alpha_1 \) and \( \alpha_2 \) representing the direction in which the new copy of the fundamental domain was shifted.

Write this system of equations as a matrix equation to find the eigenvalues.
Finding Magnetic Flux Schrodinger Operator

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

2. Define two linearly independent vectors, $\alpha_1$ and $\alpha_2$, pointing in the directions in which the fundamental domain is shifted to tile the infinite graph.

3. For each vertex $i$ define $\lambda f_i = q_i f_i - \sum_{k \in V, \ k \neq i} f_k$ where $k \neq i$, $k$ is adjacent to $i$ and $f_1, f_2, \ldots, f_n$ 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 $\alpha_1$ and $\alpha_2$ representing the direction in which the new copy of the fundamental domain was shifted.
Finding Magnetic Flux Schrödinger Operator

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

2. Define two linearly independent vectors, \( \alpha_1 \) and \( \alpha_2 \), pointing in the directions in which the fundamental domain is shifted to tile the infinite graph.

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 \( f_1, f_2, \ldots, f_n \) 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 \( \alpha_1 \) and \( \alpha_2 \) representing the direction in which the new copy of the fundamental domain was shifted.

4. Write this system of equations as a matrix equation to find the eigenvalues.
Figure: The graph representing the 2D structure of graphene, with labeled vertices and $\alpha_1, \alpha_2$. 
Finding Magnetic Flux Schrodinger Operator for Graphene

\[
\begin{pmatrix}
q_1 & -1 & 0 & -e^{i\alpha_1} & 0 \\
-1 & q_2 & -1 & 0 & -e^{i\alpha_2} \\
0 & -1 & q_3 & -1 & 0 \\
-e^{-i\alpha_1} & 0 & -1 & q_4 & -1 \\
0 & -e^{-i\alpha_2} & 0 & -1 & q_5
\end{pmatrix}
\]
Spectral Touching Point: occurs when the spectral surfaces between two eigenvalues touch
Additional Definitions

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

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.
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
Other Materials with Graphene’s Structure

- Bismuthene
- Germanene
- Silicene
- Phosphorene

Assumptions:
- Must be represented as 2-dimensional structure
- Edge lengths irrelevant
Figure: A section of the infinite periodic graph representing muscovite’s 2D structure.
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
Figure: Sodium chloride infinite periodic graph. All points of intersection are vertices where atoms are present.
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.
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.
1 Substitute all electric potential \((q)\) values, as well as \(\alpha_1\) and \(\alpha_2\) values, in the magnetic flux Schrödinger operator \(H^\alpha\).

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.
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).
Figure: Chosen sodium chloride fundamental domain. Same color & shape indicates quasi-connected vertex pairs.
Figure: Plot of the spectrum of Quartz, using the chosen fundamental domain.
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.
Conclusions

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.

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
