ABSTRACT

Necessary Conditions on Electric Potential for the Formation of Spectral Touching Points

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In recent years special attention has been given to graphene as building material and as an energy storage medium. The main property that make graphene uniquely suited to both of these concerns is that it possesses mass-less fermions, which enable loss-less electron transfer across a graphene sheet. Dirac conical points, a specialized kind of spectral touching point, are believed to be responsible for the mass-less fermions found in graphene, meaning Dirac points could be responsible for graphenes most highly sought after properties. In this work I was able to show that touching points form in graphene for all values of electrical potential, as long as certain symmetry conditions were maintained on the graph. I was then able to show how touching point formation changes as symmetry conditions were removed.

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Necessary Conditions on Electric Potential for the Formation of Spectral Touching Points

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1 Introduction

Spectral graph theory is the study of the spectrum of an operator acting on a graph. In the case of discrete graphs, the spectrum consists of eigenvalues and the corresponding eigenvectors are the eigenfunctions of the graph. These graphs can be used to study atomic and sub-atomic phenomena, biological systems, economic interactions, and any situation that can be modeled as vertices representative of objects and edges representing interactions between those objects. This work will focus, in particular, on electrical potential conditions necessary for the formation of touching points in the spectrum of a graph representation of graphene.

A touching point occurs when an eigenvalue has geometric multiplicity greater than one, or in other words, at least two linearly independent eigenvectors correspond to the same eigenvalue. In this work touching points were shown visually as the points were two spectral sheets touch, as shown in figure 1. The presence of touching points indicates that the graph in question may possess Dirac conical points, which can also be seen in figure 1 most prominently as the large conical structures that meet through a third flat spectral band.

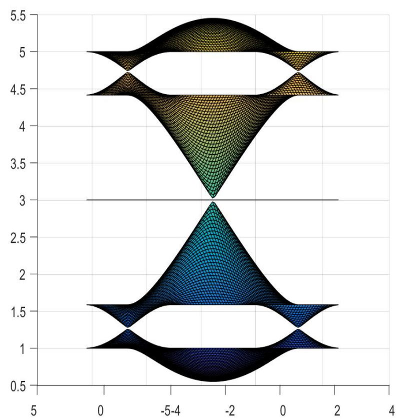

Figure 1: This figure shows several touching points between spectral sheets.

Dirac cones sometimes occur in the spectra of infinite periodic graphs and are representative of instances when the spectral surfaces of two eigenvalues form cone-like projections that touch. The key difference between touching points and Dirac cones is that touching points occur whenever two sheets touch, while Dirac cones have to have the sheets shaped in a specific, conical way. The study of Dirac cones and the conditions necessary for their formation originates from the idea that materials that have Dirac cones exhibit interesting properties, such as mass-less fermions, which leads to lossless electron transfer, and incredible tensile strength. It was posited that these qualities occur because of the Dirac conical points themselves in Dr. Novoselov's Nobel lecture [3]. A well-known example of a material that possesses Dirac cones is a single layer of carbon atoms arranged in a honeycomb pattern, known as graphene. Theses properties make graphene incredibly well suited for both energy storage and use as a building material, so the study of Dirac cones is one that is fruitful in physics, chemistry, and material sciences.

This work focuses on finding bounds on electrical potential so that Dirac cones are present in the spectrum of the infinite periodic graph representative of graphene. To study these electrical potentials, I needed to calculate the spectrum that results from the Schrödinger operator acting on the chosen infinite periodic graph. Using Floquet-Bloch theory, we can find the spectrum of the Schrödinger operator acting on the infinite periodic graph by calculating the spectrum of the magnetic Schrödinger operator on a fundamental domain of the infinite graph over all possible values of magnetic flux. The variables, α_j, introduced by the magnetic flux Schrödinger operator, correspond to the linearly independent vectors used to generate the infinite graph from the fundamental domain.

The graphs studied in this work are $\mathbb{Z}^2$-periodic which necessitates the use of two alpha variables, because two linearly independent vectors are needed to represent the shifts necessary for the fundamental domain to tile the infinite graph. The Schrödinger operator on the infinite graph is unitarily equivalent to the union over all α_j of the magnetic flux Schrödinger operator on a fundamental domain, so studying the spectrum of the magnetic flux Schrödinger operator for all α_j is equivalent to studying the spectrum of the Schrödinger operator. In Section 2, I provide necessary background information for this work. Section 3 is dedicated to the electrical potential conditions and graphene. Section 4 shows how changing symmetry conditions change touching point formation on a different graph, whose fundamental domain is shown in figure 6, and Section 5 is a conclusion and summary of the work as a whole.

2 Background

A *discrete* or *combinatorial* graph consists of a set of vertices, $\mathcal{V}$, and a set of edges, $\mathcal{E}$, with each edge connecting two vertices. The *degree* of a vertex of a graph is the number of edges connected to that vertex. On discrete graphs, functions take on values at the vertices, and therefore these functions can be represented as vectors of length $|\mathcal{V}|$.

The *Schrödinger operator*, $\mathcal{H}^o$, on a discrete graph is defined as $\mathcal{H}^o = Q$ - A where

$$Q = \begin{cases} q_u & \text{if } u = v \\ 0 & \text{otherwise} \end{cases} \tag{2.0.1}$$

with $q_u \in \mathbb{R}$ representing electrical potential of vertex u and A being the adjacency matrix.

The *magnetic Schrödinger operator*, $\mathcal{H}^A$, is defined as $\mathcal{H}^A = Q - M^A$ where Q is as before and

$$M^A = \begin{cases} q_u & \text{if } u = v \\ -e^{iA_{u,v}} & \text{if } u \text{ is connected to } v \\ 0 & \text{otherwise.} \end{cases} \tag{2.0.2}$$

An *infinite graph* is a graph with an infinite number of vertices and/or edges. An *infinite periodic graph* is an infinite graph that contains a finite subgraph that can be tessellated to produce the full infinite graph. A *fundamental domain* is a smallest subgraph of the infinite graph that can be used to generate the complete infinite graph; it is not necessarily unique. From Weyand [4], we know that the finite fundamental domain must satisfy the following properties:

1. The union of all $\mathbb{Z}^K$ shifts of the fundamental domain covers the infinite graph

2. Different shifts of the fundamental domain have no vertices in common.

A $\mathbb{Z}^K$-periodic graph is generated by shifting copies of the fundamental domain along k linearly independent vectors. As seen by the conditions above, vertices of the fundamental domain cannot overlap, and this necessitates the creation of a new vertex pair which arises from breaking an edge of the graph and defining two new vertices at the break. These newly created vertices are called *quasi-connected* vertices, and vertices that come from the same edge will be referred to as *paired quasi-connected vertices*. Due to the periodic nature of these graphs, the quasi-connected pairs must have the same conditions, such as electrical potential values, assigned to both vertices in the pair [2]. When recreating the infinite graph from the fundamental domain, the fundamental domain is shifted in such a way that paired quasi-connected vertices connect, recreating the edge in the infinite graph and removing the quasi-connected vertices.

A Dirac cone is present in the spectrum of a select few materials, such as graphene. In this project, touching points are shown to be present in the spectrum of the Schrödinger operator acting on the infinite periodic graph of graphene by calculating the spectrum of the magnetic flux Schrödinger operator on a fundamental domain after it has been unioned for all values of the variables α_1 and α_2. Visually a Dirac conical point is a point where two surfaces from the spectrum are shaped like a cone and touch each other. This phenomenon is shown clearly in figure 2.

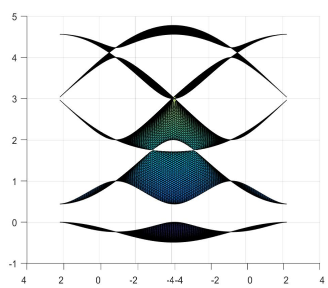

Figure 2: This figure shows several touching points between spectral bands and the shape of these touching points indicates that they are Dirac conical points.

Unitary equivalent operators have the same spectra, but different eigenfuntions. The *magnetic flux Schrödinger* operator, $\mathcal{H}^\alpha$, is defined as $\mathcal{H}^\alpha = Q - A - M^\alpha$ where

$$M^\alpha_{u,v} = \begin{cases} e^{i\alpha_j} & \text{if } (u,v) \text{ is the jth quasi-connected pair,} \\ e^{-i\alpha_j} & \text{if } (v,u) \text{ is the jth quasi-connected pair,} \\ 0 & \text{otherwise.} \end{cases} \tag{2.0.3}$$

and $\mathcal{H}^\alpha$ is an operator that is unitarily equivalent to the magnetic Schrödinger operator after summing the potentials around the jth cycle of the graph. Due to the periodicity of $e^{i\alpha}$, we can restrict each α_j to an interval of length 2π. The collection of intervals being unioned over is known as the *Brillouin zone* and is described as $[-\pi,\pi]^k$ for a $\mathbb{Z}^k$ periodic graph.

By Floquet-Bloch Theory we can recreate the spectrum of the Schrödinger operator on the infinite graph by calculating the spectrum of the $\mathcal{H}^\alpha$ operator acting on the fundamental domain of the infinite graph, and then taking the union over all α_j. This is because the operator, $\mathcal{H}^\alpha$, is unitarily equivalent to the magnetic Schrödinger operator which is unitarily equivalent to the Schrödinger operator after unioning over all α_j.

3 Graphene

In this project, spectral touching points are found by inspecting the spectrum of the magnetic flux Schrödinger operator acting on a fundamental domain. Dirac cones are a specific kind of touching points [1], so the search for touching points can help narrow the set of points that need to be evaluated to find Dirac cones. Once touching points were found numerically, the eigenvectors of the touching sheets were computationally determined. After the general form of these vectors was found, the restrictions on electrical potential values were determined using linear algebra.

The search for viable electrical potentials that produce Dirac cones in the spectrum of a hexagonal lattice graph is made easier by the need for symmetry in the infinite graph as demonstrated by Berkolaiko and Comech [1]. With a hexagonal lattice the potential symmetry necessary to have a Dirac cone is rotation by $2\pi/3$, inversion, and horizontal reflection. This means that for the chosen fundamental domain the electrical potentials at vertices one and five must be equal, similarly the electrical potentials at vertices two and four must be equal, and the electrical potential at vertex three does not need to correspond to any other vertex. Figure 3 shows these symmetry conditions being imposed on the fundamental domain, with vertices that are bound by symmetry conditions sharing an electrical potential label. The picture also shows quasi-connected pairs as vertices that have the same shape.

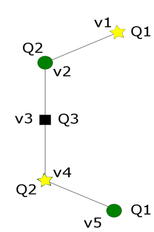

Figure 3: The chosen fundamental domain of graphene with vertices numbered, electrical potential labeled to show symmetry, and quasi-connected vertices color and shape coded.

The following matrix is the magnetic flux Schrödinger operator, $\mathcal{H}^\alpha$, acting

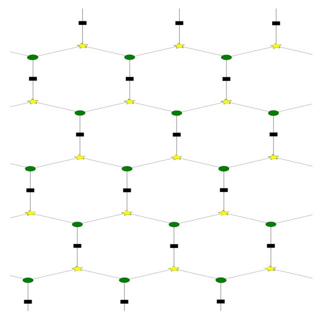

Figure 4: This is a section of the infinite graph representative of graphene. This graph has been constructed so that the same quasi-connected pairs form the fundamental domain use the same shape, in this way it is easy to see how the chosen fundamental domain generates the infinite graph

on the chosen fundamental domain of graphene:

$$H^{\alpha} = \begin{bmatrix} q_1 & -1 & 0 & -e^{i\alpha_1} & 0 \\ -1 & q_2 & -1 & 0 & -e^{i\alpha_2} \\ 0 & -1 & q_3 & -1 & 0 \\ -e^{-i\alpha_1} & 0 & -1 & q_2 & -1 \\ 0 & -e^{-i\alpha_2} & 0 & -1 & q_1 \end{bmatrix} \tag{3.0.1}$$

where $q_1, q_2, q_3 \in \mathbb{R}$ represent the electrical potential values at the corresponding vertices of the fundamental domain.

I found the eigenvectors for every touching point in the spectrum and two sets of eigenvectors were found. In the case where all electrical potentials are equal, the following three vectors formed a basis for the eigenspace:

$$v_1 = \begin{bmatrix} 0 \\ -1 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \tag{3.0.2}$$

$$v_2 = \begin{bmatrix} -1 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \tag{3.0.3}$$

and

$$v_3 = \begin{bmatrix} 1 \\ 0 \\ -2 \\ 0 \\ 1 \end{bmatrix}. \tag{3.0.4}$$

In the general case, the following vector forms were found:

$$\tilde{v}_1 = \begin{bmatrix} a \\ b \\ 0 \\ -b \\ -a \end{bmatrix} \tag{3.0.5}$$

and

$$\tilde{v}_2 = \begin{bmatrix} c \\ d \\ f \\ d \\ c \end{bmatrix}. \tag{3.0.6}$$

3.1 $q_1 = q_2 = q_3$

This section concerns the case where all three electrical potential values are equal. MATLAB reported that three linearly independent eigenvectors correspond to the same eigenvalue in this case and were of the form (3.0.2), (3.0.3), and (3.0.4). I multiplied the matrix (3.0.1) by v_1, v_2, and v_3 and then set the produced vectors equal to the eigenvectors multiplied by the eigenvalue λ which results in the following non-trivial sets of equations:

$$\begin{cases} 0 = 1 - e^{i\alpha_1} & (3.1.1) \\ \lambda = q & (3.1.2) \\ 0 = e^{-i\alpha_2} - 1 & (3.1.3) \end{cases}$$

$$\begin{cases} \lambda = q & (3.1.4) \\ 0 = e^{-i\alpha_1} - 1 & (3.1.5) \end{cases}$$

$$\begin{cases} \lambda = q & (3.1.6) \\ 0 = -1 + 2 - e^{i\alpha^2} & (3.1.7) \\ 0 = -e^{-i\alpha_1} - 1 + 2 & (3.1.8) \end{cases}$$

.

To summarize, from equations (3.1.1)-(3.1.3) we have that $\lambda = q$ and that $\alpha_1 = \alpha_2 = 0$. It is also clear that the remaining equations are satisfied by these conditions.

Conclusion: In the case where $q_1 = q_2 = q_3 = q$, all $q \in \mathbb{R}$ produce touching points at $\alpha_1 = \alpha_2 = 0$.

3.2 General Case

Here I consider the general case to be one that has no enforced relationship on the electrical potential values aside from symmetry conditions. The work in the following case does not concern the instance where $q_1 = q_2 = q_3$, as that case was addressed in the previous section. It will be demonstrated that every other combination of electrical potential values has at least one touching point with eigenvectors of the form (3.0.5) and (3.0.6).

When the matrix (3.0.1) is multiplied by $\tilde{v}_1$ and $\tilde{v}_2$ and the resulting vectors are set equal to the chosen eigenvectors multiplied by the common eigenvalue, λ, the following sets of equations are produced:

$$
\begin{cases}
a\lambda = aq_1 - b + be^{i\alpha_1} & (3.2.1)\\
b\lambda = -a + bq_2 + ae^{i\alpha_2} & (3.2.2)\\
0 = -b + b & (3.2.3)\\
-b\lambda = -bq_2 + a - ae^{-i\alpha_1} & (3.2.4)\\
-a\lambda = -aq_1 + b - be^{-i\alpha_2} & (3.2.5)
\end{cases}
$$

and

$$
\begin{cases}
c\lambda = cq_1 - d - de^{i\alpha_1} & (3.2.6)\\
d\lambda = -c + dq_2 - f - ce^{i\alpha_2} & (3.2.7)\\
f\lambda = -d + fq_3 - d & (3.2.8)\\
d\lambda = dq_2 - f - c - ce^{-i\alpha_1} & (3.2.9)\\
c\lambda = cq_1 - d - de^{-i\alpha_2} & (3.2.10)
\end{cases}
$$

Adding equations (3.2.2) and (3.2.4) gives $ae^{i\alpha_2} = ae^{-i\alpha_1}$ so either $a = 0$ or $\alpha_1 = -\alpha_2$. By adding equation (3.2.1) to equation (3.2.5) we see that $be^{i\alpha_1} = be^{-i\alpha_2}$ so either $b = 0$ or $\alpha_1 = -\alpha_2$. Since both a and b cannot be zero when $\tilde{v}_1$ is an eigenvector, $\alpha_1 = -\alpha_2$. For the remainder of this section, α will refer to α_1 (so $-\alpha$ will correspond to α_2).

When solving for the variables in these systems of equations explicitly, it appears that when $\alpha = 0$, $\alpha = \pi$, $\lambda = q_1$, $\lambda = q_2$, or $\lambda = q_3$ the variables in the eigenvectors of interest become undefined. These undefined variables will be addressed on a case by case basis in the following subsections. Aside from these values, both eigenvectors are well defined for all electrical potential values, so touching points will occur for all electrical potential values that do not occur where $\lambda = q_1$, $\lambda = q_2$, or $\lambda = q_3$ or where the electrical potential forces $\alpha = 0$ or $\alpha = \pi$ and

3.2.1 $\alpha = 0$

Solving equation (3.2.2) for a gives:

$$a = \frac{b(\lambda - q_2)}{-1 + e^{-i\alpha}}. \tag{3.2.11}$$

which is undefined at $\alpha = 0$. When $\alpha = 0$, the systems of equations given previously become the following:

$$\begin{cases} a\lambda = aq_1 & (3.2.12) \\ b\lambda = bq_2 & (3.2.13) \\ 0 = -b + b & (3.2.14) \\ -b\lambda = -bq_2 & (3.2.15) \\ -a\lambda = -aq_1 & (3.2.16) \end{cases}$$

and

$$\begin{cases} c\lambda = cq_1 - 2d & (3.2.17) \\ d\lambda = -2c + dq_2 - f & (3.2.18) \\ f\lambda = -2d + fq_3 & (3.2.19) \\ d\lambda = dq_2 - f - 2c & (3.2.20) \\ c\lambda = cq_1 - 2d & (3.2.21) \end{cases}$$

. When a does not equal zero, $\lambda = q_1$, when b does not equal zero, $\lambda = q_2$; and when neither a nor b equal zero, $\lambda = q_1 = q_2$.

If $\lambda = q_1$, by equation (3.2.17) $d = 0$, by equation (3.2.19) $\lambda = q_3$, and by equation (3.2.18) $f = -2c$ in this case $\tilde{v}_2$ is

$$\tilde{v}_2 = \begin{bmatrix} c \\ 0 \\ -2c \\ 0 \\ c \end{bmatrix} \tag{3.2.22}$$

and is still a well defined eigenvector. Otherwise, if $\lambda = q_2$, by equation (3.2.18) $f = -2c$. If $\lambda = q_1 = q_2$, then we have the same eigenvector from the $\lambda = q_1$ case. This shows that all variables are still well defined when $\alpha = 0$.

Conclusion: For the case where $\alpha = 0$, I have shown that all electrical potential values produce touching points when they are of the form $\lambda = q_1 = q_2 = q_3$.

3.2.2 $\alpha = \pi$ and $\alpha = -\pi$

Solving for d using equation (3.2.6) gives

$$d = \frac{c(\lambda - q_1)}{(-1 - e^{i\alpha})}. \tag{3.2.23}$$

This equation is undefined when $\alpha = \pi$ or $\alpha = -\pi$. Due to the periodicity of e, both of these values produce the same systems of equations so by addressing the $\alpha = \pi$ case, I will address both cases. When $\alpha = \pi$, the systems of equations given previously become:

$$\begin{cases} a\lambda = aq_1 - 2b & (3.2.24) \\ b\lambda = bq_2 - 2a & (3.2.25) \\ 0 = -b + b & (3.2.26) \\ -b\lambda = -bq_2 + 2a & (3.2.27) \\ -a\lambda = -aq_1 + 2b & (3.2.28) \end{cases}$$

and

$$\begin{cases} c\lambda = cq_1 & (3.2.29) \\ d\lambda = dq_2 - f & (3.2.30) \\ f\lambda = -d + fq_3 - d & (3.2.31) \\ d\lambda = dq_2 - f & (3.2.32) \\ c\lambda = cq_1 & (3.2.33) \end{cases}$$

. By equation (3.2.29) either $c = 0$ or $\lambda = q_1$. If $\lambda = q_1$, by equation (3.2.24) $b = 0$ and by equation (3.2.25) $a = 0$. Since this causes vector $\tilde{v}_1$ to be the zero vector, λ does not equal q_1 so we must have $c = 0$. By equation (3.2.30) $f = -d(\lambda - q_2)$ and by equation (3.2.31) $d = \frac{f(\lambda - q_3)}{-2}$. This means that λ does not equal q_2 or q_3, because that would cause the vector $\tilde{v}_2$ to be the zero vector. This means that when $\alpha = \pi$ we do have touching points for all electrical potentials but, λ does not equal q_1, q_2, or q_3.

3.2.3 $\lambda = q_1$

When solving for c using equation (3.2.6) the following equality is produced:

$$c = \frac{d(-1 + e^{i\alpha})}{\lambda - q_1}, \tag{3.2.34}$$

which is undefined when $\lambda = q_1$. When $\lambda = q_1$, the systems of equations given previously become:

$$\begin{cases} 0 = -b + be^{i\alpha} & (3.2.35) \\ b\lambda = -a + bq_2 + ae^{-i\alpha} & (3.2.36) \\ 0 = -b + b & (3.2.37) \\ -b\lambda = -bq_2 + a - ae^{-i\alpha} & (3.2.38) \\ 0 = b - be^{i\alpha} & (3.2.39) \end{cases}$$

and

$$\begin{cases} 0 = -d - de^{i\alpha} & (3.2.40) \\ d\lambda = -c + dq_2 - f - ce^{-i\alpha} & (3.2.41) \\ f\lambda = -d + fq_3 - d & (3.2.42) \\ d\lambda = dq_2 - f - c - ce^{-i\alpha} & (3.2.43) \\ 0 = -d - de^{i\alpha} & (3.2.44) \end{cases}$$

. By equation (3.2.35) $b = 0$ or $\alpha = 0$. If $b = 0$, then by equation (3.2.36) $a = 0$ or $\alpha = 0$. Since both a and b cannot equal zero, $\alpha = 0$. As shown in section 3.2.1 if $\alpha = 0$, then $\lambda = q_1 = q_2 = q_3$, $d = 0$, and $f = -2c$.

3.2.4 $\lambda = q_2$

When solving for b using equation (3.2.2), the following equality is produced:

$$b = \frac{a(-1 + e^{-i\alpha})}{\lambda - q_2}, \qquad (3.2.45)$$

which is undefined when $\lambda = q_2$. When $\lambda = q_2$ the systems of equations given previously become:

$$\begin{cases} a\lambda = aq_1 - b + be^{i\alpha} & (3.2.46) \\ 0 = -a + ae^{-i\alpha} & (3.2.47) \\ 0 = -b + b & (3.2.48) \\ -b\lambda = -bq_2 + a - ae^{-i\alpha} & (3.2.49) \\ 0 = b - be^{i\alpha} & (3.2.50) \end{cases}$$

and

$$\begin{cases} c\lambda = cq_1 - d - de^{i\alpha} & (3.2.51) \\ 0 = -c - f - ce^{-i\alpha} & (3.2.52) \\ f\lambda = -d + fq_3 - d & (3.2.53) \\ d\lambda = dq_2 - f - c - ce^{-i\alpha} & (3.2.54) \\ c\lambda = cq_1 - d - de^{i\alpha} & (3.2.55) \end{cases}$$

. By equation (3.2.47) $a = 0$ or $\alpha = 0$. If $a = 0$, then by equation (3.2.46) $b = 0$ or $\alpha = 0$. Since both a and b cannot equal zero, $\alpha = 0$. As shown in section 3.2.1 if $\alpha = 0$, then $\lambda = q_1 = q_2 = q_3$, $d = 0$, and $f = -2c$.

3.2.5 $\lambda = q_3$

when solving for f using equation (3.2.8), the following equality is produced:

$$f = \frac{-2d}{\lambda - q_3}, \tag{3.2.56}$$

which is undefined when $\lambda = q_3$. When $\lambda = q_3$, the systems of equations given previously become:

$$\begin{cases} a\lambda = aq_1 - b + be^{i\alpha} & (3.2.57) \\ b\lambda = -a + bq_2 + ae^{-i\alpha} & (3.2.58) \\ 0 = -b + b & (3.2.59) \\ -b\lambda = -bq_2 + a - ae^{-i\alpha} & (3.2.60) \\ -a\lambda = -aq_1 + b - be^{i\alpha} & (3.2.61) \end{cases}$$

and

$$\begin{cases} c\lambda = cq_1 - d - de^{i\alpha} & (3.2.62) \\ d\lambda = -c + dq_2 - f - ce^{-i\alpha} & (3.2.63) \\ 0 = -d - d & (3.2.64) \\ d\lambda = dq_2 - f - c - ce^{-i\alpha} & (3.2.65) \\ c\lambda = cq_1 - d - de^{i\alpha} & (3.2.66) \end{cases}$$

. By equation (3.2.64) $d = 0$. When $d = 0$, by equation (3.2.62) $c = 0$ or $\lambda = q_1$. If $c = 0$ and $d = 0$ then by equation (3.2.63) $f = 0$ and $\tilde{v}_2$ becomes the zero vector. This means that c cannot equal zero so $\lambda = q_1$. As shown in section 3.2.3 when $\lambda = q_1$, $\alpha = 0$ and $\lambda = q_1 = q_2 = q_3$, $d = 0$, and $f = -2c$.

3.2.6 Conclusion of the General Case

In the general case it was shown that all values of electrical potential produced tocuhing points. In the sections that followed the general case, I addressed the cases that seemed to cause variables of the chosen eigenvectors to be undefined and showed that for all of them, all $q \in \mathbb{R}$ still produced eigenvectors. However these cases we know more about the eigenvalue and where the touching point occurs. If $\alpha = 0$, $\lambda = q_1$, $\lambda = q_2$, or $\lambda = q_3$ then $\lambda = q_1 = q_2 = q_3 = q$ and it was previously shown that all $q \in \mathbb{R}$ produce touching points in this case. If $\alpha = \pi$ or $\alpha = -\pi$ then λ does not equal q_1, q_2, or q_3 and for all values of electrical potential the variables that make up the chosen eigenvectors are well defined, so all electrical potential values that satisfy these conditions produce touching points.

4 Examination of the different symmetry criteria

In this section I will be investigating the effects of applying different symmetry conditions to a novel graph, a section of which is shown in figure 5. This section will start with the most stringent of the chosen cases and then progress to the final case, where no symmetry conditions are enforced. The fundamental domain for this graph is shown in 6.

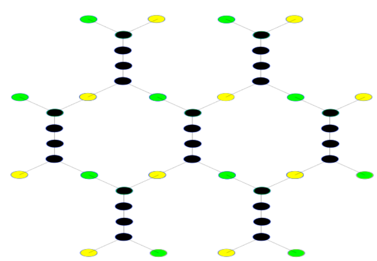

Figure 5: The chosen novel graph. This graph shares the hexagonal lattice of graphene, but has several extra vertices in each shell.

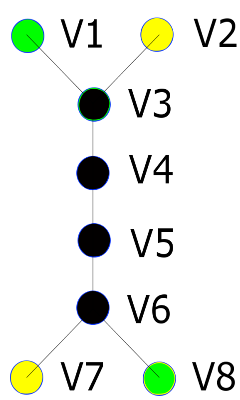

Figure 6: The chosen fundamental domain of the novel graph, with vertices numbered, and quasi-connected vertices color coded.

4.1 Rotational and Horizontal symmetry

For the chosen graph to have rotational and horizontal symmetry the elctrical potential at vertices V1, V2, V4, V5, V7, and V8 must be equal; this common value will be called q_1. The electrical potentials values at V3 and V6 must also be equal, and this common value will be called q_2. Because the electrical potentials of the quasi-connected vertex pairs V1, V8 and V2,V7 are equal this graph satisfies periodic symmetry conditions. The matrix representative of the fundamental domain of this graph being acted on by the magnetic flux Schrödinger operator, with both rotational and horizontal symmetry is

$$RH^{\alpha} = \begin{bmatrix} q_1 & 0 & -1 & 0 & 0 & 0 & 0 & -e^{i\alpha_1} \\ 0 & q_1 & -1 & 0 & 0 & 0 & -e^{i\alpha_2} & 0 \\ -1 & -1 & q_2 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & q_1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & q_1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & q_2 & -1 & -1 \\ 0 & -e^{-i\alpha_2} & 0 & 0 & 0 & -1 & q_1 & 0 \\ -e^{-i\alpha_1} & 0 & 0 & 0 & 0 & -1 & 0 & q_1 \end{bmatrix}. \tag{4.1.1}$$

It was computationally determined that two linearly independent eigenvectors corresponding to the same eigenvalue in the spectrum of this matrix were of the form:

$$x_1 = \begin{bmatrix} a \\ b \\ c \\ d \\ -d \\ -c \\ -a \\ -b \end{bmatrix} \tag{4.1.2}$$

and

$$x_2 = \begin{bmatrix} -f \\ g \\ h \\ I \\ I \\ h \\ -f \\ g \end{bmatrix}. \tag{4.1.3}$$

Multiplying the matrix (4.1.1) by the eigenvectors (4.1.2) and (4.1.3), and then setting the resulting vectors equal to (4.1.2) and (4.1.3) multiplied by the common eigenvalue, λ, gives the following sets of equations:

$$\begin{cases} a\lambda = aq_1 - c + be^{i\alpha_1} & (4.1.4) \\ b\lambda = bq_1 - c + ae^{i\alpha_2} & (4.1.5) \\ c\lambda = cq_2 - a - b - d & (4.1.6) \\ d\lambda = dq_1 - c + d & (4.1.7) \\ -d\lambda = -dq_1 + c - d & (4.1.8) \\ -c\lambda = -cq_2 + a + b + d & (4.1.9) \\ -a\lambda = -aq_1 + c - be^{-i\alpha_2} & (4.1.10) \\ -b\lambda = -bq_1 + c - ae^{-i\alpha_1} & (4.1.11) \end{cases}$$

and

$$\begin{cases} -f\lambda = -fq_1 - h - ge^{i\alpha_1} & (4.1.12) \\ g\lambda = gq_1 - h + fe^{i\alpha_2} & (4.1.13) \\ h\lambda = hq_2 + f - g - I & (4.1.14) \\ I\lambda = Iq_1 - h - I & (4.1.15) \\ I\lambda = Iq_1 - h - I & (4.1.16) \\ h\lambda = hq_2 + f - g - I & (4.1.17) \\ -f\lambda = -fq_1 - h - ge^{-i\alpha_2} & (4.1.18) \\ g\lambda = gq_1 - h + fe^{-i\alpha_1} & (4.1.19) \end{cases}$$

.

By adding equation (4.1.4) to equation (4.1.10) we see that $be^{i\alpha_1} = be^{-i\alpha_2}$. If b does not equal zero, then $\alpha_1 = -\alpha_2$. By adding equation (4.1.5) to equation (4.1.11) $ae^{i\alpha_2} = ae^{-i\alpha_1}$. If a does not equal zero, then $\alpha_2 = -\alpha_1$. If $a = b = 0$, then by equation (4.1.4) $c = 0$, and by (4.1.6) $d = 0$. Hence, if $a = b = 0$, the vector (4.1.2) is equal to the zero vector, and is not an eigenvector. This means that $\alpha_1 = -\alpha_2$. For the rest of this section, $\alpha = \alpha_1 = -\alpha_2$.

From equation (4.1.4) $b = (a(\lambda - q_1) + c)e^{-i\alpha}$.
From equation (4.1.5) $a = -(b(\lambda - q_1) + c)e^{-i\alpha}$.
From equation (4.1.6) $d = -c(\lambda - q_2) - a - b$.
From equation (4.1.7) $c = -d(\lambda - q_2) + d$.
From equation (4.1.12) $g = (f(\lambda - q_1) - h)e^{-i\alpha}$.
From equation (4.1.13) $f = (g(\lambda - q_1) + h)e^{-i\alpha}$.
From equation (4.1.14) $I = -h(\lambda - q_2) + f - g$.
From equation (4.1.15) $h = -I(\lambda - q_1 + 1)$.

Conclusion: Because all variables that make up the chosen general eigenvectors for this matrix are well defined for all values of electrical potential, all electrical potential values will produce touching points when both rotational and horizontal symmetry are enforced along the line $\alpha_1 = -\alpha_2$. *Remark*: It is worth noting that horizontal symmetry on its own will not be addressed, because it enforces conditions equivalent to rotational and horizontal symmetry.

4.2 Rotational symmetry

For the chosen graph to have rotational symmetry, the elctrical potential at vertices V1,V2 and V4 must be equal; this common values will be called q_1. Because of the required periodic symmetry of this graph, the electrical potential at verticies V5, V7, and V8 must be also be equal to q_1. The electrical potentials at vertices V3 and V6 are free and will be called q_2 and q_3 respectively. The matrix representative of the fundamental domain of this graph being acted on by the magnetic flux Schrödinger operator, with only rotational symmetry enforced is

$$R^\alpha = \begin{bmatrix} q_1 & 0 & -1 & 0 & 0 & 0 & 0 & -e^{i\alpha_1} \\ 0 & q_1 & -1 & 0 & 0 & 0 & -e^{i\alpha_2} & 0 \\ -1 & -1 & q_2 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & q_1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & q_1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & q_3 & -1 & -1 \\ 0 & -e^{-i\alpha_2} & 0 & 0 & 0 & -1 & q_1 & 0 \\ -e^{-i\alpha_1} & 0 & 0 & 0 & 0 & -1 & 0 & q_1 \end{bmatrix}. \tag{4.2.1}$$

It was computationally determined that the linearly independent eigenvectors corresponding to the same eigenvalue for this graph have the following forms:

$$\tilde{v}_1 = \begin{bmatrix} a \\ b \\ 0 \\ c \\ c \\ 0 \\ b \\ a \end{bmatrix} \tag{4.2.2}$$

and

$$\tilde{v}_2 = \begin{bmatrix} 0 \\ d \\ 0 \\ f \\ f \\ 0 \\ d \\ 0 \end{bmatrix}. \tag{4.2.3}$$

Multiplying the matrix (4.2.1) by the eigenvectors (4.2.2) and (4.2.3), and then setting the resulting vectors equal to (4.2.2) and (4.2.3) multiplied by the common eigenvalue, λ, gives the following sets of non-trivial equations:

$$\begin{cases} a\lambda = aq_1 - ae^{i\alpha_1} & (4.2.4) \\ b\lambda = bq_1 - be^{i\alpha_2} & (4.2.5) \\ 0 = -a - b - c & (4.2.6) \\ c\lambda = cq_1 - c & (4.2.7) \\ b\lambda = bq_1 - be^{-i\alpha_2} & (4.2.8) \\ a\lambda = aq_1 - ae^{-i\alpha_1} & (4.2.9) \end{cases}$$

and

$$\begin{cases} d\lambda = dq_1 - de^{i\alpha_2} & (4.2.10) \\ 0 = -d - f & (4.2.11) \\ f\lambda = fq_1 - f & (4.2.12) \\ d\lambda = dq_1 - de^{-i\alpha_2} & (4.2.13) \end{cases}$$

From equation (4.2.11) if either $f = 0$ or $d = 0$, then the vector (4.2.3) is the zero vector and not an eigenvector. Since both f and d are non-zero equation (4.2.10) becomes $\lambda = q_1 - e^{i\alpha_2}$ and equation (4.2.12) becomes $\lambda = q_1 - 1$. For these equations to be satisfied $\alpha_2 = 0$.

From equation (4.2.6) $a = -b - c$. For vector (4.2.2) to be an eigenvector, at least two of the variables a, b, and c must be non-zero. If $a = 0$, then $b = -c$ and no new information is made available from the systems of equations. If a is not equal to zero and either $b = 0$ or $c = 0$, then from equation (4.2.4) $\lambda = q_1 - e^{i\alpha_1}$, so $\alpha_1 = 0$.

Conclusion: Since all variables that constitute the eigenvectors of interest in this case are not dependent on the values of electrical potential, all electrical potential values will produce a touching point in this case. Further more, all of these touching points can be shown to happen where $\alpha_2 = 0$, and when a does not equal zero $\alpha_1 = 0$. This is significantly more restrictive than the rotational and horizontal symmetry case, indicating that as fewer symmetry conditions are applied, touching points occur in fewer places.

4.3 No Symmetry

This section will only have the periodic symmetry of the graph enforced. This means that the electrical potentials at V1 and V8 must be equal, this common value will be called q_1. The electrical potential at vertices V2 and V7 also must be equal, and this alue will be called q_2. Vertice V3, V4, V5, and V6 are all free and the electrical potential values at those vertices will be referred to as q_3, q_4, q_5, and q_6 respectively. The matrix representative of the magnetic flux Schrödinger operator acting on the chosen fundamental domain with no symmetry conditions enforced is:

$$NS^{\alpha} = \begin{bmatrix} q_1 & 0 & -1 & 0 & 0 & 0 & 0 & -e^{i\alpha_1} \\ 0 & q_2 & -1 & 0 & 0 & 0 & -e^{i\alpha_2} & 0 \\ -1 & -1 & q_3 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & q_4 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & q_5 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & q_6 & -1 & -1 \\ 0 & -e^{-i\alpha_2} & 0 & 0 & 0 & -1 & q_2 & 0 \\ -e^{-i\alpha_1} & 0 & 0 & 0 & 0 & -1 & 0 & q_1 \end{bmatrix}. \tag{4.3.1}$$

The linearly independent eigenvectors corresponding to the same eigenvalue in this case have the following forms:

$$\tilde{z}_1 = \begin{bmatrix} a \\ -a \\ 0 \\ 0 \\ 0 \\ 0 \\ b \\ -b \end{bmatrix} \tag{4.3.2}$$

and

$$\tilde{z}_2 = \begin{bmatrix} c \\ c \\ d \\ f \\ g \\ h \\ I \\ I \end{bmatrix}. \tag{4.3.3}$$

Multiplying the matrix (4.3.1) by the eigenvectors (4.3.2) and (4.3.3), and then setting the resulting vectors equal to (4.3.2) and (4.3.3) multiplied by the common eigenvalue, λ, gives the following sets of non-trivial equations:

$$\begin{cases} a\lambda = aq_1 + be^{i\alpha_1} & (4.3.4) \\ -a\lambda = -aq_2 - be^{i\alpha_2} & (4.3.5) \\ b\lambda = bq_2 + ae^{-i\alpha_2} & (4.3.6) \\ -b\lambda = -bq_1 - ae^{-i\alpha_1} & (4.3.7) \end{cases}$$

and

$$\begin{cases} c\lambda = cq_1 - d - Ie^{i\alpha_a} & (4.3.8) \\ c\lambda = cq_2 - d - Ie^{i\alpha_2} & (4.3.9) \\ d\lambda = -2c + dq_3 - f & (4.3.10) \\ f\lambda = -g - d + fq_4 & (4.3.11) \\ g\lambda = gq_5 - f - h & (4.3.12) \\ h\lambda = -g - 2I + hq_6 & (4.3.13) \\ I\lambda = Iq_2 - h - ce^{-i\alpha_2} & (4.3.14) \\ I\lambda = Iq_1 - h - ce^{-i\alpha_1}. & (4.3.15) \end{cases}$$

From (4.3.6) $(\lambda - q_2) = \frac{a}{be^{i\alpha_2}}$, and from (4.3.5) $(\lambda - q_2) = \frac{be^{i\alpha_2}}{a}$ which means that $a = be^{i\alpha_2}$. Next, from (4.3.4) $(\lambda - q_1) = \frac{be^{i\alpha_1}}{a}$, and from(4.3.7) $(\lambda - q_1) = \frac{a}{be^{i\alpha_1}}$so we also have $a = be^{i\alpha_1}$. Since $a = be^{i\alpha_1}$ and $a = be^{i\alpha_2}$, $\alpha_1 = \alpha_2$ if b does not equal zero. If $b = 0$ by equation (4.3.7) $a = 0$ and the vector (4.3.2) is the zero vector, so b does not equal zero and $\alpha_1 = \alpha_2$. For the rest of this section, α_1 and α_2 will be referred to as α.

From (4.3.4) $(\lambda - q_1) = \frac{be^{i\alpha}}{a}$, and from(4.3.7) $(\lambda - q_1) = \frac{a}{be^{i\alpha}}$. Setting the two equations equal and solving for a yields $a = be^{i\alpha}$. Combining this with equation (4.3.4) gives $a\lambda = aq_1 + a$ and because a does not equal zero, $\lambda = q_1 + 1$. Combining this with equation (4.3.5) gives $a\lambda = aq_2 + a$. If $a = 0$, then $b = 0$ so the vector (4.3.2) is the zero vector. Since a does not equal zero $\lambda = q_2 + 1$. Since both q_1 and q_2 are equal to $\lambda - 1$, $q_1 = q_2$.

From (4.3.8) $I = (-c(\lambda - q_1) - d)e^{-i\alpha}$.
From (4.3.10) $f = -d(\lambda - q_3) - 2c$
From (4.3.11) $d = -f(\lambda - q_4) - g$.
From (4.3.12) $h = -q(\lambda - q_5) - f$
From (4.3.13) $g = -h(\lambda - q_6) - 2I$.
From (4.3.14) $c = (-I(\lambda - q_1) - h)e^{i\alpha}$.

Conclusion: All variables that make up the chosen general eigenvectors for this matrix are well defined for all values of electrical potential, seemingly indicating that all electrical potential values will produce touching points. However, touching points only occur when $q_1 = q_2$, along the line $\alpha_1 = \alpha_2$. So in the case of no symmetry conditions being applied (other than those required by the periodicity of the graph) touching points will still occur, but they only occur when a stricter symmetry has been applied to the graph. *Remark*: This forced equality between q_1 and q_2 is equivalent to lateral symmetry, so lateral symmetry will not be addressed individually in this work.

5 Summary and Conclusion

In section 3, I was able to show that touching points will occur in the spectrum of the infinite graph representative of graphene for all possible real values of electrical potential. Different cases, like all electrical potentials being equal, caused touching points to occur at different values of α_1 and α_2, but all values of electrical potential cause touching points to occur at some α_1,α_2 coordinate. Since touching points indicate that Dirac cones could be present, all values of electrical potential have the possibility of producing Dirac cones, meaning that graphene could potentially possess Dirac cones at all electrical potential values (which it appears to visually).

In section 4, I demonstrated the loss of generality associated with reducing symmetry conditions. In the initial case of rotational and horizontal symmetry, all electrical potential values produce touching points along the line $\alpha_1 = -\alpha_2$. The case of strictly rotational symmetry still produced touching points for all electrical potential values however, all touching points occur at $\alpha_1 = \alpha_2 = 0$. Finally in the case of only periodic symmetry, touching points would only occur under conditions that mimicked a stricter symmetry condition, specifically that $q_1 = q_2$, which in this graph would be lateral symmetry. As long as lateral symmetry is met, all electrical potentials will produce touching points.

As a continuation of this project, I would like to mathematically determine which touching points were true Dirac cones, and which were touching points of a different topological nature. A second project extending this work would be to create a graph that has touching points, but no Dirac cones. Once this graph had been concocted, creating a material representative of that graph and and investigating its physical properties would be an interesting way to investigate the nature of the changes caused by Dirac cones compared to those caused by touching points.

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