Dirac Points in the Spectrum of Periodic Planar Networks

Michael Goldberg
University of Cincinnati

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Hamiltonian for Graphene: $H = -\Delta + V, \quad V(x) = \sum_{y \in \Lambda} V_0(x - y)$
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Translation symmetry is not quite transitive.
Each fundamental domain has two vertices.
General Properties:

For each $k$ in the Brillouin zone $\mathbb{R}^2/\Lambda^*$, there is a countably infinite set of real eigenvalues $E_1(k) \leq E_2(k) \leq \cdots$.

Functions $E_b(k)$ give energy bands and dispersion relations of $H$.

Multiplicities $E_n(k_0) = E_{n+1}(k_0)$ certainly occur, especially if you vary $V_0$ over a family of admissible potentials.
Two types of eigenvalue multiplicity:

1. “Incidental” band crossing as $V_0$ is varied.
Two types of eigenvalue multiplicity:

2. “Dirac points” or conical singularity of $E_{n,k}$.

The red graph is forbidden because $H$ is self-adjoint.

So Dirac points appear to be an edge case of spectral behavior...
But Fefferman, Weinstein (2012) showed that Dirac points occur for generic Hamiltonians with honeycomb symmetry.

Energy bands joined at a Dirac point cannot be pulled apart by small perturbations of the system.

[i.e. the figure is misleading.]
Our goal: Examine this phenomenon with a toy model.

Identify symmetries that might/might not be responsible for the remarkable stability of Dirac points in the honeycomb lattice.

Extrapolate, if possible, to other planar periodic materials.
Vertices of the toy model: 2 copies of a lattice, $L$ and $L + d$. 

\[ \begin{array}{c c c c c c c c c c c} 
\end{array} \]
Weighted edges of the toy model:

Edges from $x$ to $x + y$ in $L$ have weight $\lambda_y$.

Edges from $x + d$ to $x + y + d$ in $L + d$ have weight $\mu_y$.

Edges from $x$ to $x + y + d$ have weight $\nu_y$.

Connections don't need to be to closest neighbors.
This yields a graph Laplacian

$$\Delta \psi(x) = \begin{cases} 
\sum_{y \in L_0} \left[ \frac{1}{2} \lambda_y (\psi(x+y) + \psi(x-y) - 2\psi(x)) 
+ \nu_y (\psi(x+d+y) - \psi(x)) \right] & \text{if } x \in L_0, \\
\sum_{y \in L_0} \left[ \frac{1}{2} \mu_y (\psi(x+y) + \psi(x-y) - 2\psi(x)) 
+ \nu_y (\psi(x-d-y) - \psi(x)) \right] & \text{if } x \in L_d.
\end{cases}$$

Note that $\ell^2(L \cup L + d)$ has a basis of plane wave eigenfunctions.
Characterization of plane waves with frequency $k$.

$$\phi(x) = \begin{cases} 
  c_1e^{ik \cdot x} & \text{if } x \in L \\
  c_2e^{ik \cdot x} & \text{if } x \in L + d
\end{cases}$$

We can represent $\phi$ by the vector $\begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$.

Graph Laplacian is linear, preserves frequency of plane waves, so 
\[-\Delta \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = M(k) \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}\] for some $2 \times 2$ matrix $M(k)$. 
The exact formula is
\[-\Delta \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} \sum_{y \in L} (\lambda_y (1 - \cos(k \cdot y)) + \nu_y) & \sum_{y \in L} \nu_y e^{ik \cdot (y+d)} \\ \sum_{y \in L} \nu_y e^{-ik \cdot (y+d)} & \sum_{y \in L} (\nu_y + \mu_y (1 - \cos(k \cdot y))) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix},\]

and the band dispersion functions are eigenvalues of \( M(k) \).

Two energy bands given by \( E^\pm(k) = \)
\[
\left( \sum_{y \in L} (\lambda_y + \mu_y) \sin^2\left(\frac{k \cdot y}{2}\right) + \nu_y \right) \pm \sqrt{\left( \sum_{y \in L} (\lambda_y - \mu_y) \sin^2\left(\frac{k \cdot y}{2}\right) \right)^2 + \left| \sum_{y \in L} \nu_y e^{ik \cdot y} \right|^2}
\]

Discriminant has the form \( \sqrt{A(k)^2 + |B(k)|^2} \)

Side note: \( E^\pm(k) \) does not depend on \( d \).
Dirac points occur if discriminant goes to zero in nondegenerate way.

Naive analysis: Need $A(k)$, $\text{Re}(B(k))$, and $\text{Im}(B(k))$ to vanish for some $k$ in the Brillouin zone $\mathbb{R}^2/L^*$. That’s 3 equations, 2 variables.

Suppose internal connections on $L$ and $L + d$ are identical. This is the symmetry condition $\lambda_y = \mu_y$ for all $y \in L$. Then $A(k) \equiv 0$, so discriminant simplifies to $|B(k)|$. 
Under this assumption, Dirac points occur precisely when \( B(k) \) has a simple root. In other words, when the vector field
\[
B(k) = \begin{bmatrix} \text{Re}(B(k)) \\ \text{Im}(B(k)) \end{bmatrix}
\]
has a simple zero.

Simple zeros are locally stable under \( C^1 \) perturbations of \( B(k) \).

Conclusion: If Laplacian has a Dirac point for a particular choice of graph parameters \( \{\lambda_y = \mu_y, \nu_y\}_{y \in L} \), then it continues to do so for all nearby choices in an open neighborhood.
Example: Regular Graphene

\[ v_1 = \begin{bmatrix} \frac{3}{2} \\ \frac{\sqrt{3}}{2} \end{bmatrix}, \quad v_2 = \begin{bmatrix} \frac{3}{2} \\ -\frac{\sqrt{3}}{2} \end{bmatrix} \]

\[ d = \begin{bmatrix} -1 \\ 0 \end{bmatrix} \]

\[ \lambda_y = \mu_y = 0 \text{ for all } y \in L. \]

\[ \nu_0 = \nu_{v_1} = \nu_{v_2} = 1. \]

All other \( \nu_y = 0. \)

\[ B(k) = 1 + 2e^{i\left(\frac{3}{2}k_1\right)}\cos\left(\frac{\sqrt{3}}{2}k_2\right) \text{ has simple zeros at } k_0 = \begin{bmatrix} 0 \\ \pm \frac{4\pi}{3\sqrt{3}} \end{bmatrix}. \]
Existence of Dirac points does not require $\nu_0 = \nu_{v_1} = \nu_{v_2}$ exactly or the absence of interactions between other vertices.

It doesn’t depend on geometry of $v_1, v_2$, or $d$ at all.

All toy models sufficiently close also have a pair of Dirac points. (the frequency $k_0$ where they occur may vary)
Current project (joint work with V. Borovyk): Toy models with 3 or more copies of $L$ as vertices. What symmetry condition should take the place of $\lambda_y = \mu_y$?

Algebra becomes a major concern...the discriminant of a characteristic polynomial of even a $3 \times 3$ self-adjoint matrix $M(k)$ is ugly. Sum-of-squares trick is hard to reproduce.

Big question: Do these toy models provide any insight for Hamiltonians with periodic potentials on $\mathbb{R}^2$?