Dirac Points in the Spectrum of Periodic Planar Networks

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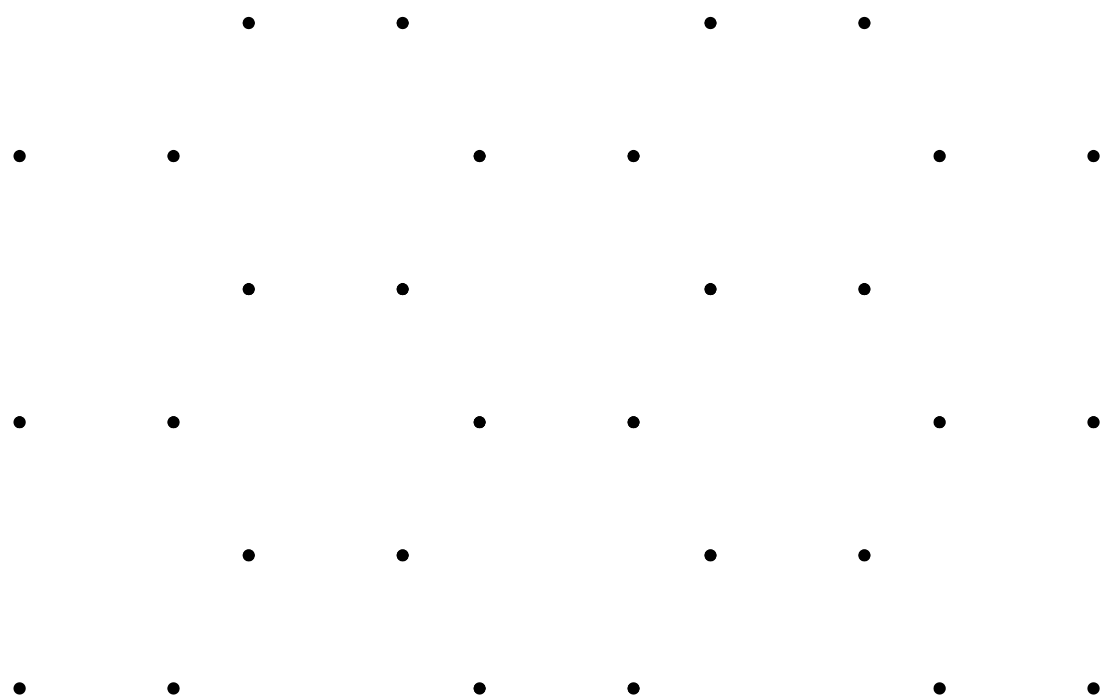
Hamiltonian for Graphene: $H = -\Delta + V, \;\; V(x) = \sum_{y \in \Lambda} V_0(x-y)$



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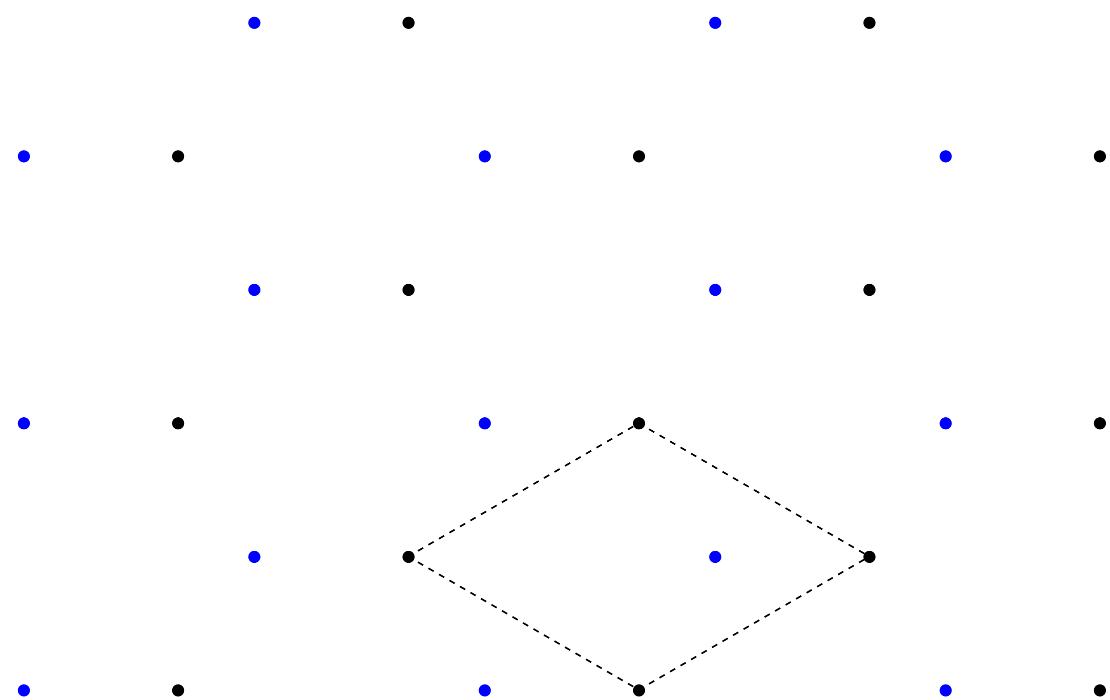


Translation symmetry is not quite transitive.
Each fundamental domain has two vertices.

General Properties:

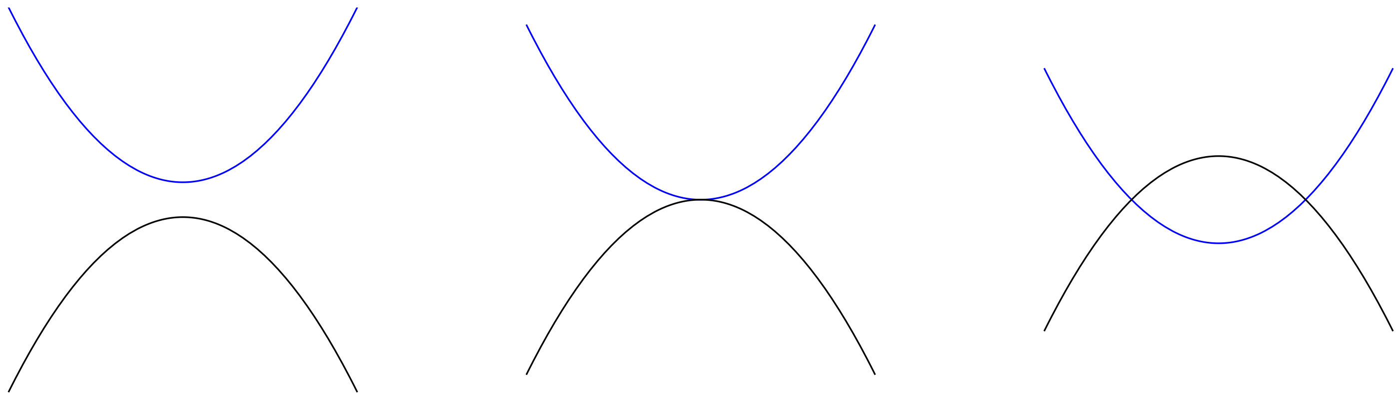
For each $\mathbf{k}$ in the Brillouin zone $\mathbb{R}^2/\Lambda^*$, there is a countably infinite set of real eigenvalues $E_1(\mathbf{k}) \leq E_2(\mathbf{k}) \leq \cdots$

Functions $E_b(\mathbf{k})$ give energy bands and dispersion relations of H.

Multiplicities $E_n(\mathbf{k}_0) = E_{n+1}(\mathbf{k}_0)$ certainly occur, especially if you vary V_0 over a family of admissible potentials.

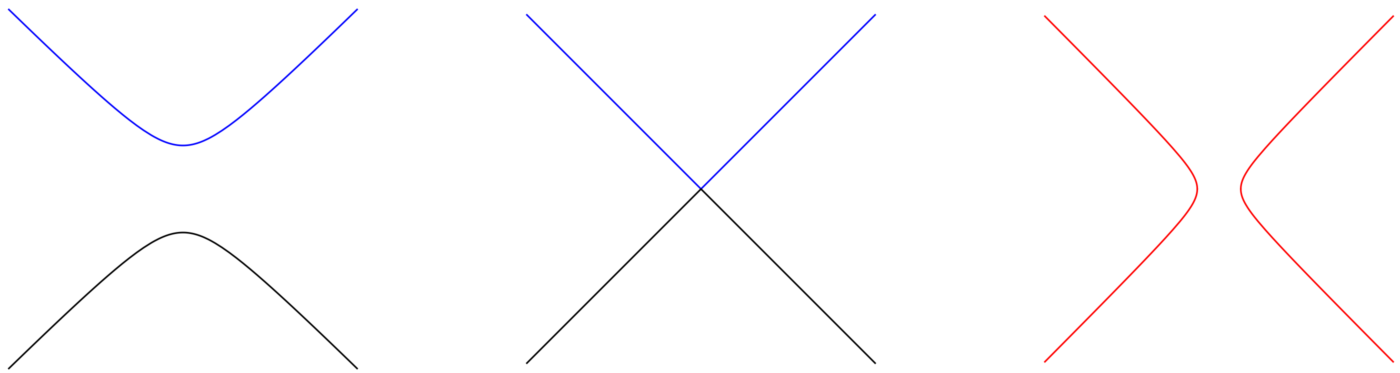
Two types of eigenvalue multiplicity:

1. "Incidental" band crossing as V_0 is varied.



Two types of eigenvalue multiplicity:

2. "Dirac points" or conical singularity of $E_n\mathbf{k}$.

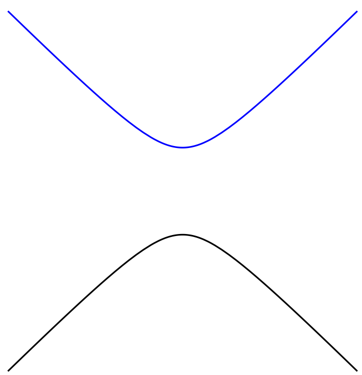
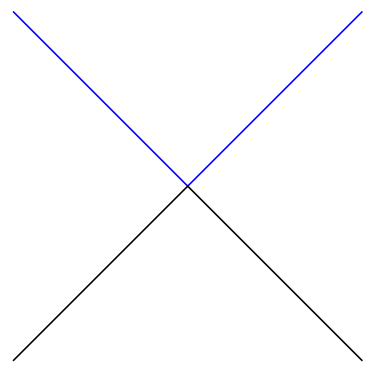


The red graph is forbidden because H is self-adjoint.

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.

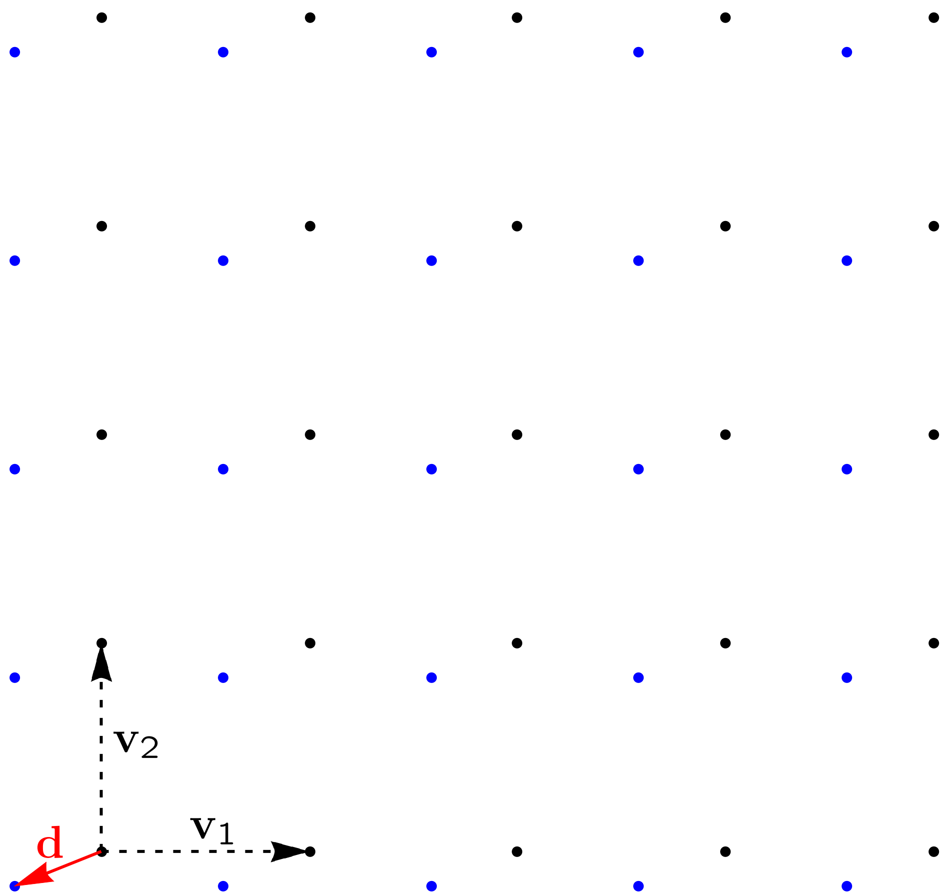
[i.e. the figure  $\Longleftrightarrow$  is misleading.]

Our goal: Examine this phenomenon with a toy model.

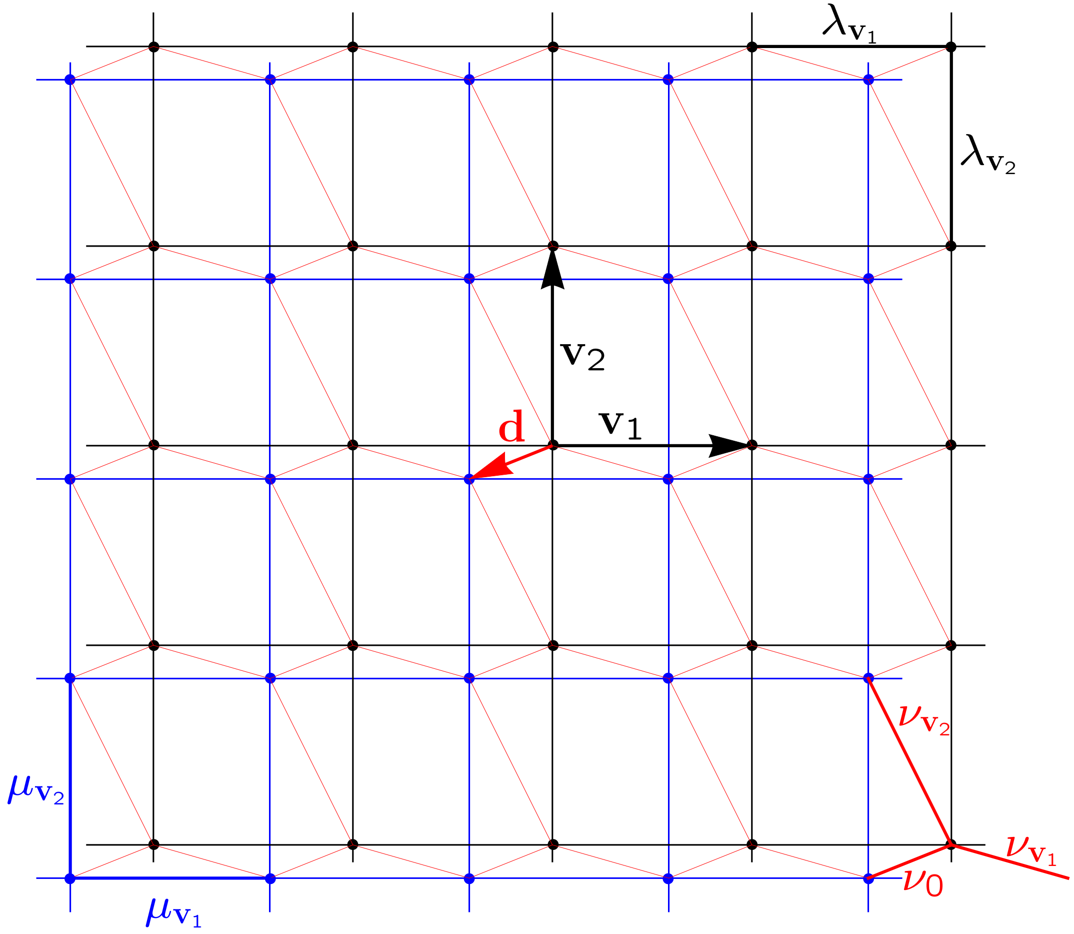
Identify symmetries that might/might not be responsible for the remarkable stability of Dirac points in the honeycomb lattice.

Extrapolate, if possible, to other planar periodic materials.

Vertices of the toy model: 2 copies of a lattice, L and $L + \mathbf{d}$.



Weighted edges of the toy model:



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

Edges from $x+\mathbf{d}$ to $x+y+\mathbf{d}$ in $L + \mathbf{d}$ have weight μ_y.

Edges from x to $x + y + \mathbf{d}$ have weight ν_y.

Connections don't need to be to closest neighbors.

This yields a graph Laplacian

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

Note that $\ell^2(L\cup L+\mathbf{d})$ has a basis of plane wave eigenfunctions.

Characterization of plane waves with frequency $\mathbf{k}$.

$$\phi(x) = \begin{cases} c_1 e^{i\mathbf{k}\cdot x} & \text{if } x \in L \\ c_2 e^{i\mathbf{k}\cdot x} & \text{if } x \in L + \mathbf{d} \end{cases}$$

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

Graph Laplacian is linear, preserves frequency of plane waves, so $-\Delta \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = M(\mathbf{k}) \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$ for some 2×2 matrix $M(\mathbf{k})$.

The exact formula is

$$-\Delta \begin{bmatrix} c_1 \\ \\ c_2 \end{bmatrix} = \underbrace{\begin{bmatrix} \sum_{y \in L} (\lambda_y (1 - \cos(\mathbf{k} \cdot y)) + \nu_y) & \sum_{y \in L} \nu_y e^{i\mathbf{k} \cdot (y+d)} \\ \sum_{y \in L} \nu_y e^{-i\mathbf{k} \cdot (y+d)} & \sum_{y \in L} (\nu_y + \mu_y (1 - \cos(\mathbf{k} \cdot y))) \end{bmatrix}}_{M(\mathbf{k})} \begin{bmatrix} c_1 \\ \\ c_2 \end{bmatrix}$$

and the band dispersion functions are eigenvalues of $M(\mathbf{k})$.

Two energy bands given by $E^{\pm}(\mathbf{k}) =$

$$\Big(\sum_{y \in L} (\lambda_y + \mu_y) \sin^2(\tfrac{\mathbf{k} \cdot y}{2}) + \nu_y \Big) \pm \sqrt{\Big(\sum_{y \in L} (\lambda_y - \mu_y) \sin^2(\tfrac{\mathbf{k} \cdot y}{2}) \Big)^2 + \Big| \sum_{y \in L} \nu_y e^{i\mathbf{k} \cdot y} \Big|^2}$$

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

Side note: $E^{\pm}(\mathbf{k})$ does not depend on $\mathbf{d}$.

Dirac points occur if discriminant goes to zero in nondegenerate way.

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

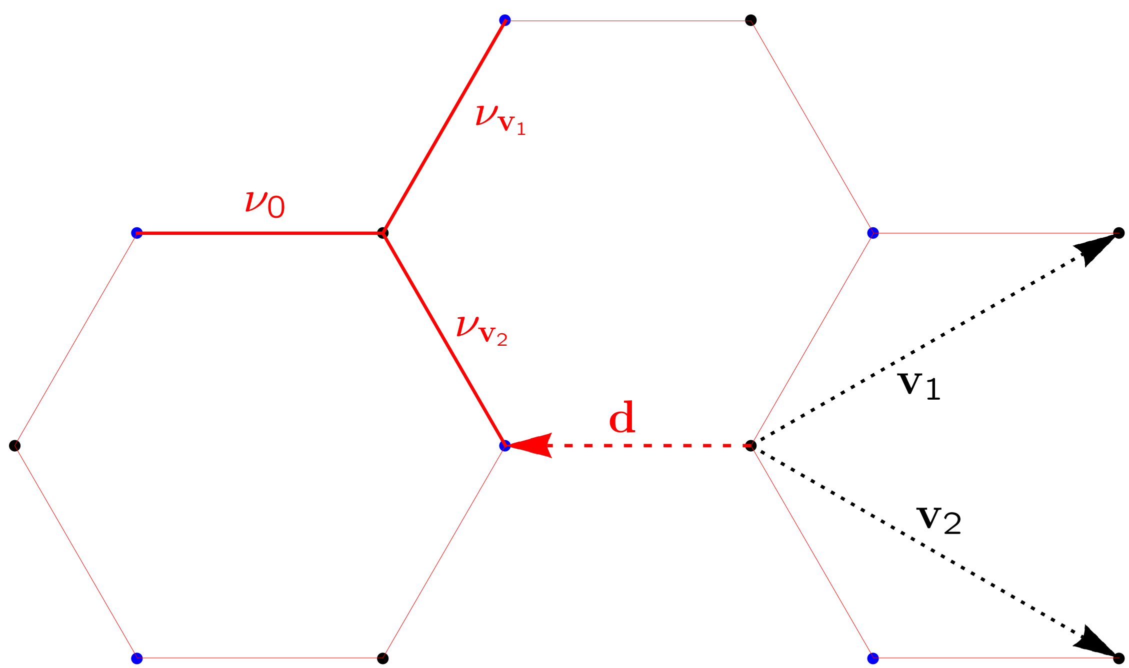
Suppose internal connections on L and $L + \mathbf{d}$ are identical.
This is the symmetry condition $\lambda_y = \mu_y$ for all $y \in L$.
Then $A(\mathbf{k}) \equiv 0$, so discriminant simplifies to $|B(\mathbf{k})|$.

Under this assumption, Dirac points occur precisely when $B(\mathbf{k})$ has a simple root. In other words, when the vector field $\mathbf{B}(\mathbf{k}) = \begin{bmatrix} \mathrm{Re}(B(\mathbf{k})) \\ \mathrm{Im}(B(\mathbf{k})) \end{bmatrix}$ has a simple zero.

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

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



$$\mathbf{v}_1 = \begin{bmatrix} \frac{3}{2} \\ \frac{\sqrt{3}}{2} \end{bmatrix}, \ \mathbf{v}_2 = \begin{bmatrix} \frac{3}{2} \\ -\frac{\sqrt{3}}{2} \end{bmatrix}$$

$$\mathbf{d} = \begin{bmatrix} -1 \\ 0 \end{bmatrix}$$

$\lambda_y = \mu_y = 0$ for all $y \in L$.

$\nu_0 = \nu_{\mathbf{v}_1} = \nu_{\mathbf{v}_2} = 1$.

All other $\nu_y = 0$.

$B(\mathbf{k}) = 1 + 2e^{i(\frac{3}{2}k_1)}\cos(\frac{\sqrt{3}}{2}k_2)$ 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 $\nu_0 = \nu_{\mathbf{v}_1} = \nu_{\mathbf{v}_2}$ exactly or the absence of interactions between other vertices.

It doesn't depend on geometry of $\mathbf{v}_1, \mathbf{v}_2$, or $\mathbf{d}$ at all.

All toy models sufficiently close also have a pair of Dirac points. (the frequency $\mathbf{k}_0$ 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 characterstic polynomial of even a 3×3 self-adjoint matrix $M(\mathbf{k})$ 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 $\mathbb{R}^2$?