Symmetry and Dirac points in the spectrum of graphene Laplacians

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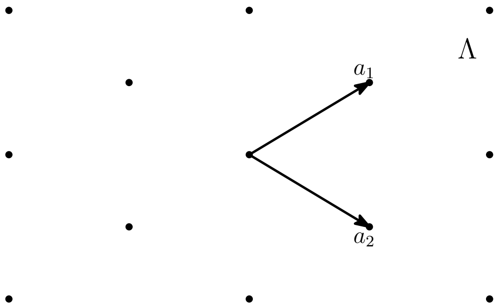
Based on `arXiv:1412.8096 [math-ph]`
(with A.Comech)

BIRS, Banff, Mar 2015

Consider lattice Λ generated by the vectors

$$\vec{a}_1 = \begin{pmatrix} \sqrt{3}/2 \\ 1/2 \end{pmatrix}, \qquad \vec{a}_2 = \begin{pmatrix} \sqrt{3}/2 \\ -1/2 \end{pmatrix}.$$



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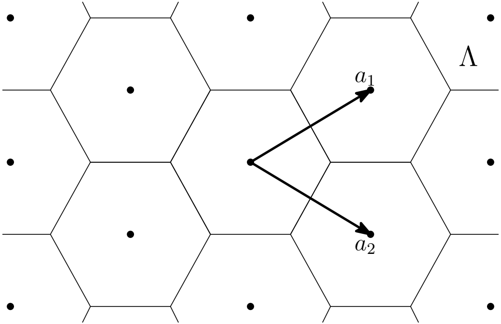

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Consider operators symmetric with respect to shifts by Λ (plus other symmetries to be specified)

- Schrödinger operator in $\mathbb{R}^2$

$$H = -\Delta + Q(x)$$

- discrete Schrödinger operator on a discrete graph

$$(Hf)_v = -\sum_{u \sim v} m_{u,v}(f_u - f_v) + Q_v f_v.$$

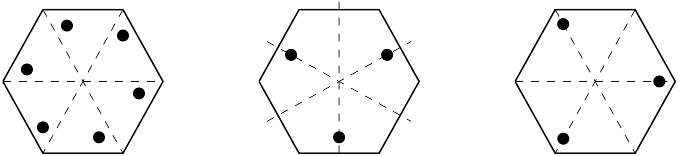
- Schrödinger operator on a quantum graph

Hexagonal lattice: symmetries

Potential Q is Λ-invariant + other symmetries:

We will consider subgroups of D_6 generated by subsets of:

- R — rotation by $2\pi/3$
- V — inversion, $(x_1, x_2) \mapsto (-x_1, -x_2)$
- F — horizontal reflection, $(x_1, x_2) \mapsto (-x_1, x_2)$
- F_V — vertical reflection, $(x_1, x_2) \mapsto (x_1, -x_2)$



$R + V$ $\quad$ $R + F$ $\quad$ $R + F_V$

Floquet-Bloch theory

Let H be periodic with respect to shifts by Λ.

- Space $X(\vec{k})$ of Bloch functions ("quasi-periodic"):

$$\psi(\vec{x} + n_1\vec{a}_1 + n_2\vec{a}_2) = e^{i(n_1k_1+n_2k_2)}\psi(\vec{x}), \qquad n_1, n_2 \in \mathbb{Z}.$$

  Here $\psi \in L^2_{loc}$, quasi-momentum $\vec{k} = (k_1, k_2) \in (-\pi, \pi]^2$.

- Let

$$H(\vec{k}) := H\Big|_{X(\vec{k})}$$

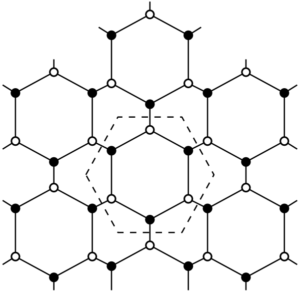
- then

$$\sigma(H) = \bigcup_{\vec{k}\in(-\pi,\pi]^2} \sigma(H(\vec{k})).$$

Dispersion relation

$$\psi(\vec{x} + n_1\vec{a}_1 + n_2\vec{a}_2) = e^{i(n_1k_1+n_2k_2)}\psi(\vec{x}).$$

- $\sigma(H(\vec{k}))$ as a function of $\vec{k}$ is *dispersion relation*.
- Example:



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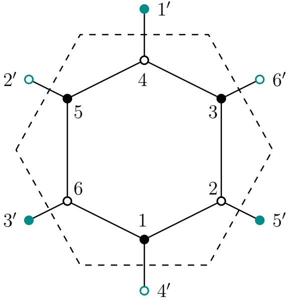

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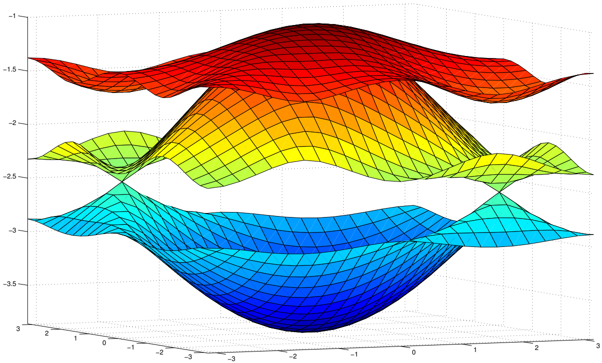
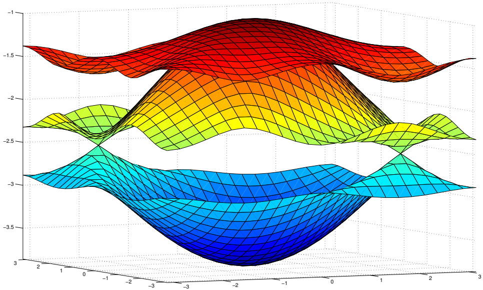


Dirac points



Important physical properties of graphene are due to *conical* or *Dirac points* in the dispersion relation. Proofs of existence:

- tight-binding model (Wallace 1947 etc)
- quantum graphs (Kuchment–Post 2007)
- $-\Delta + \epsilon Q$, small ϵ (Grushin 2009)
- $-\Delta + \epsilon Q$, almost all ϵ (Fefferman– Weinstein 2012).

My motivation: couting zeros

(joint wih R.Band and T.Weyand)

- Let ψ_n be the n-th eigenfunction of a quantum graph
- ϕ_n — the number of its zeros
- then

$$0 \leq \phi_n - (n-1) \leq \beta,$$

  where β is the number of cycles.
- call $\sigma_n = \phi_n - (n-1)$ the *nodal surplus*.

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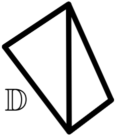
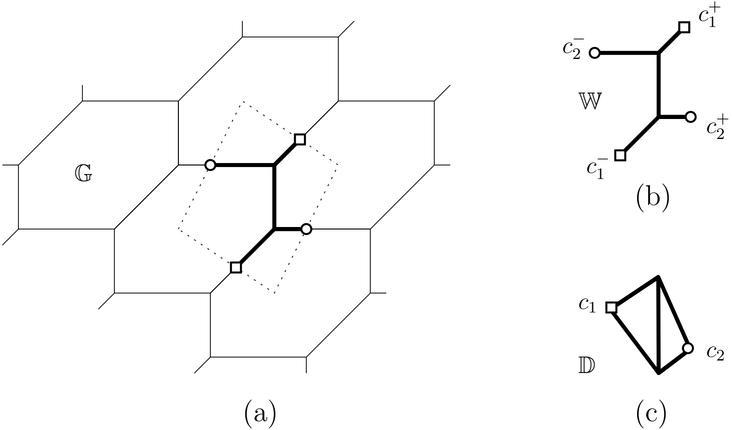


Theorem

The mandarin graph has nodal surplus $\{0, 1, 1, 1, \ldots\}$.



Theorem

- *The dispersion relation has a critical point at* $\vec{k} = (0, 0)$
- *For the graph* $\mathbb{G}$ *the Morse index of the critical point at* $(0, 0)$ *is equal to the nodal surplus* σ_n *of* $\mathbb{D}$.

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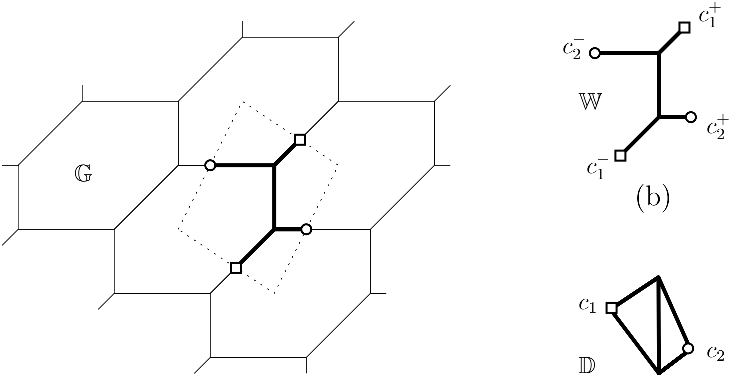

(a) (b) (c)

Corollary

The dispersion relation of $\mathbb{G}$ has only saddle points at $(0,0)$. (The same applies to critical points at $(0,\pi)$, $(\pi,0)$ and (π,π).

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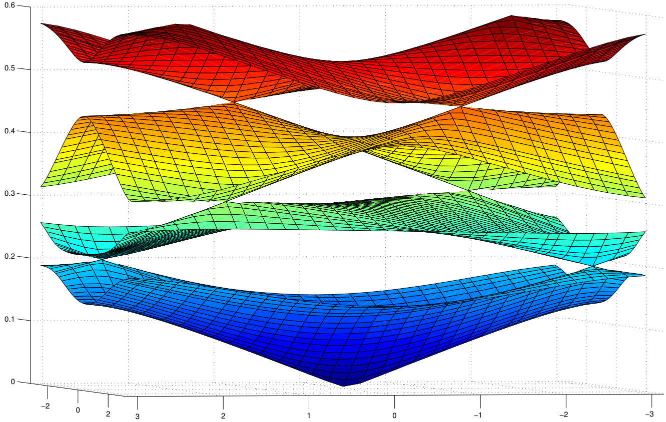

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Dirac points for graphene: results

Previous results for $-\Delta + \epsilon Q$ (Grushin 2009) Fefferman–Weinstein 2012:

1. $R + V \Rightarrow$ at $\pm\vec{k}^*$ there are 2-degenerate eigenvalues,
2. $R + V \Rightarrow$ at $\pm\vec{k}^*$ the dispersion relation is a circular cone
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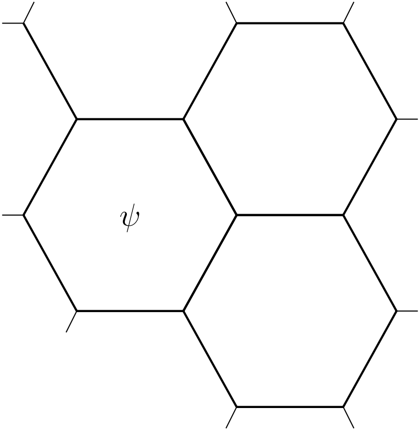
Our results (B–Comech):

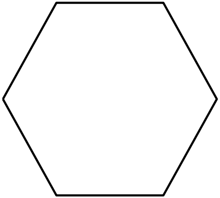
1. simpler proofs that work for
   - other operators H
   - symmetry $R + F$ or $R + V$
   - point $\vec{k} = (0, 0)$
2. for (weakly $\not{R}$) $+ F$ Dirac points move but restricted to a line.

Description of $H(\vec{k})$

Bloch functions:

$$\psi(\vec{x} + n_1\vec{a}_1 + n_2\vec{a}_2) = e^{i(n_1 k_1 + n_2 k_2)}\psi(\vec{x}), \qquad n_1, n_2 \in \mathbb{Z}.$$





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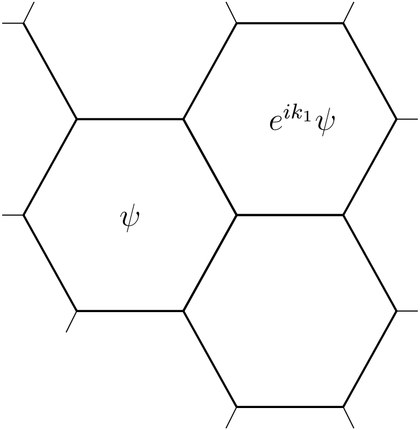

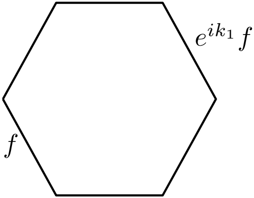

$$\psi\big|_{ur} = e^{ik_1}\psi\big|_{ll}$$

$$\partial_n\psi\big|_{ur} = -e^{ik_1}\partial_n\psi\big|_{ll}$$

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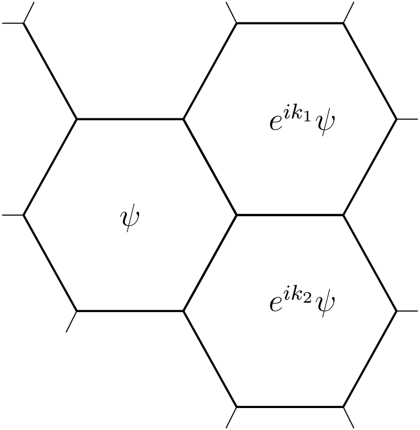

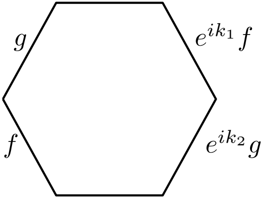

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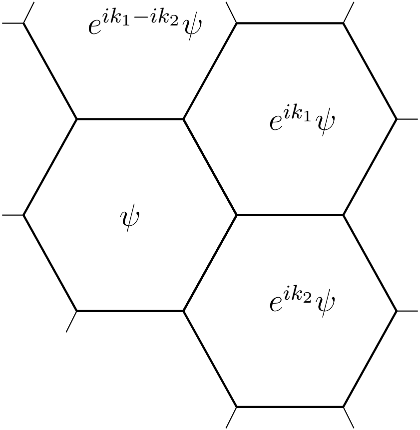

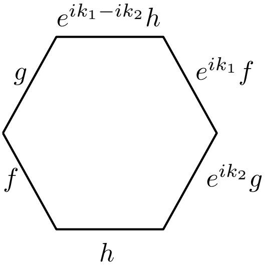

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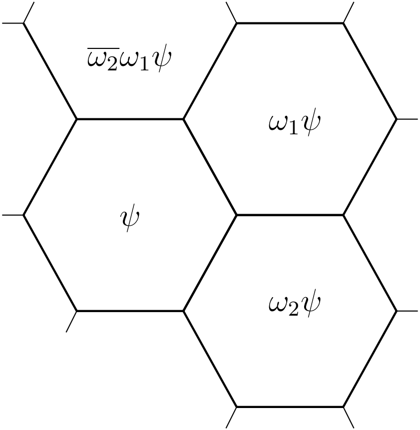
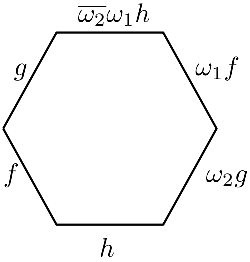
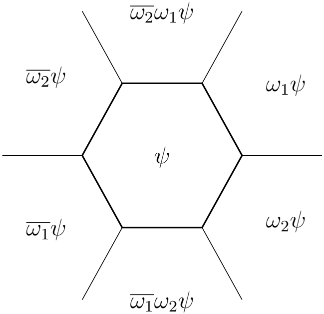




where $\omega_j = e^{ik_j}$

Why $\vec{k}^*$?



- $RX(\vec{k}) = X(\vec{k}')$, where

$$\omega_1' = \overline{\omega}_1\omega_2, \quad \omega_2' = \overline{\omega}_1.$$

Fixed points: $\omega_1^3 = 1$, $\omega_2 = \overline{\omega}_1$,

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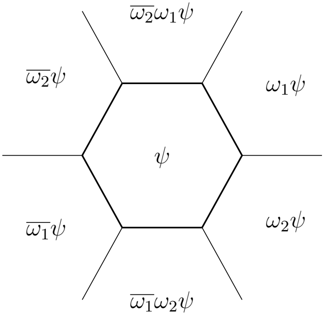

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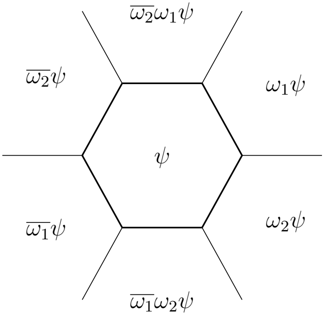

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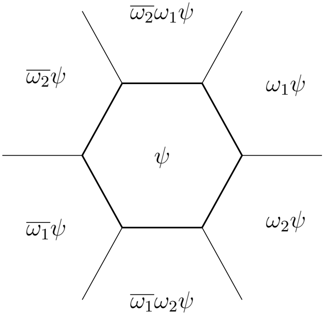

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- Fixed points of $\overline{V}$: all $\vec{k}$.

Degeneracies at $\vec{k} = \pm\vec{k}^*$: idea

Let operator H has symmetries $\{S_1, S_2, \dots\}$,

$$HS_j = S_j H.$$

- Irrep of dim $d \Rightarrow$ (usually) d-fold eigenvalue.
- $\langle R, F \rangle \simeq S_3$ has 2-dim irrep
- $\left\langle R, \overline{V} \right\rangle \simeq C_6$ abelian ?!?

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- but $\overline{V}$ is antiunitary, look at "corepresentations" (Wigner)

$$R : \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \mapsto \begin{pmatrix} \tau z_1 \\ \overline{\tau} z_2 \end{pmatrix}, \qquad \overline{V} : \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \mapsto \begin{pmatrix} \overline{z_2} \\ \overline{z_1} \end{pmatrix},$$

where $\tau = e^{2\pi i/3}$.

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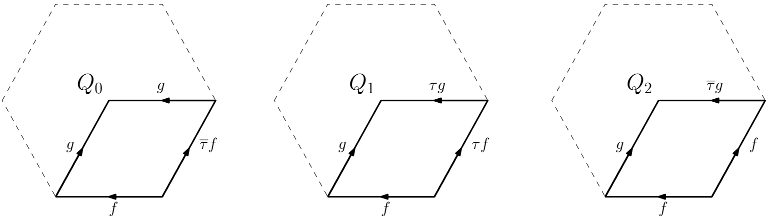

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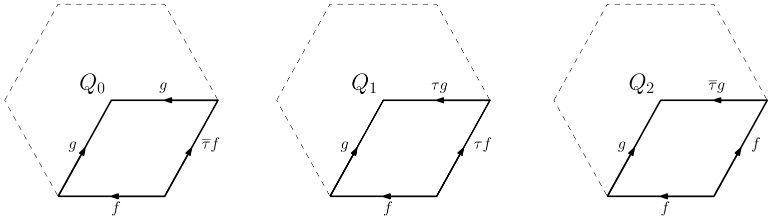

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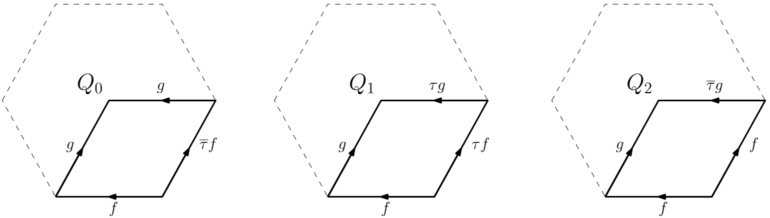

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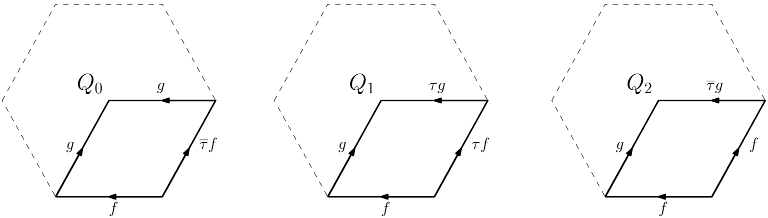

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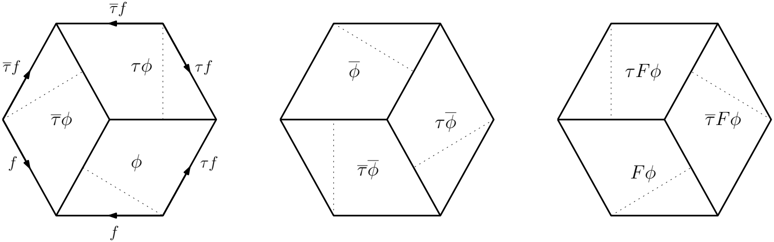
- *operators Q_1 and Q_2 are isospectral,*
- *and therefore every eigenvalue of Q_1 is a double (or more) eigenvalue of $H(\vec{k}^*)$.*

Transplantation proof

- Start with an eigenfunction ϕ of Q_1.
- Fill the whole hexagonal domain
- Apply $\overline{V}$ or F.



Algebraic proof

Use Band–Parzanchevski–Ben-Shach criterion,

$$\mathrm{Ind}_{\mathcal{R}}^{\mathcal{G}}\,\rho_1 = \mathrm{Ind}_{\mathcal{R}}^{\mathcal{G}}\,\rho_2,$$

where

$$\mathcal{R} = \left\langle R | R^3 = 1 \right\rangle, \qquad \rho_j : R \mapsto (\tau^j)$$

and

$$\mathcal{G} = \left\langle R, F | F^2 = 1, FR = R^2 F \right\rangle$$

or

$$\mathcal{G} = \left\langle R, \overline{V} | \overline{V}^2 = 1, \overline{V} R = R \overline{V} \right\rangle$$

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Note that the criterion fails on

$$\mathcal{G} = \left\langle R, \overline{F_V} | \overline{F_V}^2 = 1, \overline{F_V} R = R \overline{F_V} \right\rangle$$

"therefore" no degeneracy for $R + F_V$ symmetry.

Proof of conical shape: symmetries

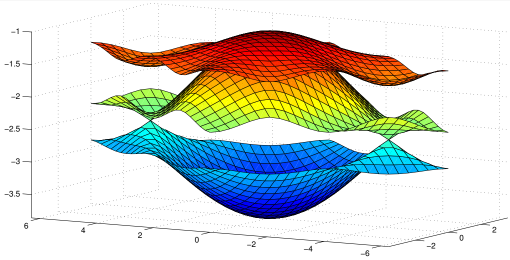
Define “correct” coordinates,

$$\vec{\kappa} = \begin{pmatrix} 1/\sqrt{3} & 1/\sqrt{3} \\ 1 & -1 \end{pmatrix} \vec{k} \quad \text{and} \quad \vec{k}^* \mapsto \vec{\kappa}^*.$$

Lemma

If H has rotational R and time-reversal (complex conjugation) T symmetries, the dispersion relation is symmetric with respect to

- *rotation by* $\pi/3$ *around* $\vec{\kappa} = (0, 0)$,
- *rotation by* $2\pi/3$ *around* $\pm\vec{\kappa}$.



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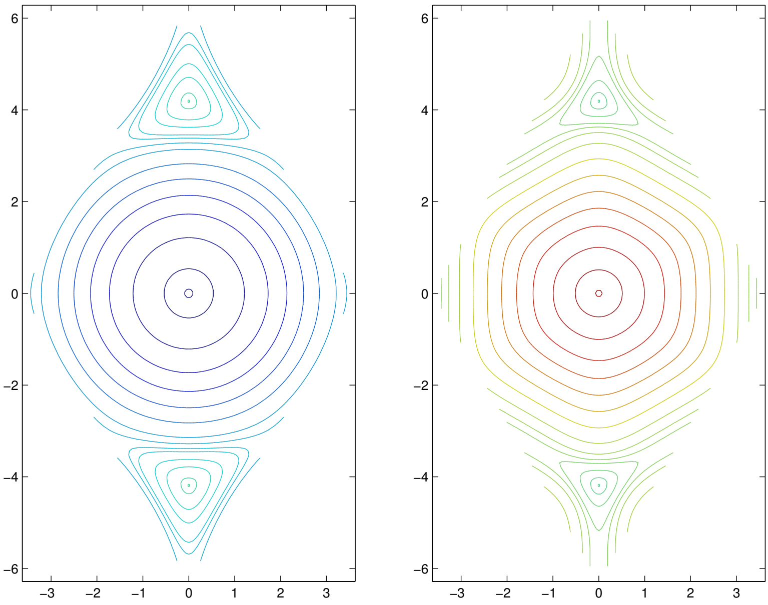

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- Expand to 2nd order: a quadric surface.
- Double root at $(0, 0) \Rightarrow$ intersecting planes or coinciding planes or cone.
- Rotation by $2\pi/3 \Rightarrow$ circular cone or coinciding planes.

A non-degeneracy condition to rule out coinciding planes.

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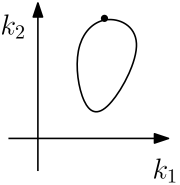

- Choose a contour in parameter space.
- Along the contour, choose continuously n-th eigenfunction.
- Upon return, the eigenfunction may be multiplied by a phase — this is "Berry phase" $e^{i\beta}$.

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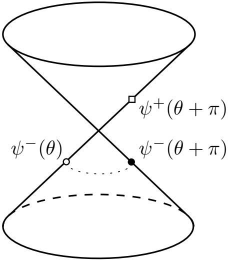

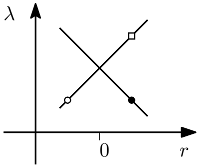

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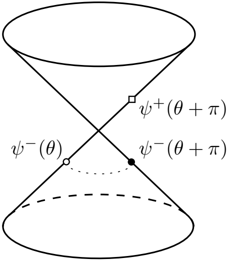

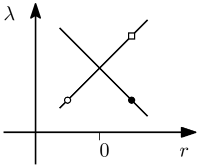

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For $\not{R} + F$ proof is different, implies a Dirac point on $k_2 = -k_1$.

Conclusions

- Simpler proofs that work for
  - different operators H
  - symmetry $R + F$ or $R + V$
  - point $\vec{k} = (0, 0)$.
- Role of symmetry is made explicit.
- For (weakly $\not{R}$) $+ F$ Dirac points move but restricted to a line.