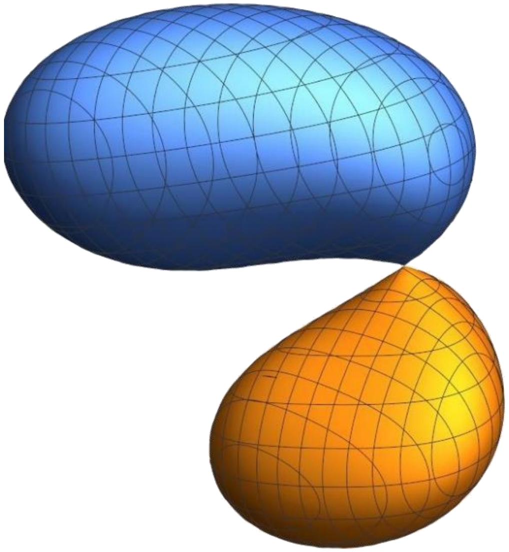

Master semester project: Type-II Weyl points with closed Fermi surface

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Supervisor: Alexey Soluyanov (UZH)

Weyl fermions

- Dirac equation: $(i\gamma^{\mu}\partial_{\mu} - m)\psi = 0$

  γ^{μ} satisfy Clifford algebra

- Helicity operator: $h_{\boldsymbol{p}} = 2\frac{\boldsymbol{L}\cdot\boldsymbol{p}}{p}$

  Chirality operator: $\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3$

- In case of $m = 0$:

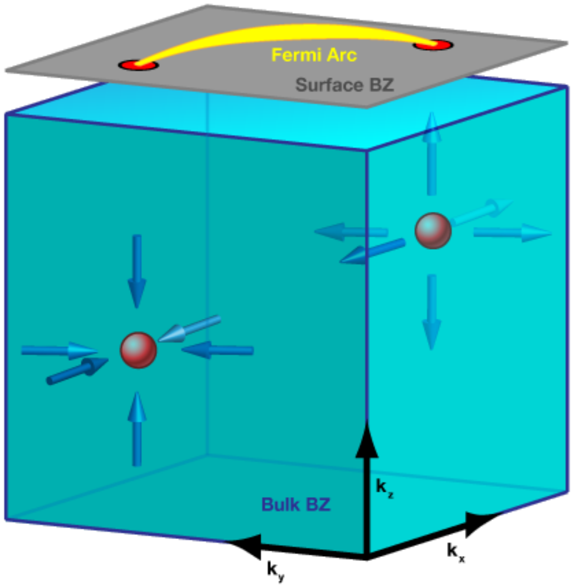
  helicity = chirality (conserved in time, Lorentz invariant)

  Solutions can be represented by 2-component spinors:
  <u>left-handed and right-handed Weyl fermions</u>

Weyl semimetals

Experimental signatures:

1. Fermi arc: surface states connecting projections of Weyl points
2. Anomalous transport properties: negative magnetoresistance



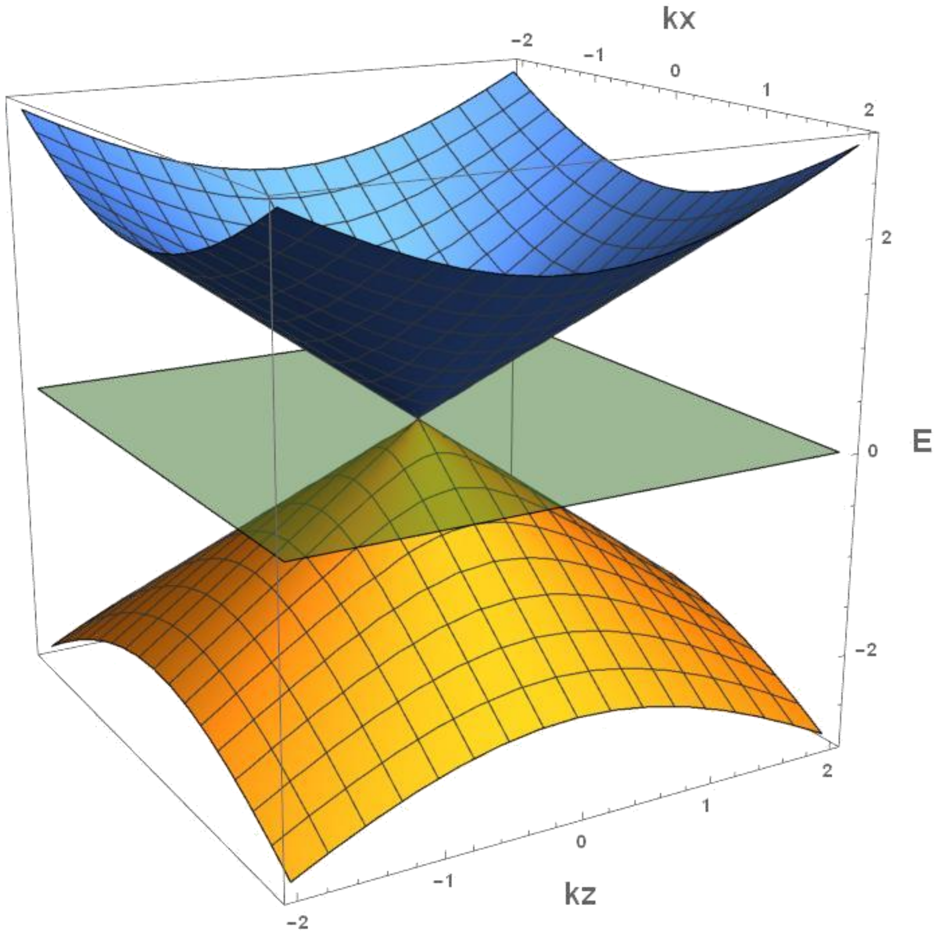
Weyl points: monopoles and antimonopoles of Berry curvature

ETH zürich

Linear Hamiltonian

- Simplest case:

$$\widehat{H}(\boldsymbol{k}) = \boldsymbol{k} \cdot \boldsymbol{\sigma}$$



Fermi surface is a point

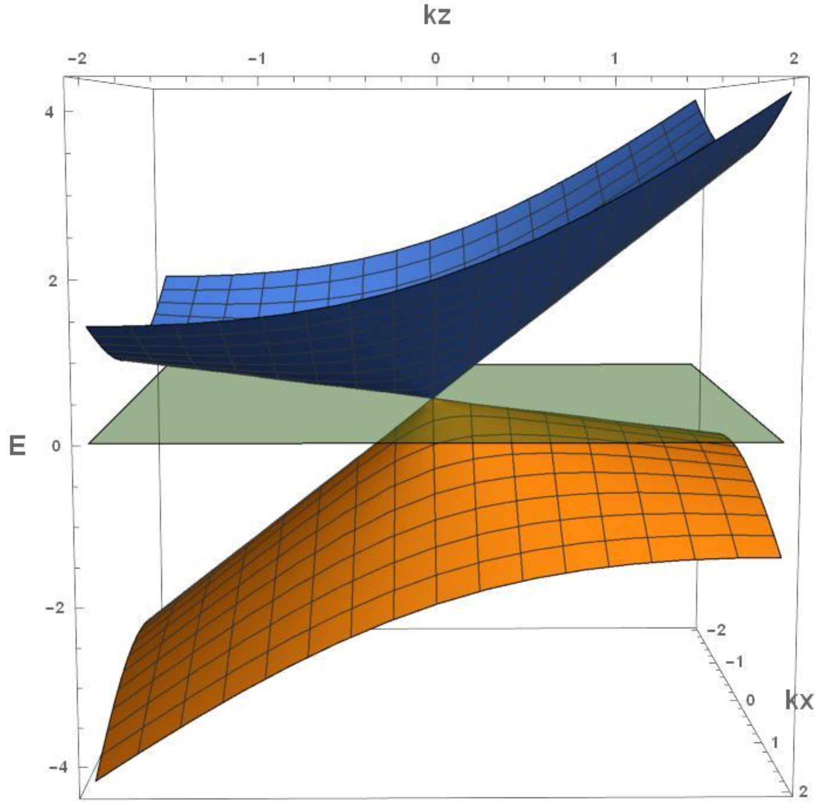
Linear Hamiltonian

- General case:

$$\hat{H}(\boldsymbol{k}) = \sum_{i=1}^{3} v_i k_i \sigma_0 + \sum_{i,j=1}^{3} k_i A_{ij} \sigma_j$$

"kinetic" term

"potential" term

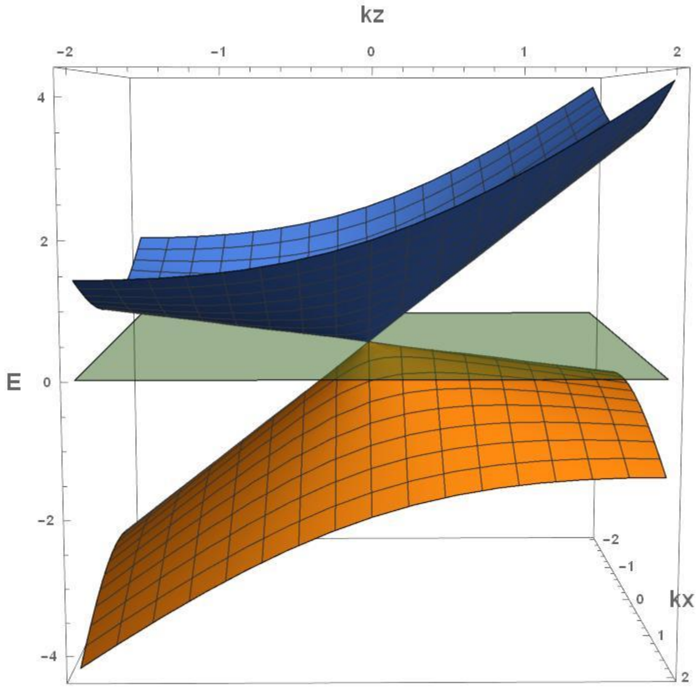


Which Fermi surfaces are possible?

Linear Hamiltonian: type-I and type-II Weyl points

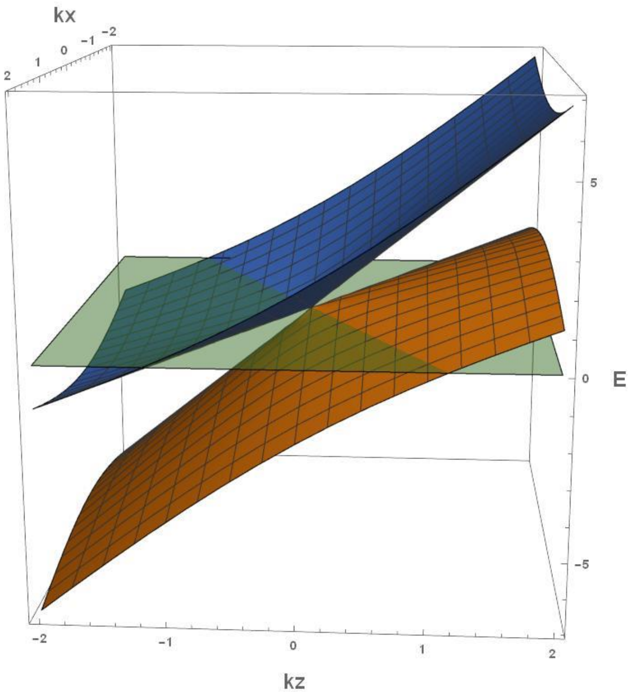
Type-I

- “kinetic” term is small enough
- Fermi surface is a point



Type-II

- “kinetic” term is large enough
- Fermi surface is open
- Weyl point is a touching between electron and hole pockets



Linear Hamiltonian with magnetic field (z-dir.)

$$\widehat{H}(\boldsymbol{k}) = C k_z \sigma_0 + \boldsymbol{k} \cdot \boldsymbol{\sigma}$$

- Add magnetic field along z-direction:

$$B = (0, 0, B)$$
$$A = (0, Bx, 0)$$

$$k_x \to k_x$$
$$k_y \to k_y - i\frac{e}{c}B\hat{x} = k_y - i\frac{e}{c}B\frac{\partial}{\partial k_x}$$
$$k_z \to k_z$$

$$\widehat{H}(\boldsymbol{k}) = \begin{pmatrix} k_z(C+1) & k_x - ik_y - \frac{e}{c}B\frac{\partial}{\partial k_x} \\ k_x + ik_y + \frac{e}{c}B\frac{\partial}{\partial k_x} & k_z(C-1) \end{pmatrix}$$

Linear Hamiltonian with magnetic field (z-dir.)

- Introduce creation and annihilation operators:

$$\begin{cases} \hat{a} = \frac{l}{\sqrt{2}}\left(\frac{1}{l^2}\frac{\partial}{\partial k_x} + k_x + ik_y\right) \\ \hat{a}^\dagger = \frac{l}{\sqrt{2}}\left(-\frac{1}{l^2}\frac{\partial}{\partial k_x} + k_x - ik_y\right) \end{cases}$$

$$[\hat{a}, \hat{a}^\dagger] = 1$$

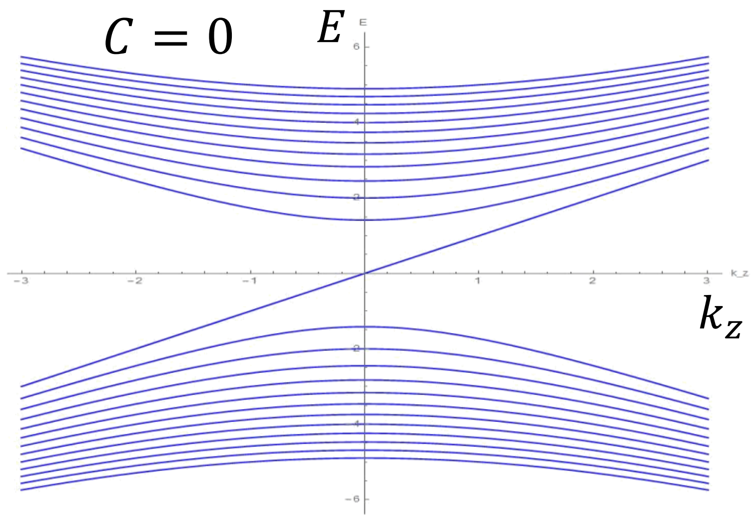
$$l = \sqrt{\frac{c}{eB}}$$

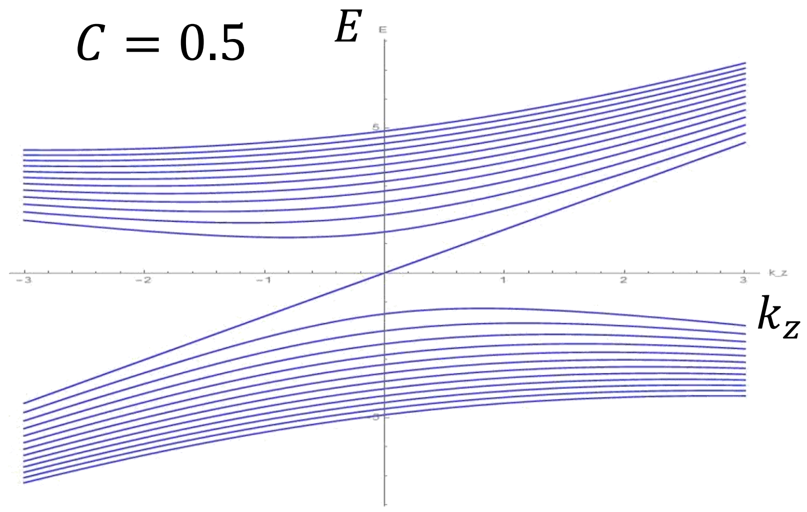
$$\hat{H} = \begin{pmatrix} k_z(C+1) & \frac{\sqrt{2}}{l}\hat{a}^\dagger \\ \frac{\sqrt{2}}{l}\hat{a} & k_z(C-1) \end{pmatrix}$$

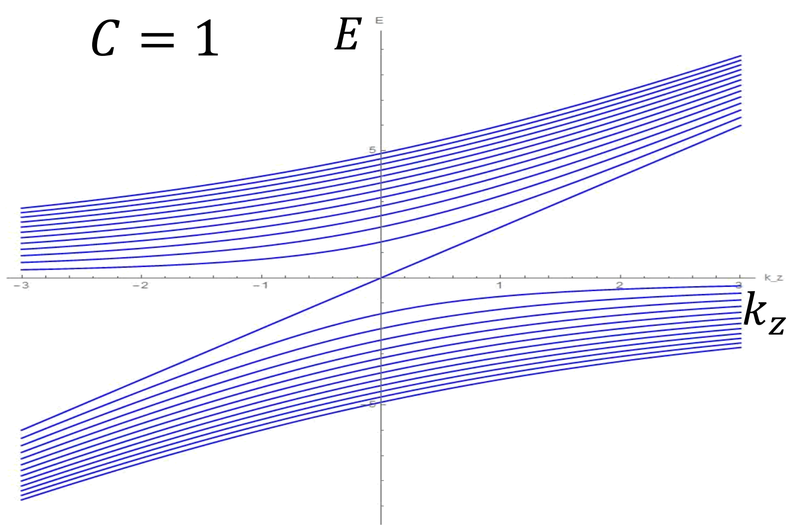
- Search for solutions in the form:

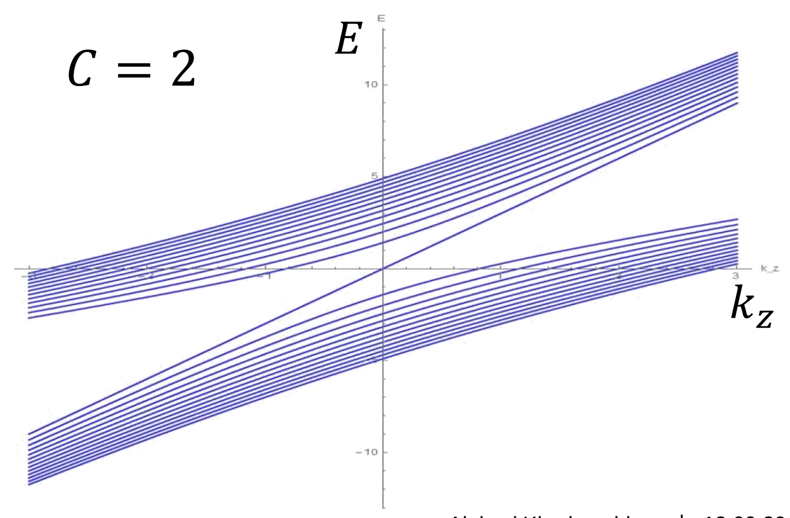
$$\psi = \begin{pmatrix} C_1|n\rangle \\ C_2|m\rangle \end{pmatrix}$$

Linear Hamiltonian with magnetic field (z-dir.)









Linear Hamiltonian with magnetic field (x-dir.)

$$\hat{H}(\boldsymbol{k}) = Ck_x\sigma_0 + \boldsymbol{k}\cdot\boldsymbol{\sigma}$$

Instead of rotating the magnetic field, we rotate the coordinate system together with the basis of Pauli matrices

- We again use the same procedure of "Landau quantization":

$$\hat{H} = \begin{pmatrix} C\frac{\sqrt{2}}{2l}\left(\hat{a}+\hat{a}^\dagger\right)+k_z & \frac{\sqrt{2}}{l}\hat{a}^\dagger \\ \frac{\sqrt{2}}{l}\hat{a} & C\frac{\sqrt{2}}{2l}\left(\hat{a}+\hat{a}^\dagger\right)-k_z \end{pmatrix}$$

Linear Hamiltonian with magnetic field (x-dir.)

- There is no solution in the form $\psi = \begin{pmatrix} C_1|n\rangle \\ C_2|m\rangle \end{pmatrix}$
- We will search it in the form of a linear combination:

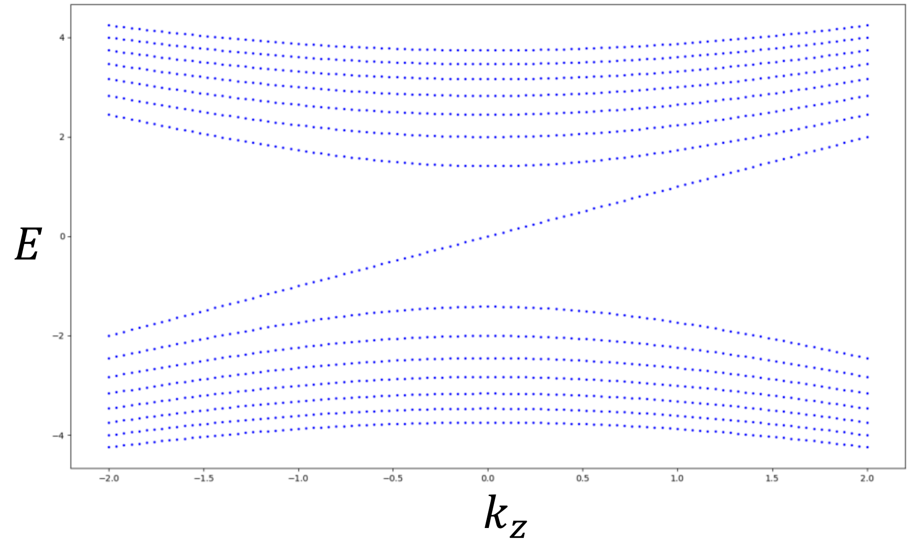
$$\psi = A_0\begin{pmatrix}|0\rangle \\ 0\end{pmatrix} + B_0\begin{pmatrix}0 \\ |0\rangle\end{pmatrix} + A_1\begin{pmatrix}|1\rangle \\ 0\end{pmatrix} + B_1\begin{pmatrix}0 \\ |1\rangle\end{pmatrix} + \cdots + A_N\begin{pmatrix}|N\rangle \\ 0\end{pmatrix} + B_N\begin{pmatrix}0 \\ |N\rangle\end{pmatrix} + \cdots$$

$$\begin{pmatrix}
k_z & 0 & C\frac{\sqrt{2}}{2l} & 0 & \cdots & \cdots & \cdots & 0 \\
0 & -k_z & \frac{\sqrt{2}}{l} & C\frac{\sqrt{2}}{2l} & \ddots & & & \vdots \\
C\frac{\sqrt{2}}{2l} & \frac{\sqrt{2}}{l} & k_z & 0 & \ddots & \ddots & & \vdots \\
0 & C\frac{\sqrt{2}}{2l} & 0 & -k_z & \ddots & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & k_z & 0 & C\frac{\sqrt{2}}{2l}\sqrt{N} & 0 \\
\vdots & & \ddots & \ddots & 0 & -k_z & \frac{\sqrt{2}}{l}\sqrt{N} & C\frac{\sqrt{2}}{2l}\sqrt{N} \\
\vdots & & & \ddots & C\frac{\sqrt{2}}{2l}\sqrt{N} & \frac{\sqrt{2}}{l}\sqrt{N} & k_z & 0 \\
0 & \cdots & \cdots & \cdots & 0 & C\frac{\sqrt{2}}{2l}\sqrt{N} & 0 & -k_z
\end{pmatrix}
\begin{pmatrix} A_0 \\ B_0 \\ A_1 \\ B_1 \\ \vdots \\ \vdots \\ A_N \\ B_N \end{pmatrix}
= E \begin{pmatrix} A_0 \\ B_0 \\ A_1 \\ B_1 \\ \vdots \\ \vdots \\ A_N \\ B_N \end{pmatrix}$$

Linear Hamiltonian with magnetic field (x-dir.)

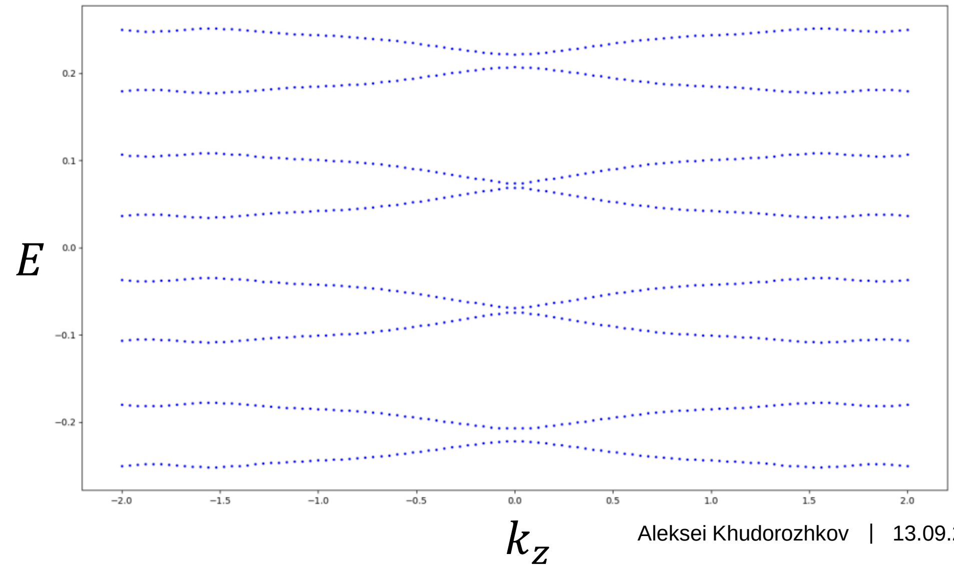
- For $0 \leq C < 1$:

  same as for $C = 0$
  with magnetic field
  along z-direction



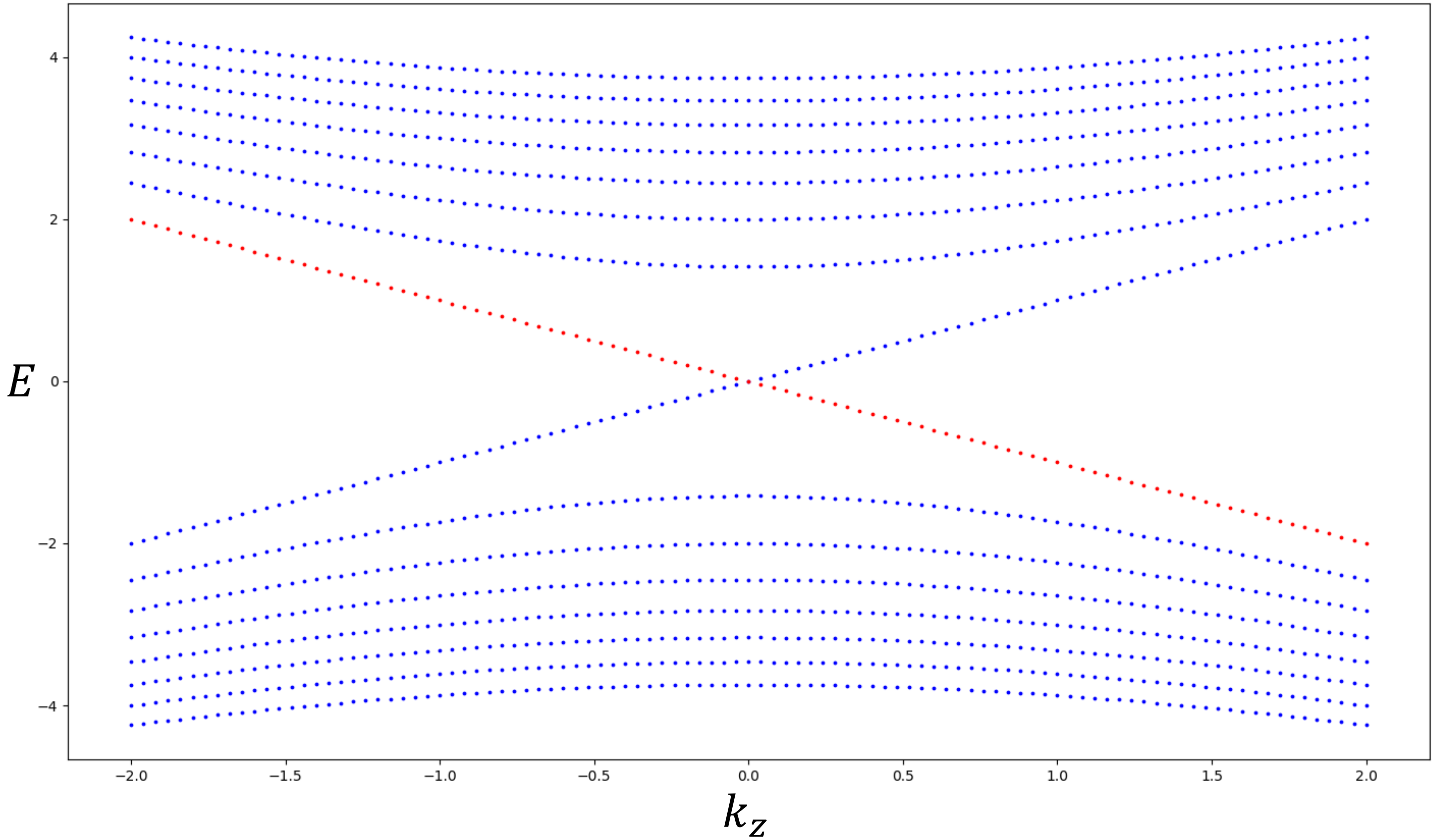
- For $C > 1$:

  gap opens



Linear Hamiltonian with magnetic field (x-dir.)

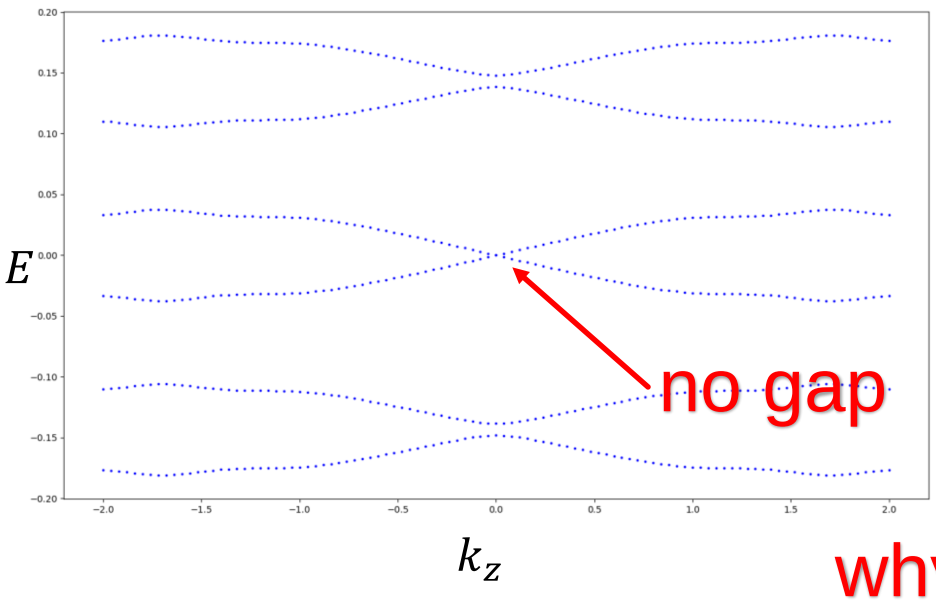
- Several flaws of numerical solution:
  1. Ghost states: states where the contribution from $|N\rangle$ states is dominant



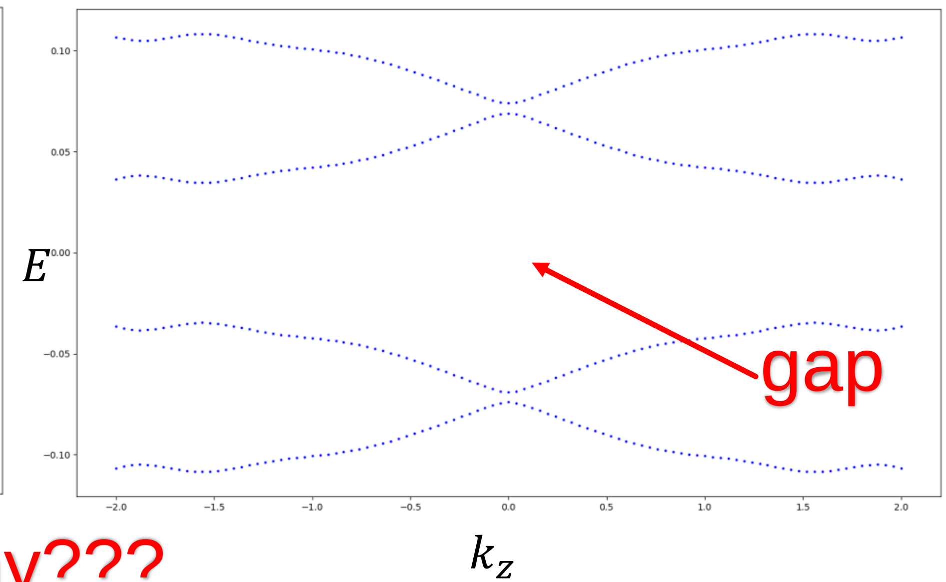
Linear Hamiltonian with magnetic field (x-dir.)

- Several flaws of numerical solution:
  2. Replacement of an infinite system of equations with a finite one

$C = 1.5; N = 300$



$C = 1.5; N = 301$

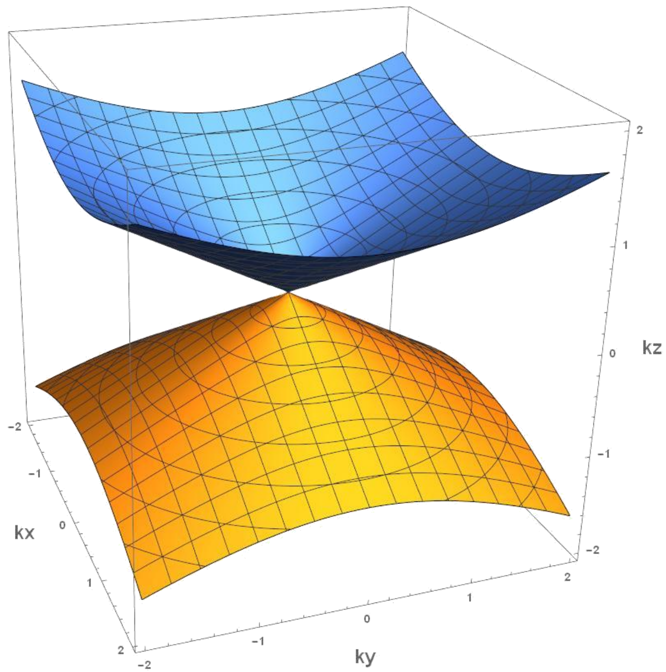


why???

Analytically proven that with $|C| > 1$, there is no solution with $E = 0, k_z = 0$.

Non-linear Hamiltonian

- We try to avoid an infinite number of LLs “diving” under the Fermi level (which is bad for transport properties).
- For this, we want to close Fermi surface by adding non-linear terms to $\widehat{H}$.



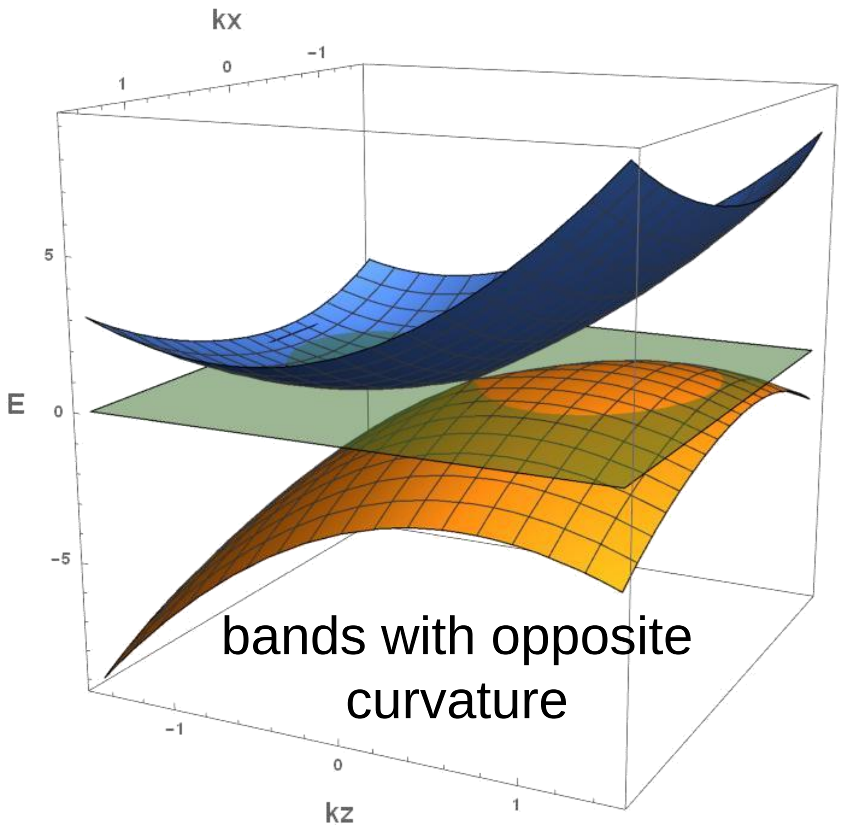
FS for linear $\widehat{H}$
(type-II Weyl point)

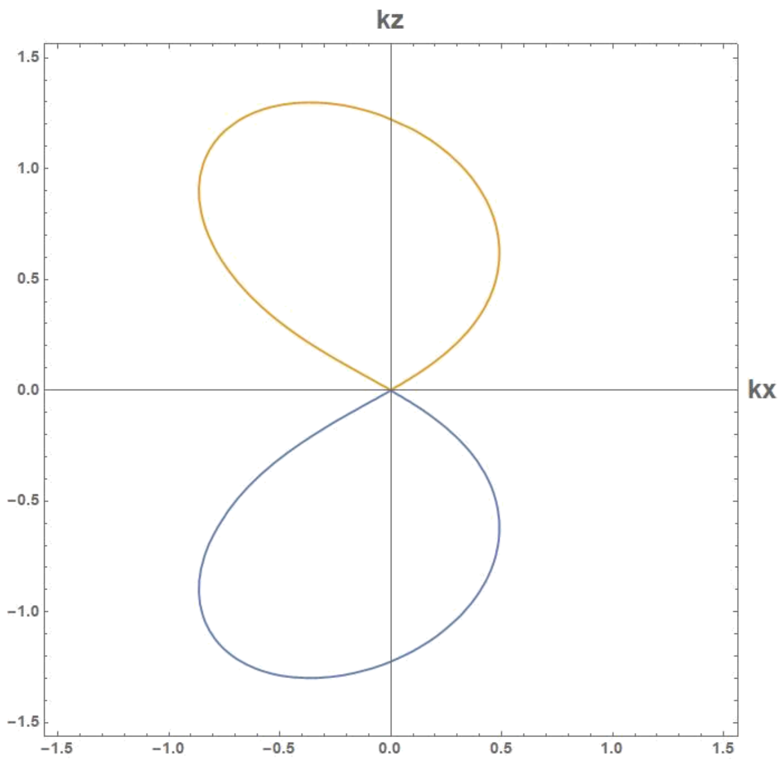
+ non-linear terms

?

Non-linear Hamiltonian (example 1)

$$\hat{H}(\boldsymbol{k}) = Ck_z\sigma_0 + (k_x + k_y^2 + k_z^2)\sigma_x + (k_y + k_x^2 + k_z^2)\sigma_y + (k_z - k_x k_y)\sigma_z$$

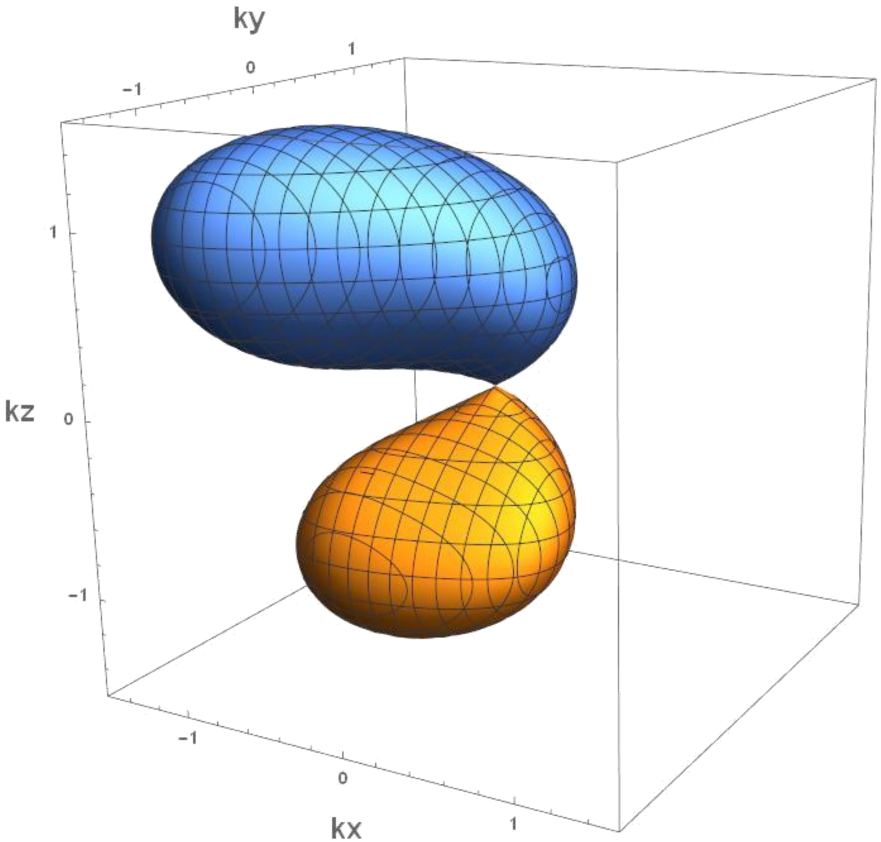




dispersion relation

Non-linear Hamiltonian (example 1)

$$\hat{H}(\boldsymbol{k}) = Ck_z\sigma_0 + (k_x + k_y^2 + k_z^2)\sigma_x + (k_y + k_x^2 + k_z^2)\sigma_y + (k_z - k_x k_y)\sigma_z$$

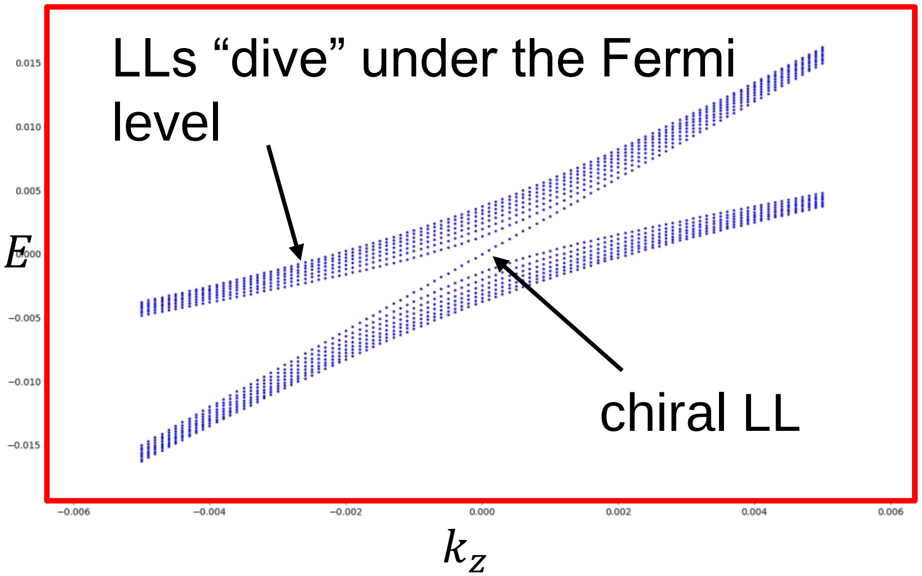


Fermi surface

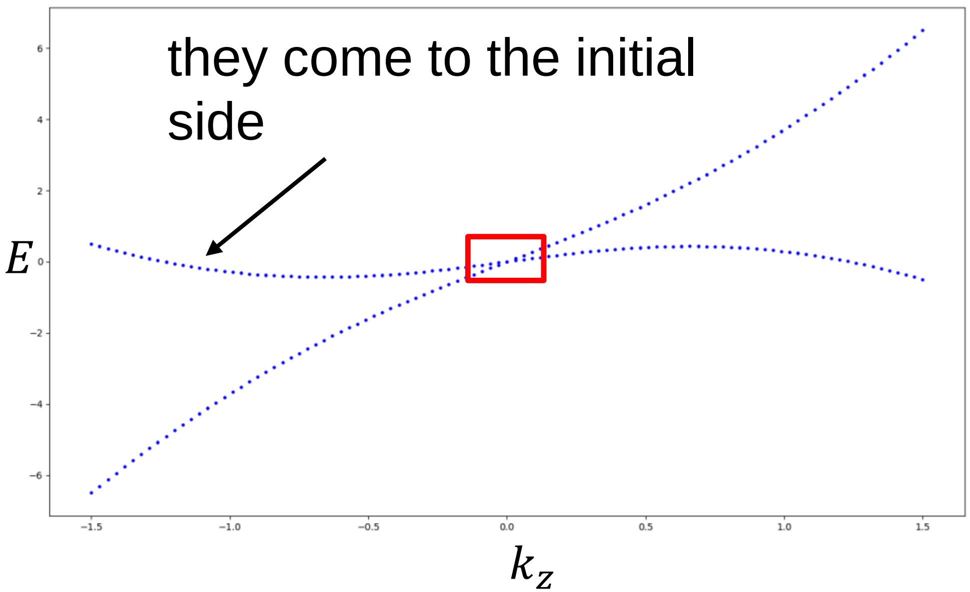
Non-linear Hamiltonian (example 1)

$$\hat{H}(\boldsymbol{k}) = Ck_z\sigma_0 + (k_x + k_y^2 + k_z^2)\sigma_x + (k_y + k_x^2 + k_z^2)\sigma_y + (k_z - k_x k_y)\sigma_z$$

- With magnetic field:



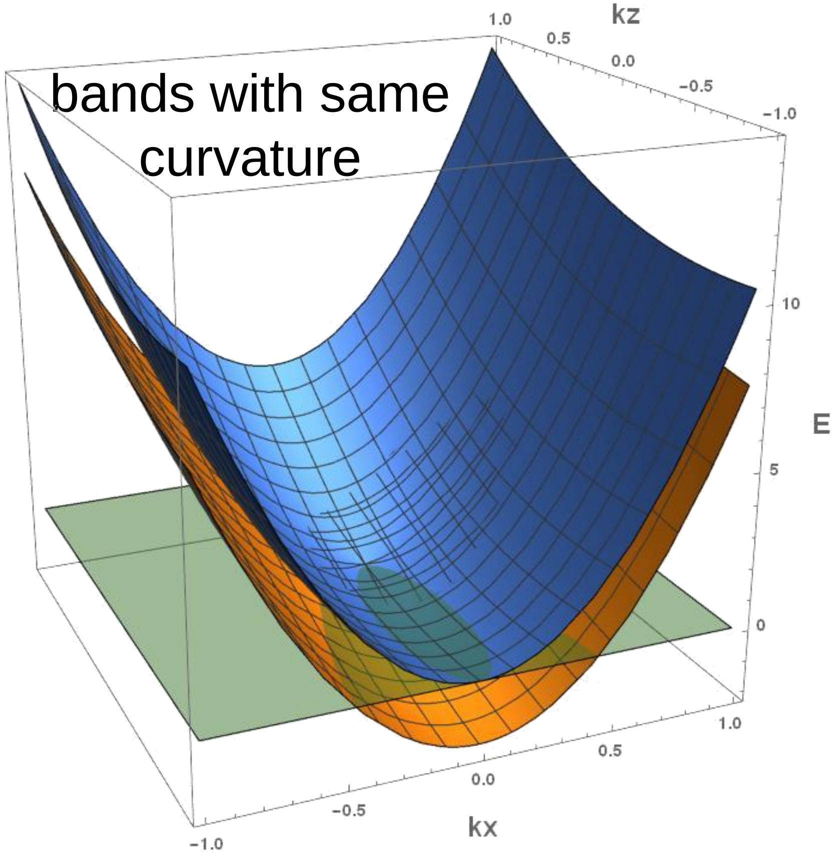
close-up view

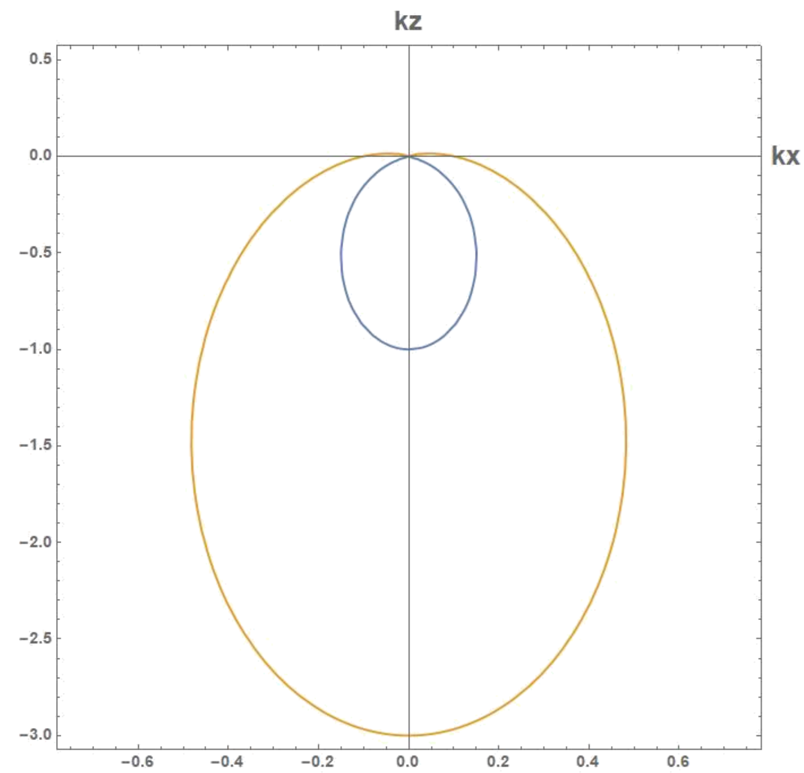


far-away view

Non-linear Hamiltonian (example 2)

$$\hat{H}(\boldsymbol{k}) = (Ck_z + 10k_x^2 + 4k_y^2 + k_z^2)\sigma_0 + \boldsymbol{k}\cdot\boldsymbol{\sigma}$$

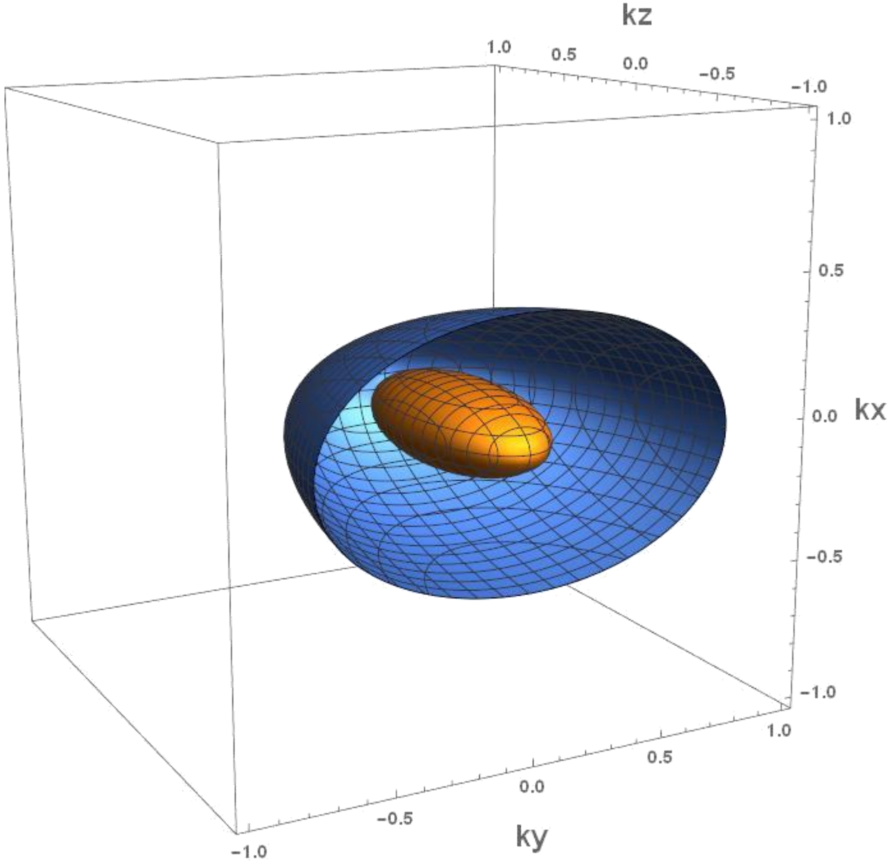




dispersion relation

Non-linear Hamiltonian (example 2)

$$\hat{H}(\boldsymbol{k}) = (Ck_z + 10k_x^2 + 4k_y^2 + k_z^2)\sigma_0 + \boldsymbol{k}\cdot\boldsymbol{\sigma}$$

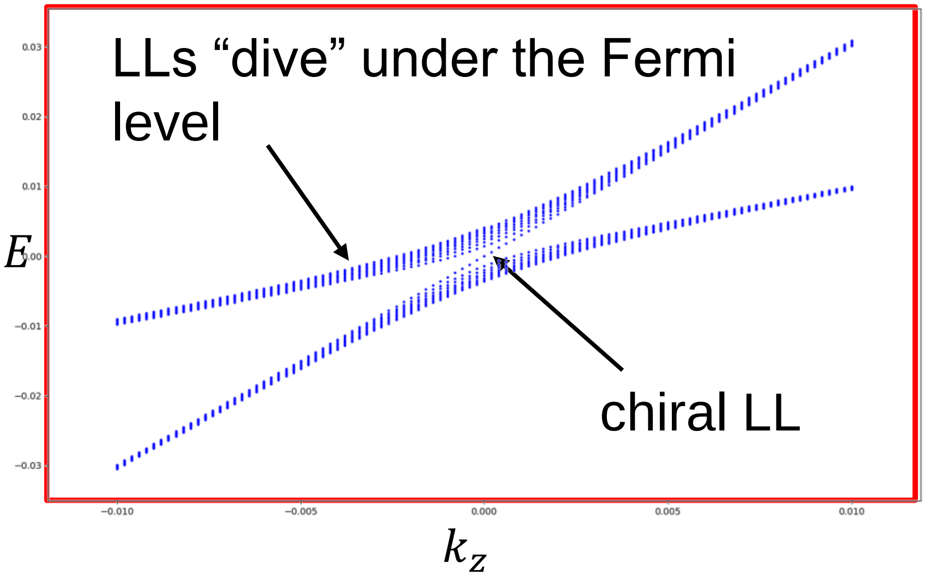


Fermi surface

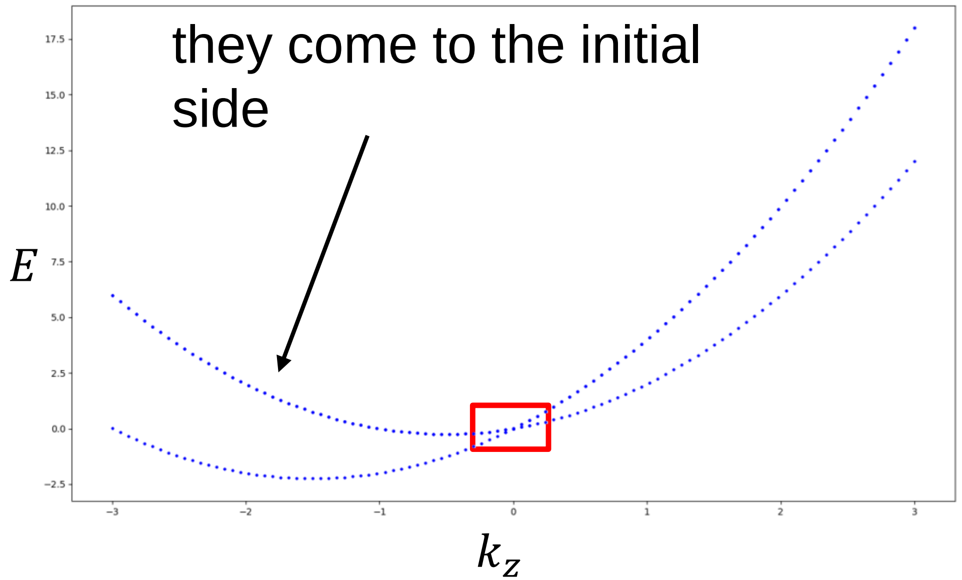
Non-linear Hamiltonian (example 2)

$$\hat{H}(\boldsymbol{k}) = (Ck_z + 10k_x^2 + 4k_y^2 + k_z^2)\sigma_0 + \boldsymbol{k}\cdot\boldsymbol{\sigma}$$

- With magnetic field:



close-up view



far-away view

Further steps

- Study other possible variants of higher-order terms to find closed Fermi surfaces.
- Calculate magnetoelectric response (essentially, conductivity tensor depending on B), knowing LLs structure.
  - Using semi-classical Boltzmann transport theory or
  - Using fully quantum approach with the use of Green's functions
- See if this model can explain any experimental results.
- Maybe study the model describing 2 Weyl points with opposite chiralities or try tight-binding approach.