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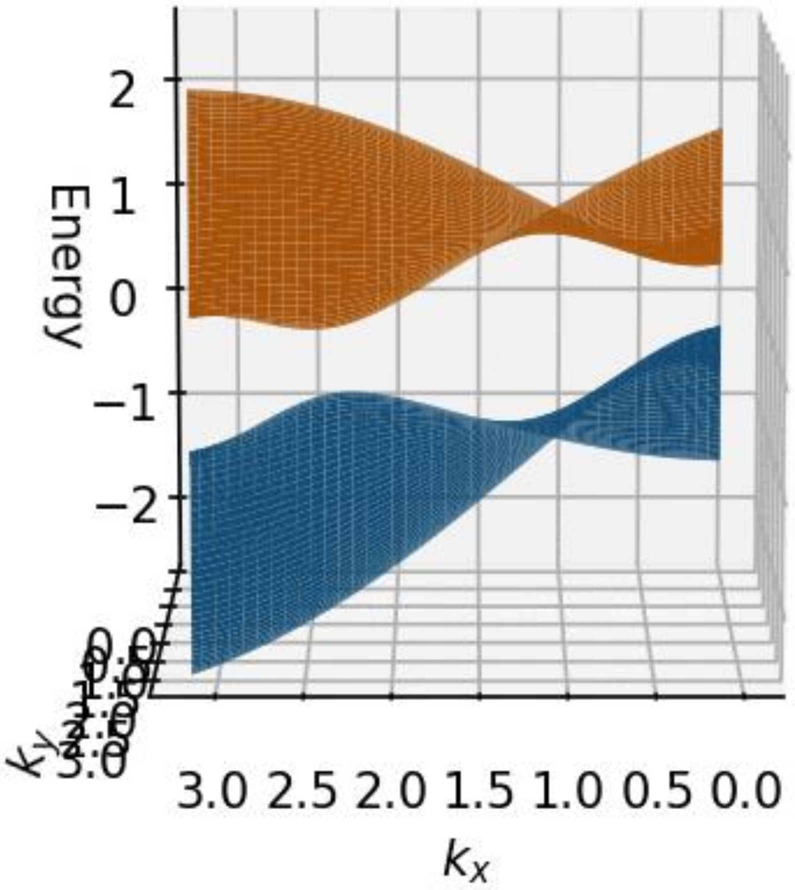
MŰEGYETEM 1782

Weyl nodes at a topological phase transition in 2D



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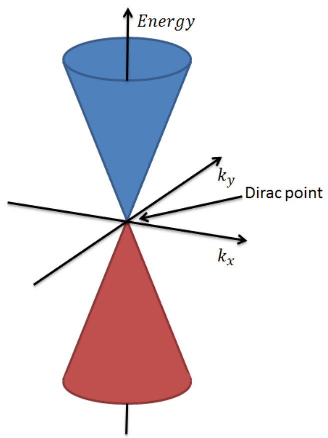
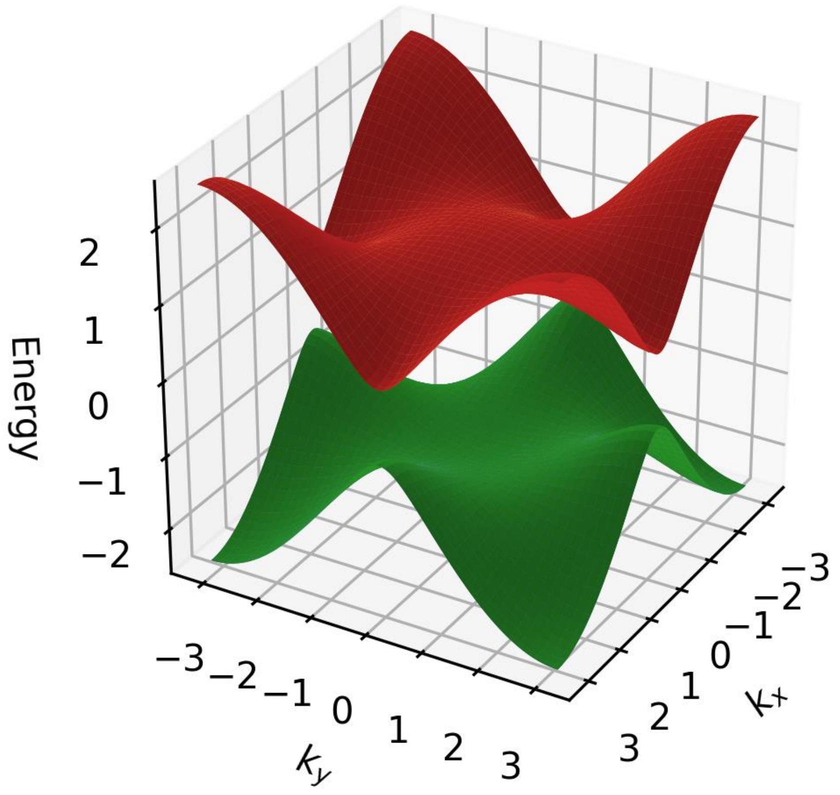
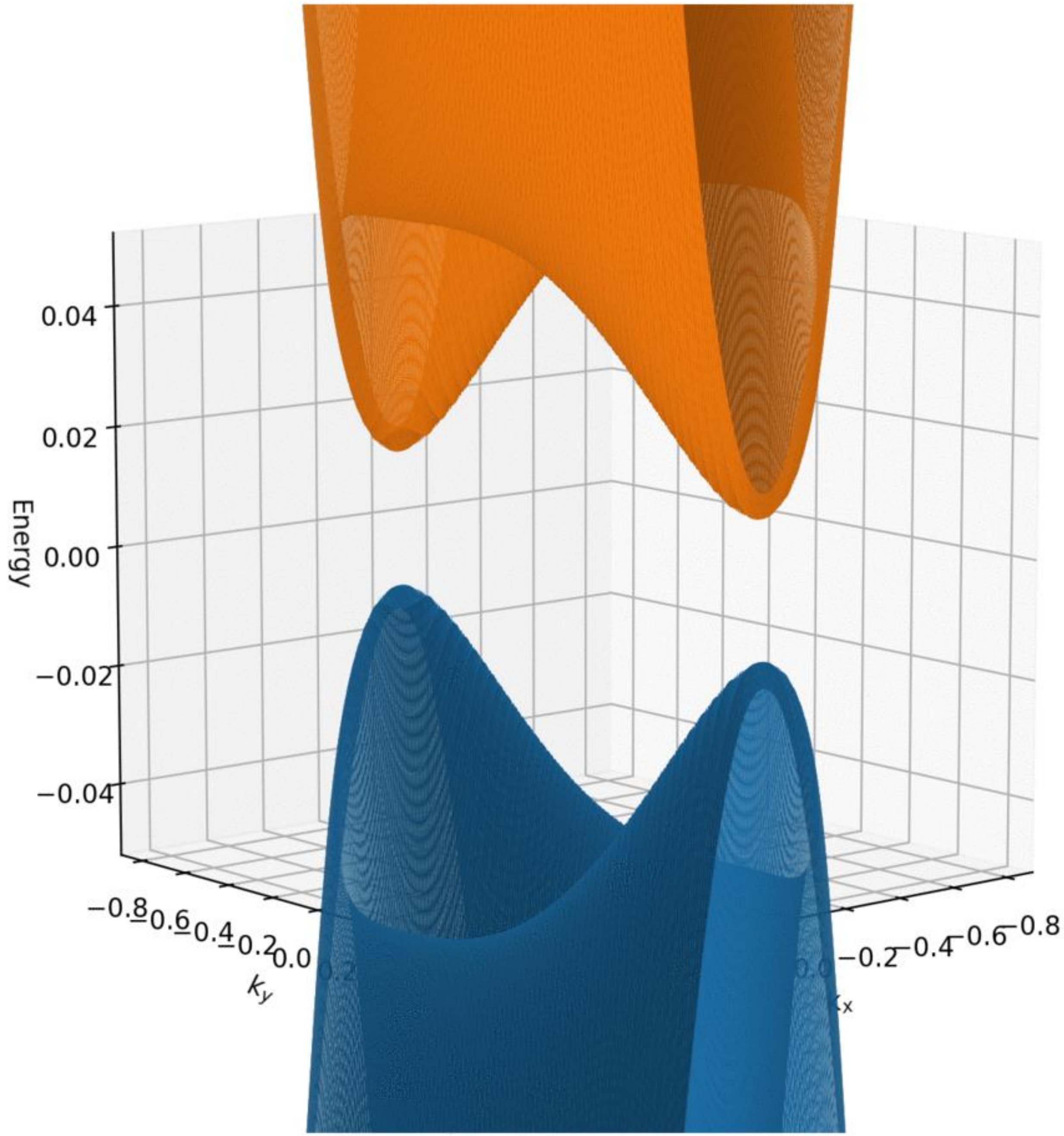
Weyl nodes are points where bands touch

- H(k), reciprocal space
- size of Hamiltonian = no. of bands
- Bands can touch, overlap, cross
- Weyl nodes are special band touching points:
  - touching only occurs in 1 point
  - carries topological charge (‚chirality'), can be ± 1
  - dispersion relation linear in all directions: Dirac cone





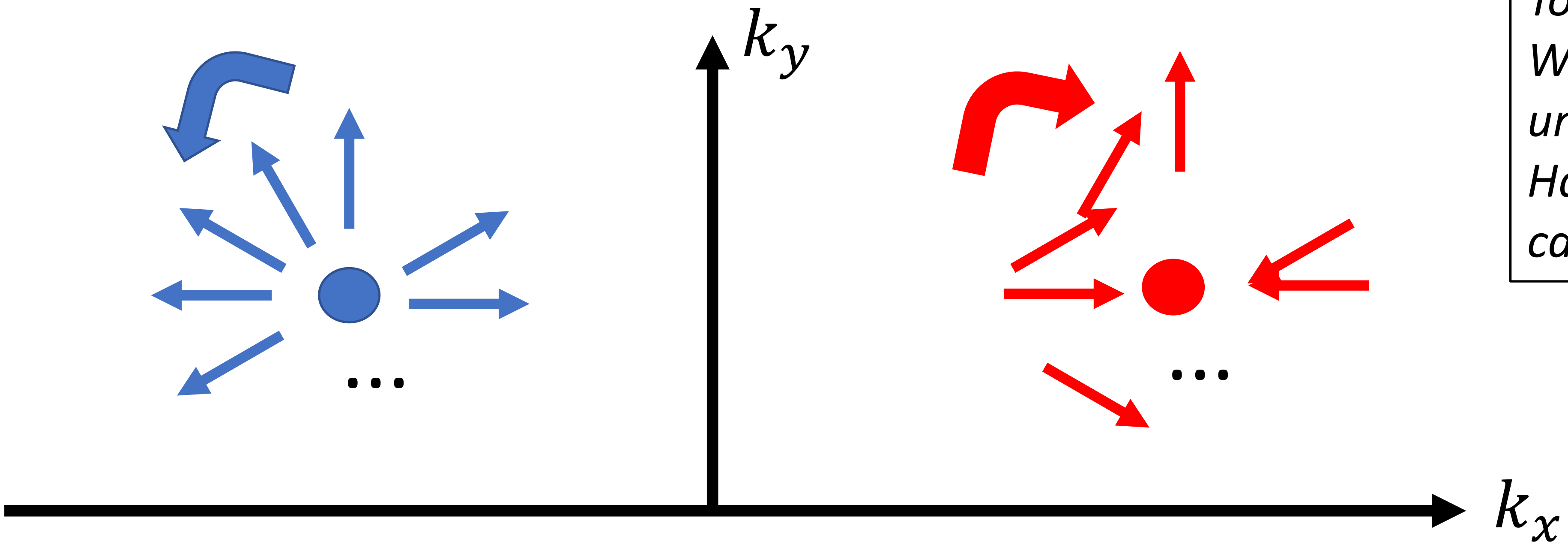
$$\hat{H}(k) = \sin k_x \hat{\sigma}_x + \sin k_y \hat{\sigma}_y + [u + \cos k_x + \cos k_y] \hat{\sigma}_z$$



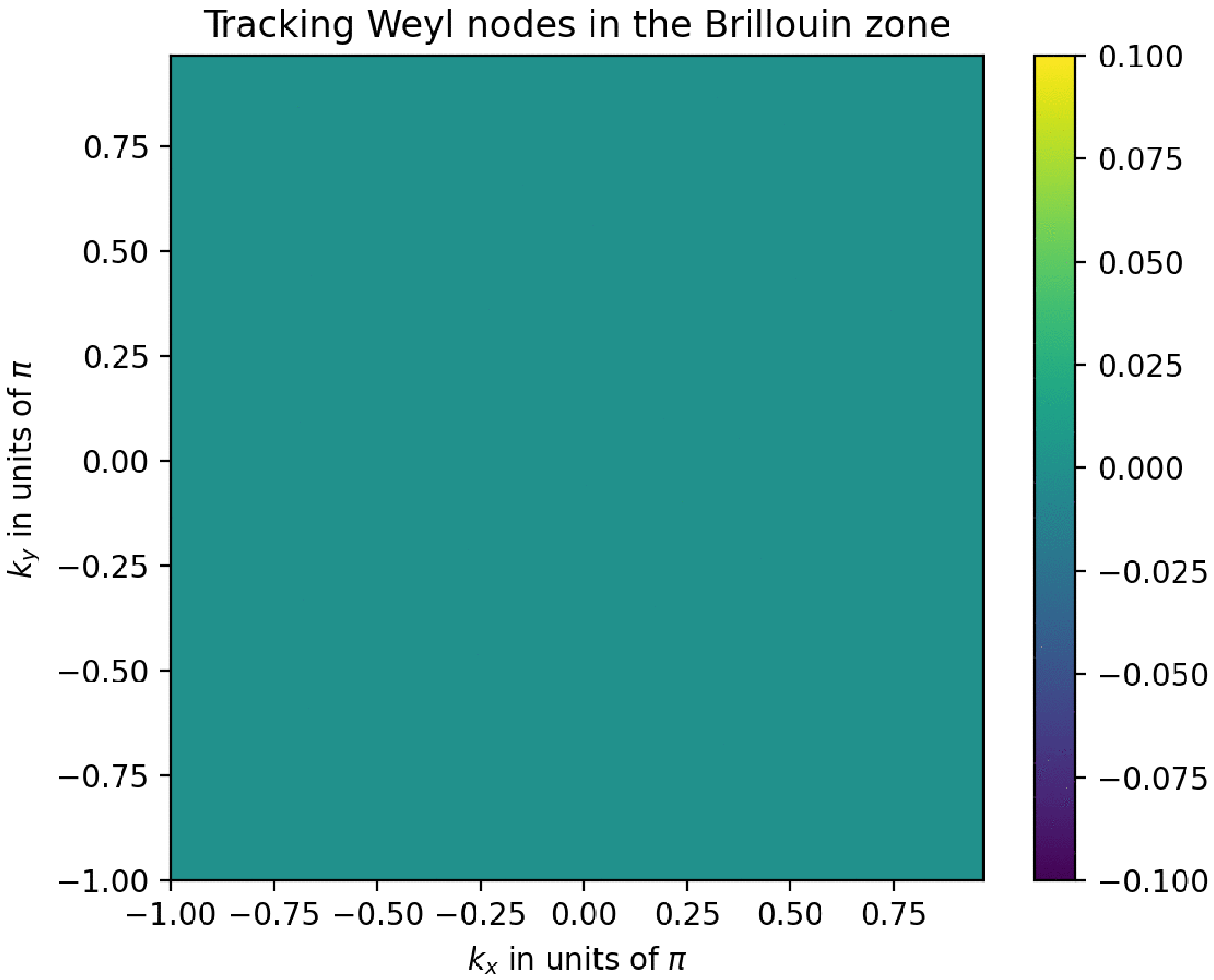
Energy
0.04
0.02
0.00
−0.02
−0.04
k_y
−0.8
0.6
0.4
0.2
0.0
k_x
−0.2
−0.4
−0.6
−0.8

Finding Weyl nodes in reciprocal space

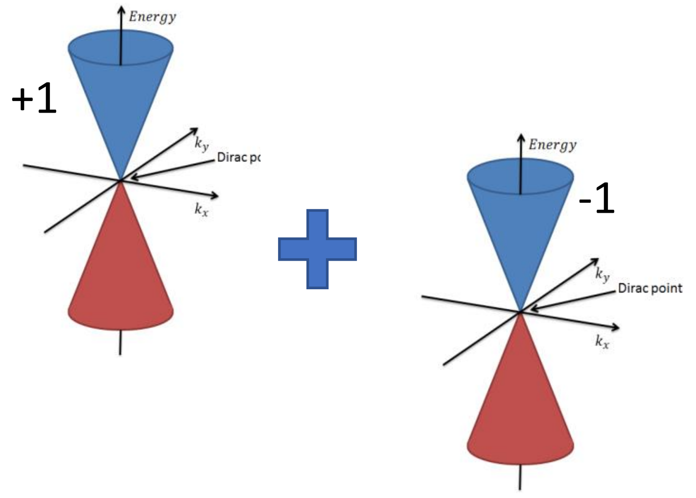
- Bring Hamiltonian to block off-diagonal form: $\hat{H} = \begin{bmatrix} 0 & h(k) \\ h(k)^{*T} & 0 \end{bmatrix}$
- $\det h(k)$ is complex vector-field, winds around Weyl nodes
- direction of winding: chirality



Topological protection: Weyl node has $\det h = 0$, under perturbation of the Hamiltonian these points can move but are robust

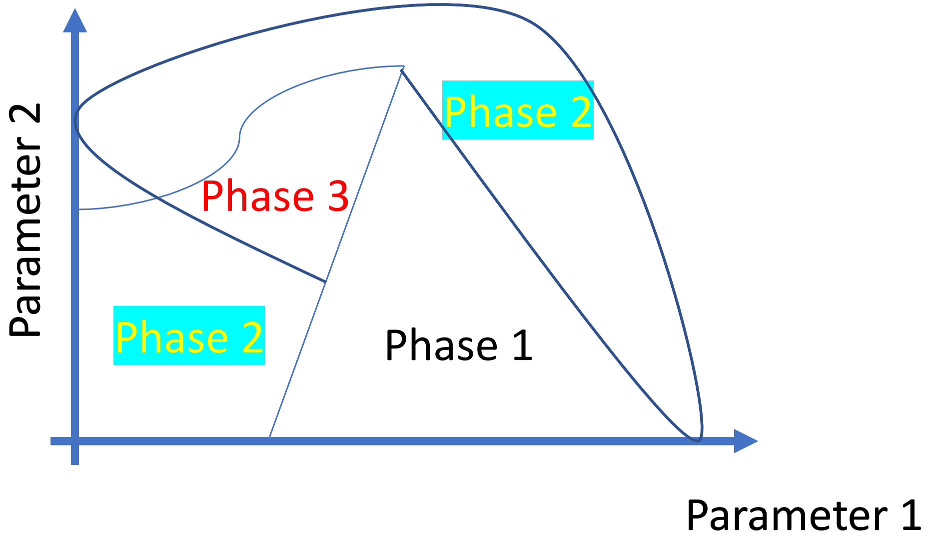

Tracking Weyl nodes in the Brillouin zone
k_y in units of π
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
k_x in units of π
0.100
0.075
0.050
0.025
0.000
−0.025
−0.050
−0.075
−0.100

Weyl semimetals have Weyl nodes



- Weyl nodes pair-create and annihilate
  - Zero net chirality both before and after ($0 \rightarrow \pm 1$ and $\pm 1 \rightarrow 0$)
- No band-gap so it is not an insulator
- Weyl semimetallic phase:

  A connected set of points in phase space with finite dimensions in all directions that have associated Weyl nodes



Our general goal: investigate in 2D

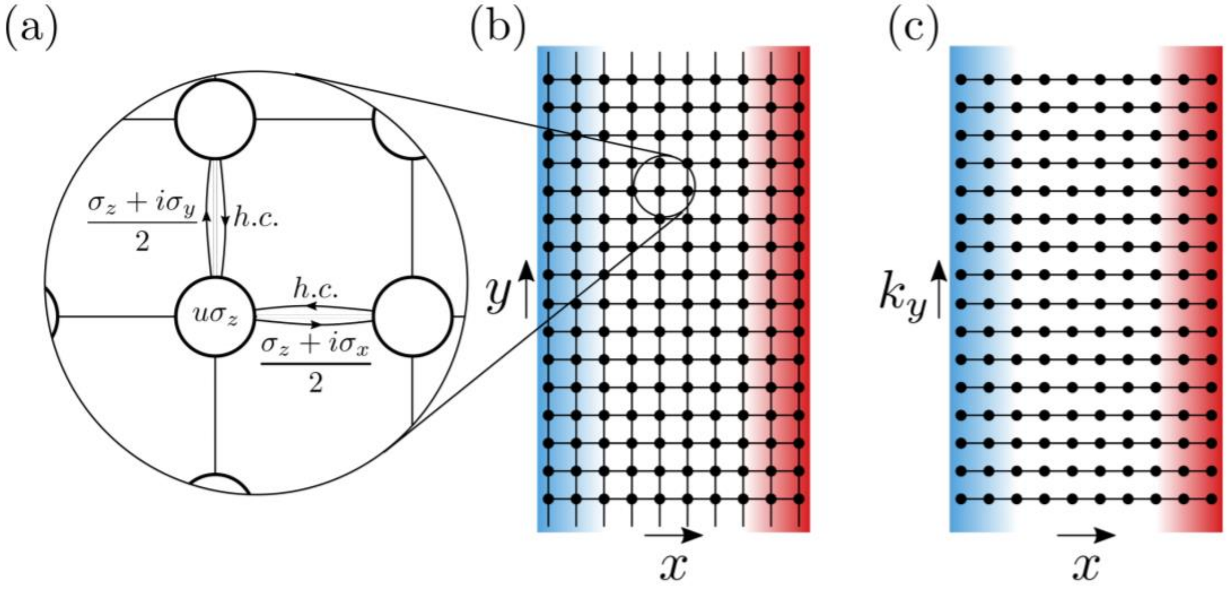
- Question: for a 2D Hamiltonian **with chiral and time-reversal** symmetry with **broken inversion symmetry** we expect to have **Weyl semimetallic regions** between different topological classes

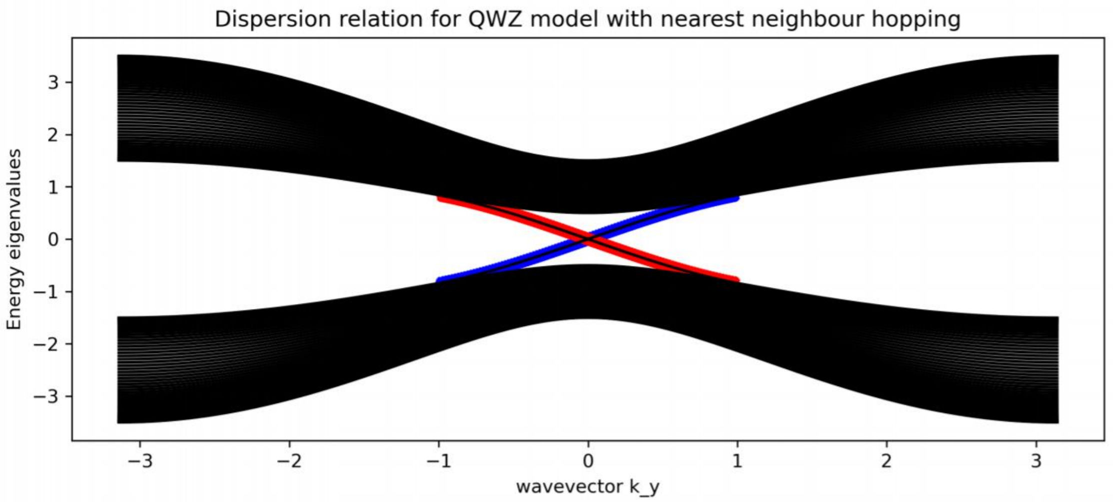
- idea comes from the 3D case, similar but without chiral symmetry

- First step: investigate the generalized anistropic Bernevig-Hughes-Zhang model (abbr. BHZ)

The QWZ model is a Chern insulator I.

- Chern insulator: 2D insulator with nonzero Chern number
- guaranteed low-energy (≈ 0) states at boundary
- Edge state: localized to edge, can conduct





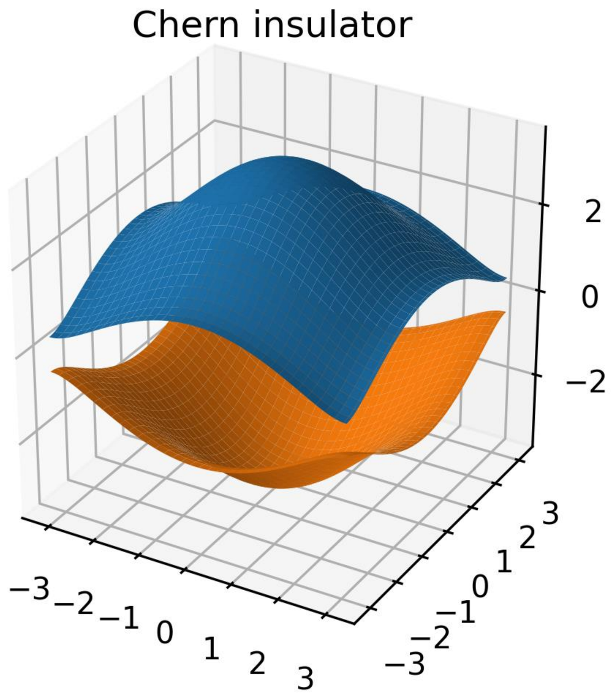
The QWZ model is a Chern insulator II.

- Can be described in reciprocal space by:

$$\hat{H}(k) = \sin k_x \hat{\sigma}_x + \sin k_y \hat{\sigma}_y + [u + \cos k_x + \cos k_y]\hat{\sigma}_z$$

- Depending on u, either trivial or topological insulator
  - Topological insulator: some edge states cross bandgap

- Bulk band structure not enough to distinguish Chern from trivial

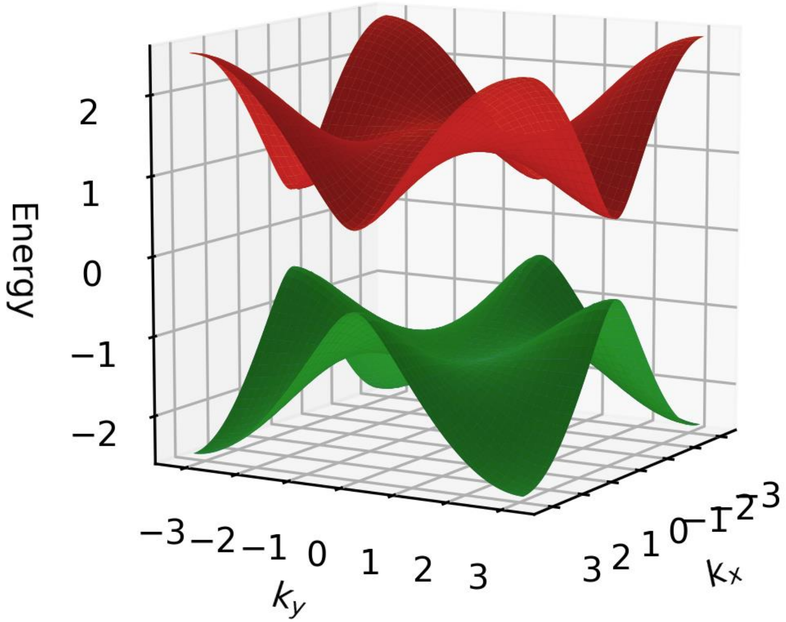


BHZ model = 2x QWZ + coupling

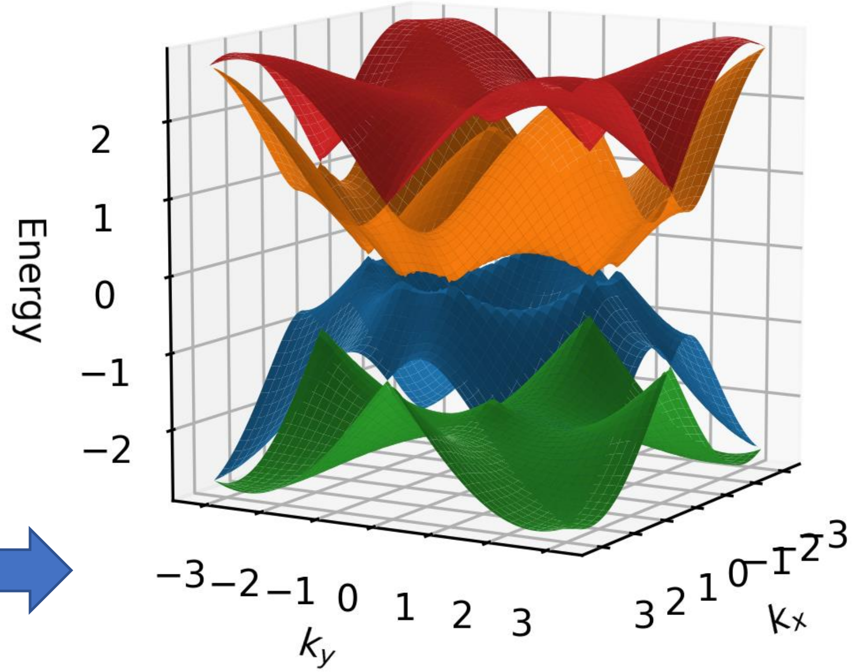
- couple two QWZ models with **inversion-breaking term**, add in **anisotropy** in x/k_x directions (v_x)
- Reciprocal-space Hamiltonian:

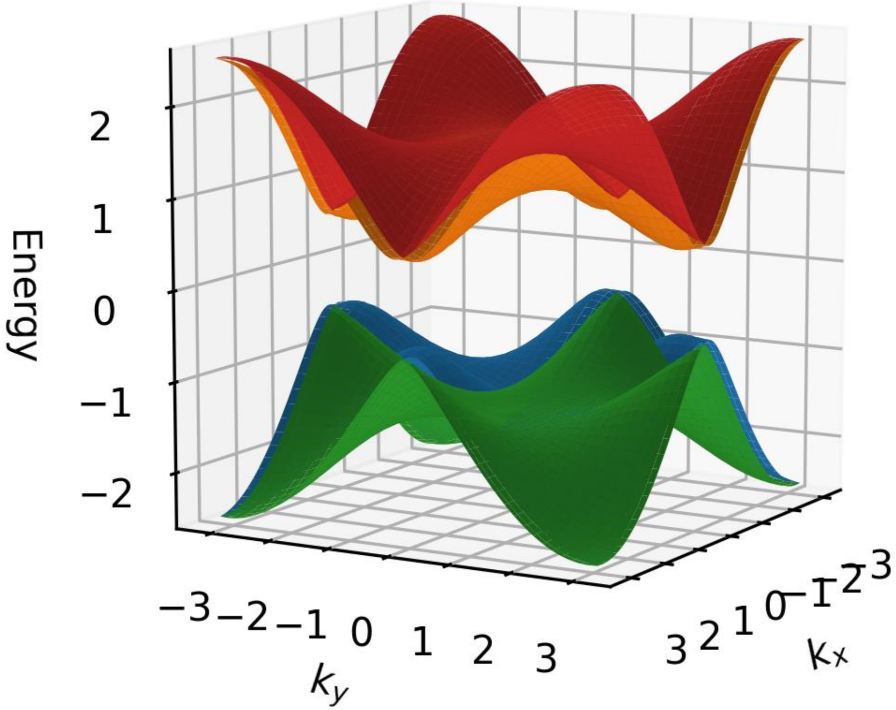
$$\hat{H} = \begin{bmatrix} \boxed{u} + v_x c_x + c_y & v_x s_x - i s_y & 0 & -C \\ v_x s_x + i s_y & -(\boxed{u} + v_x c_x + c_y) & C & 0 \\ 0 & C & \boxed{u} + v_x c_x + c_y & -v_x s_x - i s_y \\ -C & 0 & -v_x s_x + i s_y & -(\boxed{u} + v_x c_x + c_y) \end{bmatrix}$$

where $c_x = \cos(k_x)$, $c_y = \cos(k_y)$, $s_x = \sin(k_x)$, $s_y = \sin(k_y)$.



Interlayer coupling increases



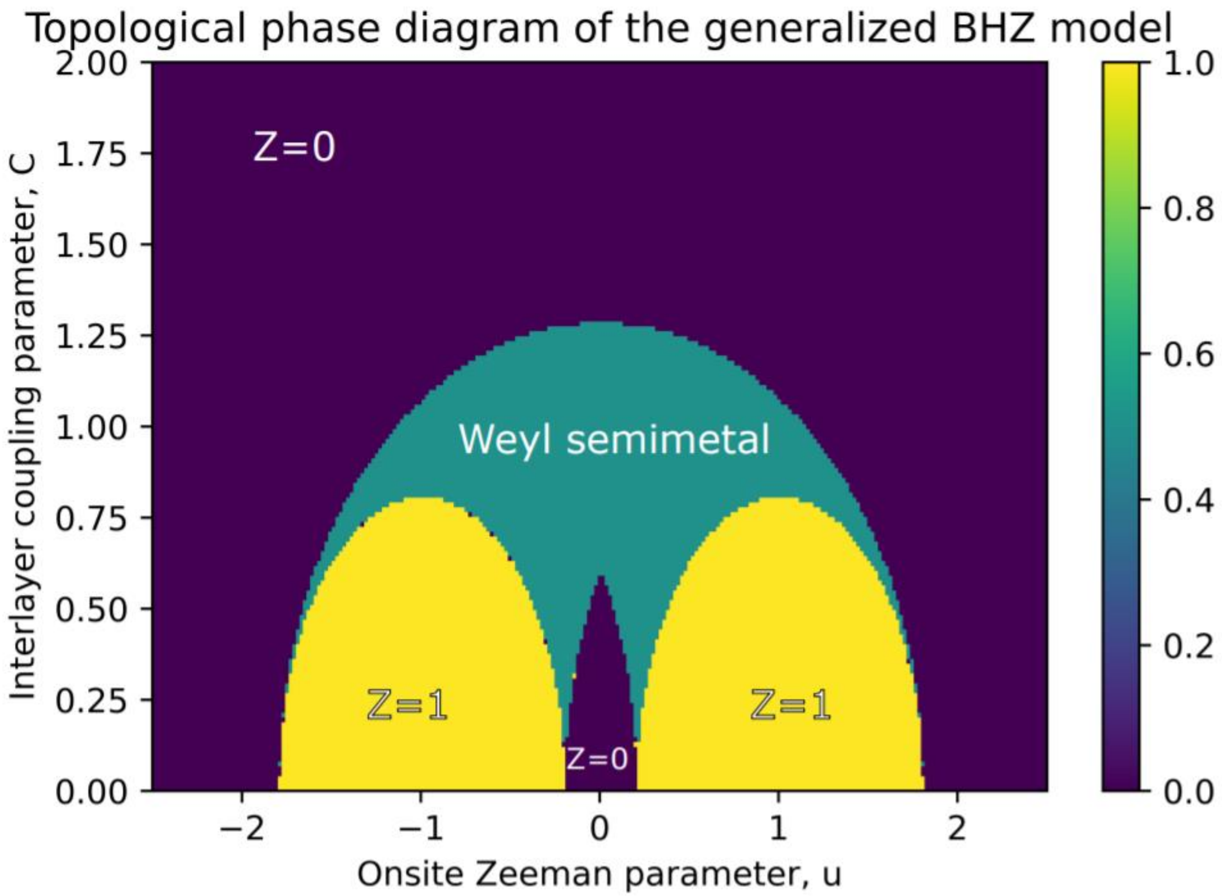


Phase diagram of BHZ model has Weyl phase

- Purely numerical calculation based on Z_2 and bandgap calculation:

$C > 0$

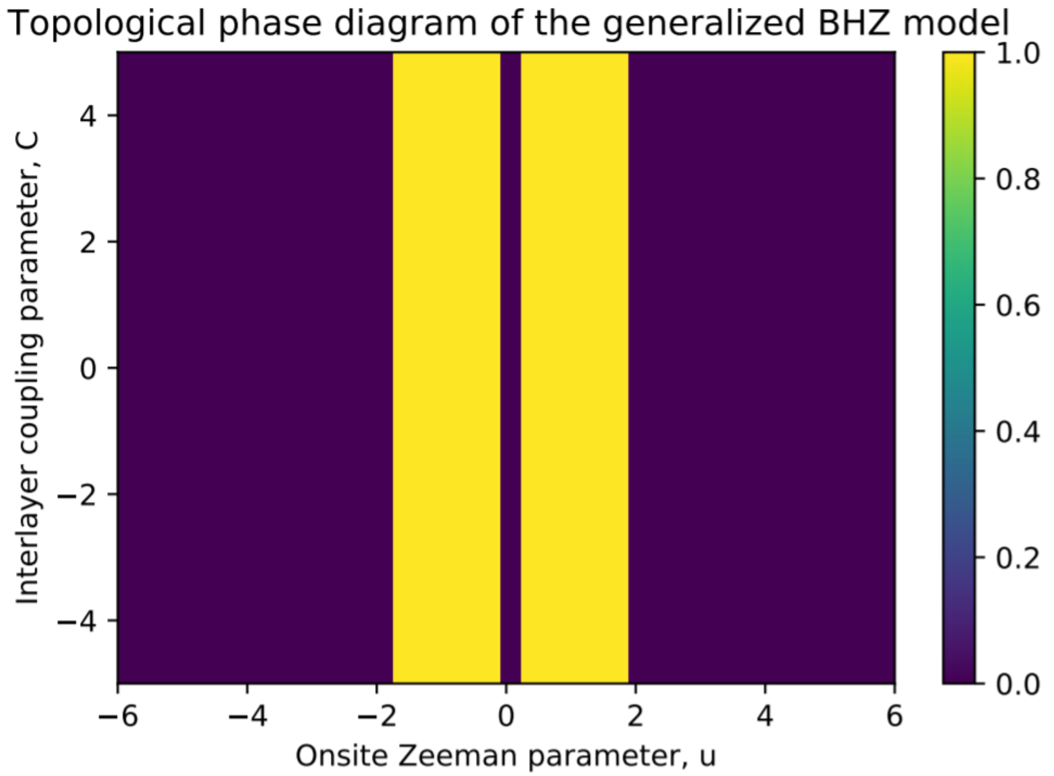
$C = 0$



vx = 0.8

Inversion-respecting coupling: no Weyl phases

- We can alternative use a coupling that preserves inversion symmetry. In this case we do not expect Weyl-semimetallic phases at all. Using $C_2 t_x \sigma_x \prod(k_x, k_y)$ for coupling, indeed we get:



$\prod(k_x, k_y)$ is odd

Chiral basis for analytic calculations

$$\hat{U} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & -i \\ 0 & 1 & -i & 0 \\ 0 & 1 & i & 0 \\ 1 & 0 & 0 & i \end{bmatrix}$$

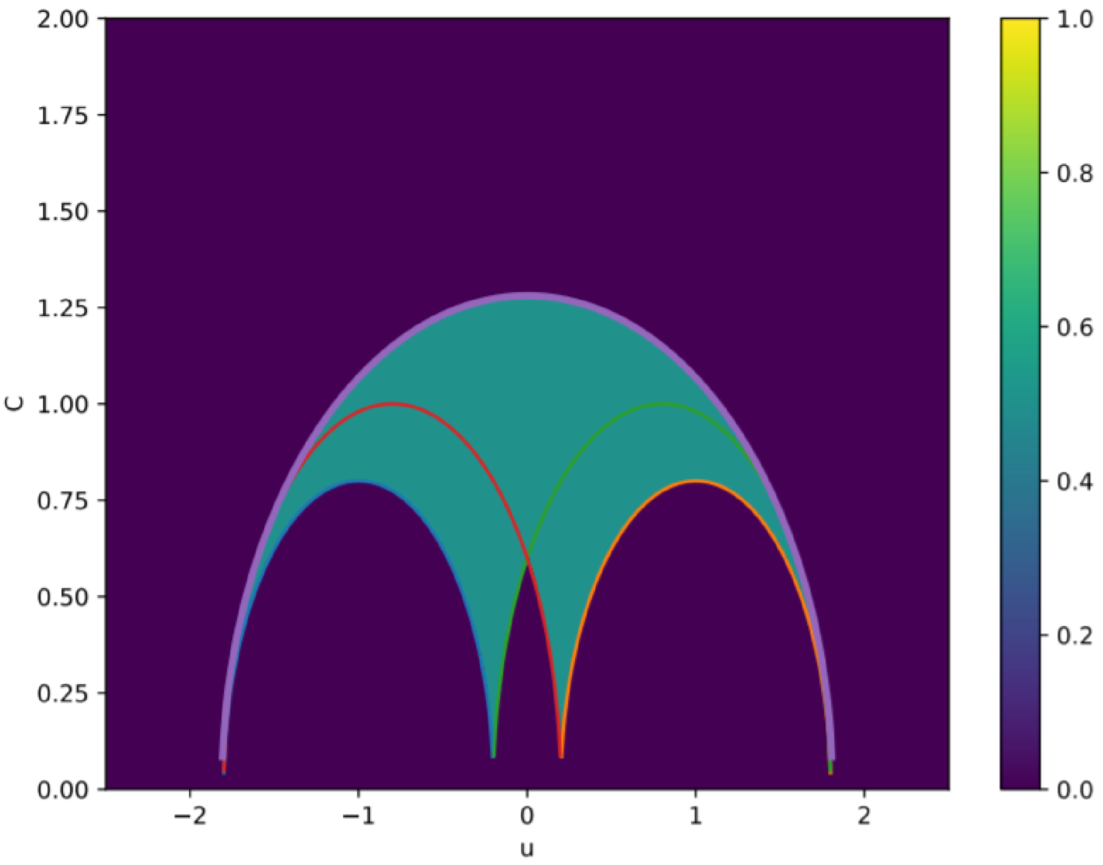
- Can rewrite $H = \begin{bmatrix} 0 & h(k) \\ h(k)^{*T} & 0 \end{bmatrix}$ by a unitary transformation with U

$$\hat{h}(C_1) = \begin{bmatrix} v_x \sin(k_x) - i \sin(k_y) & u + v_x \cos(k_x) + \cos(k_y) + iC_1 \\ -\left(u + v_x \cos(k_x) + \cos(k_y) + iC_1\right) & v_x \sin(k_x) + i \sin(k_y) \end{bmatrix}$$

Have Weyl points when $\det h(k) = 0$

Analytical boundaries are ellipses (+ combinations)

- Calculate where $\det h(k)$ gives $\cos k = \pm 1 \mid \sin k = \pm 1$: this gives boundary



$$u^2 + 2C^2 = 2v_x^2 + 2$$

$$(u \pm 1)^2 + C^2 = v_x^2$$

$$(u \pm v_x)^2 + C^2 = 1$$

vx = 0.8

shows very good agreement with numerical results

Inversion: no Weyl, broken inversion: Weyl

$C \neq 0$: „inversion” symmetry is broken, between any topological phase we have a Weyl semimetallic region

$C = 0$: „inversion” symmetry is not broken, topological phases have no Weyl semimetallic regions between them

Better to formulate Mathematically...

Mathematical explanation

1. The presence of time-reversal symmetry sets $\det(h(k)) = \det(h(-k))$ [12] meaning that the nodes at k and $-k$ have the same chirality (this is true in general). This is indeed what we observe in the generalized BHZ model without inversion symmetry.

2. If $C = 0$ in the generalized BHZ model, we find that

$$\det(h_{BHZ}(k)) = \det(h_{BHZ}(-k))^* \tag{24}$$

from which it follows that the chiralities at k and $-k$ are opposite. Combined with 1., this means that there can be no Weyl nodes when both inversion and TR symmetry is present in the generalized BHZ model.

Quotation marks around „inversion symmetry”

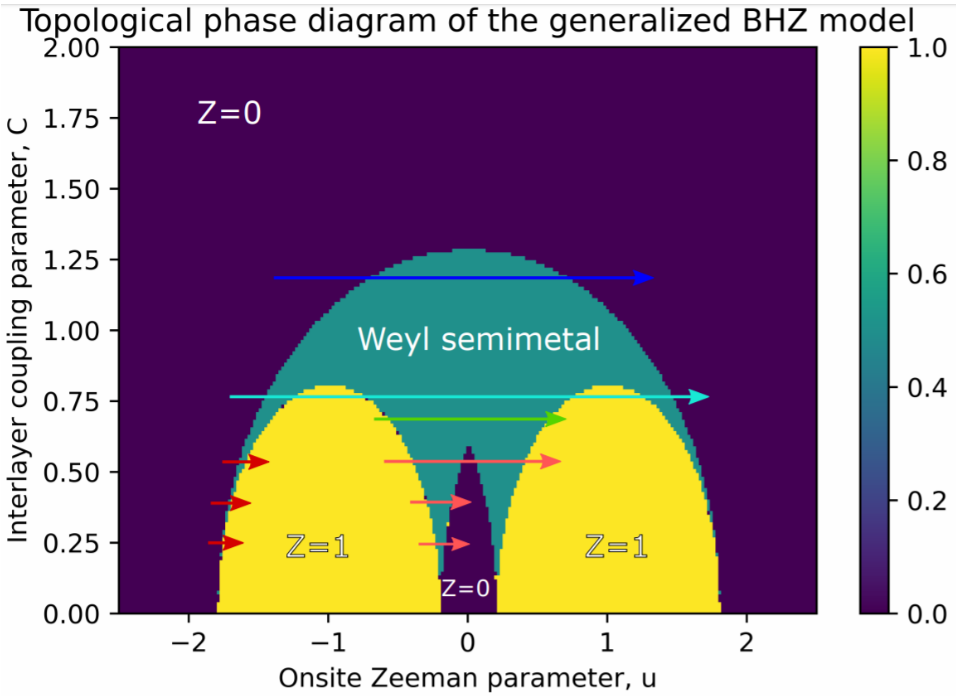
- a generic inversion symmetry would give:

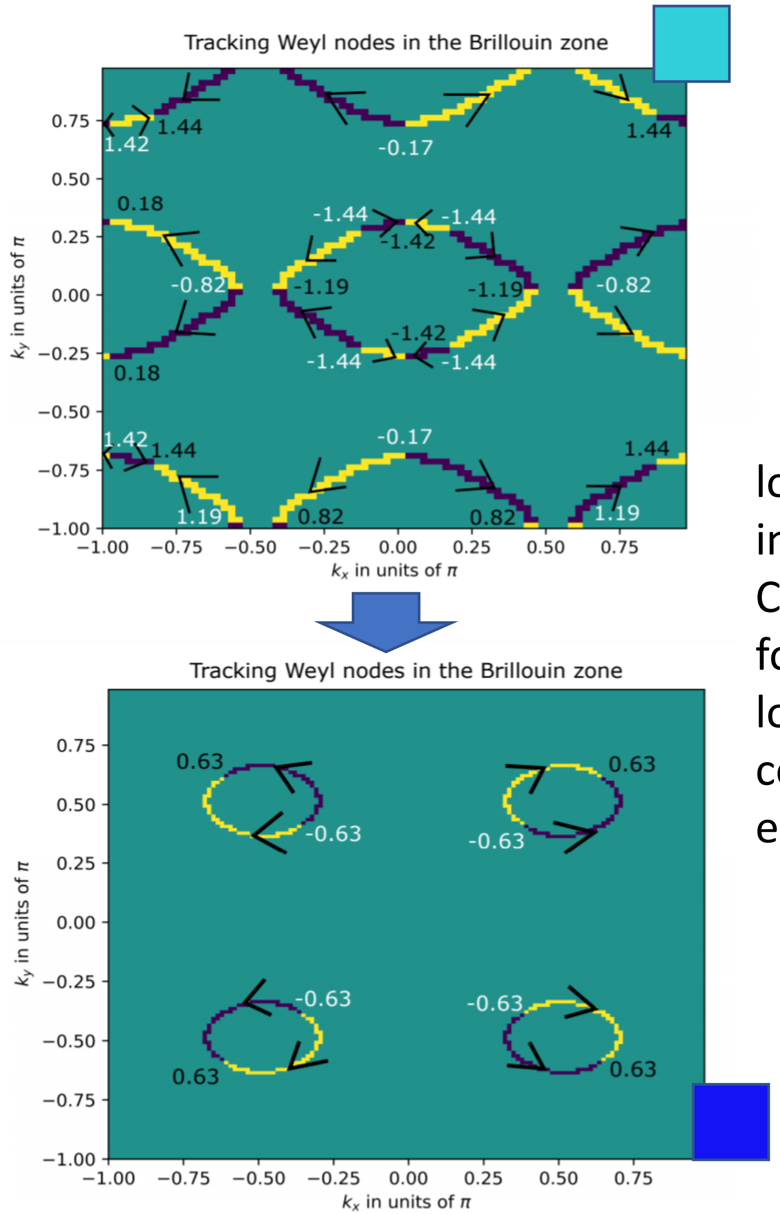
$$\det h(k) = \det h(-k)$$

so these inversion symmetries do not prohibit the existence of Weyl phases.

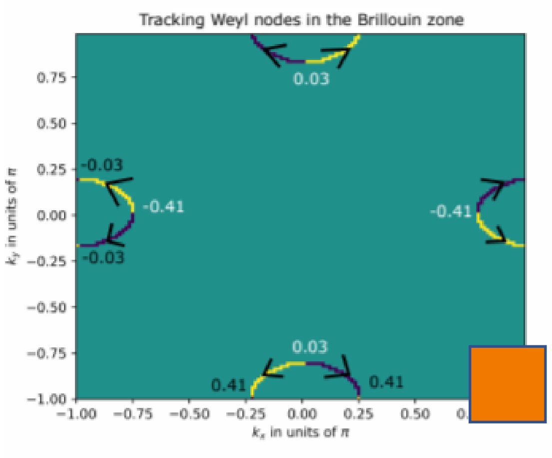
- Our ‚inversion symmetry’ is different from the generally expected one
    - What property of our inversion symmetry counts?

Paths in the phase diagram → trajectories of Weyl nodes

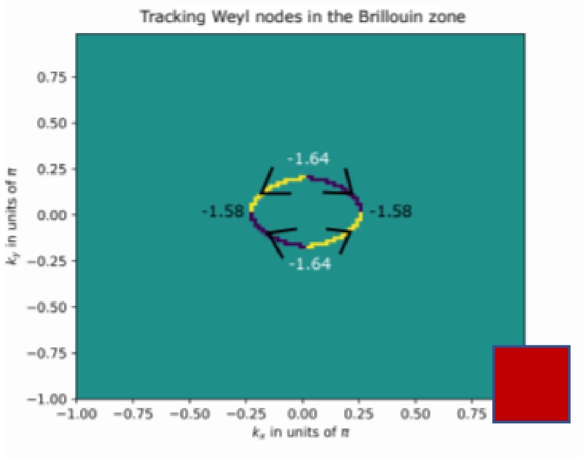




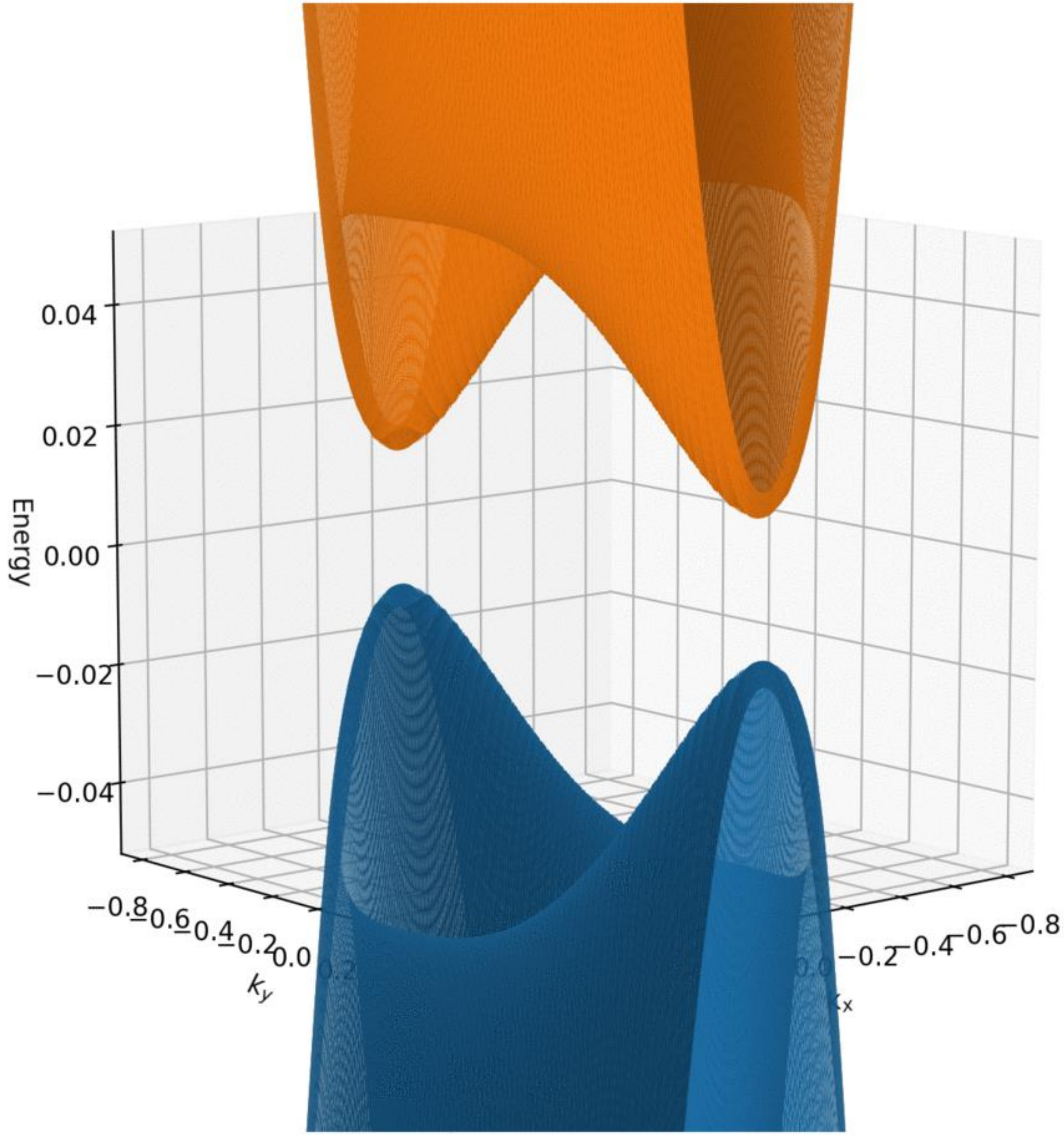
loops interact as C grows to form new loops centred elsewhere

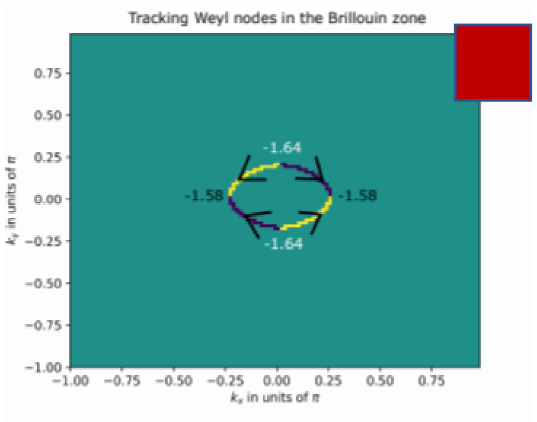


(c) $C = 0.55$, centre



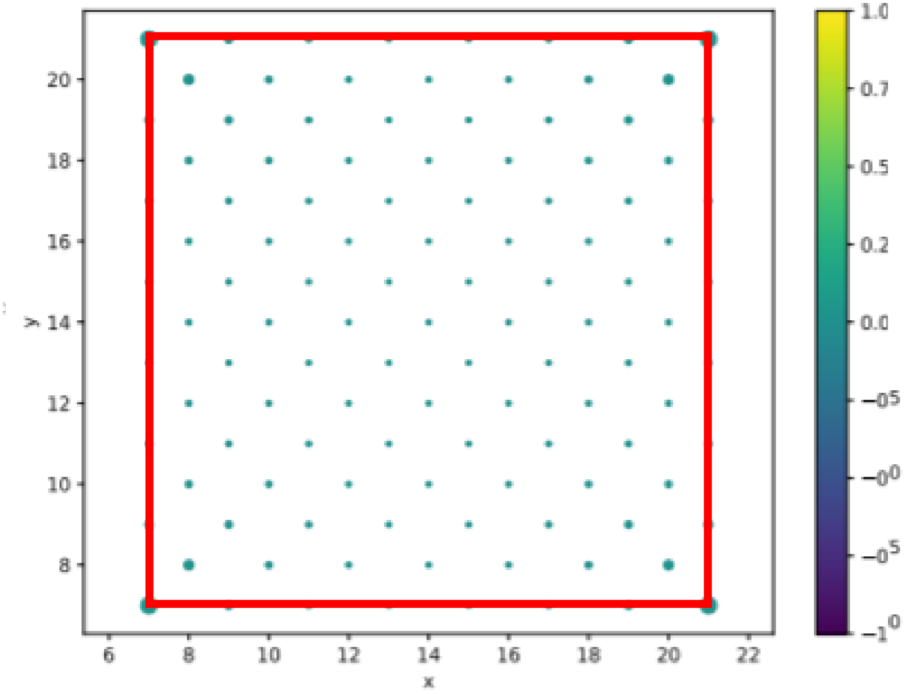
(f) $C = 0.55$, left

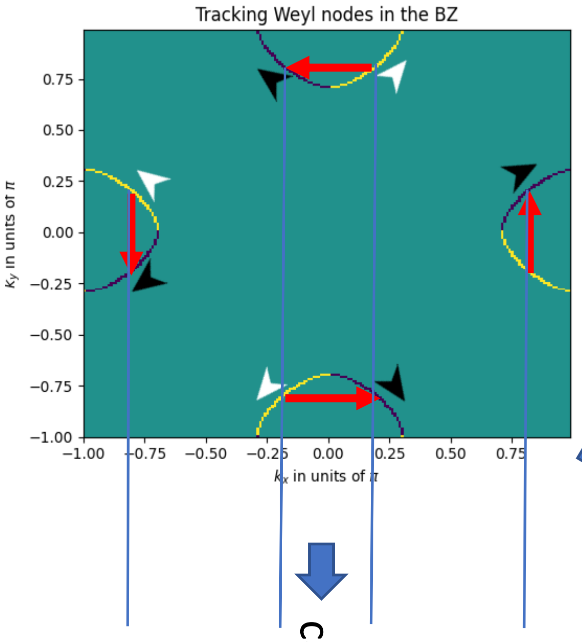

0.04
0.02
Energy
0.00
−0.02
−0.04
−0.8 0.6 0.4 0.2 0.0
k_y
0.0 −0.2 −0.4 −0.6 −0.8
k_x


Tracking Weyl nodes in the Brillouin zone
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
k_y in units of π
-1.64
-1.58
-1.58
-1.64
−1.00 −0.75 −0.50 −0.25 0.00 0.25 0.50 0.75
k_x in units of π

(f) $C = 0.55$, left

Real-space Hamiltonian determines edge state density





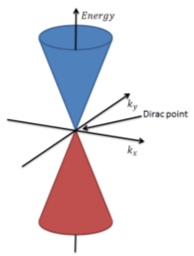
cancel

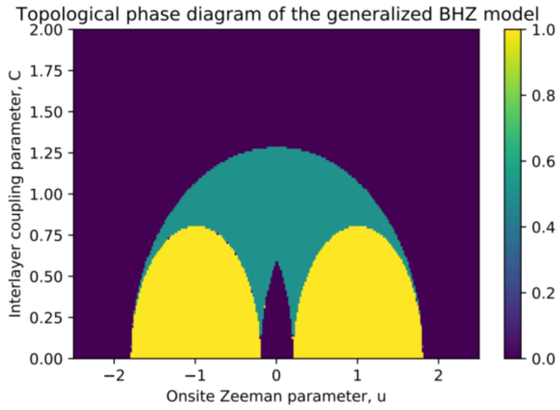
doesn't cancel

cancel

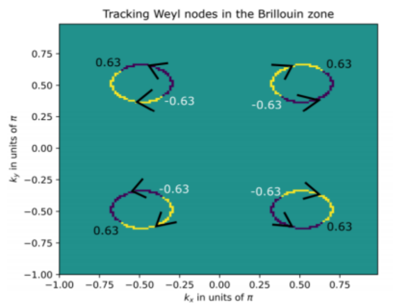
red arrows indicate Fermi arcs

Summary





1. Weyl nodes are special, topologically protected band-touching points
2. The generalized anisotropic BHZ model has the properties of 3D system:
   - inversion symmetry respected: no Weyl phases
   - inversion symmetry broken: Weyl phases
3. General 2D system behaves differently than in 3D (regarding Weyl phases)
4. Topological phase transitions in the BHZ model have associated Weyl node trajectories in phase space



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List of useful papers

[1] W. P. Su, J. R. Schrieffer, A. J. Heeger: *Solitons in Polyacetylene*. Physical Review Letters, Vol. 45, No. 25 (1979)

[2] J. K. Asbóth, L. Oroszlány, A. Pályi: *A Short Course on Topological Insulators*. Springer (2016)

[3] M. Koshino, T. Morimoto, M. Sato: *Topological zero modes and Dirac points protected by spatial symmetry and chiral symmetry*. Physical Review B 90, 115207 (2014)

[4] L. Li, C. Yang, S. Chen: *Winding numbers of phase transition points for one-dimensional topological systems*. Europhysics Letters, Vol. 112, No. 1 (2015)

[5] A. Essin, V. Gurarie: *Bulk-boundary correspondence of topological insulators from their respective Green's functions*. Physical Review B 84, 125132 (2011)

[6] G. H. Wannier: *Dynamics of Band Electrons in Electric and Magnetic Fields*. Reviews of Modern Physics 34, 645 (1962)

[7] M. J. Rice, E. J. Mele: *Elementary Excitations of a Linearly Conjugated Diatomic Polymer*. Physical Review Letters 49, 1455 (1982)

[8] X.-L. Qi, Y.-S. Wu, S.-C. Zhang: *Topological quantization of the spin Hall effect in two-dimensional paramagnetic semiconductors*. Physical Review B 74, 085308 (2006)

[9] B. A. Bernevig, T. L. Hughes, S.-C. Zhang *Quantum Spin Hall Effect and Topological Phase Transition in HgTe Quantum Wells* Science Vol. 314, Iss. 5806 (2006)

[10] T. Fukui, Y. Hatsugai: *Quantum Spin Hall Effect in Three Dimensional Materials: Lattice Computation of Z_2 Topological Invariants and Its Application to Bi and Sb*. J. Phys. Soc. Jpn, Vol. 76, No. 5 (2007)

[11] T. Fukui, Y. Hatsugai, H. Suzuki: *Chern Numbers in Discretized Brillouin Zone: Efficient Method of Computing (Spin) Hall Conductances*. J. Phys. Soc. Jpn. Vol. 74, No. 6 (2005)

[12] B. Béri *Topologically stable gapless phases of time-reversal invariant superconductors*. Physical Review B 81, 134515 (2009)

BHZ model in real space

- inverse Fourier-transform:

$$
\begin{aligned}
\hat{H} = u \sum_{m_x=1}^{M_x} |m_x\rangle\langle m_x| \sum_{m_y=1}^{M_y} |m_y\rangle\langle m_y| \, \tau_0 \otimes \sigma_z \\
+C \sum_{m_x=1}^{M_x} |m_x\rangle\langle m_x| \sum_{m_y=1}^{M_y} |m_y\rangle\langle m_y| \, \tau_y \otimes \sigma_y \\
+\frac{1}{2} \sum_{m_x=1}^{M_x} |m_x\rangle\langle m_x| \sum_{m_y=1}^{M_y-1} \big(|m_y\rangle\langle m_y+1| + |m_y+1\rangle\langle m_y| \big) \tau_0 \otimes \sigma_z \\
+\frac{1}{2i} \sum_{m_x=1}^{M_x} |m_x\rangle\langle m_x| \sum_{m_y=1}^{M_y-1} \big(|m_y\rangle\langle m_y+1| - |m_y+1\rangle\langle m_y| \big) \tau_0 \otimes \sigma_y \\
+\frac{1}{2} \sum_{m_y=1}^{M_y} |m_y\rangle\langle m_y| \sum_{m_x=1}^{M_x-1} \big(|m_x\rangle\langle m_x+1| + |m_x+1\rangle\langle m| \big) \tau_0 \otimes \sigma_z \\
+\frac{1}{2i} \sum_{m_y=1}^{M_y} |m_y\rangle\langle m_y| \sum_{m_x=1}^{M_x-1} \big(|m_x\rangle\langle m_x+1| - |m_x+1\rangle\langle m_x| \big) \tau_z \otimes \sigma_x
\end{aligned}
$$

Numerical methods for Chern number and Z_2 invariant

- Chern number
  - discretize Brillouin zone into plaquettes, calculate Berry flux (Berry phase of going around each plaquette in a fixed direction) for each plaquette
  - sum all Berry fluxes of plaquettes to get Chern number
  - works in arbitrary (local) gauge
- Z_2 invariant
  - fix gauges at TRIM and non-TRIM boundary points of inversion-half BZ
  - calculate Berry potential (A) and curvature (F) for each plaquette
  - $Z_2 = \frac{1}{2\pi \mathrm{i}} \left[\sum_{k_\ell \in \partial \mathcal{B}^-} A_1(k_\ell) - \sum_{k_\ell \in \mathcal{B}^-} F_{12}(k_\ell) \right]$ (sum A over boundary and F over whole inversion-half BHZ)

see more: *„Chern Numbers in Discretized Brillouin Zone: Efficient Method of Computing (Spin) Hall Conductances”* and *„Quantum Spin Hall Effect in Three Dimensional Materials: Lattice Computation of Z2 Topological Invariants and Its Application to Bi and Sb”*