

Weyl semimetals from noncentrosymmetric topological superconductors

1) Standard route to Weyl semimetals: at transition between weak topological phases

2D: Transition between trivial and topological insulator: Quantum Phase transition, critical state

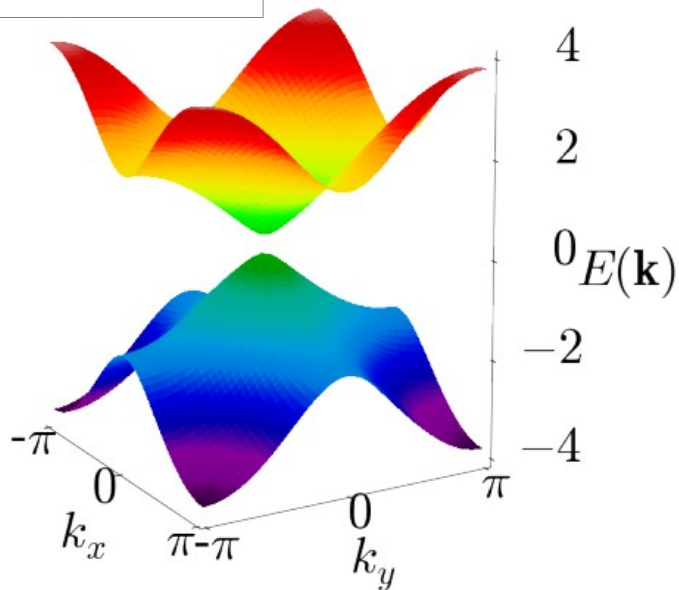
$$\hat{H}(k_x, k_y) = \sin k_x \hat{\sigma}_x + \sin k_y \hat{\sigma}_y + [u + \cos k_x + \cos k_y] \hat{\sigma}_z$$

trivial insulator

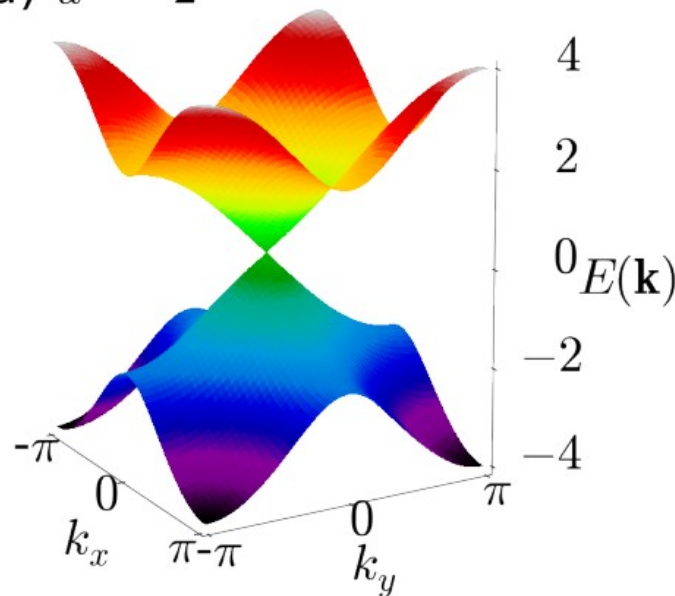
critical state (semimetal)

Chern insulator

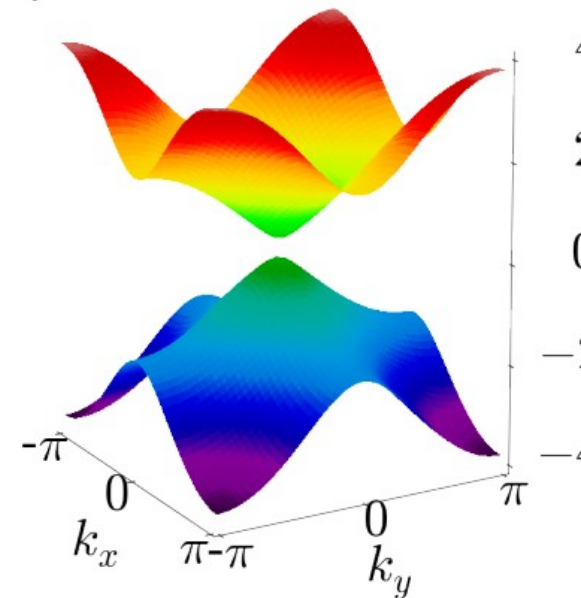
$u = -2.2$



(a) $u = -2$

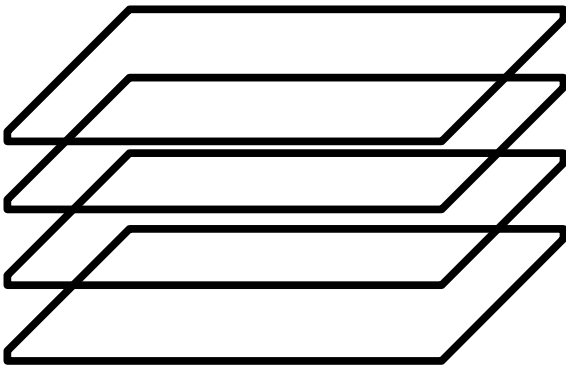


(d) $u = -1.8$

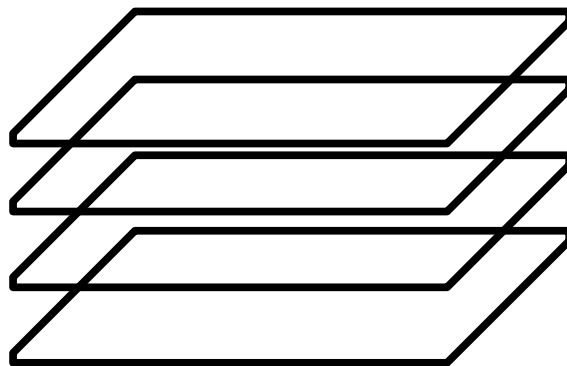


Stack of 2D insulators: transition via a line of nodes

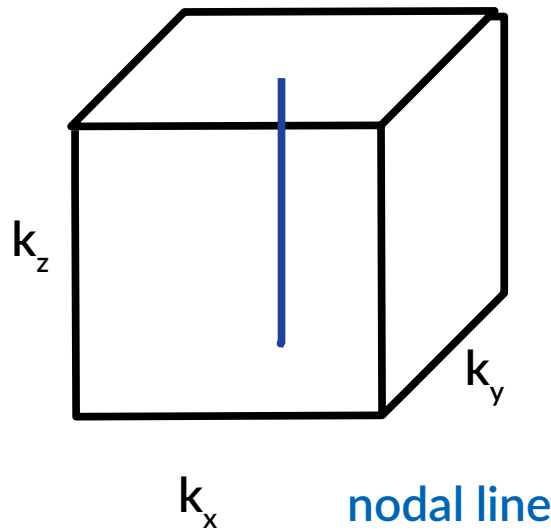
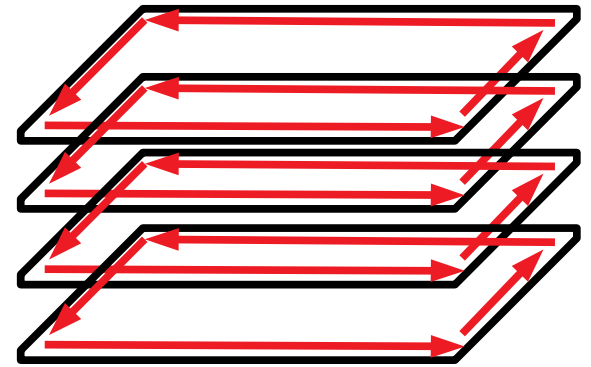
stack of trivial insulators



stack of critical systems
(gap closing at Γ)

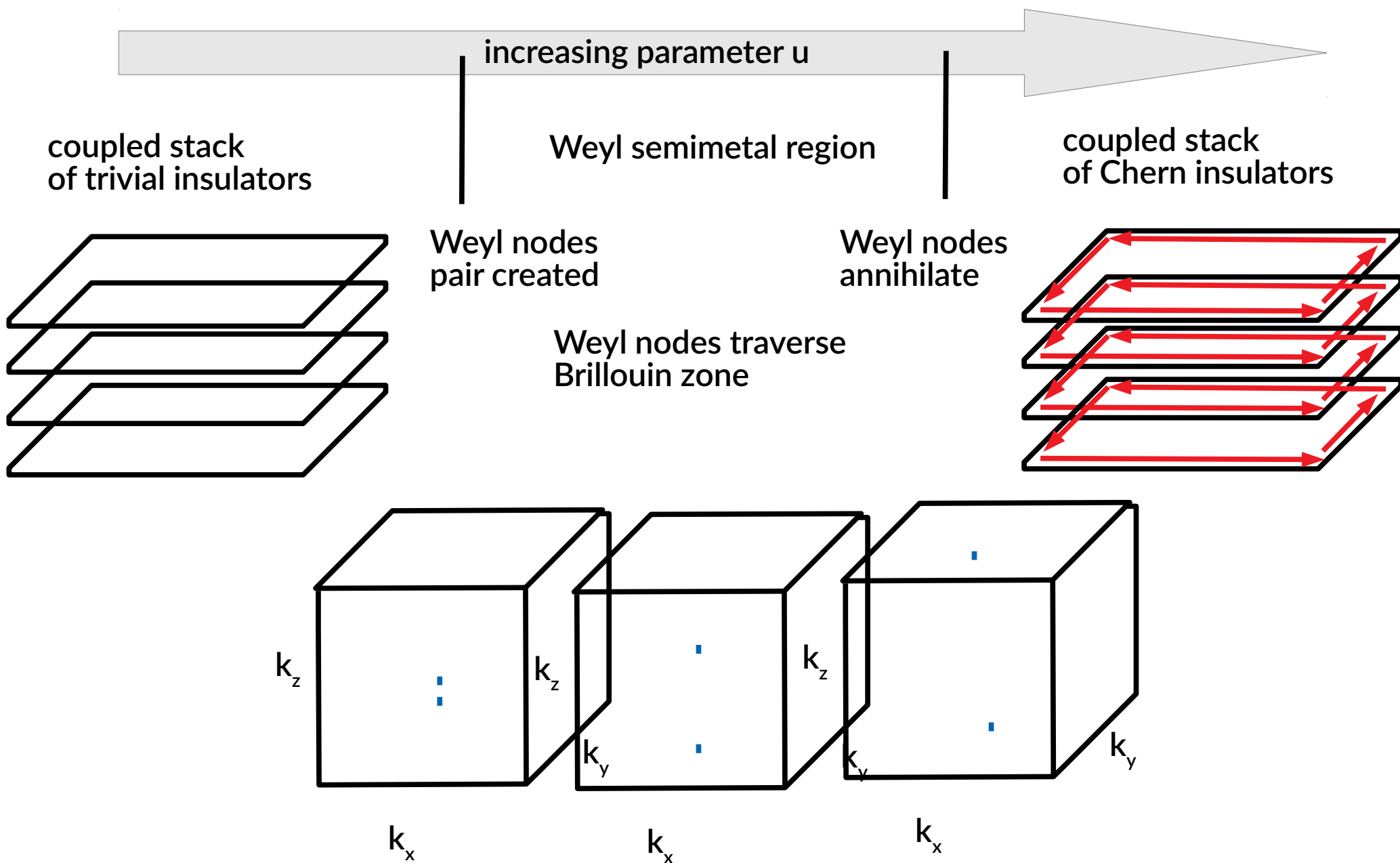


stack of Chern insulators



nodal line

Coupling the stacks \rightarrow transition happens by pair of Weyl nodes traversing the Brillouin Zone = Weyl semimetal



2) Liu & Vanderbilt 2014: Weyl semimetals also at transition between trivial and Z2 topological insulators, if no inversion symmetry

PHYSICAL REVIEW B **90**, 155316 (2014)



Weyl semimetals from noncentrosymmetric topological insulators

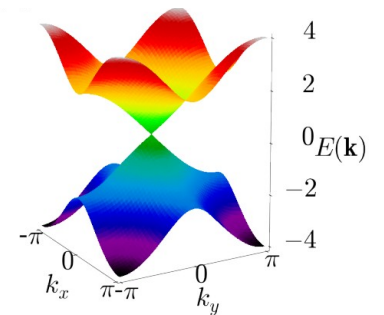
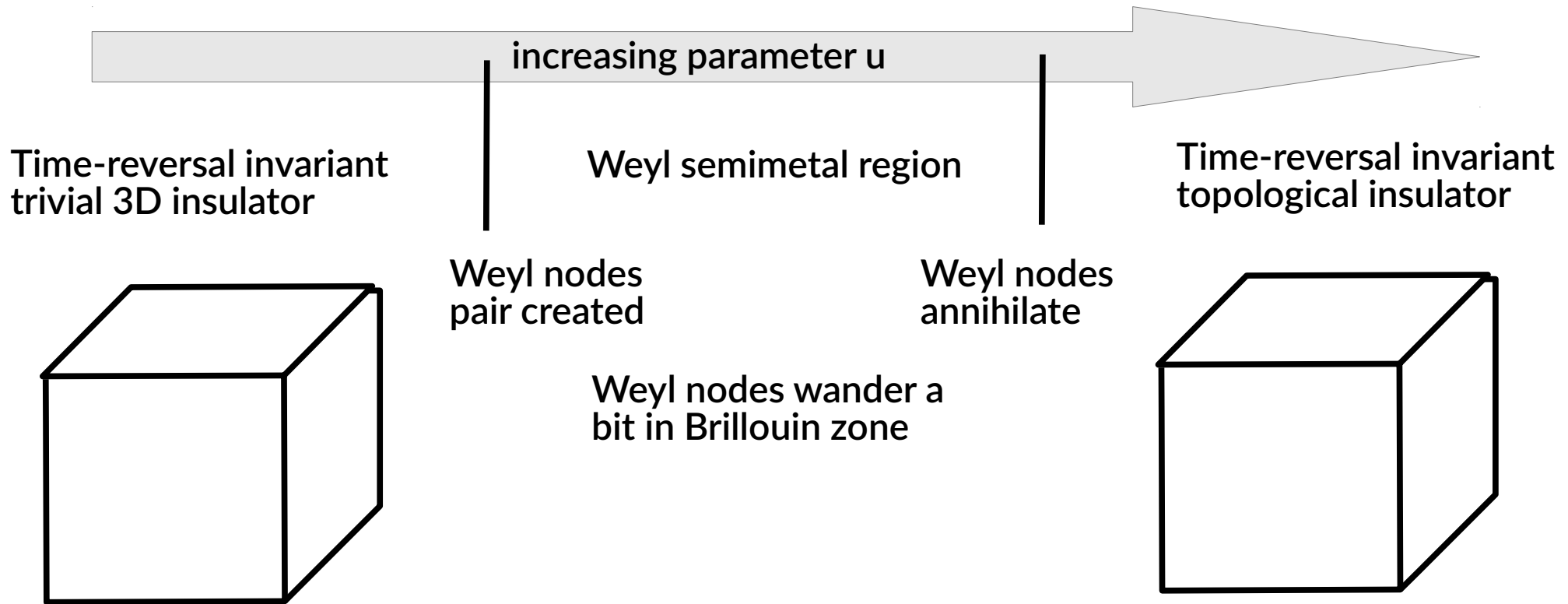
We consider the problem of TPTs in noncentrosymmetric insulators in the most general case. In the space of the two bands which touch at the TPT, the system can be described by the effective Hamiltonian

$$H(\mathbf{k}, \lambda) = f_x(\mathbf{k}, \lambda)\sigma_x + f_y(\mathbf{k}, \lambda)\sigma_y + f_z(\mathbf{k}, \lambda)\sigma_z, \quad (1)$$

where λ is the parameter that drives the TPT and $\sigma_{x,y,z}$ are the three Pauli matrices defined in the space spanned by the highest occupied and the lowest unoccupied states at \mathbf{k} . Since we study the TPT between two insulating phases, we can assume without loss of generality that the system is gapped for $\lambda < \lambda_0$, and that the first touching that occurs at $\lambda = \lambda_0$ takes place at $\mathbf{k} = \mathbf{k}_0$. In other words, $f_i(\mathbf{k}_0, \lambda_0) = 0, i = x, y, z$.

Then we ask what happens if $\mathbf{k}_0 \rightarrow \mathbf{k}_0 + \mathbf{q}$ and $\lambda_0 \rightarrow \lambda_0 + \delta\lambda$.

Liu & Vanderbilt conclusion: in the generic case, transition to 3D Z2 top.ins. via Weyl semimetal



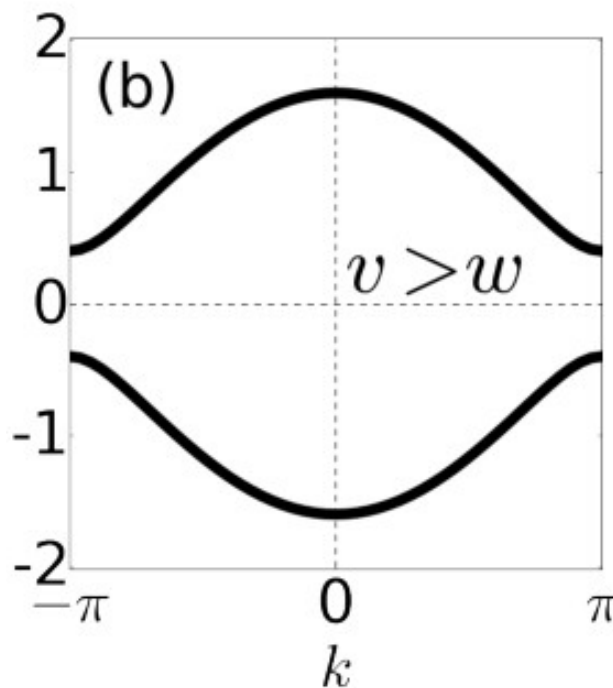
odd number of
Weyl cones on
surface

3) Weyl semimetals between weak topological insulators in 2D, with chiral symmetry

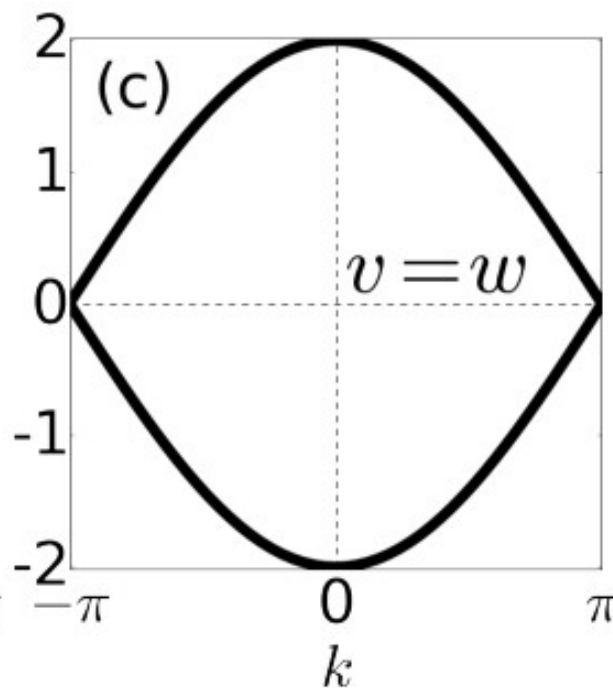
1D: Transition between trivial and topological insulator: Quantum Phase transition, critical state

$$\hat{H}_{\text{SSH}}(k) = (v + w_x \cos k_x) \hat{\sigma}_x + (w_x \sin k_x) \hat{\sigma}_y$$

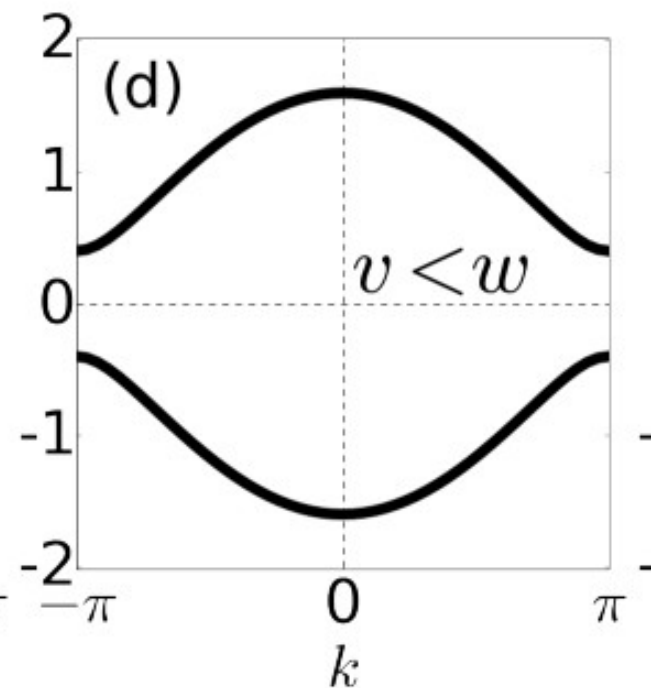
trivial insulator



critical state (semimetal)

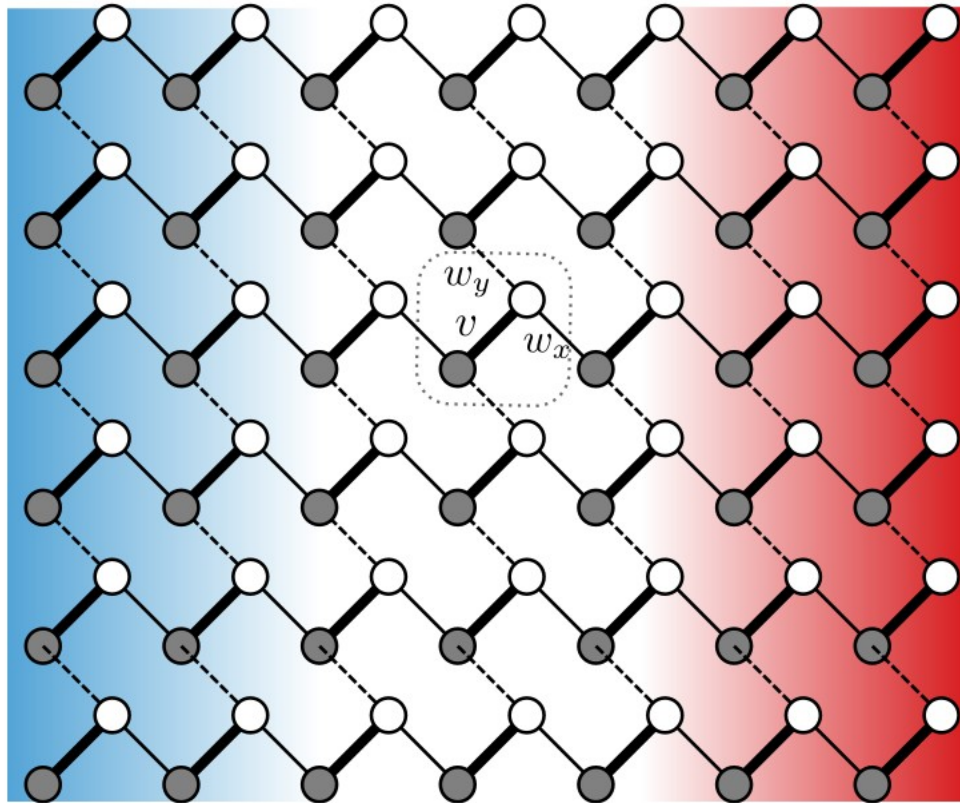


topological insulator

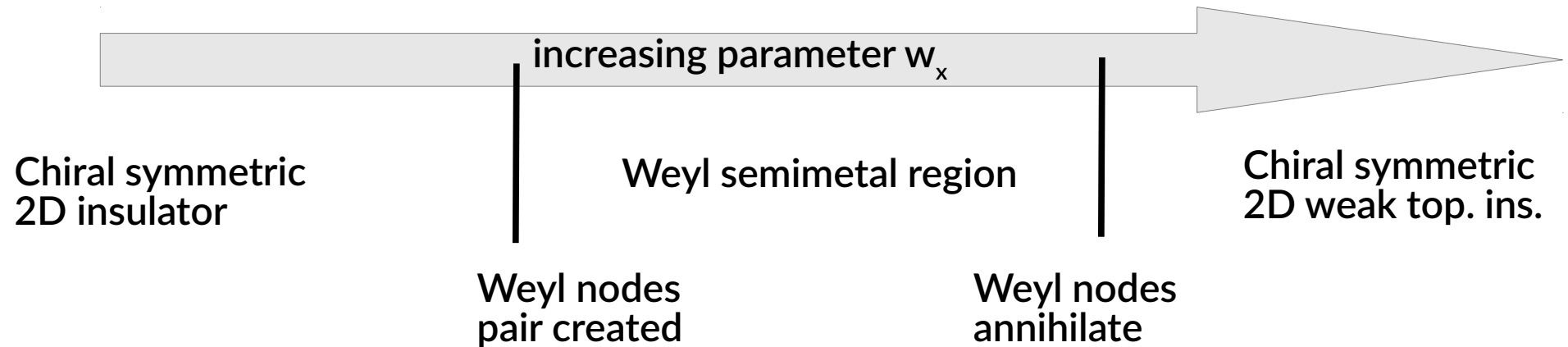


Stack of coupled SSH chains – respecting chiral symmetry

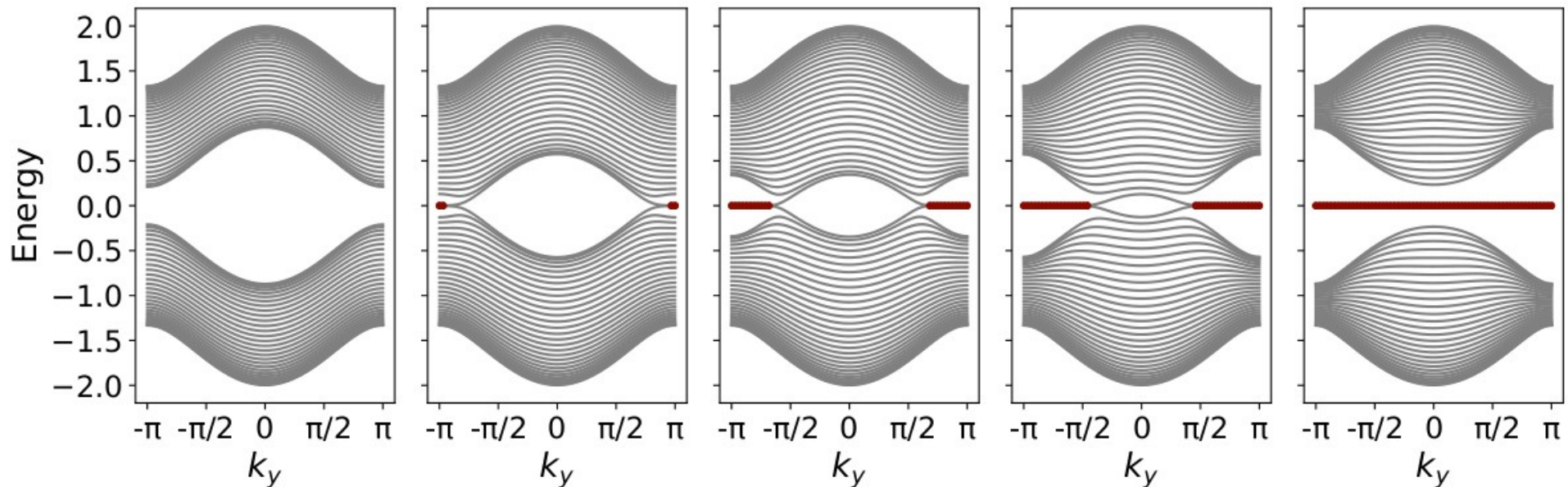
$$\hat{H}_{\text{C2D}}(k) = (v + w_x \cos k_x + w_y \cos k_y) \hat{\sigma}_x + (w_x \sin k_x + w_y \sin k_y) \hat{\sigma}_y$$



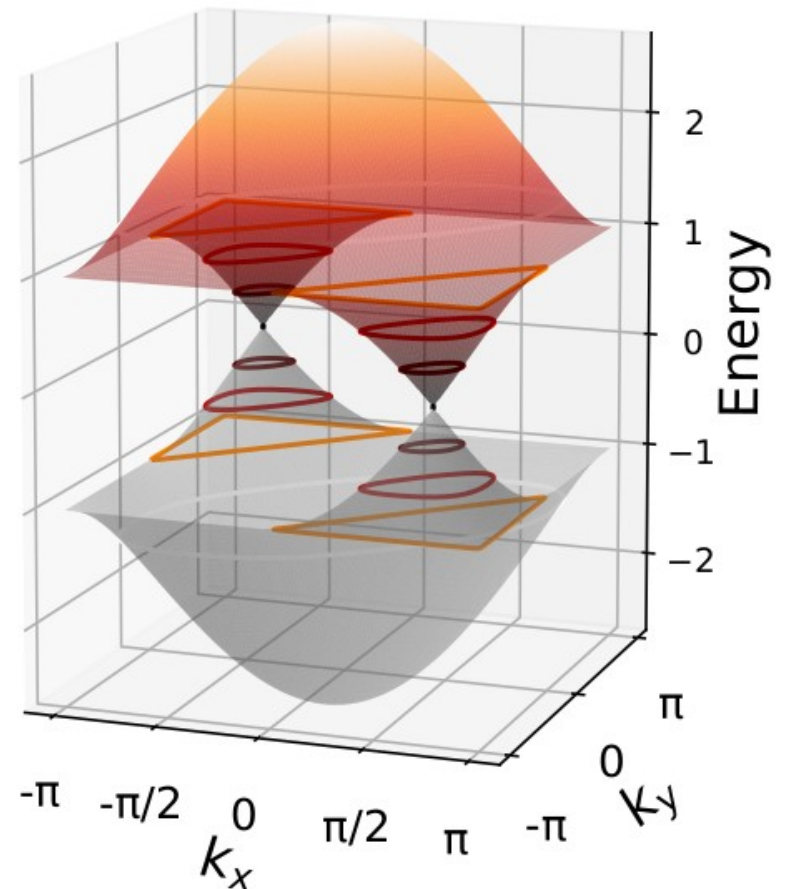
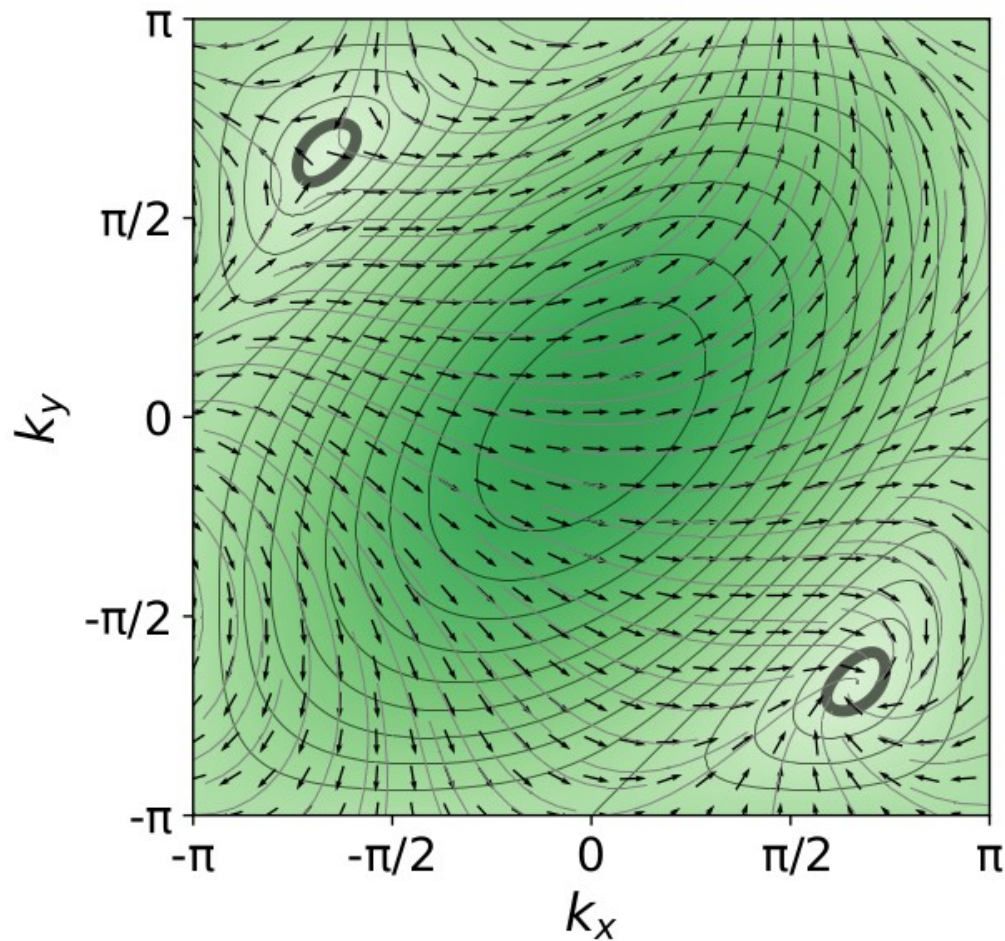
Transition between phases broadens: Weyl nodes, traverse Brillouin zone, annihilate



Weyl nodes traverse Brillouin zone



The charge of Weyl nodes is not Chern number, but a winding number



4) So what about the Liu-Vanderbilt story in 2D? chiral symmetric + time-reversal symmetric 2D topological insulators = time-reversal invariant topological superconductors

BHZ = two layers of QWZ model (particle-hole symmetric Chern insulator layer
+ time-reversed partner), with appropriate coupling

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

$$H_{\text{TRI}} = \begin{bmatrix} H & C \\ C^\dagger & H^* \end{bmatrix}$$



σ matrices: particle-hole
 τ matrices: layer

$\hat{\tau}_y \hat{K}$ - Time reversal

$\hat{\sigma}_x \hat{K}$ - Particle-hole

$\hat{\tau}_y \hat{\sigma}_x$ - Chiral

BHZ model also has inversion symmetry, we need to break it

$$\begin{pmatrix} (u + \cos k_x + \cos k_y)\hat{\sigma}_z + \sin k_x \hat{\sigma}_x + \sin k_y \hat{\sigma}_y & -i\hat{\sigma}_y \\ i\hat{\sigma}_y & (u + \cos k_x + \cos k_y)\hat{\sigma}_z - \sin k_x \hat{\sigma}_x + \sin k_y \hat{\sigma}_y \end{pmatrix}$$

$$\hat{H}_{\text{BHZ}} = (u + \cos k_x + \cos k_y)\hat{\sigma}_z \hat{\tau}_0 + \sin k_x \hat{\sigma}_x \hat{\tau}_z + \sin k_y \hat{\sigma}_y \hat{\tau}_0 + \hat{\sigma}_y \hat{\tau}_y$$

$\hat{\tau}_y \hat{\sigma}_x$ - Chiral

	τ_0	τ_x	τ_y	τ_z
σ_0				
σ_x				S
σ_y	S		C	
σ_z	C			

$\hat{\tau}_y \hat{K}$ - Time reversal

	τ_0	τ_x	τ_y	τ_z
σ_0	+	-	-	-
σ_x	+	-	-	-
σ_y	-	+	+	+
σ_z	+	-	-	-

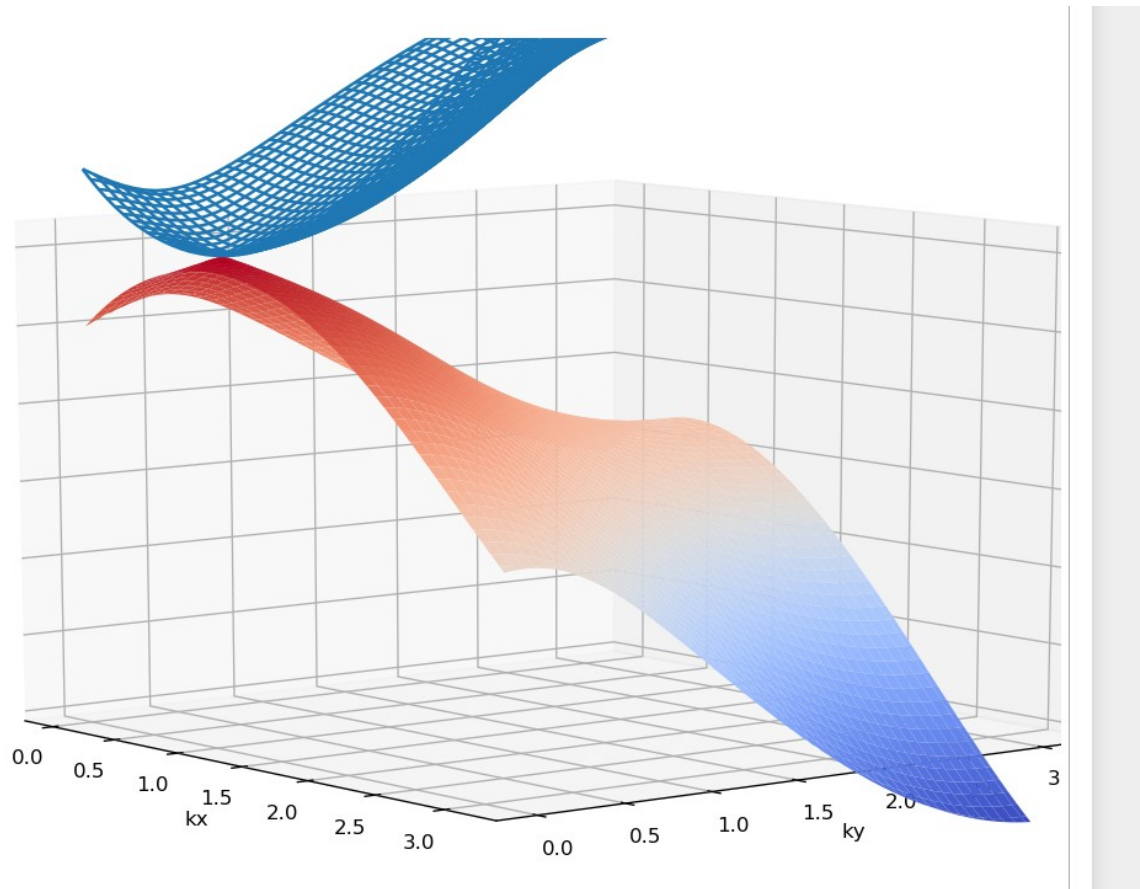
$\hat{\tau}_z \hat{\sigma}_z$ - Inversion

Extra terms allowed by chiral & TR symmetries:

$\sin(k) \tau_x$, $\sin(k) \tau_z$, $\sin(k) \tau_x \sigma_x$, $\sin(k) \tau_y \sigma_z$

Inversion symmetry broken by red terms

I tried it numerically, and the story seems to work



To-do

- Numerically explore simple model
 - Linearize around band touching point
 - ?Find possible candidate material
-
- Play around with disorder? Robustness? What if only disorder breaks inversion symmetry?