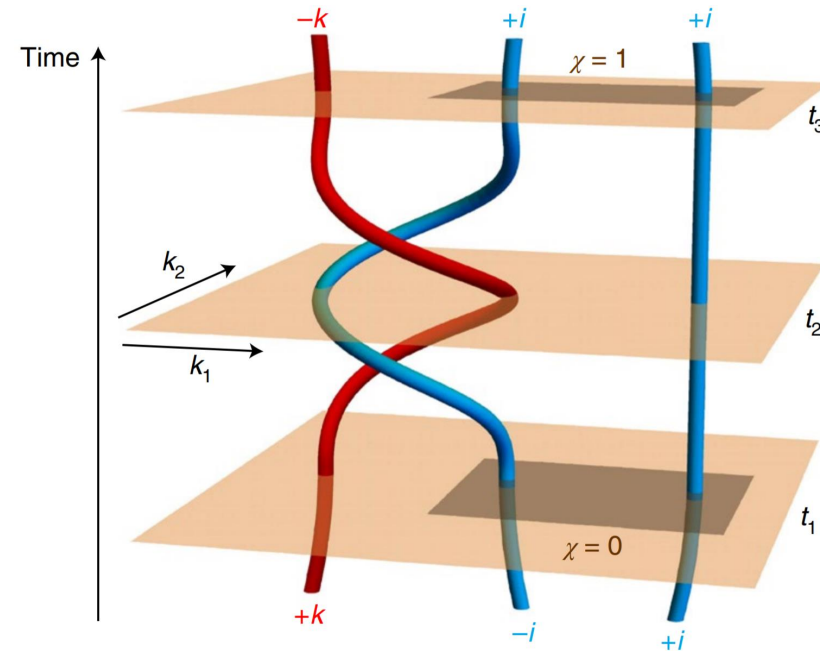
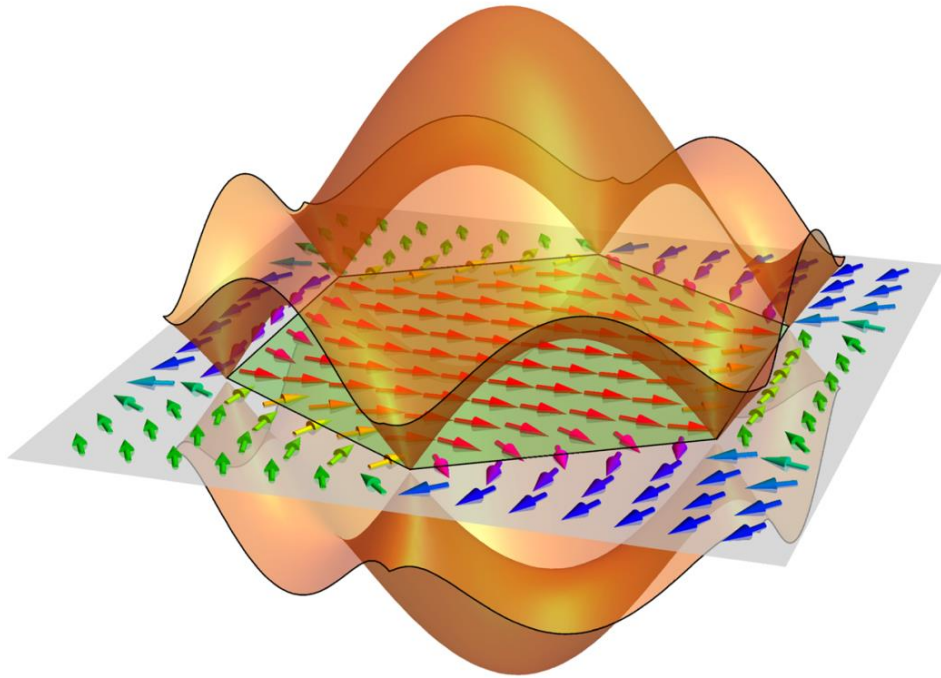


Homotopic insights into topological band invariants

Tomáš Bzdušek; 22. July 2021

KITP Program: Interacting Topological Matter



PAUL SCHERRER INSTITUT



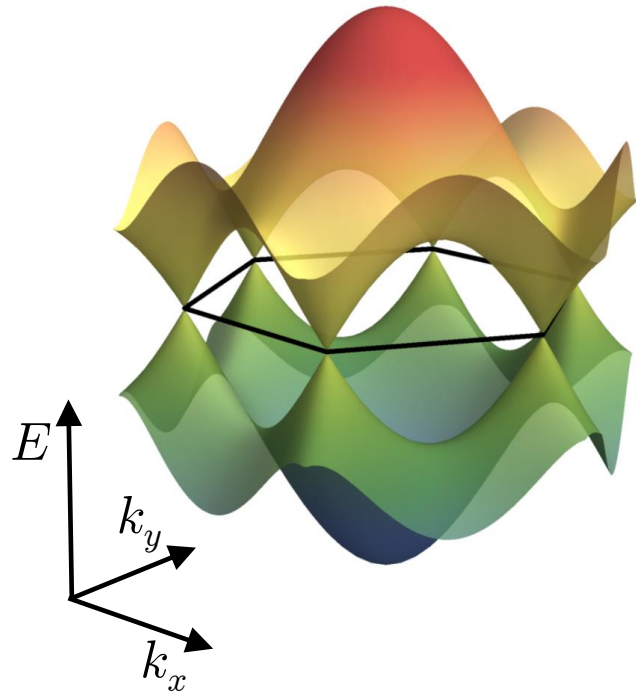
University of
Zurich^{UZH}



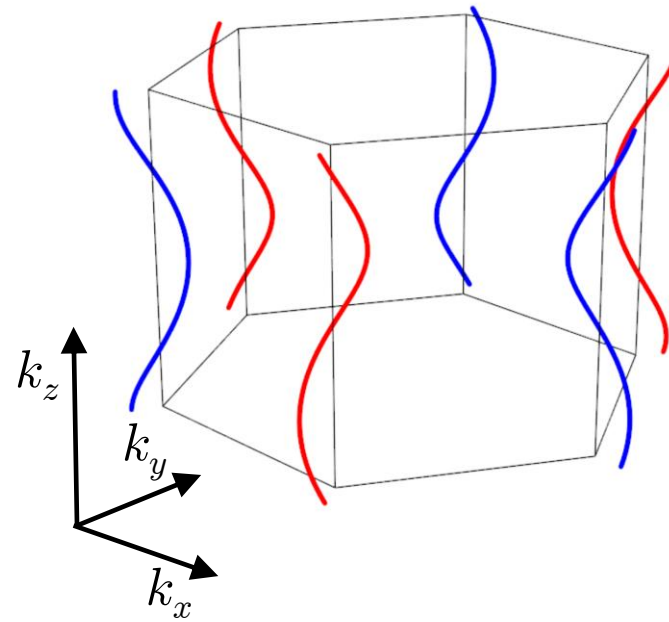
SWISS NATIONAL SCIENCE FOUNDATION

Band degeneracies (“nodes”) in energy spectra

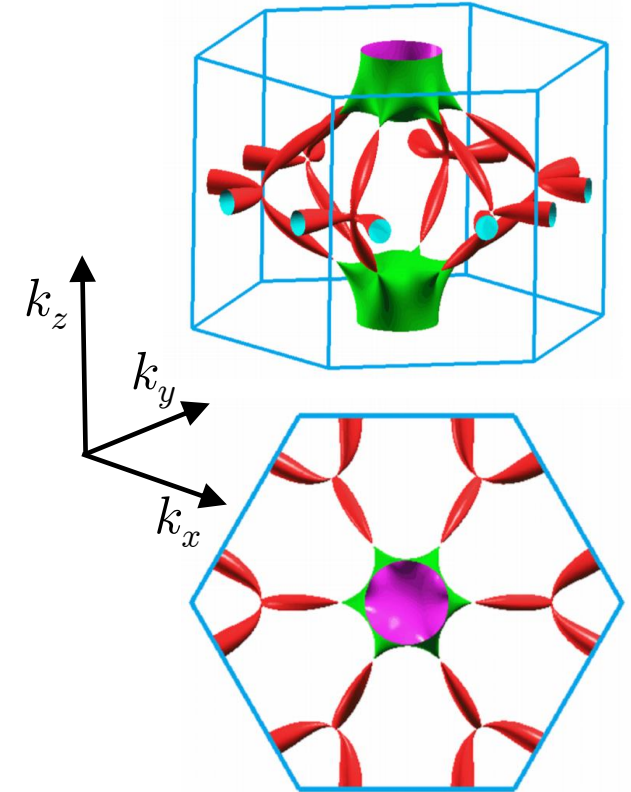
[X. Feng et al., *Phys. Rev. Mat.* **2**, 014202 (2018)]



Nodal points
in graphene



Nodal lines
in ABC-graphite



Nodal chain
in ZrB_2

Techniques to characterize band topology

K-theory

- assumes ∞ of bands
- uses complete information
- handles crystalline symmetry

Homotopy theory

- for arbitrarily many bands
- uses complete information
- hard to handle symmetries

Few-band (fragile/delicate) topologies,
 k -local obstructions (nodes),
symmetry non-indicated phases, ...

Symmetry indicators / TQC

- for arbitrarily many bands
- uses reduced information
- built around symmetries

INFINITE

BANDS

FEW

LOW

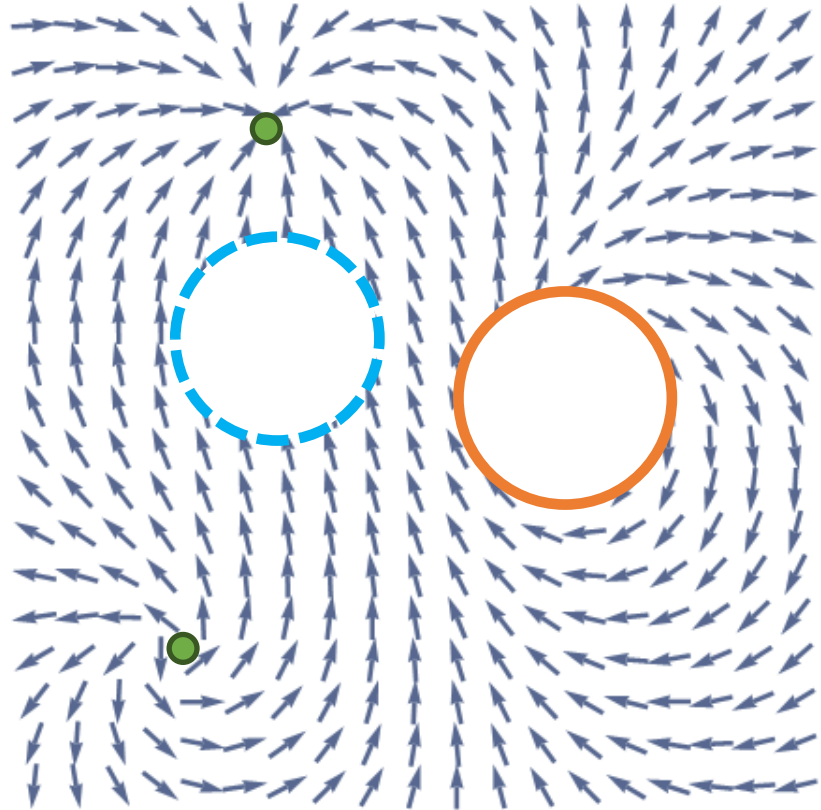
SYMMETRY

HIGH

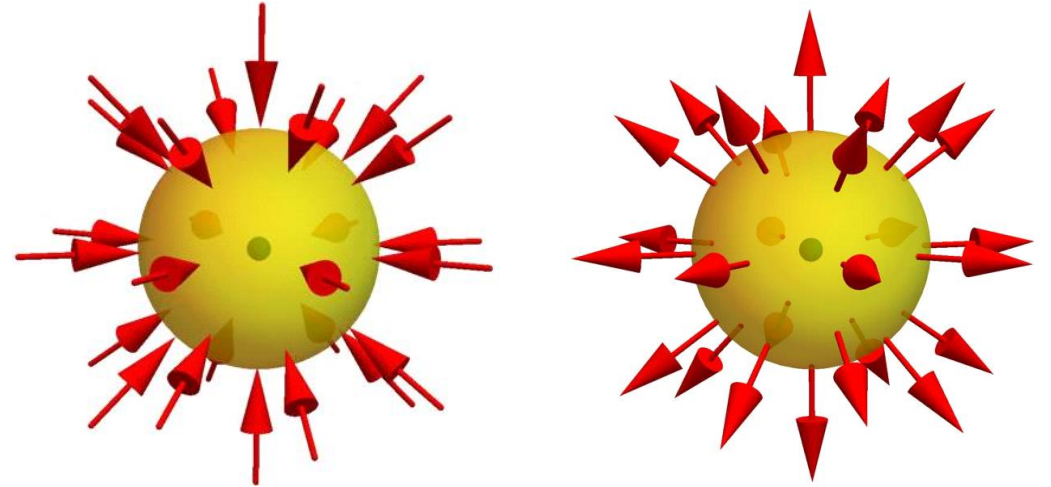
Structure of the presentation

- I. Intro to **topological defects in ordered media**
(vortices, hedgehogs, disclinations, etc.)
- II. Formalization using **homotopy groups**
(mathematical theory of defects developed in late 1970s)
- III. Use mathematical analogy to **characterize band nodes in k -space**
(classification of band nodes + their non-Abelian properties)
- IV. Introduce “**delicate**” **topological insulators**
(Few-band topologies invisible to both K-theory and symmetry indicators)

Topological defects in ordered media

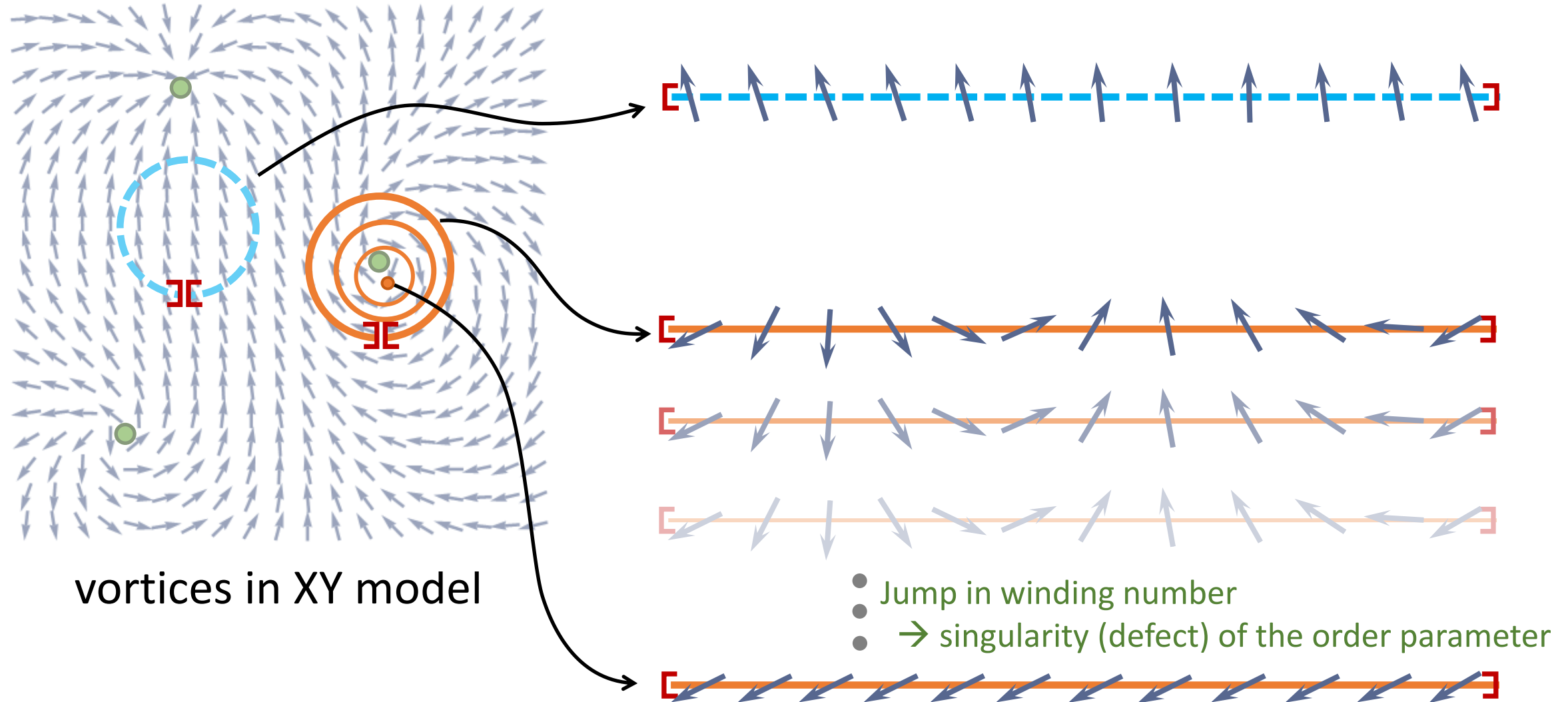


vortices in XY model
(detected on a closed loop)

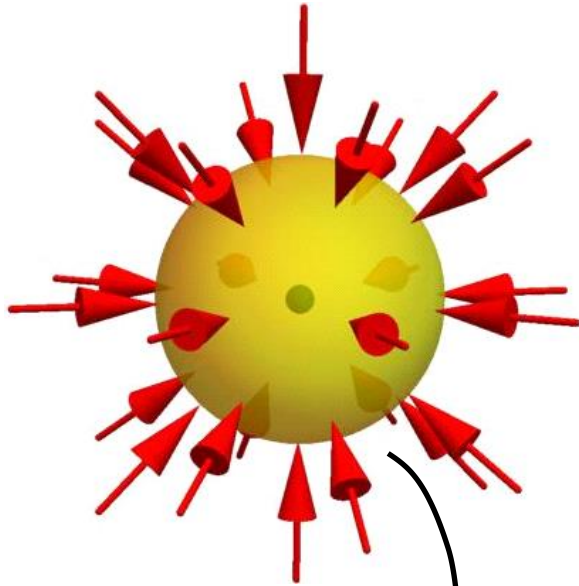


hedgehogs in Heisenberg model
(detected on a sphere)

Relation of topological *defects* to topological *textures*

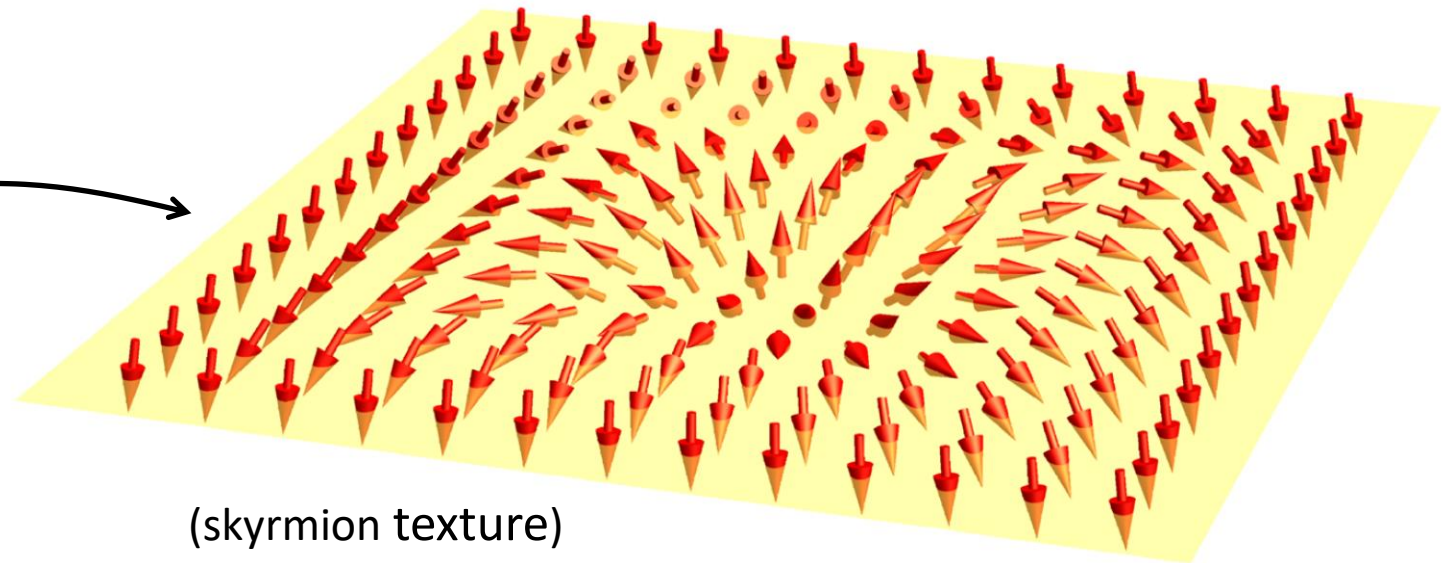


Relation of topological *defects* to topological *textures*



Analogous analysis for the Heisenberg model:

- 1.) Imagine the enclosing sphere is made of rubber
- 2.) Puncture a hole at the bottom point of the sphere
- 3.) Stretch the punctured sphere into a square shape

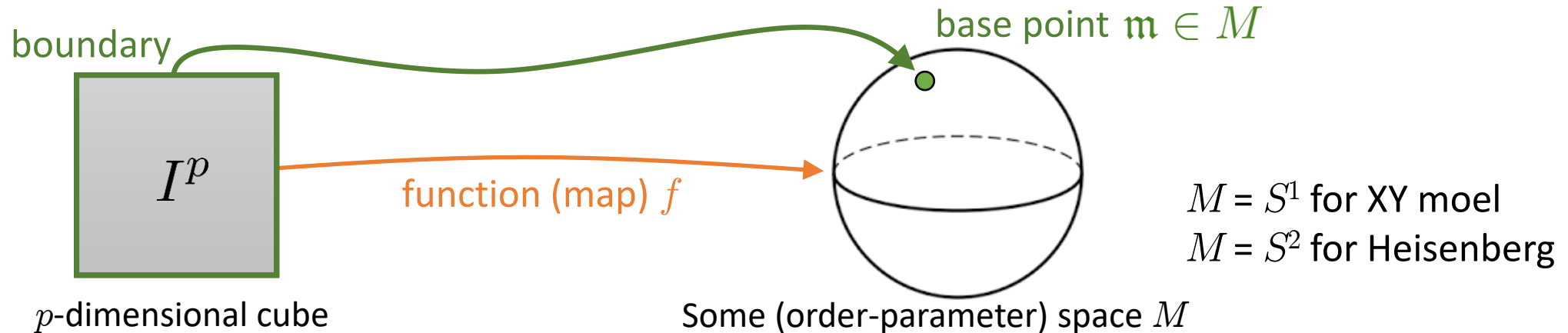


(skyrmion texture)

Basics of homotopy theory

[Review: N. D. Mermin, *The topological theory of defects in ordered media*, Rev. Mod. Phys. **51**, 591–648 (1979)]

- Formal definition of p^{th} based homotopy group $\pi_p(M, \mathfrak{m})$:



- **Group structure:** Composition rule is *stacking*:

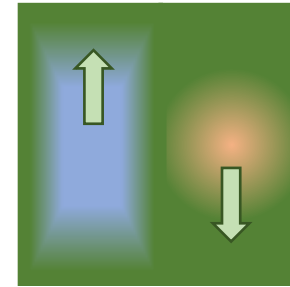
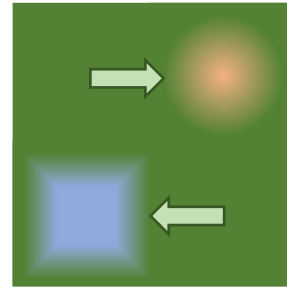
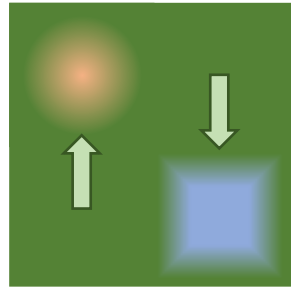
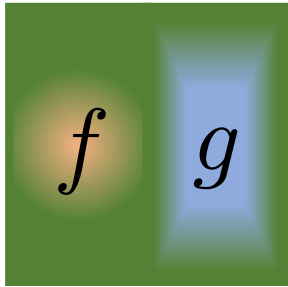


(equivalence class $[f]$ = continuous deformations of f ; identity & inverse element left for homework!)

Basics of homotopy theory

[Review: N. D. Mermin, *The topological theory of defects in ordered media*, Rev. Mod. Phys. **51**, 591–648 (1979)]

- Second (and higher) based homotopy groups are Abelian:



$f \circ g \sim g \circ f$ → The two stacking of functions f and g are equivalent under continuous deformations.

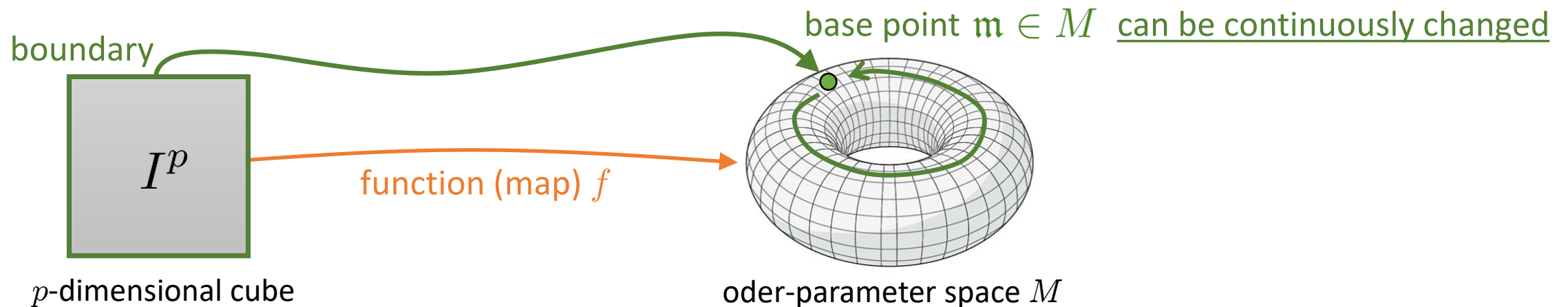
$[f] \circ [g] = [g] \circ [f]$ → Equivalence classes $[f]$ of f and $[g]$ of g (elements of the homotopy group) commute.

Basics of homotopy theory

[Review: N. D. Mermin, *The topological theory of defects in ordered media*, Rev. Mod. Phys. **51**, 591–648 (1979)]

- First homotopy group may be non-Abelian

- In practice: free homotopy classes $\pi_p(M, \mathfrak{m})$; may lose group structure



Key notion in constructing the free homotopy group: *action of* $\pi_1(M, \mathfrak{m})$ *on* $\pi_p(M, \mathfrak{m})$.

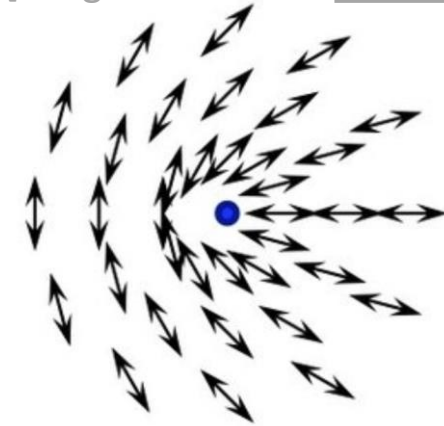
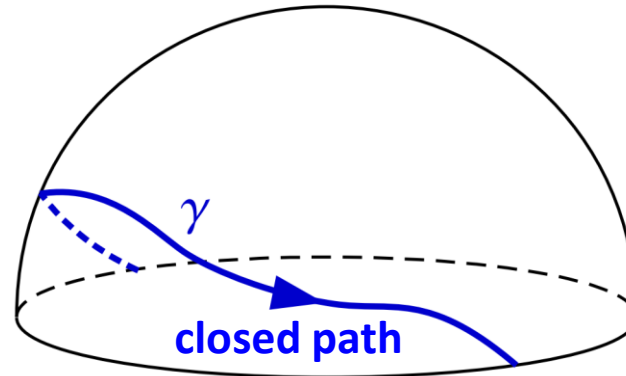
Non-trivial example #1: Uniaxial nematic liquid

Orientational order; order parameter space: $M = S^2 / \mathbb{Z}_2 \simeq \mathbb{R}P^2$

[image source DOI:[10.1117/12.2007269](https://doi.org/10.1117/12.2007269)]

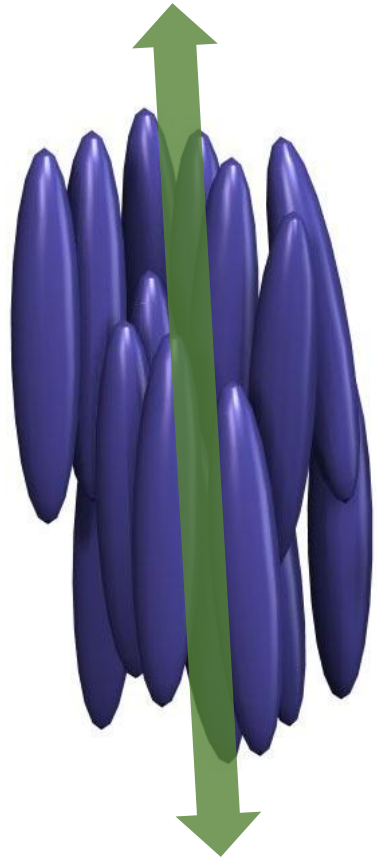
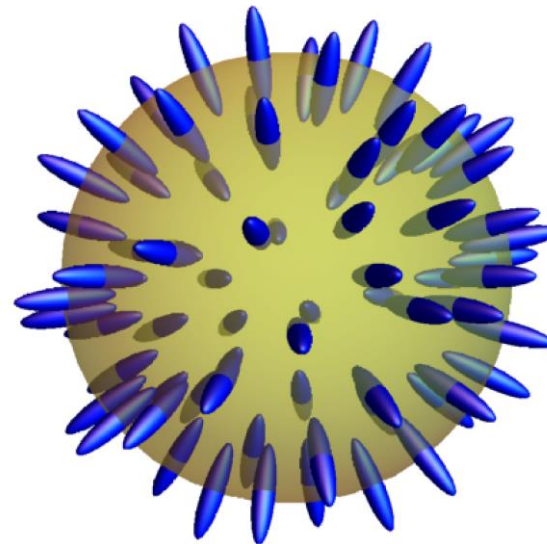
$$\pi_1(\mathbb{R}P^2, \mathfrak{m}) = \mathbb{Z}_2$$

results in disclination defects (lines in 3D)



$$\pi_2(\mathbb{R}P^2, \mathfrak{m}) = \mathbb{Z}$$

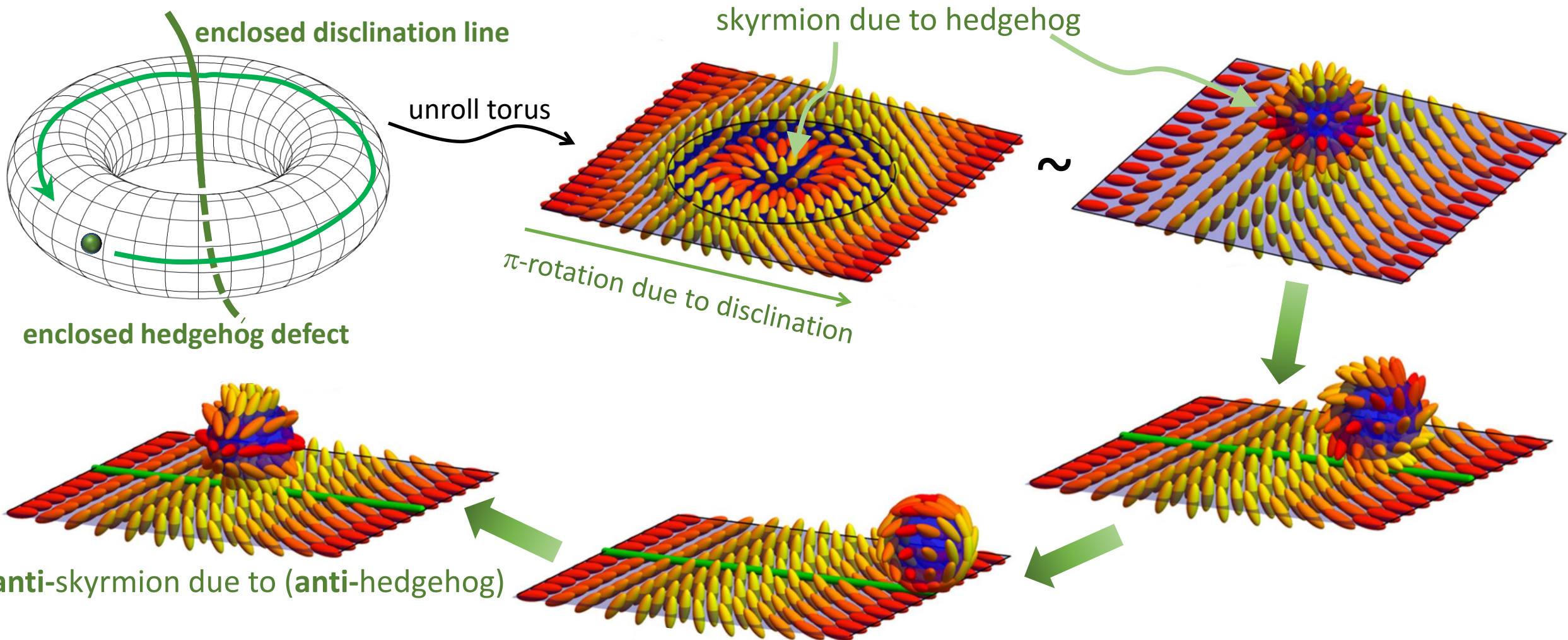
results in hedgehog defects



“director” d
(headless arrow)

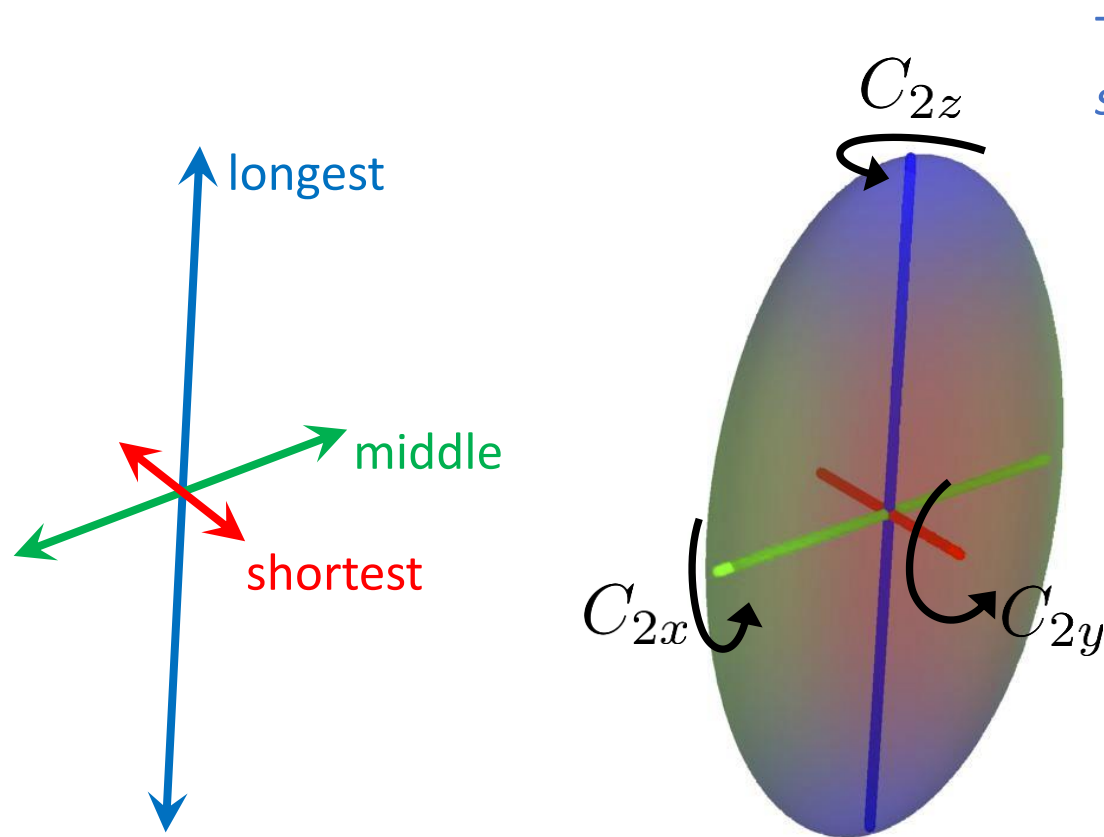
Non-trivial example #1: Uniaxial nematic liquid

Action of π_1 on π_2 results in *non-trivial braiding effects!*



Non-trivial example #2: Biaxial nematic liquid

Orientational order; order parameter space: $M = SO(3)/D_2$



The quotient is the stabilizer subgroup.

$$= \{E, C_{2x}, C_{2y}, C_{2z}\}$$

“dihedral group”

spin-½ representations of the pi-rotation.

$$= \{\pm \mathbf{1}, \mp i\sigma_x, \mp i\sigma_y, \mp i\sigma_z\}$$

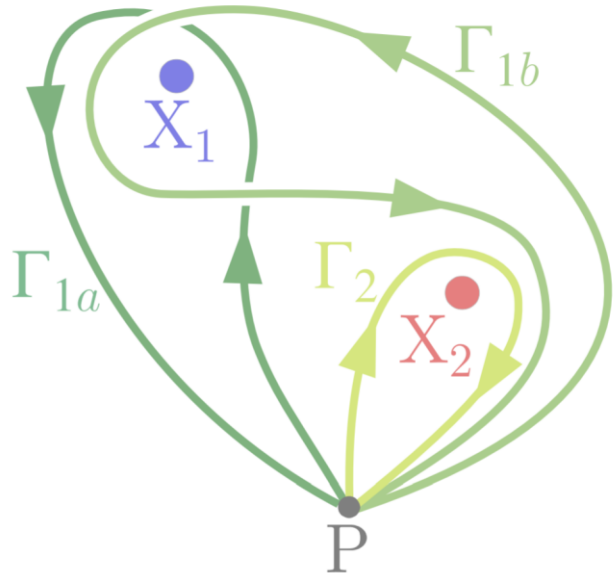
$$= \{\pm 1, \pm i, \pm j, \pm k\}$$

“quaternion group”

It can be shown that $\pi_1(\dots) = \bar{D}_2$.

Non-trivial example #2: Biaxial nematic liquid

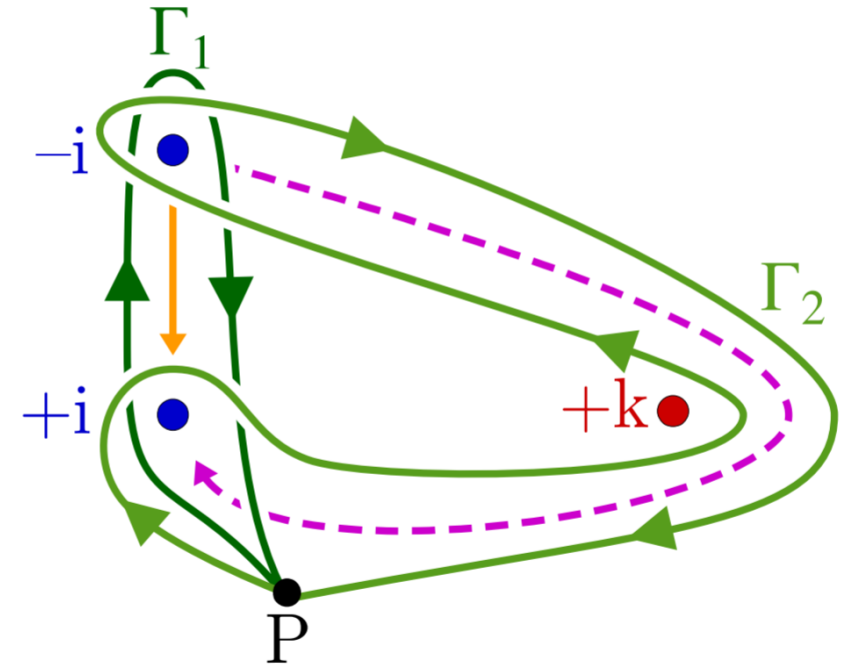
To study *braiding of defects*, let us fix a base point P in the coordinate space.



$$\Gamma_{1b} \sim \Gamma_2 \circ \Gamma_{1a} \circ \Gamma_2^{-1}$$

$$c_{1b} = c_2 \cdot c_{1a} \cdot c_2^{-1}$$

$$-i = k \cdot i \cdot (-k)$$



It can be shown that $\pi_1(\dots) = \bar{D}_2 = \{\pm 1, \pm i, \pm j, \pm k\}$.

This group is *non-commutative*, e.g. $i \cdot j = k = -j \cdot i$.

From topological defects to band-structure nodes

Isomorphism:

Playground: coordinate space \rightarrow momentum space

Texture: order parameter \rightarrow gapped Hamiltonian

Target space: order-parameter space \rightarrow classifying space

Mathematical intermezzo: Grassmannian spaces

Consider Hamiltonian with N filled and M empty bands with no symmetry:

eigensystem decomposition

$$\mathcal{H}(\mathbf{k}) = \sum_{a=1}^{N+M} |u_a(\mathbf{k})\rangle \varepsilon_a(\mathbf{k}) \langle u_a(\mathbf{k})|$$



spectral normalization

$$\mathcal{H}(\mathbf{k}) = \sum_{a=1}^{N+M} |u_a(\mathbf{k})\rangle \text{sign}[\varepsilon_a(\mathbf{k})] \langle u_a(\mathbf{k})|$$



space of spectrally normalized Hamiltonians

$$M = \text{U}(N + M) / \text{U}(N) \times \text{U}(M)$$

Some symmetries (C_2T , spinless PT) impose *reality condition*, in which case:

$$M = \text{O}(N + M) / \text{O}(N) \times \text{O}(M)$$

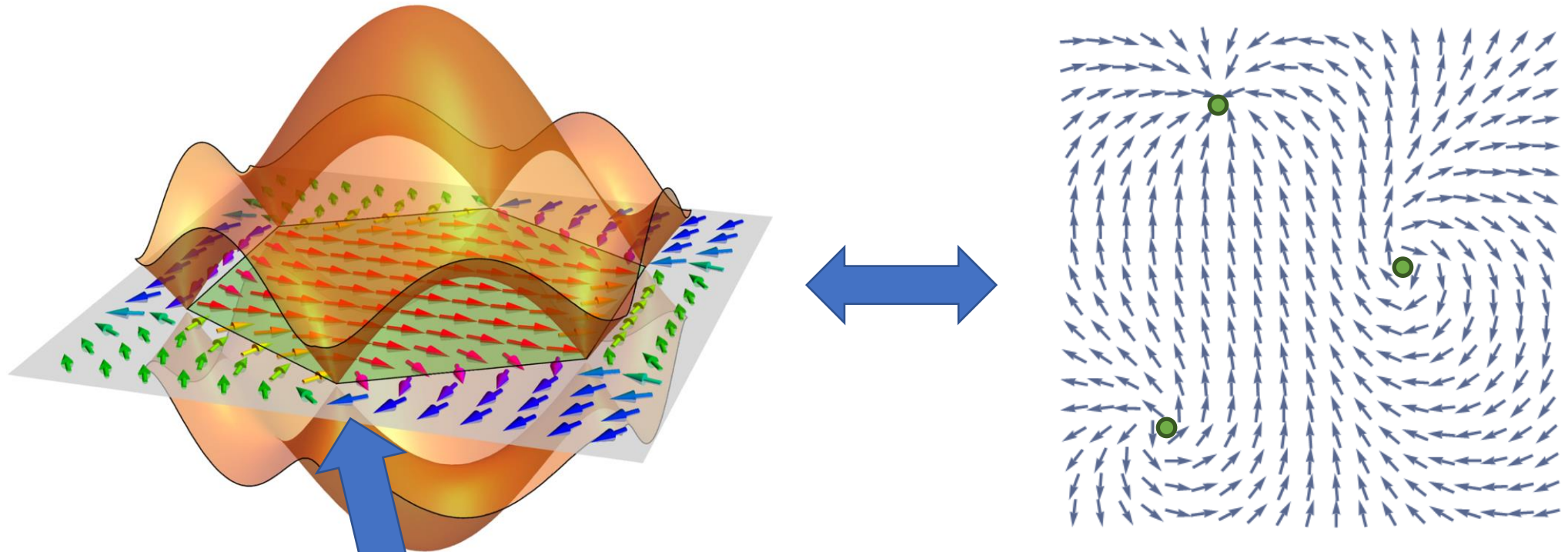
Simple instances: $\text{Gr}_{\mathbb{C}}(1, 2) \simeq S^2$
like Heisenberg model

$\text{Gr}_{\mathbb{R}}(1, 2) \simeq S^1$
like XY model

$\text{Gr}_{\mathbb{R}}(1, 3) = \text{Gr}_{\mathbb{R}}(2, 3) \simeq S^2 / \mathbb{Z}_2 \simeq \mathbb{R}P^2$
like uniaxial nematic liquid

$\text{Gr}_{\mathbb{R}}(2, 4) \simeq (S^2 \times S^2) / \mathbb{Z}_2$

Graphene vs. the XY model



Some symmetries (C_2T spinless PT) impose *reality condition*, in which case:

$$M = O(N + M)/O(N) \times O(M)$$

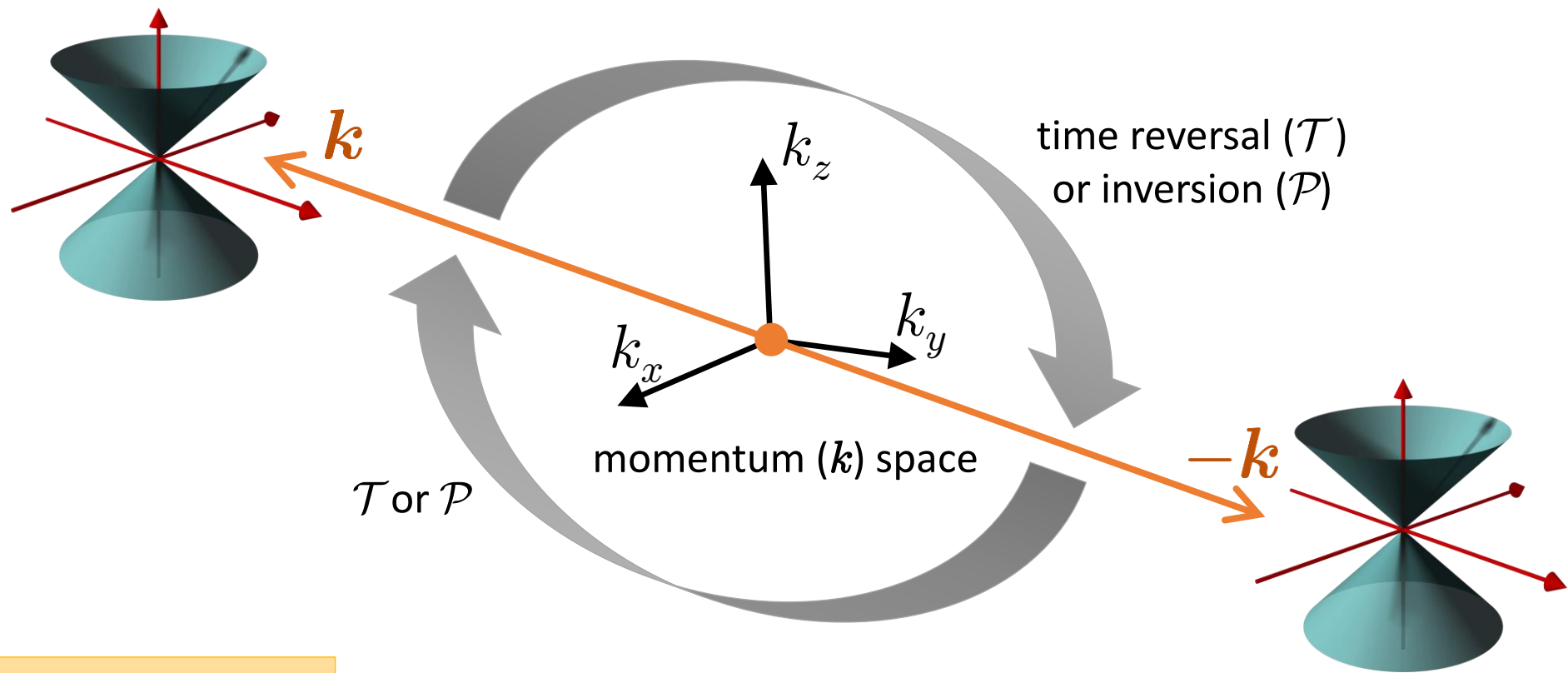
$$\text{Gr}_{\mathbb{R}}(1, 3) = \text{Gr}_{\mathbb{R}}(2, 3) \simeq S^2/\mathbb{Z}_2 \simeq \mathbb{R}P^2$$

like uniaxial nematic liquid

$$\text{Gr}_{\mathbb{R}}(1, 2) \simeq S^1$$

like XY model

Band nodes protected by local-in- \mathbf{k} symmetries



Three such symmetries

\mathcal{PT} , \mathcal{PC} , and \mathcal{CT}

$$(\mathcal{PT})\mathcal{H}(\mathbf{k})(\mathcal{PT})^{-1} = \mathcal{H}(\mathbf{k})$$

local-in- \mathbf{k} symmetry

Band nodes protected by local-in- k symmetries

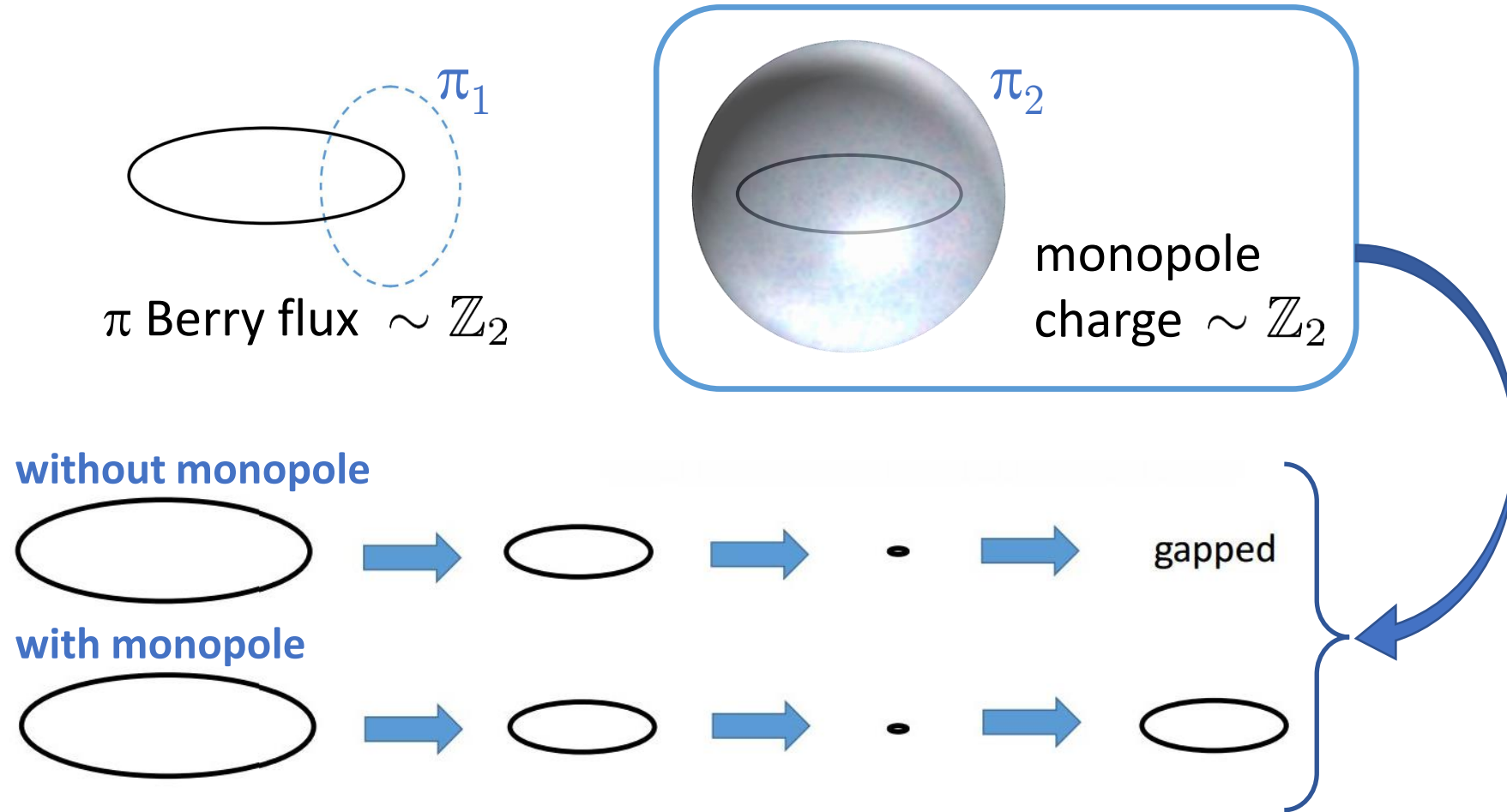
label	\mathcal{PT}	\mathcal{PC}	\mathcal{CT}	Space M of Hamiltonians	(stable) homotopy group of M				
					π_0	π_1	π_2	π_3	π_4
A	\times	\times	\times	$U(n + \ell)/U(n) \times U(\ell)$			\mathbb{Z}		\mathbb{Z}
AIII	\times	\times	1	$U(n)$		\mathbb{Z}		\mathbb{Z}	
AI	+1	\times	\times	$O(n + \ell)/O(n) \times O(\ell)$		\mathbb{Z}_2	\mathbb{Z}_2		$2\mathbb{Z}$
BDI	+1	+1	1	$O(n)$	\mathbb{Z}_2	\mathbb{Z}_2		$2\mathbb{Z}$	
D	\times	+1	\times	$O(2n)/U(n)$	\mathbb{Z}_2		$2\mathbb{Z}$		
DIII	-1	+1	1	$U(2n)/Sp(n)$		$2\mathbb{Z}$			
AII	-1	\times	\times	$Sp(n + \ell)/Sp(n) \times Sp(\ell)$					\mathbb{Z}
CII	-1	-1	1	$Sp(n)$				\mathbb{Z}	\mathbb{Z}_2
C	\times	-1	\times	$Sp(n)/U(n)$			\mathbb{Z}	\mathbb{Z}_2	\mathbb{Z}_2
CI	+1	-1	1	$U(n)/O(n)$		\mathbb{Z}	\mathbb{Z}_2	\mathbb{Z}_2	

band nodes nodal points
PAIR nodal lines
nodal surfaces
 Interpret as topological charges carried by the band nodes

Band nodes protected by local-in- k symmetries

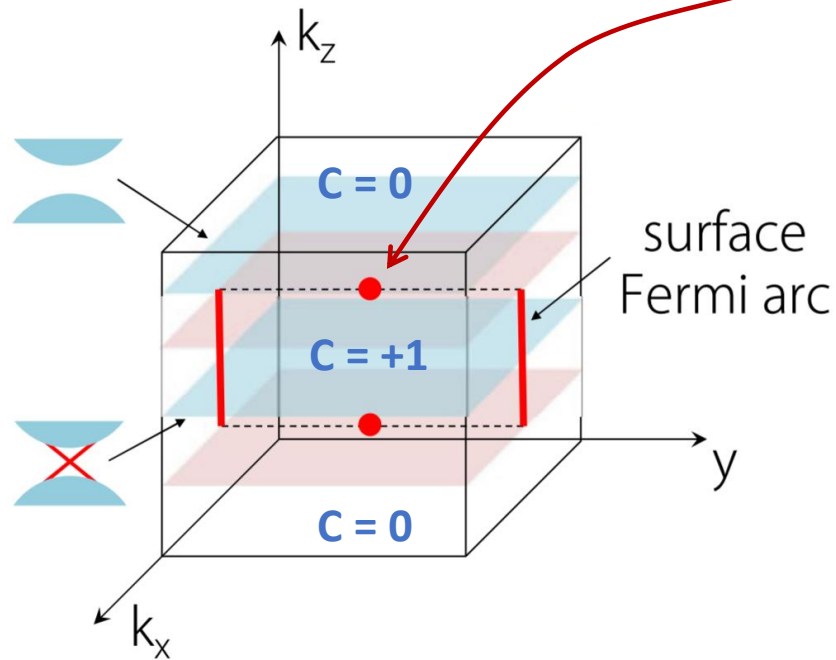
label	\mathcal{PT}	\mathcal{PC}	\mathcal{CT}	Space M of Hamiltonians	(stable) homotopy group of M				
					π_0	π_1	π_2	π_3	π_4
A	\times	\times	\times	$U(n+l)/U(n) \times U(l)$			\mathbb{Z}		\mathbb{Z}
AIII	\times	\times	1	$U(n)$		\mathbb{Z}		\mathbb{Z}	
AI	+1	\times	\times	$O(n+l)/O(n) \times O(l)$		\mathbb{Z}_2	\mathbb{Z}_2		$2\mathbb{Z}$
BDI	+1	+1	1	$O(n)$	\mathbb{Z}_2	\mathbb{Z}_2		$2\mathbb{Z}$	
D	\times	+1	\times	$O(2n)/U(n)$	\mathbb{Z}_2		$2\mathbb{Z}$		
DIII	-1	+1	1	$U(2n)/Sp(n)$		$2\mathbb{Z}$			
AII	-1	\times	\times	$Sp(n+l)/Sp(n) \times Sp(l)$					\mathbb{Z}
CII	-1	-1	1	$Sp(n)$				\mathbb{Z}	\mathbb{Z}_2
C	\times	-1	\times	$Sp(n)/U(n)$			\mathbb{Z}	\mathbb{Z}_2	\mathbb{Z}_2
CI	+1	-1	1	$U(n)/O(n)$		\mathbb{Z}	\mathbb{Z}_2	\mathbb{Z}_2	

Nodal-line rings with **two** topological charges



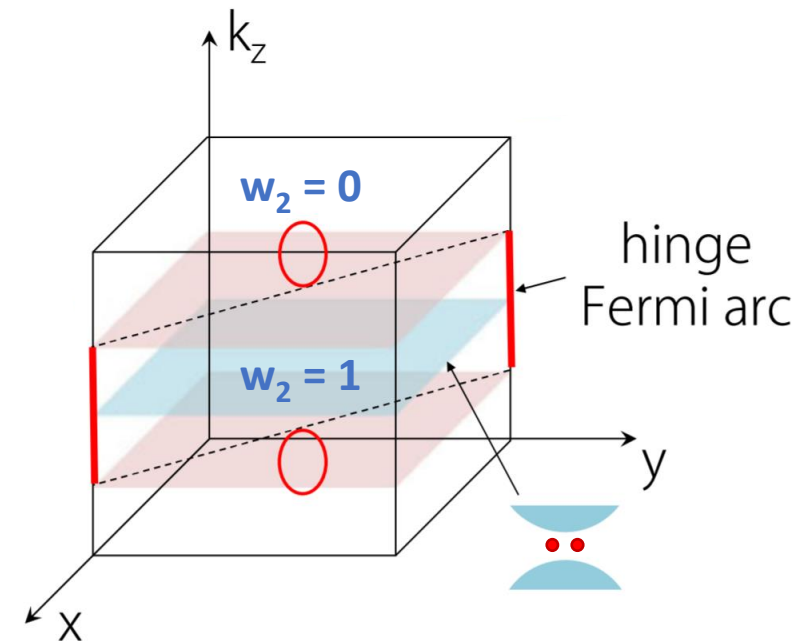
Manifestation of the monopole charge: higher-order topology

Recall the case of **Weyl points**,
which separate 2D sheets
with different *Chern class*.



Manifested by **surface Fermi arcs**.

Similarly, **nodal loops with monopole charge**
separate 2D sheets with different values of
second Stiefel-Whitney class.



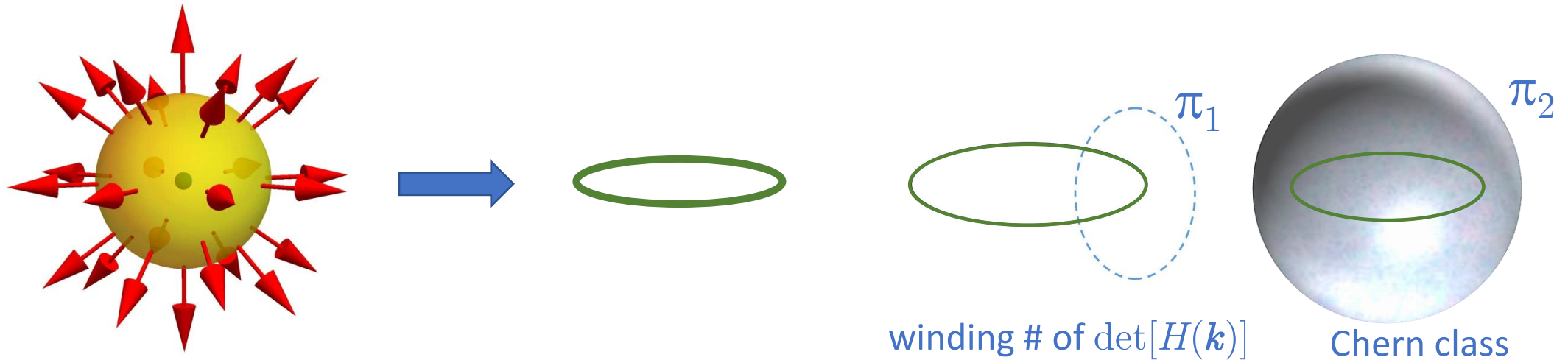
Manifested by **hinge Fermi arcs** or by **filling anomaly**.

Non-trivial band node braiding example #1: Chern class vs. exceptional lines of non-Hermitian models

(my only slide about non-Herm. models!)

Consider Hermitian model with no local-in- k symmetries \rightarrow *Weyl points*.

Non-Hermitian perturbation expands the WP into an *exceptional ring*.



Space of spectrally normalized (non-degenerate, two-band) non-Hermitian Hamiltonians

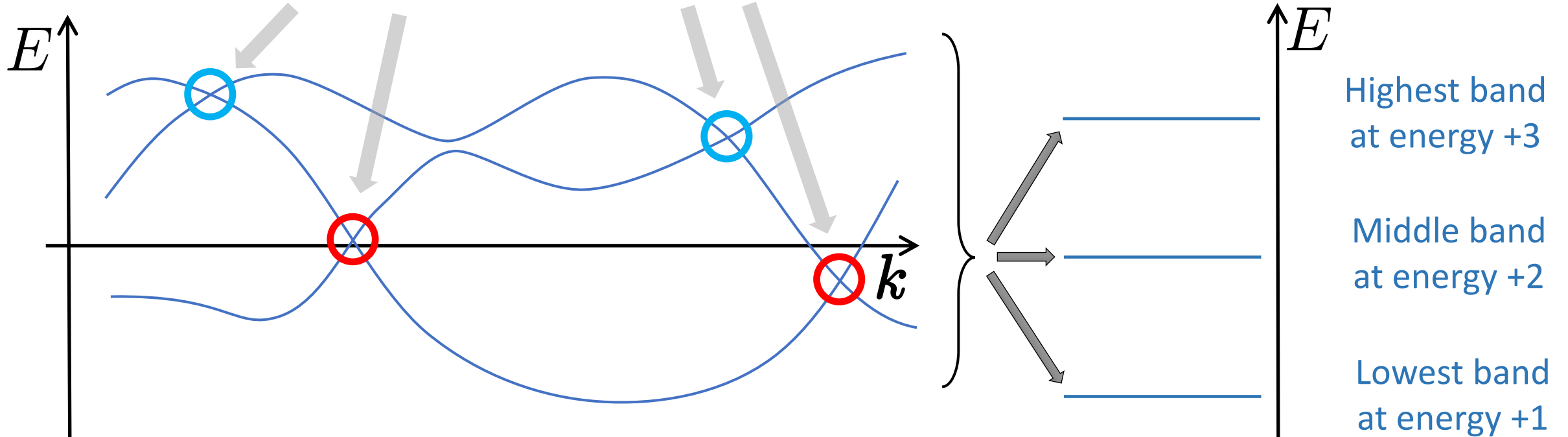
$$M = (S^2 \times S^1) / \mathbb{Z}_2 \quad \pi_1(\dots) = \mathbb{Z} \quad \pi_2(\dots) = \mathbb{Z}$$

... and there is a non-trivial action of π_1 (its parity) on π_2 (sign reversal)

Non-trivial band node braiding example #2: Nodal points of C_2T -symmetric 3-band model.

Find mathematical operation that
treats all nodes as topological defects.

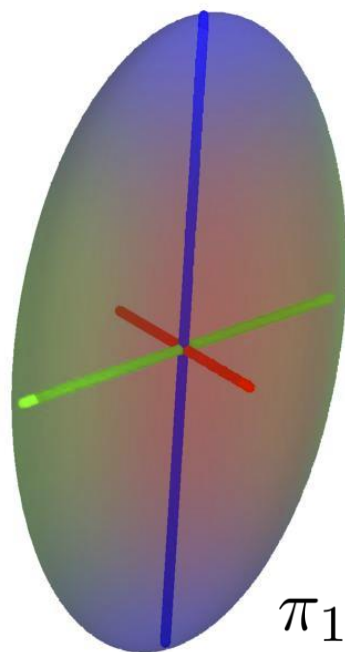
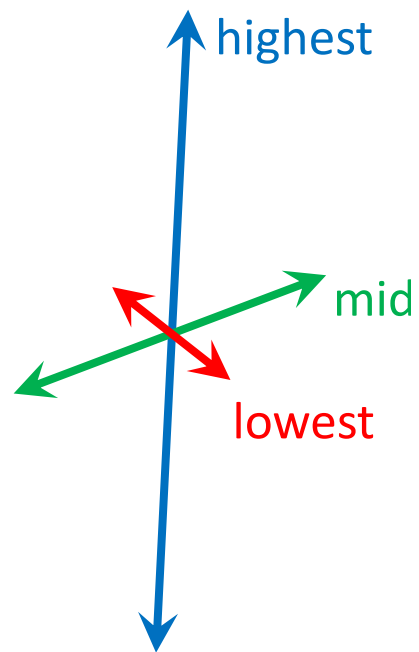
Normalize the band energies!



Mathematically: Normalize the spectral decomposition of the Hamiltonian

$$\mathcal{H}(\mathbf{k}) = \sum_{n=1}^3 |u_{\mathbf{k}}^n\rangle E_{\mathbf{k}}^n \langle u_{\mathbf{k}}^n| \quad \longrightarrow \quad \mathcal{H}(\mathbf{k}) = \sum_{n=1}^3 |u_{\mathbf{k}}^n\rangle n \langle u_{\mathbf{k}}^n|$$

Non-trivial band node braiding example #2: Nodal points of C_2T -symmetric 3-band model.

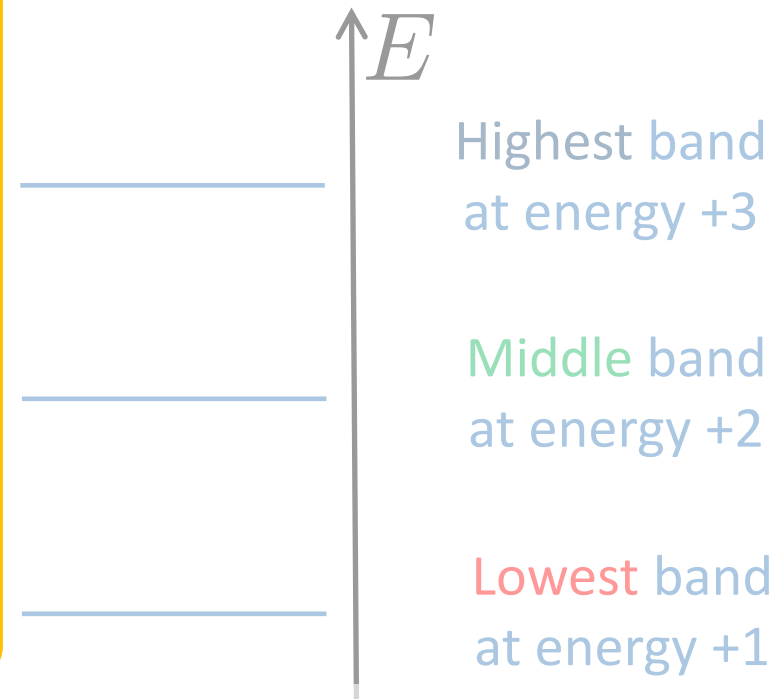


(reality condition!)

$$M = \text{SO}(3)/\text{D}_2$$

$$\pi_1(M) = \{\pm 1, \pm i, \pm j, \pm k\}$$

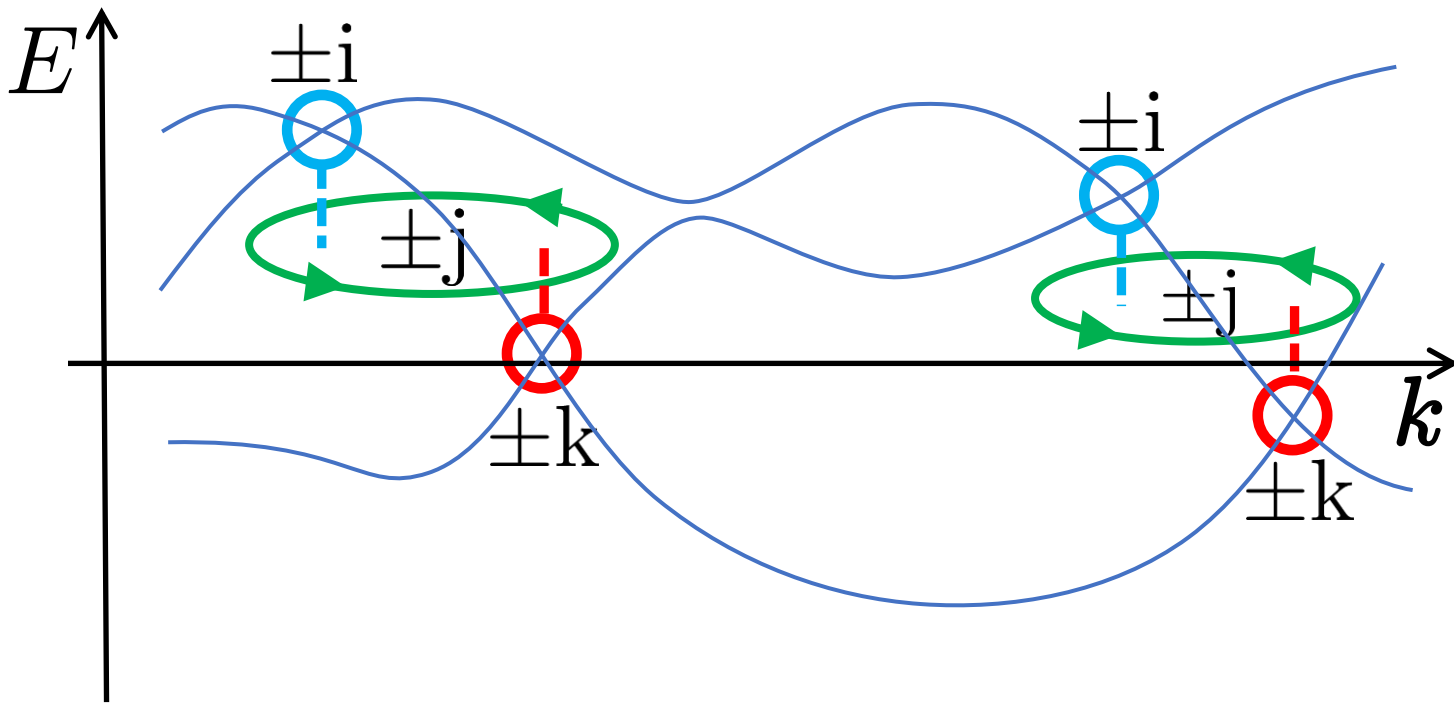
Three real orthogonal states – each defined up to overall sign!



Mathematically: Normalize the spectral decomposition of the Hamiltonian

$$\mathcal{H}(\mathbf{k}) = \sum_{n=1}^3 |u_{\mathbf{k}}^n\rangle E_{\mathbf{k}}^n \langle u_{\mathbf{k}}^n| \quad \longrightarrow \quad \mathcal{H}(\mathbf{k}) = \sum_{n=1}^3 |u_{\mathbf{k}}^n\rangle n \langle u_{\mathbf{k}}^n|$$

Non-Abelian charges of band nodes

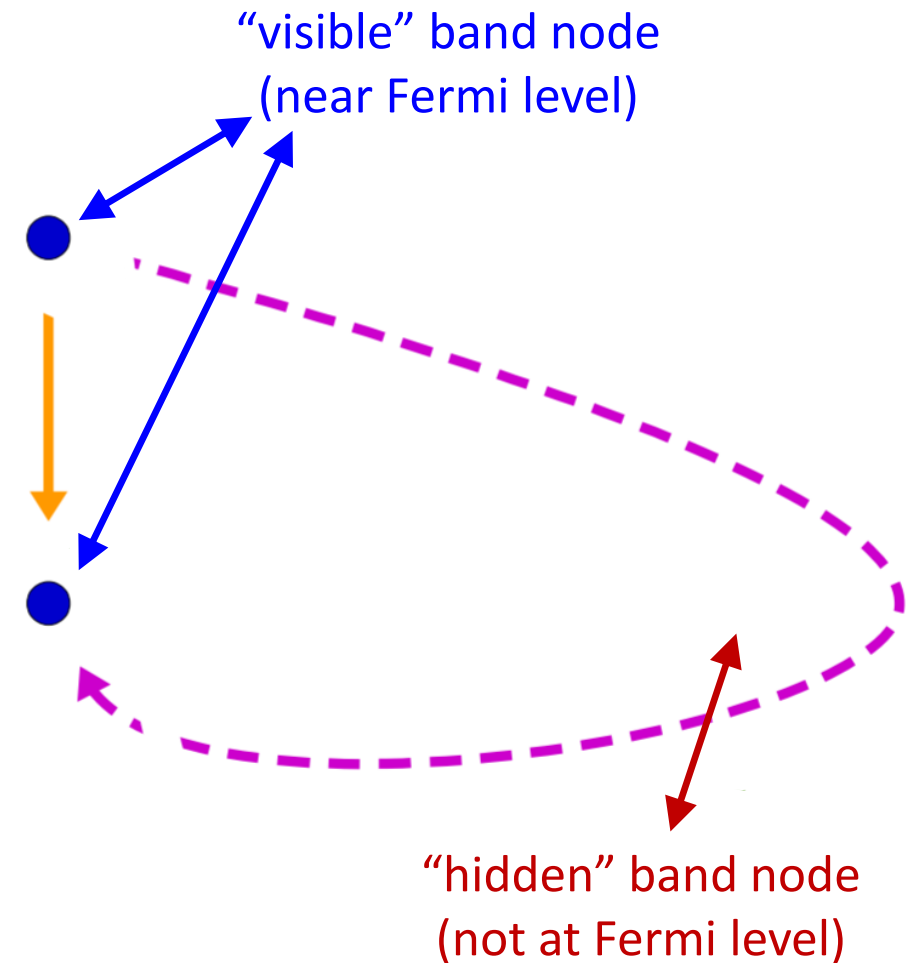


$$M = \text{SO}(3)/\text{D}_2$$

$$\pi_1(M, \mathfrak{m}) = \{\pm 1, \pm i, \pm j, \pm k\}$$

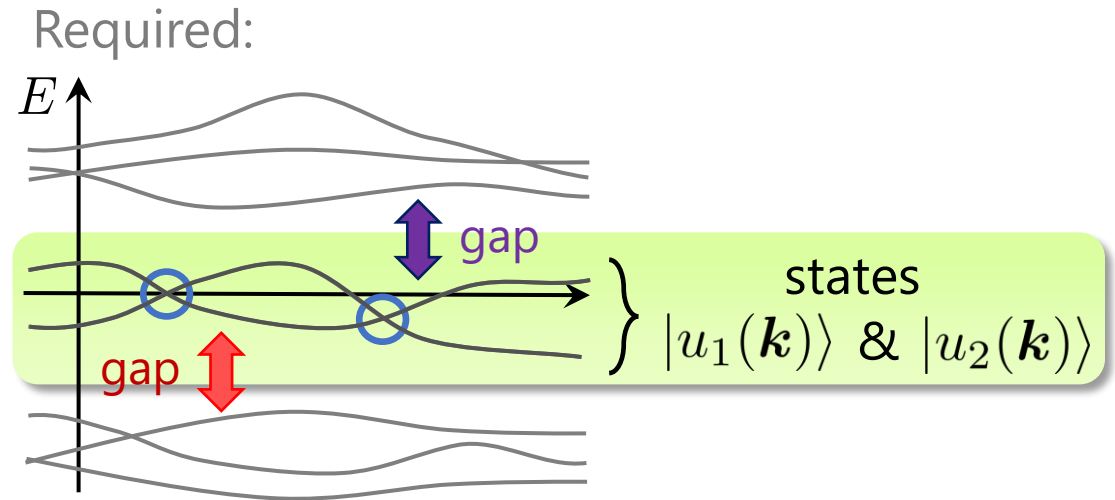
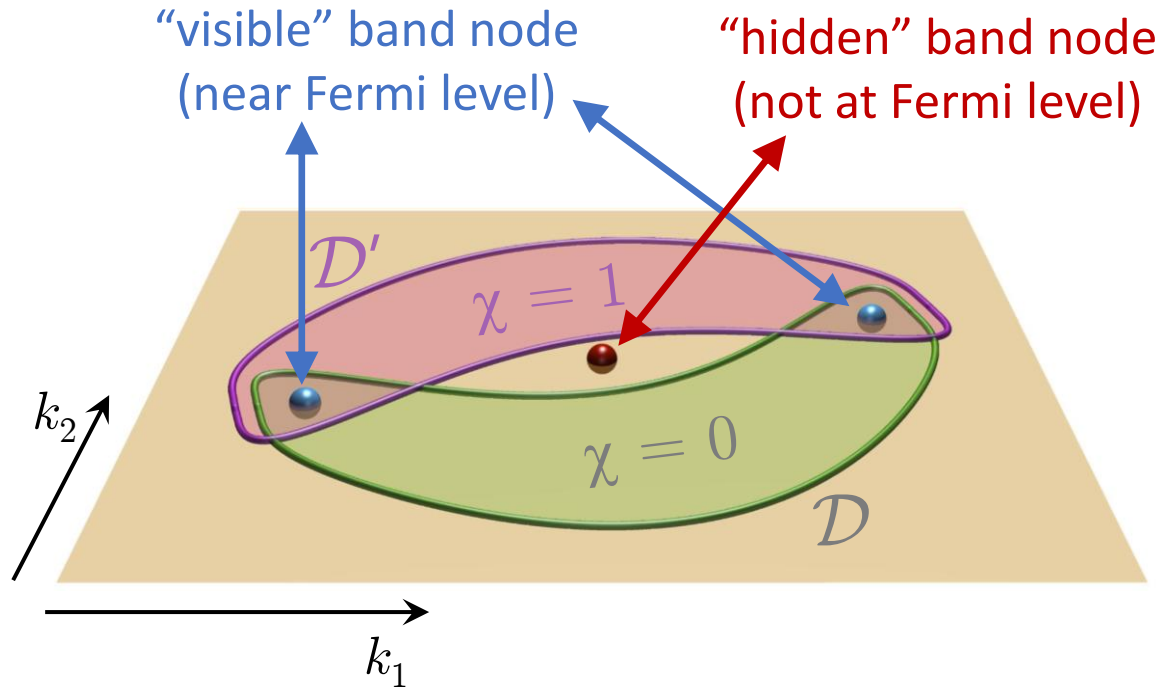
Nodes characterized by the conjugacy classes

$$\pi_1(M) = \left\{ \{+1\}, \{\pm i\}, \{\pm j\}, \{\pm k\}, \{-1\} \right\}$$



Note: energy (E) and time progression (t) in principle correspond to additional dimensions (not plotted).

Generalization to many bands: *patch Euler class*



$$\chi(\mathcal{D}) = \frac{1}{2\pi} \left[\int_{\mathcal{D}} \text{Eu}(\mathbf{k}) dk_1 dk_2 - \oint_{\partial\mathcal{D}} \mathbf{a}(\mathbf{k}) \cdot d\mathbf{k} \right]$$

Required:

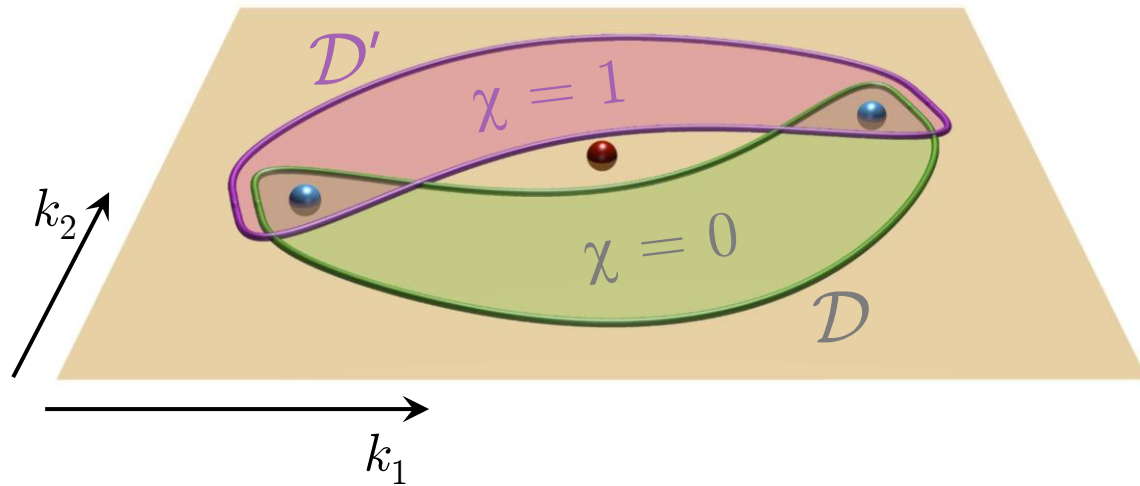
Euler connection

$$\mathbf{a}(\mathbf{k}) = \langle u_1(\mathbf{k}) | \nabla u_2(\mathbf{k}) \rangle$$

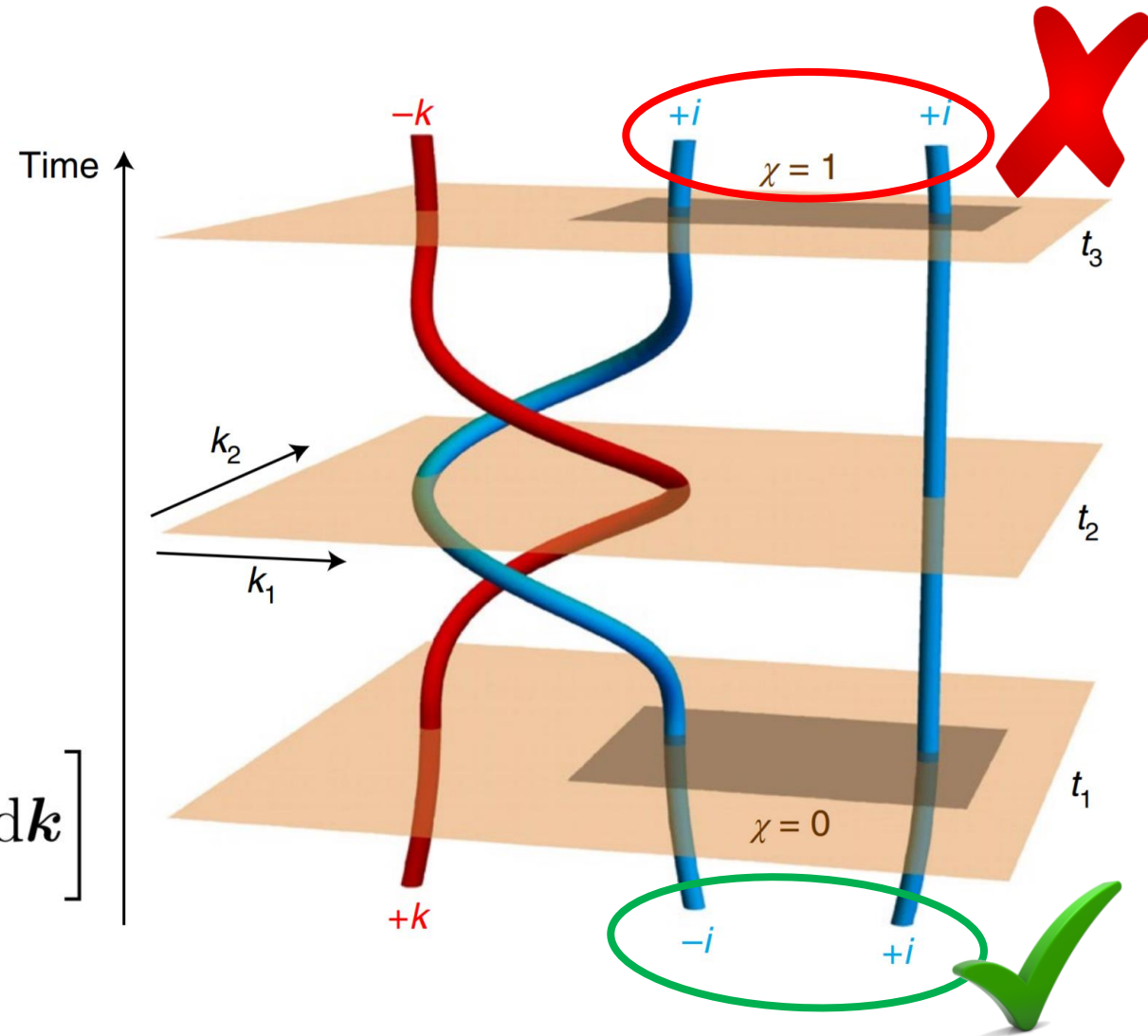
Euler curvature

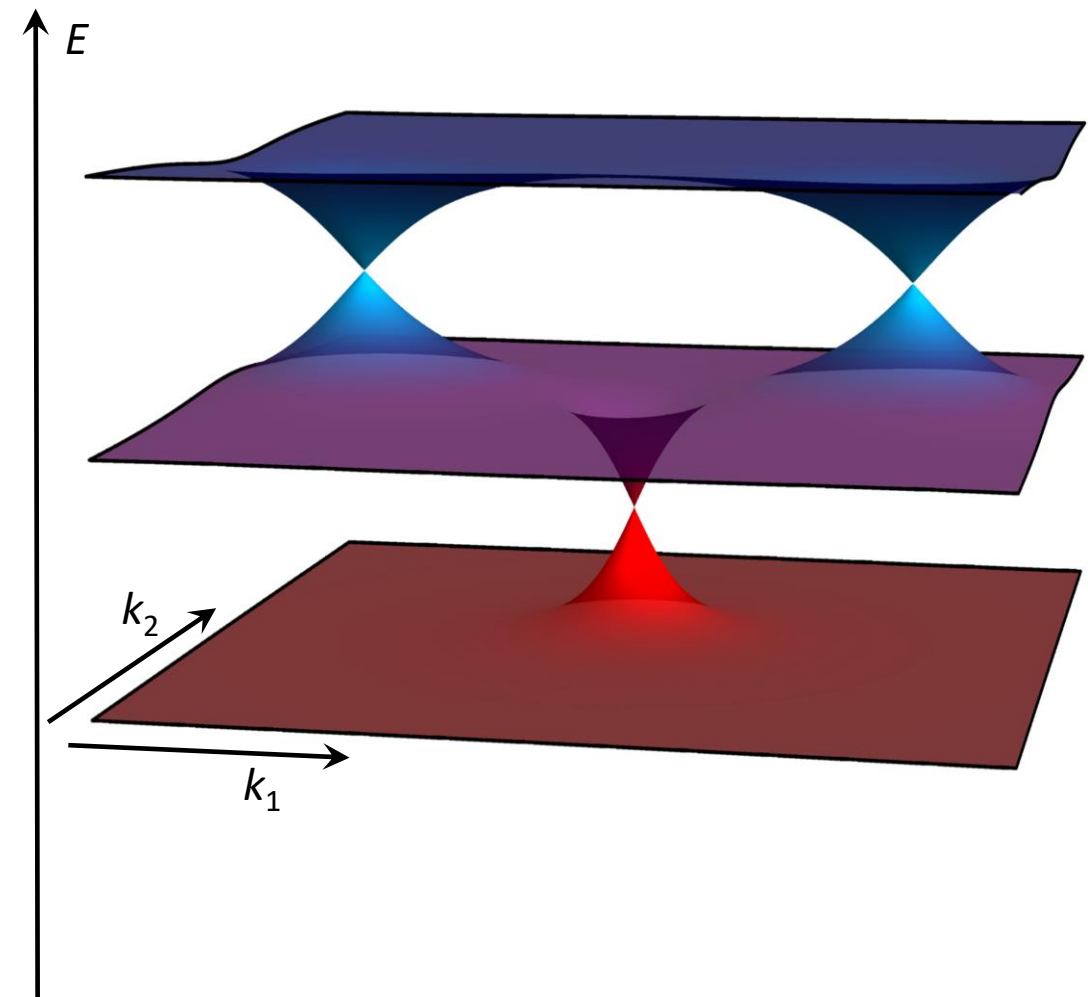
$$\text{Eu}(\mathbf{k}) = \nabla \times \mathbf{a}(\mathbf{k})$$

Generalization to many bands: *patch Euler class*

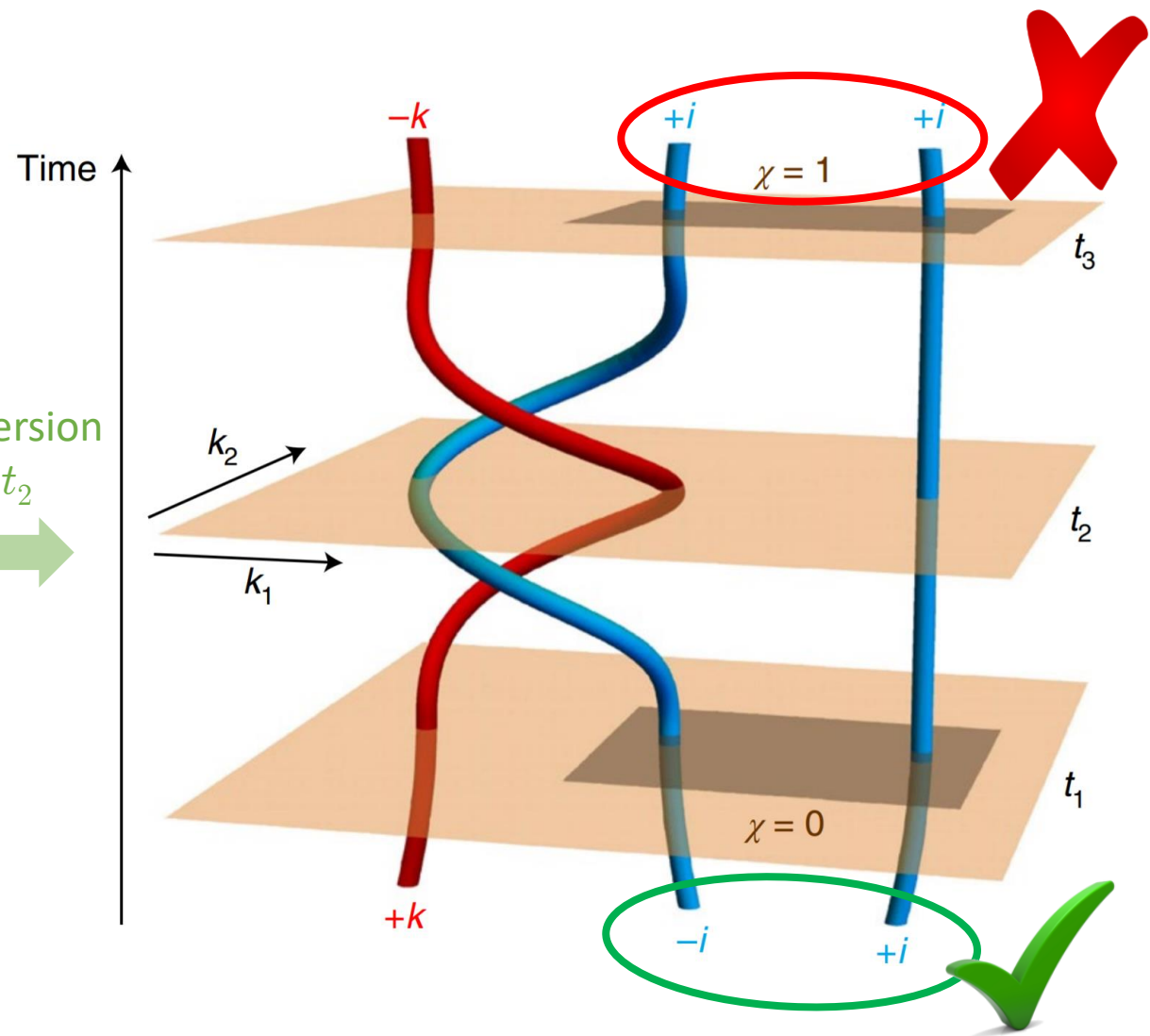


$$\chi(\mathcal{D}) = \frac{1}{2\pi} \left[\int_{\mathcal{D}} \text{Eu}(\mathbf{k}) dk_1 dk_2 - \oint_{\partial\mathcal{D}} \mathbf{a}(\mathbf{k}) \cdot d\mathbf{k} \right]$$

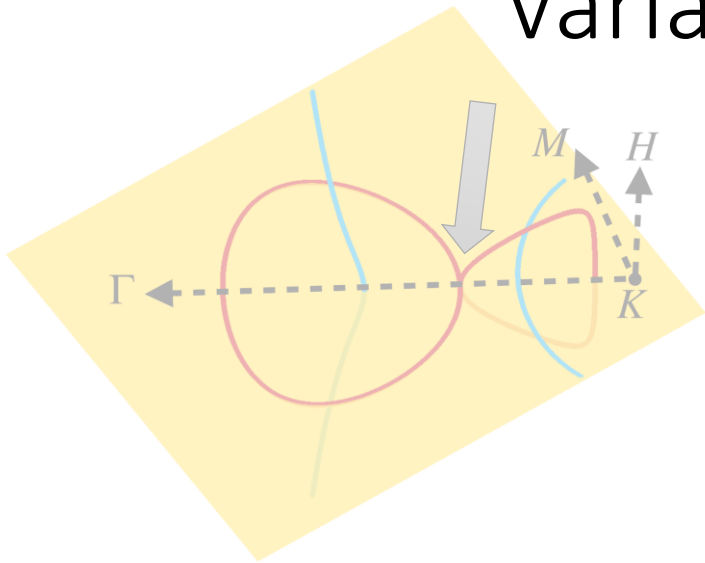




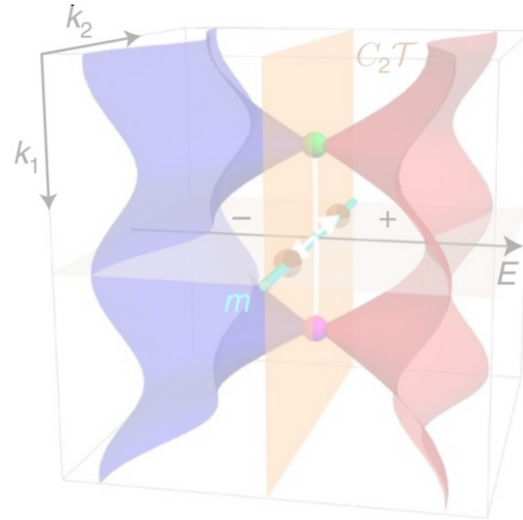
Energy dispersion
at time t_2



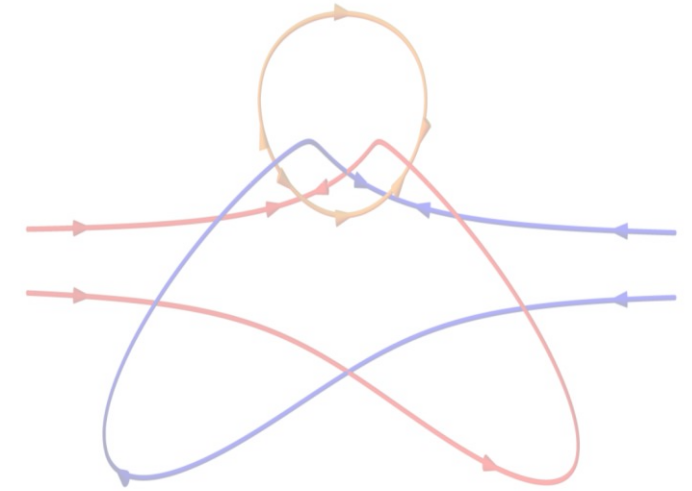
Variations on the non-Abelian story



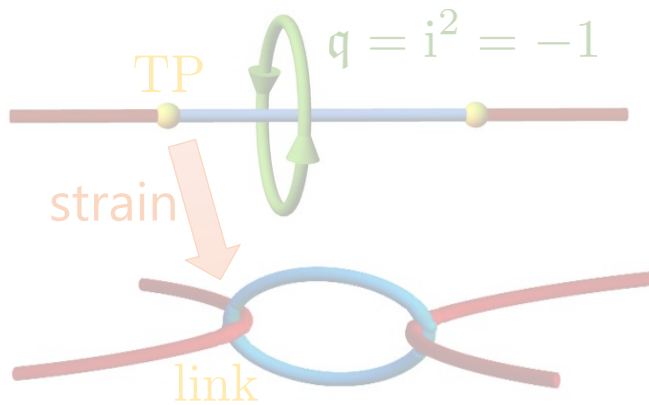
Topological stability of nodal chains; application to elemental Sc. [Science **365**, 1273-1277 (2019)]



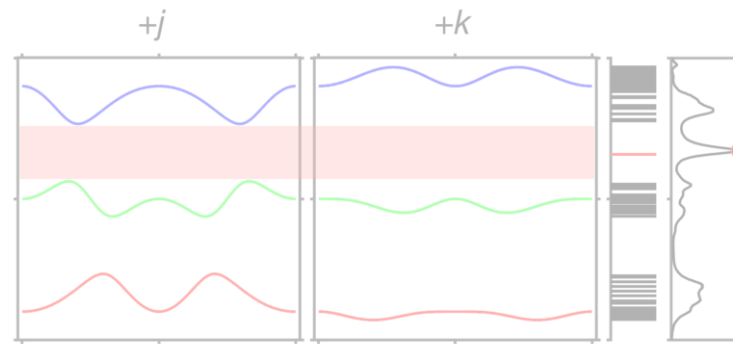
Colliding Weyl points of opposite chirality in ZrTe *fail to annihilate*. [Nat. Phys. **16**, 1137–1143 (2020)]



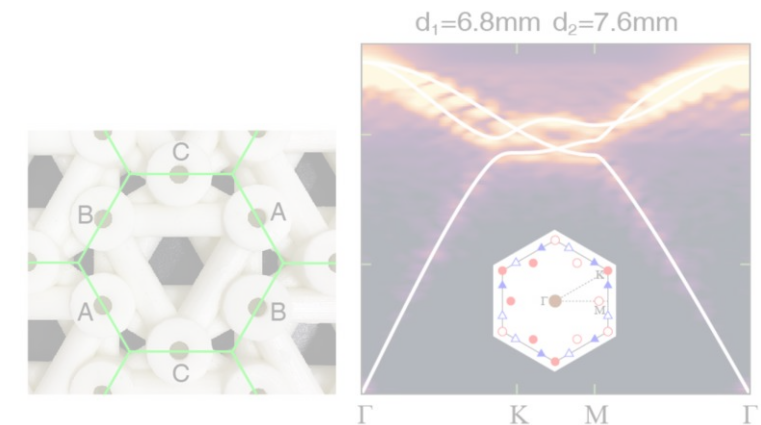
Non-trivial braiding of Dirac points in twisted bilayer graphene. [Phys. Rev B **102**, 035161 (2020)]



Conversion of triple nodal points into linked nodal rings (Li₂NaN). [Phys. Rev. B **103**, 1121101 (2021)]



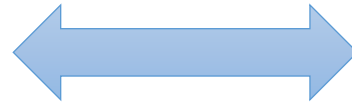
Photonics realization of “non-Abelian 1D topological Insulators”. [Nature **594**, 195–200 (2021)]



Observed non-trivial braiding of Dirac points in metamaterial phonons. [arXiv:2104.13397 (2021)]

Mathematical analogies:

Defects of order parameter
in coordinates space.



Degeneracies of spectral gap
in momentum space.

XY-model vortices \longleftrightarrow Dirac points in graphene
[non-trivial π_1]

Heisenberg hedgehogs \longleftrightarrow Weyl points
[trivial π_1 and non-trivial π_2]

hedgehogs & disclinations of uniaxial nematics \longleftrightarrow Chern # & exceptional lines of non-Herm. Hamiltonian
[non-trivial action of π_1 on π_2]

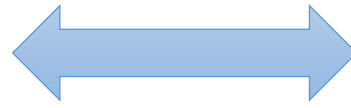
disclination defects of biaxial nematics \longleftrightarrow band nodes of three-band real-sym. Hamiltonian
[non-Abelian π_1]

Domain walls \longleftrightarrow (Bogoliubov-Fermi) nodal surfaces
[non-trivial π_0]

Mathematical analogies:

[see also: R. Kennedy, *et al.*, Phys. Rev. B **91**, 245148 (2015)]

Topological textures of order parameter in coordinates space.

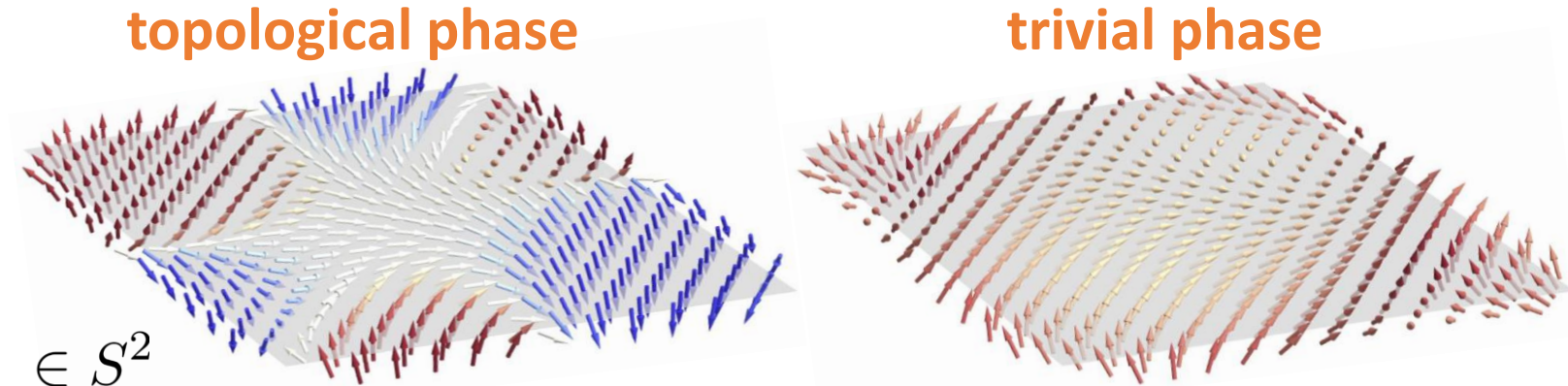


Topological insulators in momentum space.

Example #1: Haldane model

$$H(\mathbf{k}) = h_0(\mathbf{k})\mathbf{1} + \mathbf{h}(\mathbf{k}) \cdot \boldsymbol{\sigma}$$

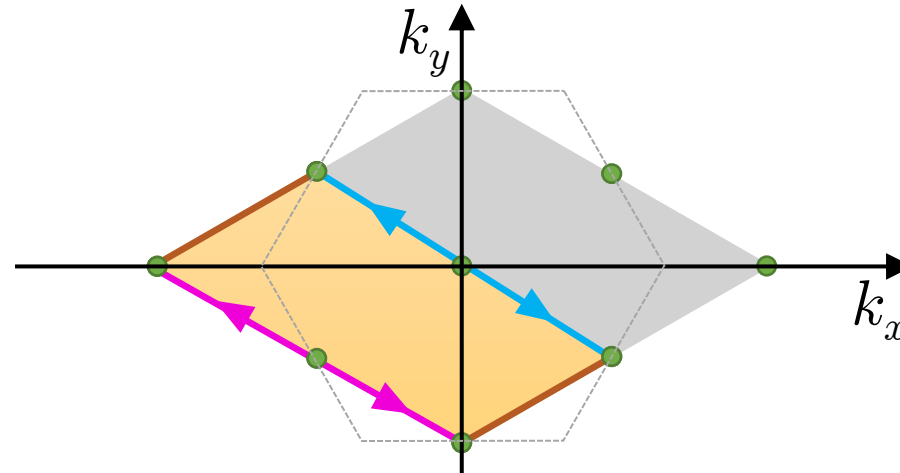
$$(n_x, n_y, n_z) := \frac{(h_x, h_y, h_z)}{\sqrt{h_x^2 + h_y^2 + h_z^2}} \in S^2$$



Homotopy group $\pi_2(\text{Gr}_{\mathbb{C}}) = \mathbb{Z}$ detects the Chern number.

Example #2: Kane-Mele model

$$\mathcal{T}^{-1}H(\mathbf{k})\mathcal{T}^{-1} = H(-\mathbf{k})!$$



Techniques to characterize band topology

INFINITE

BANDS

FEW

K-theory

- assumes ∞ of bands
- uses complete information
- handles crystalline symmetry

Homotopy theory

- for arbitrarily many bands
- uses complete information
- hard to handle symmetries

Symmetry indicators / TQC

- for arbitrarily many bands
- uses reduced information
- built around symmetries

LOW

SYMMETRY

HIGH

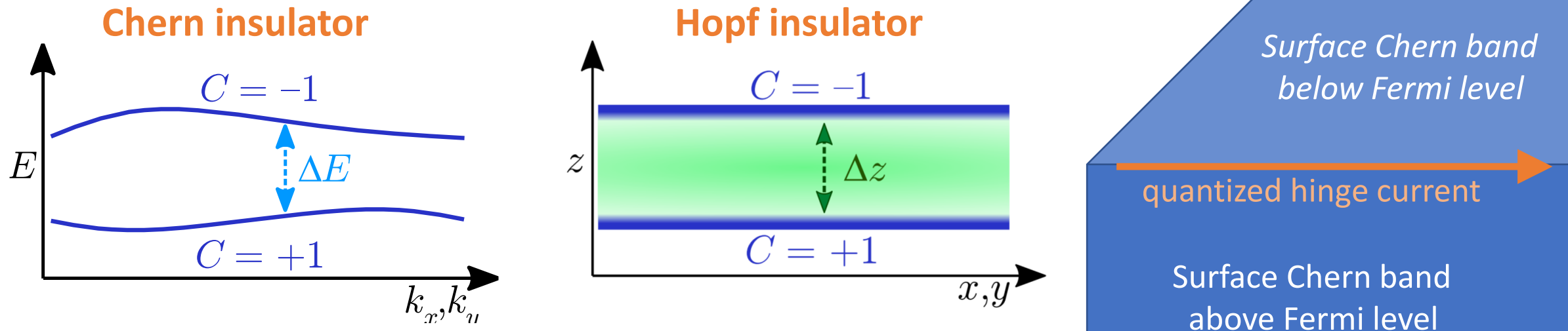
Canonical model of “unstable” topology

Hopf insulator: Two-band class-A model in 3D, based on $\pi_3(S^2) = \mathbb{Z}$.

[J. E. Moore, Y. Ran, and X.-G. Wen, Phys. Rev. Lett. **101**, 186805 (2008)]

$$z(\mathbf{k}) = \begin{pmatrix} \sin k_x + i \sin k_y \\ \sin k_z + i[\cos k_x + \cos k_y + \cos k_z - m] \end{pmatrix} \quad H(\mathbf{k}) = [z^\dagger \boldsymbol{\sigma} z] \cdot \boldsymbol{\sigma}$$

New paradigm for topological boundary anomaly:



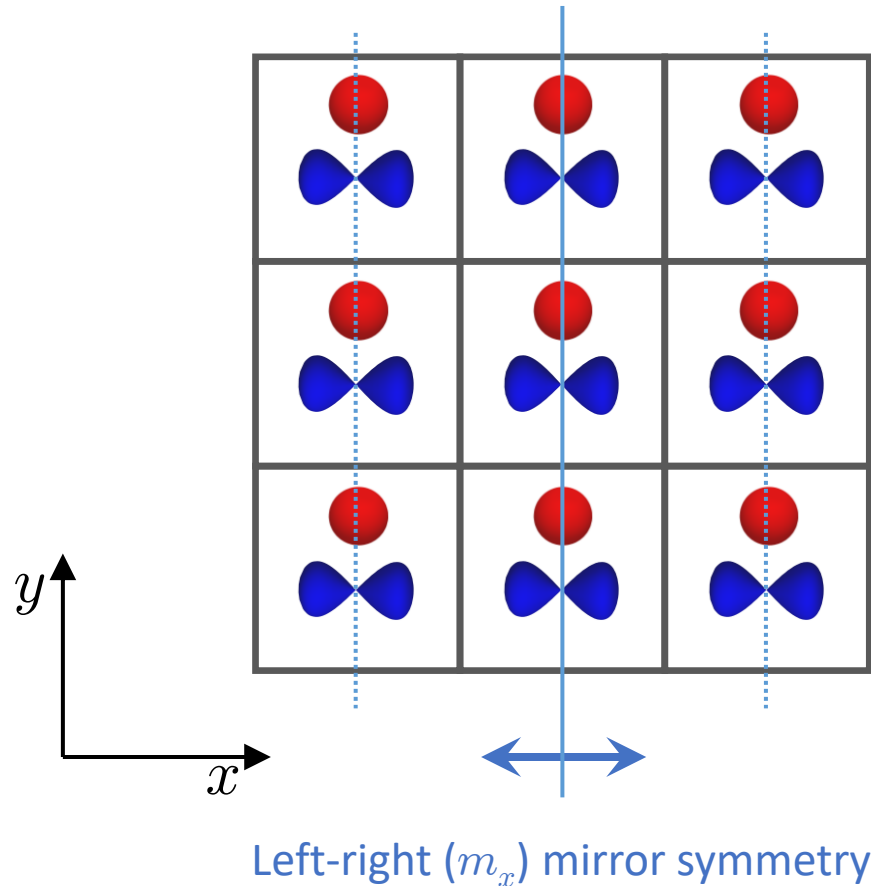
A. Alexandradinata *et al.*, Phys. Rev. B **103**, 045107 (2021)

B. Lapierre *et al.*, Phys. Rev. Research **3**, 033045 (2021)

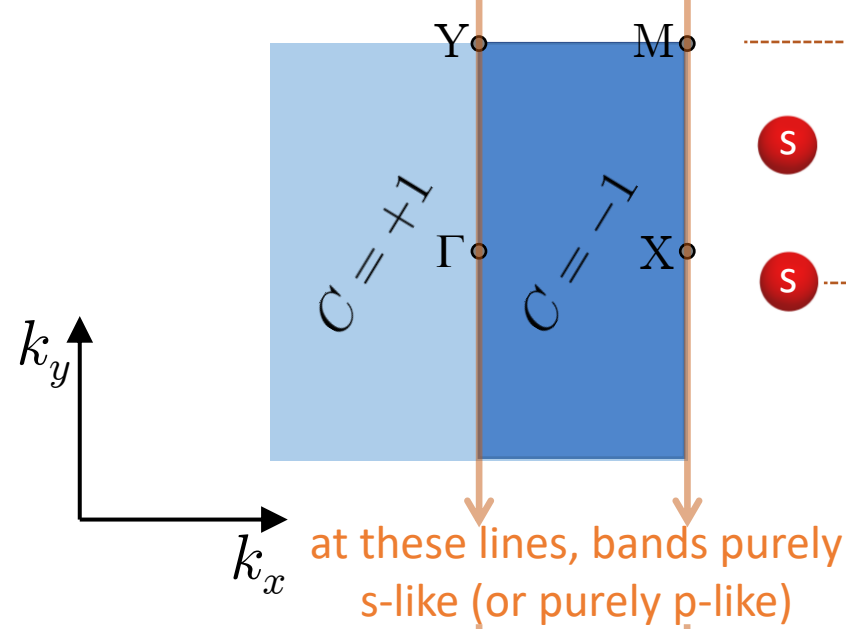
P. Zhu *et al.*, Phys. Rev. B **103**, 014417 (2021)

Returning Thouless pump in 2D

real space:



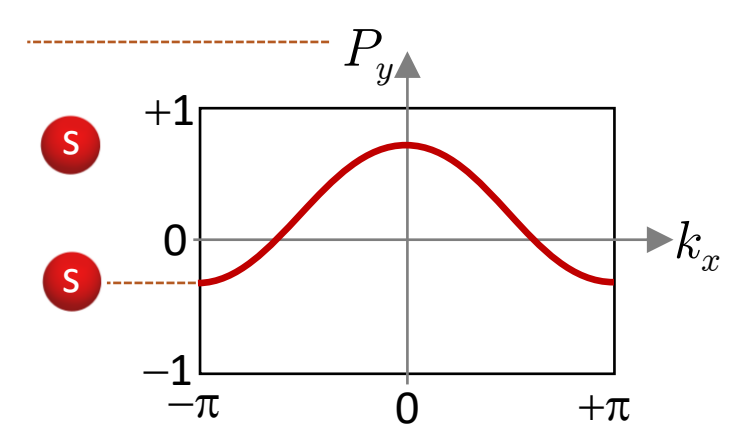
momentum space:



Assume: valence s-like & conduction p-like at both high-sym. lines.

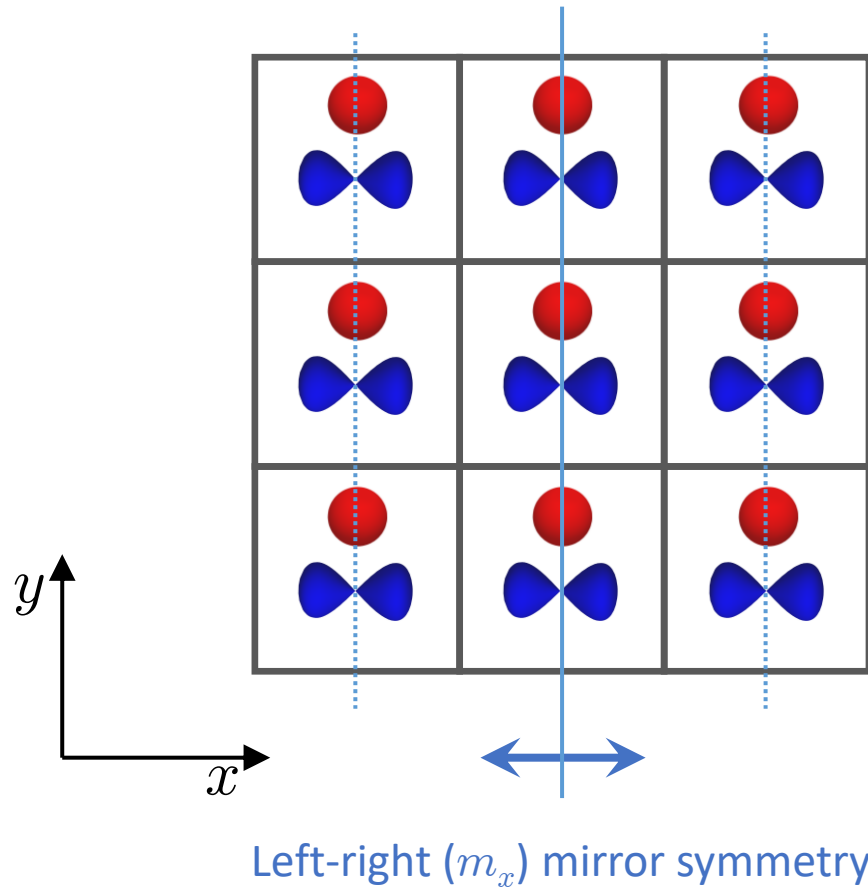
The same (projected) Hamiltonian

polarization:

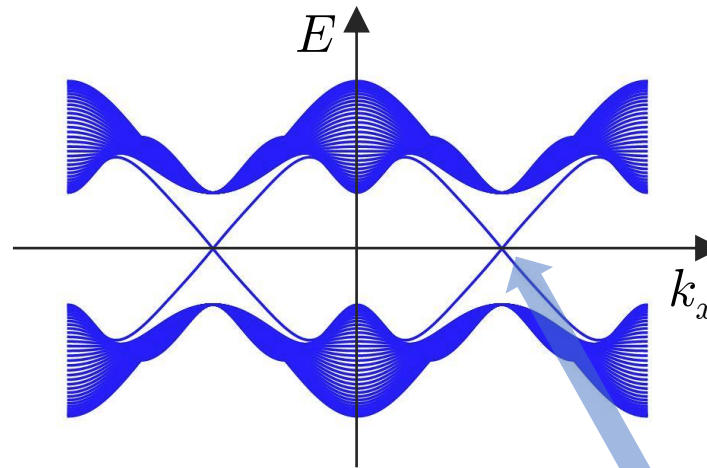


Returning Thouless pump in 2D

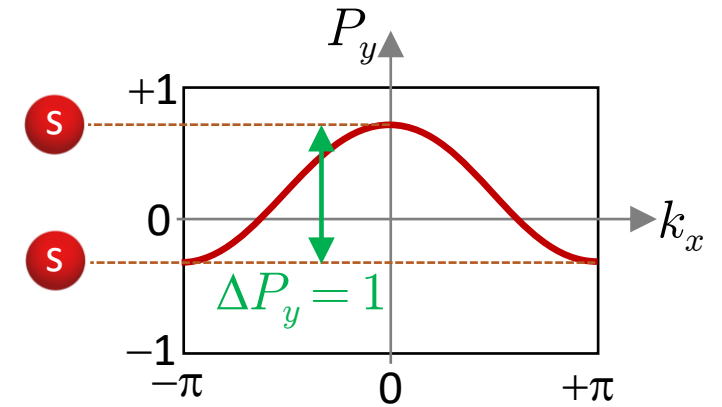
real space:



surface states:



polarization:



To be shown in A. Nelson, T.B., *et. al.* (in preparation):

- Enforces metallic in-gap states at sharp boundaries.
- In 2D leads to edge-localized Zak-phase.
- In 3D leads to surface-localized Chern number (like Hopf).

The topological obstruction *remains stable* if added conduction/valence bands respect the mirror-even/odd dichotomy → neither stable, nor fragile, but delicate topology.

Open questions...

Observable fingerprints of the non-commutative exchange of band nodes?

Cataloguing homotopy-revealed delicate topologies?

Stability against disorder & interactions?

Material realizations?

(...)

Works in collaborations with:

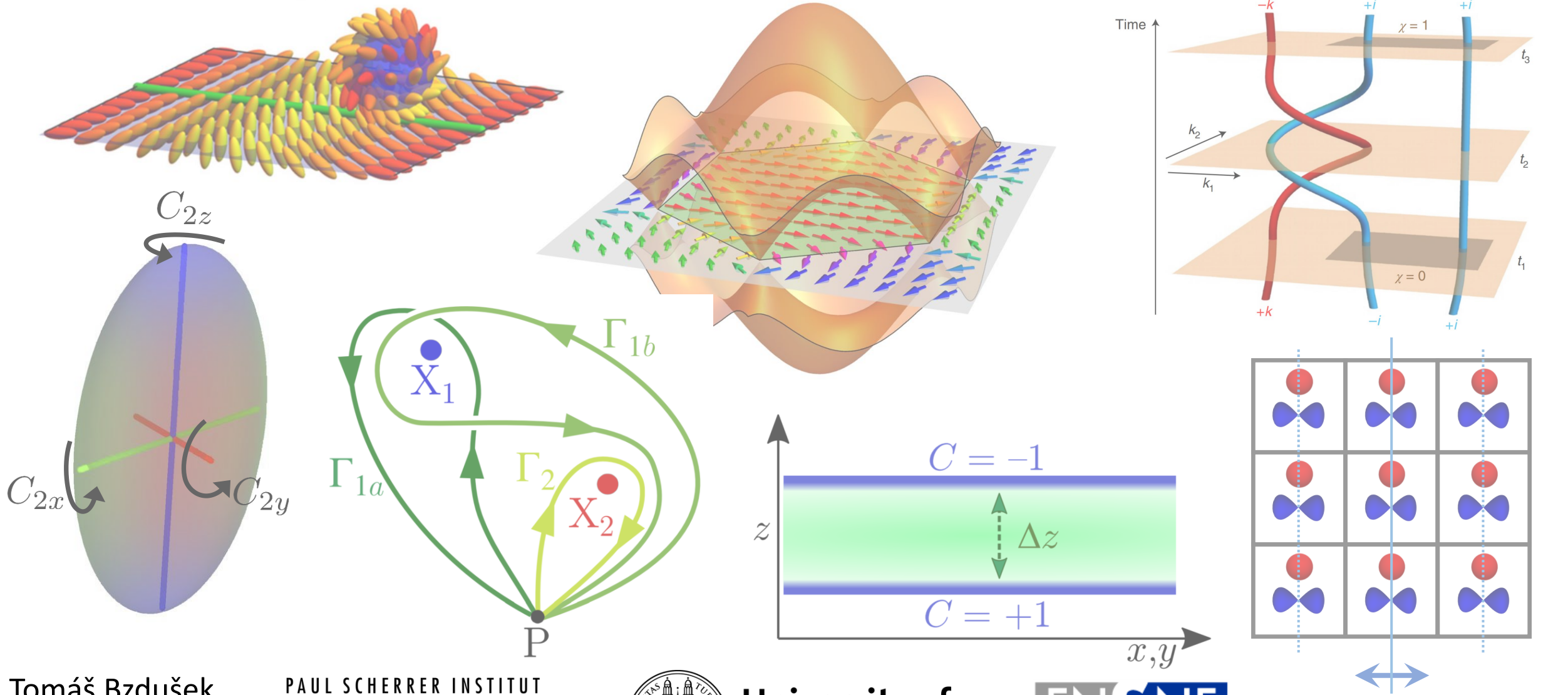
Theory:

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S. Fan (Stanford, USA)
P. M. Lenggenhager (PSI, Switzerland)
A. Nelson (Uni Zürich, Switzerland)
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M. Sigrist (ETH Zürich, Switzerland)
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A. A. Soluyanov[†] (Uni Zürich, Switzerland)
X.-Q. Sun (Stanford → UIUC)
A. Tiwari (PSI, Switzerland)
C. C. Wojcik (Stanford, USA)

First-principles calculations:

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S. S. Tsirkin (Uni Zürich, Switzerland)
H. Weng (IoP Beijing, China)
Q.S. Wu (EPFL, Switzerland)
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Summary & thank you for attention!



Tomáš Bzdušek

22. July 2021

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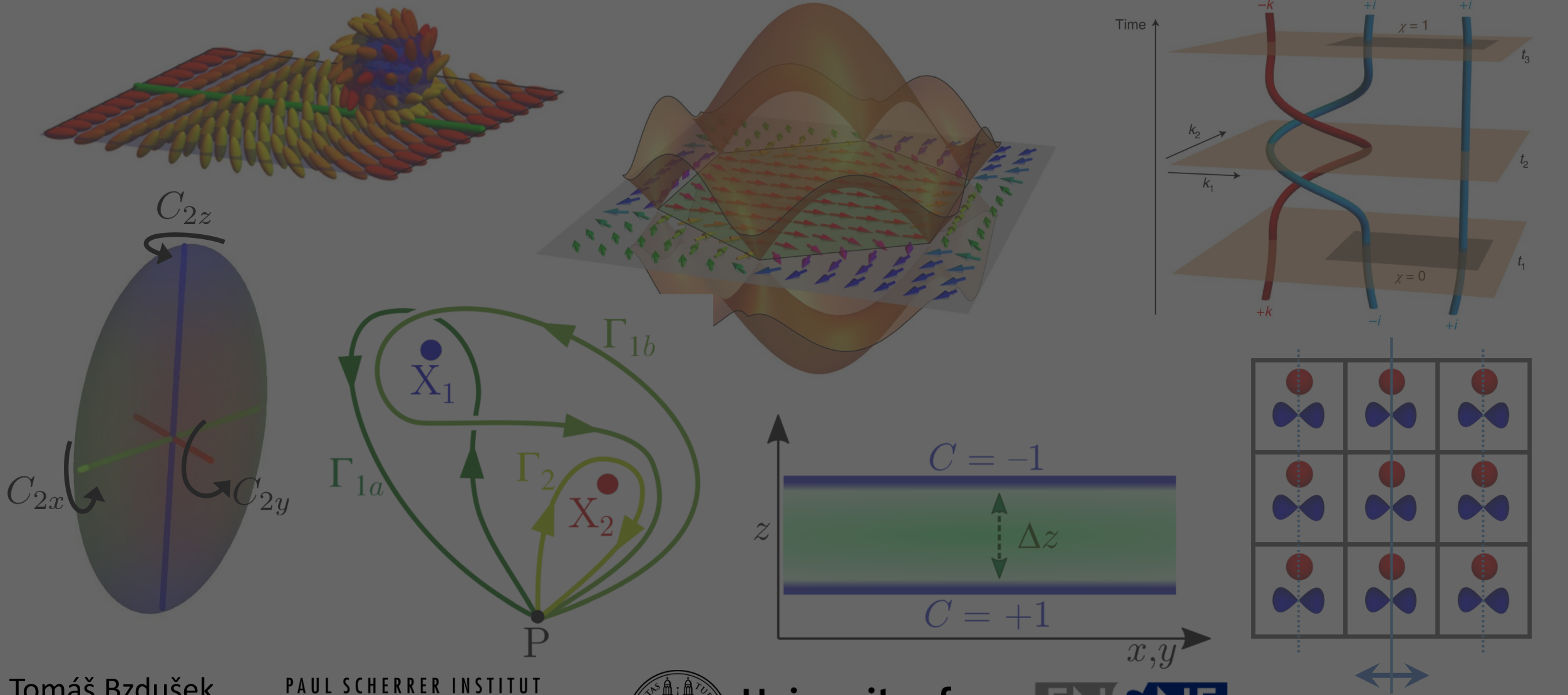


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Summary & thank you for attention!



Tomáš Bzdušek

22. July 2021

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