Non-Abelian Band Topology in Noninteracting Metals

(topological band theory beyond tenfold way)

Tomáš Bzdušek

SPICE Mainz, 30 September 2019

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Science

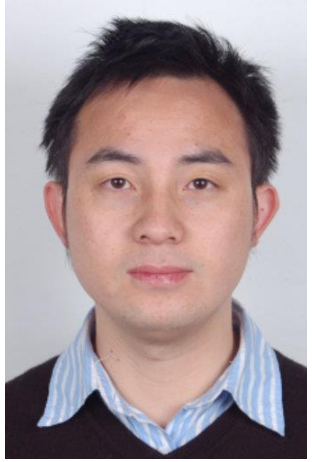
RESEARCH ARTICLES

Non-Abelian band topology in noninteracting metals

QuanSheng Wu[1,2], Alexey A. Soluyanov[3,4], Tomáš Bzdušek[5,6]*

[…] we introduce non-Abelian topological charges that characterize line nodes inside the momentum space of $\mathcal{PT}$-symmetric crystalline metals with weak spin-orbit coupling. We show that these are quaternion charges, similar to those describing disclinations in biaxial nematics. […]

(published 20 Sep 2019)



QuanSheng Wu

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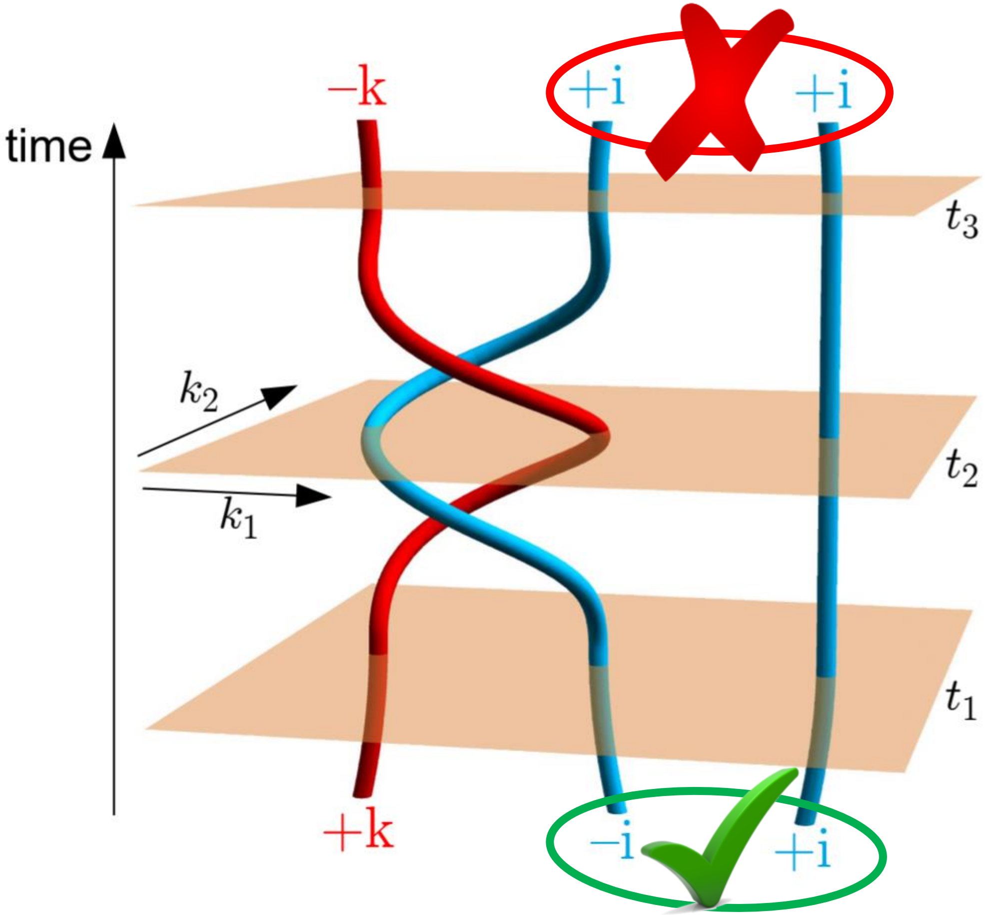
Alexey Soluyanov

Universität
Zürich UZH

Non-abelian “reciprocal” braiding of band nodes



(trajectories in k-space vs. time)

arXiv: 1903.0018 & 1907.10611

Robert-Jan Slager

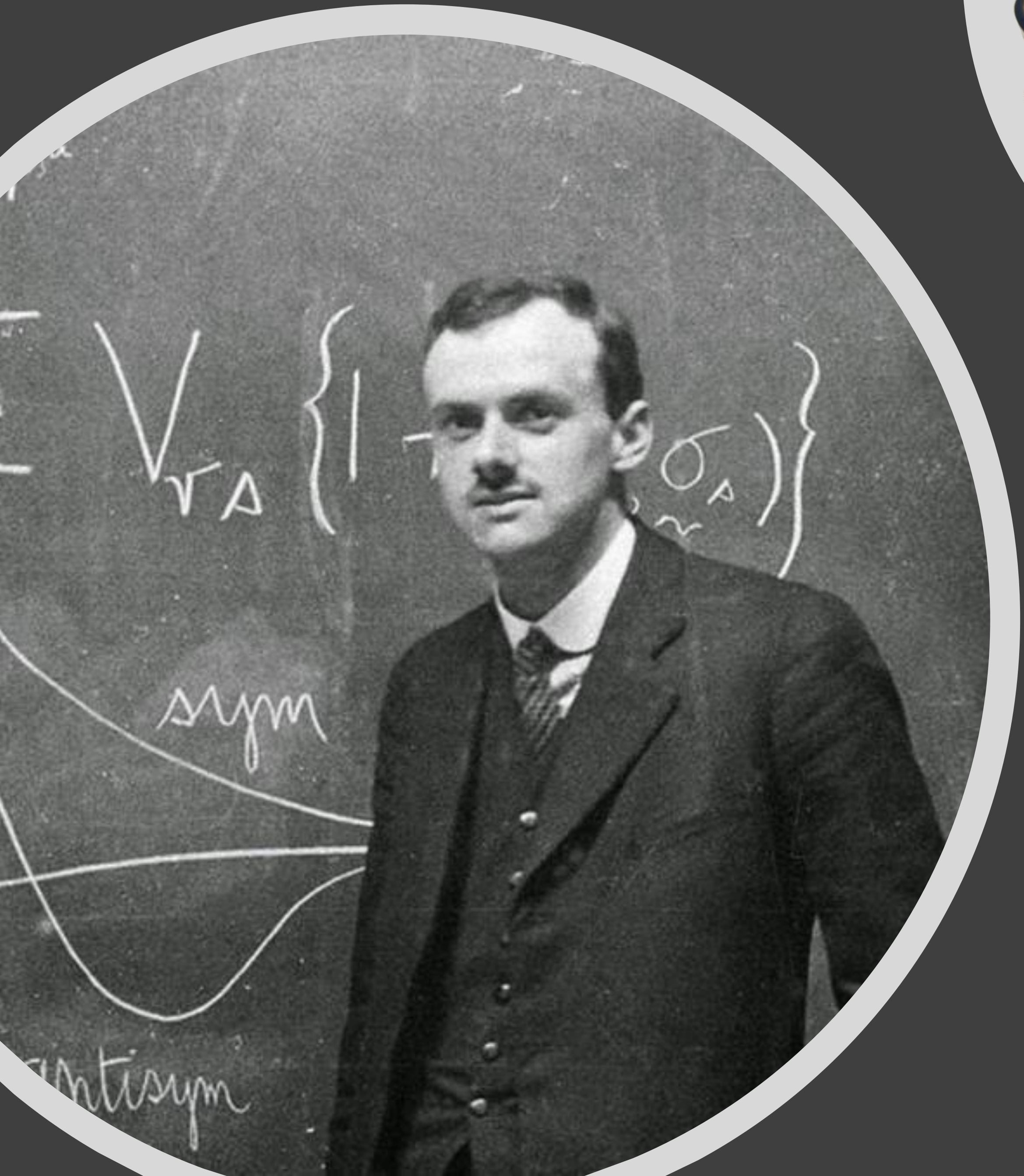
HARVARD
UNIVERSITY

Adrien Bouhon

NORDITA
The Nordic Institute for Theoretical Physics

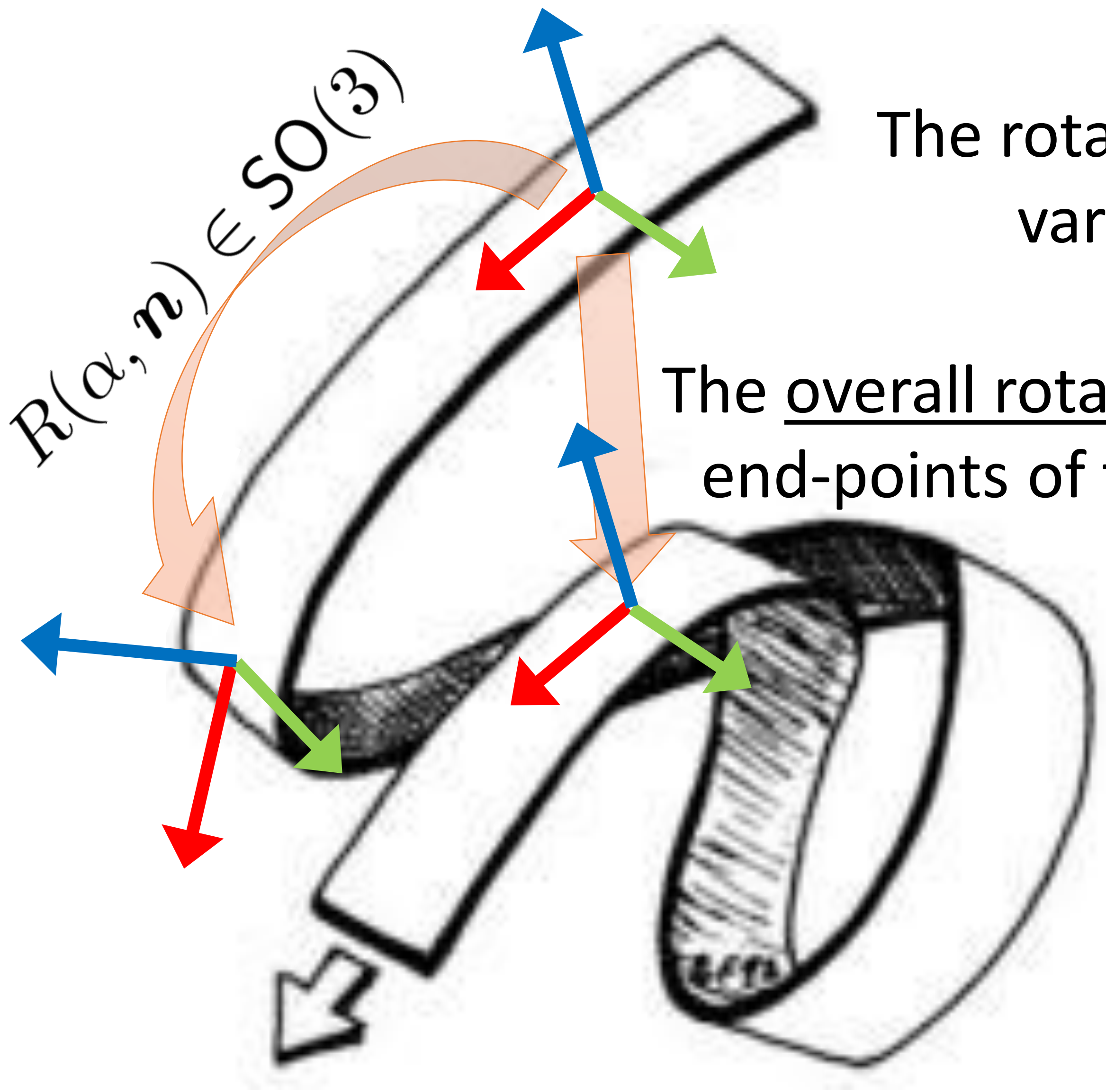
Apoorv Tiwari

University of
Zurich$^{\text{UZH}}$



The Dirac’s belt trick

How to describe a twisted belt



The rotation $R(\alpha,\boldsymbol{n})$ smoothly varies along the belt.

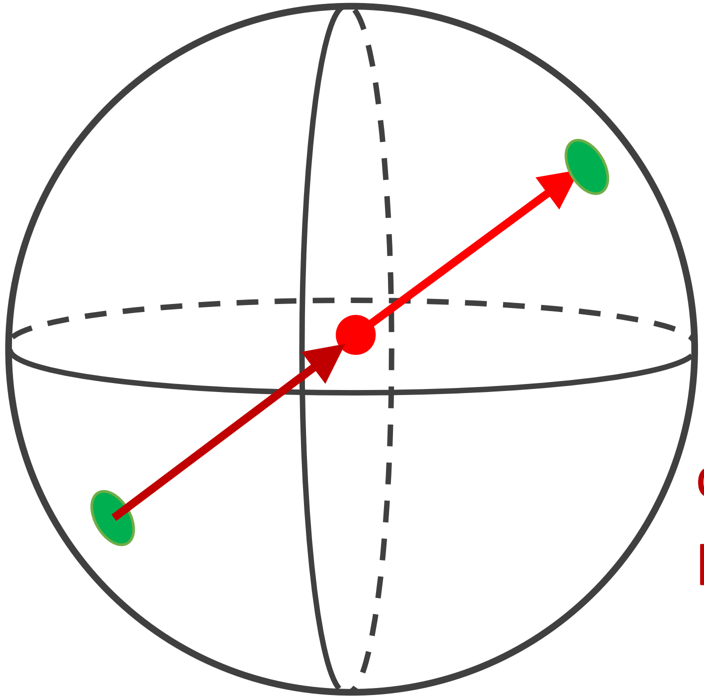
The overall rotation between the end-points of the belt is trivial.

Visualizing the “SO(3)” manifold of rotations

Rotation around axis $\boldsymbol{n}$ by angle $0 \leq \alpha \leq \pi$: $R(\boldsymbol{n}, \alpha) \mapsto \alpha \boldsymbol{n} \in \mathbb{R}^3$

(constitute a 3D ball with radius π)

+ identify antipodal points on the ball surface because $R(\boldsymbol{n}, \pi) = R(-\boldsymbol{n}, \pi)$



closed **non-contractible** path inside the ball

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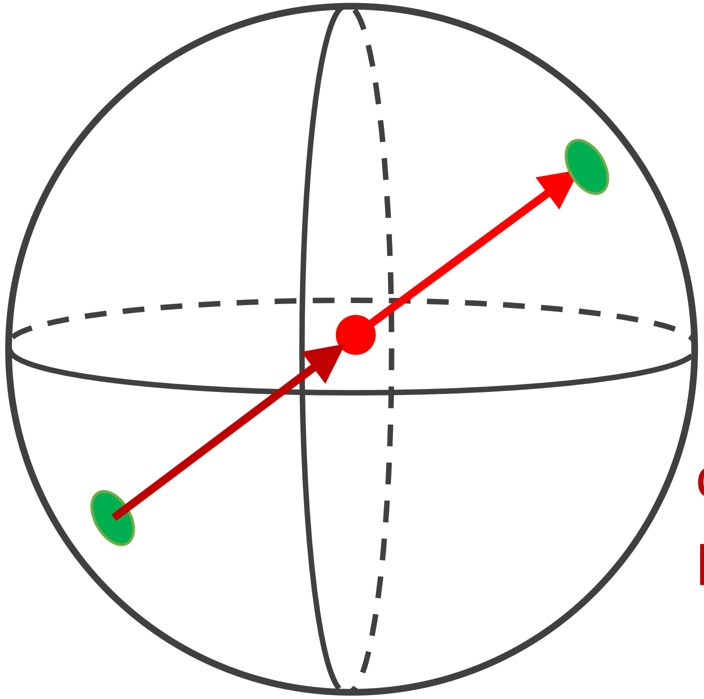
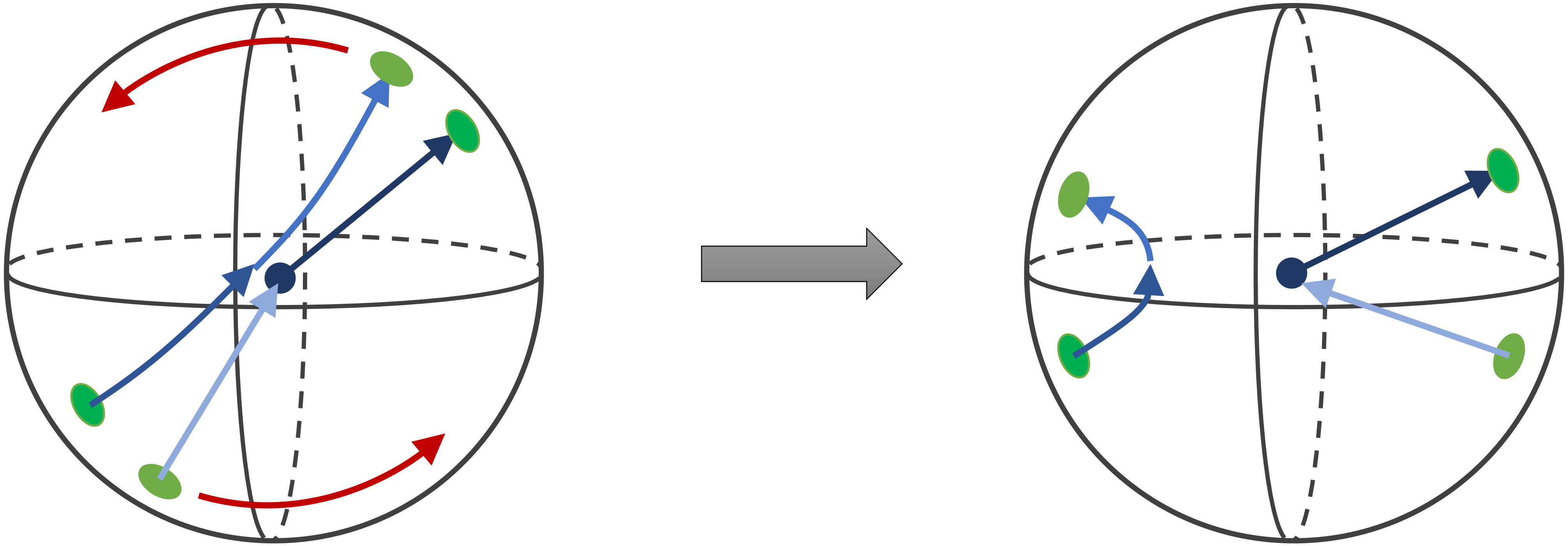


closed **non-contractible** path inside the ball

Visualizing the “SO(3)” manifold of rotations

4π rotation of the belt



What about π rotations (C_{2x} and C_{2y})?

As geometric transformations: $C_{2x} \circ C_{2y} = C_{2y} \circ C_{2x}$

As paths that keep memory: $C_{2x} \circ C_{2y} \neq C_{2y} \circ C_{2x}$

$$\Downarrow$$

$$C_{2x} \circ C_{2y} \circ C_{2x}^{-1} \circ C_{2y}^{-1} = 2\pi\text{-rotation}$$

How does it matter for band structures?

~~Hermitian~~ Bloch Hamiltonians

Real symmetric?

Yes, if there is an antiunitary symmetry S such that:

$$S\mathcal{H}(\boldsymbol{k})S^{-1} = \mathcal{H}(\boldsymbol{k}) \qquad S^2 = +1$$

In 2D: $C_2\mathcal{T}$ (irrespective of spin-orbit coupling)

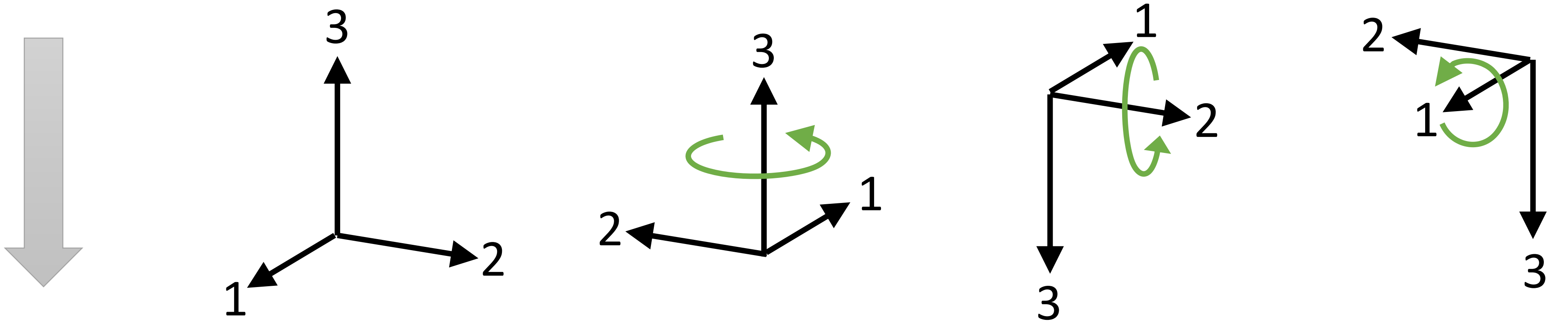
In 3D: $\mathcal{PT}$ (without spin-orbit coupling)

~~Hermitian~~ Bloch Hamiltonians

Real symmetric?

Then eigenstates are real (but sign ambiguity)

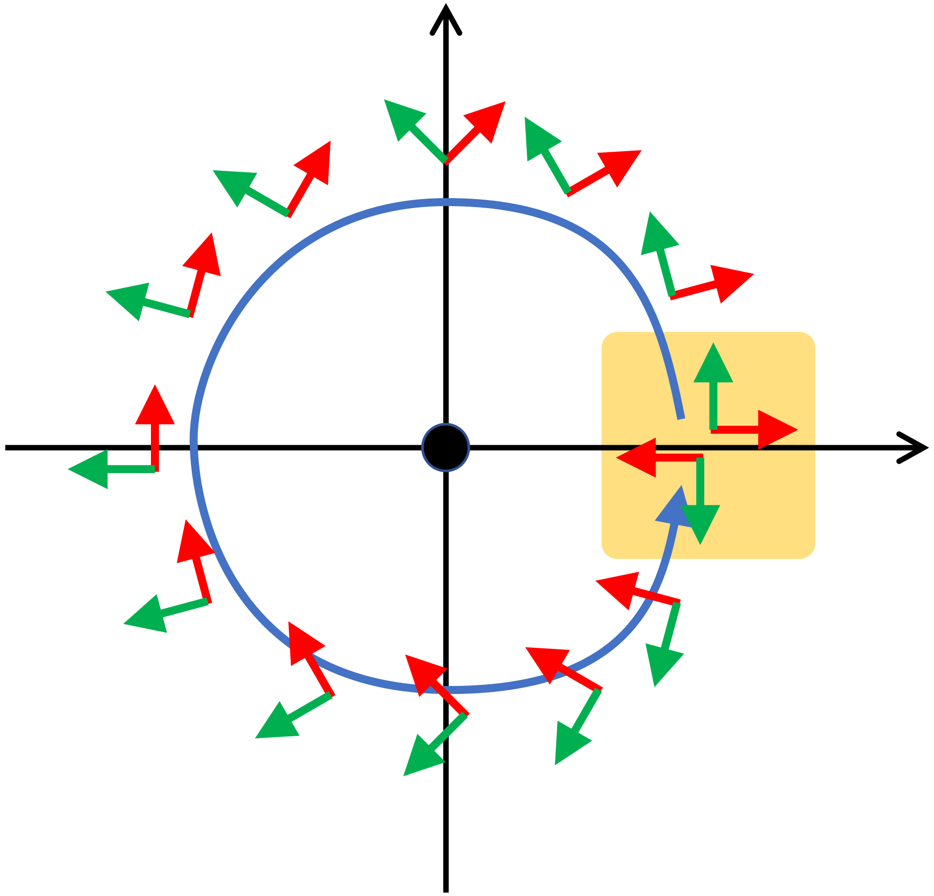
and orthogonal to each other.



the complete set of eigenstates span an orthonormal frame

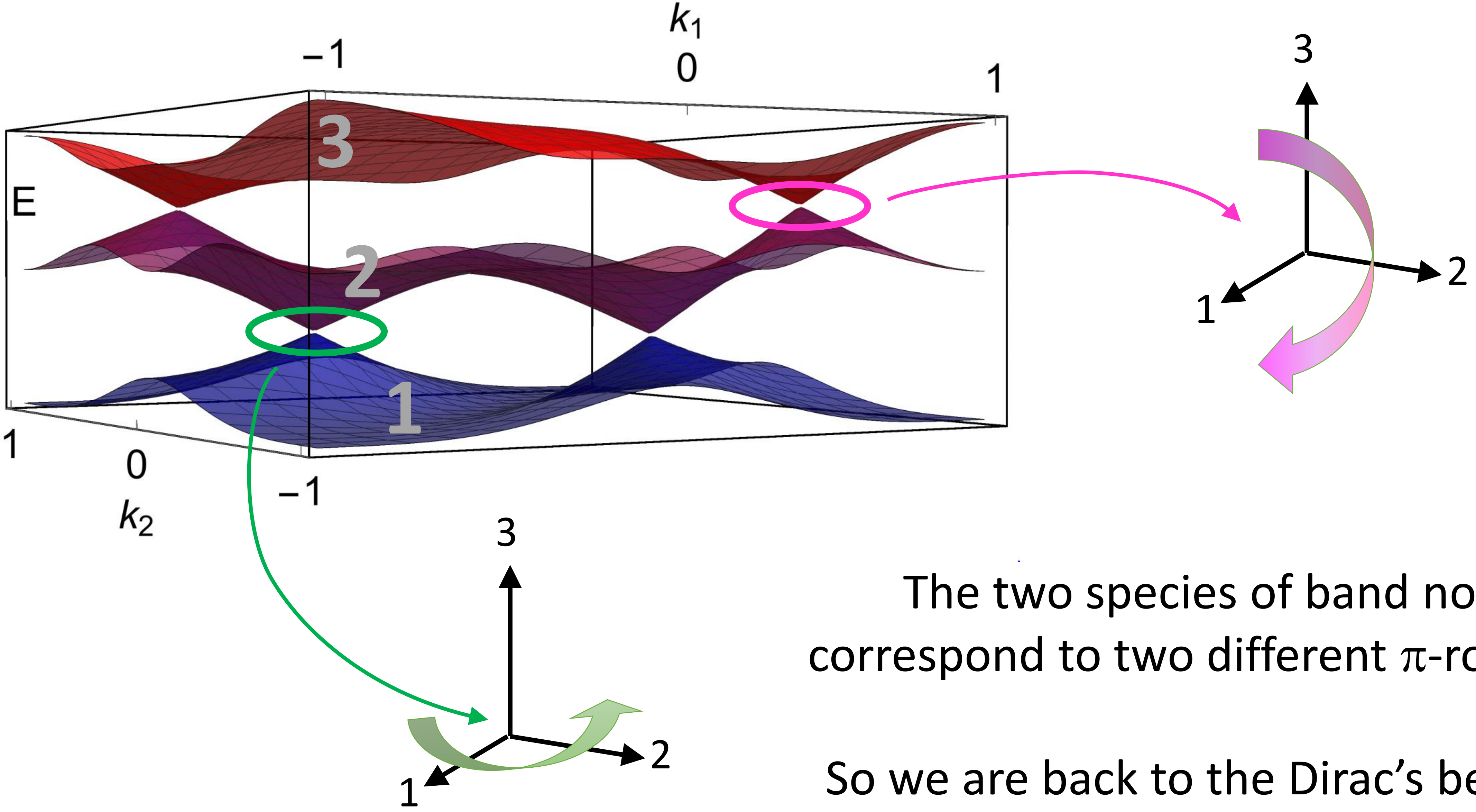
Band node in a 2-band model

$$\mathcal{H}(\boldsymbol{k}) = k_x \sigma_z + k_y \sigma_x$$



The band degeneracy
is associated with
a π-rotation of the frame

Band nodes in a 3-band model

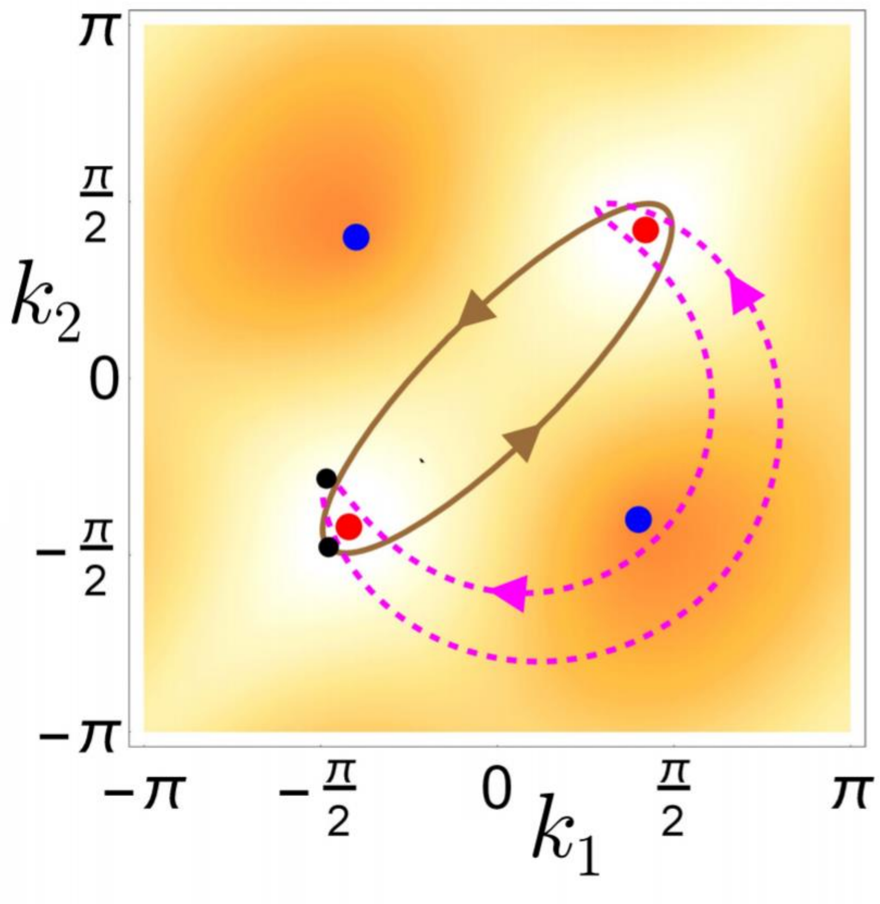


The two species of band nodes correspond to two different π-rotations.

So we are back to the Dirac's belt trick!

R.-J. Slager, A. Bouhon, and T. Bzdušek, arXiv:1907.10611 (2019)

Band nodes in a 3-band model



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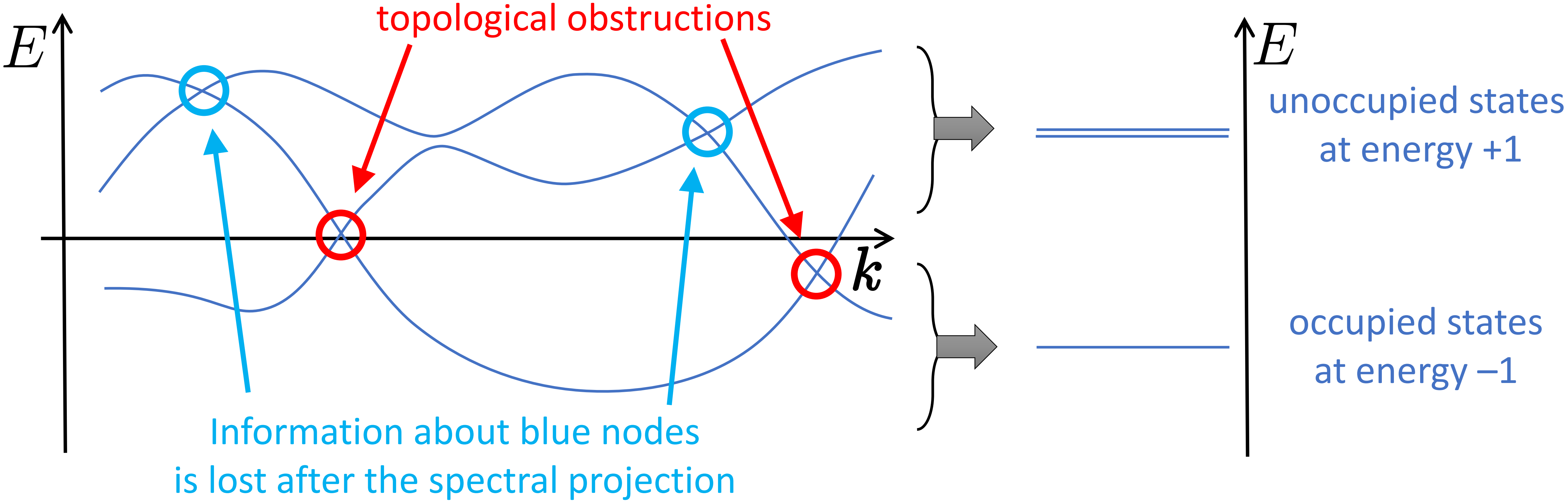


topological obstructions

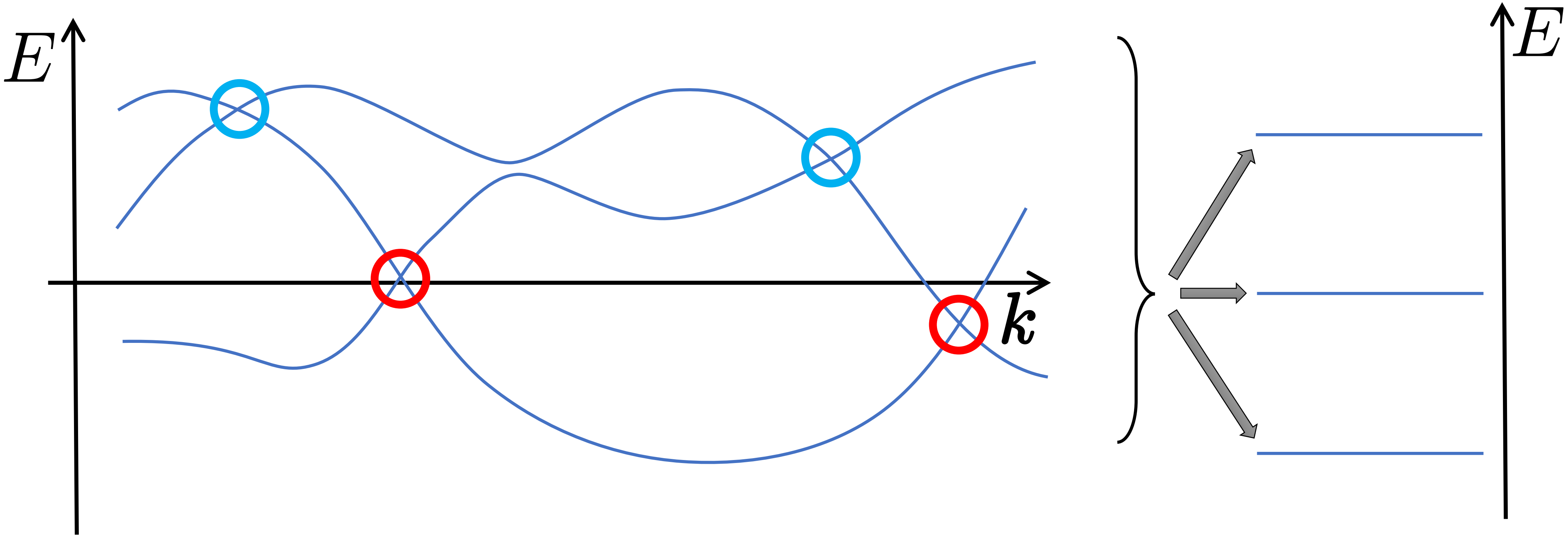
Information about blue nodes
is lost after the spectral projection

unoccupied states
at energy +1

occupied states
at energy –1

Q.S. Wu, A. A. Soluyanov, T. Bzdušek, Science **365**, 1273 (2019)

Band nodes in a 3-band model



Third band
at **energy +3**

Second band
at **energy +2**

Lowest band
at **energy +1**

Q.S. Wu, A. A. Soluyanov, T. Bzdušek, Science **365**, 1273 (2019)

Non-commutative
“frame-rotation charge”
(arbitrarily many bands)

Generalizes Z_2 **Berry phase** + new 1D topological phases.

Explains the topological stability of **nodal chains**

Relates **monopole charge** (on S^2) to the linking structure

Governs **node conversions** between Weyl points and Nodal loops

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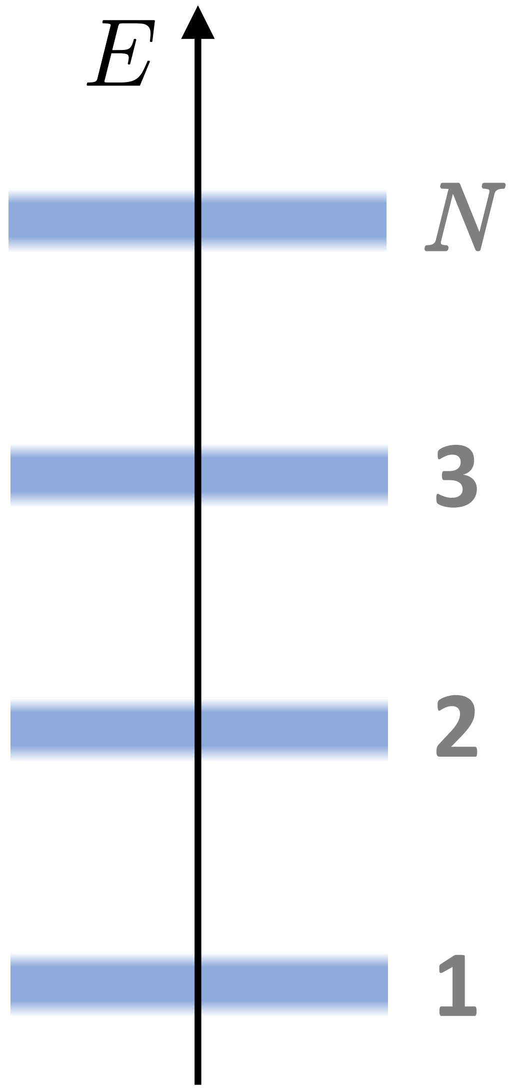
The non-Abelian topological charge



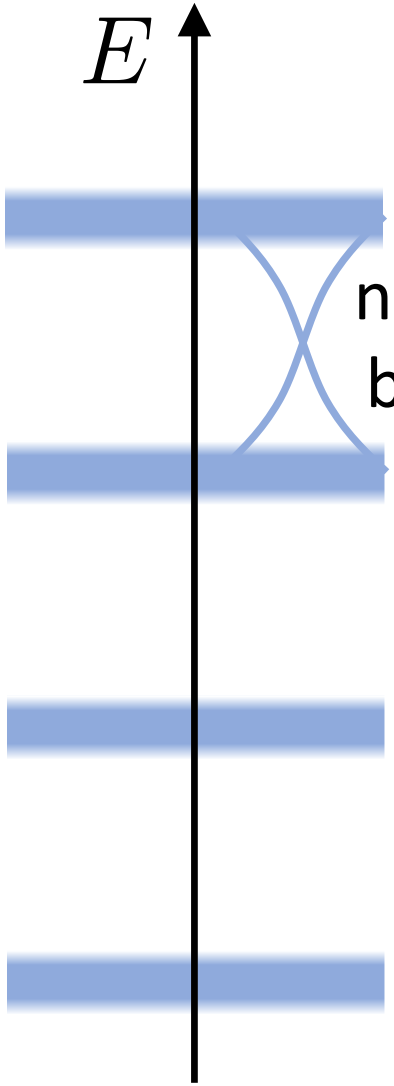
On a closed path in $\boldsymbol{k}$-space (also 1D BZ):

Quantization of Berry phase on N bands:
$2^{N\text{-}1}$ possibilities

The generalized “frame-rotation charge”:
2^N possibilities

Q.S. Wu, A. A. Soluyanov, T. Bzdušek, Science **365**, 1273 (2019)

The non-Abelian topological charge



node inside band gap j

topological charge g_j in group G that obeys:

$$(1)\ \ \exists!(-1)\in G:(-1)^2=+1$$

$$(2)\ \ \forall j:(g_j)^2=-1$$

$$(3)\ \ \forall j: g_j\cdot g_{j+1}=-g_{j+1}\cdot g_j$$

$$(4)\ \ \forall\,|i-j|\neq 1: g_i\cdot g_j=+g_j\cdot g_i$$

A. Tiwari and T. Bzdušek, arXiv:1903.0018 (2019)

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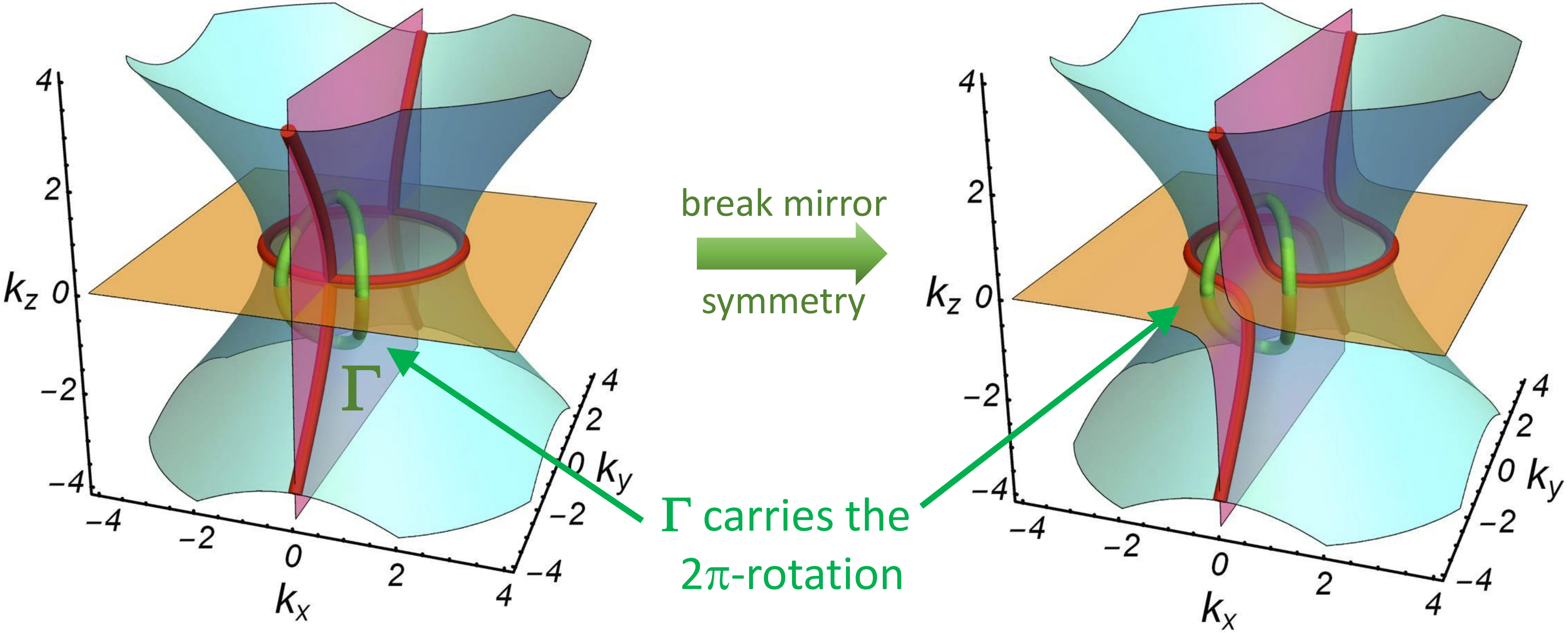
Nodal chains in two-band models

We assume space-time inversion $\mathcal{PT} = \mathcal{K}$ and mirror symmetry $m_z = \sigma_z$

$$\mathcal{H}(\boldsymbol{k}) = \boxed{h_x(\boldsymbol{k})}\sigma_x + \boxed{h_z(\boldsymbol{k})}\sigma_z \qquad \pi_1(S^1) = \mathbb{Z}$$

odd in k_z even in k_z

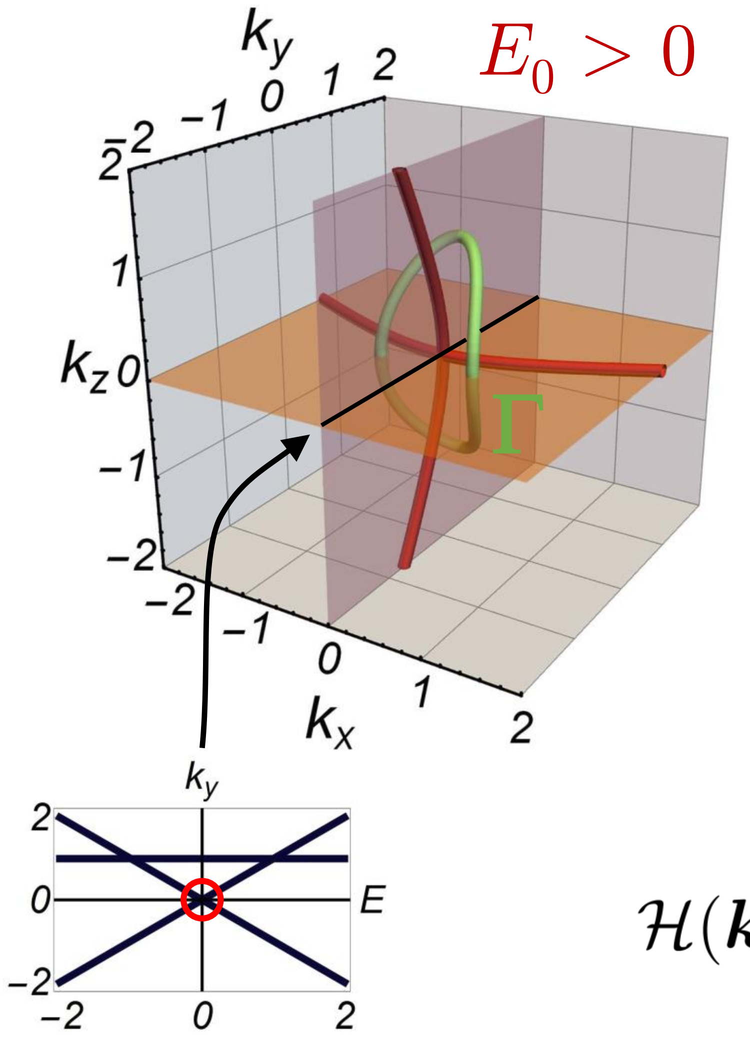


break mirror symmetry

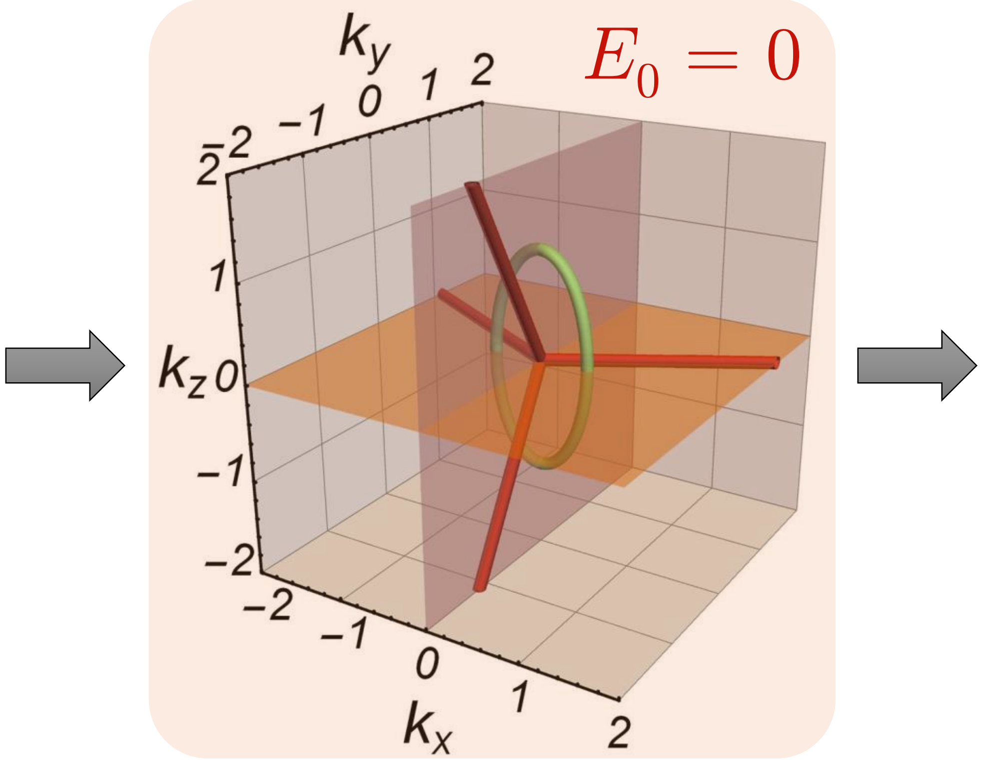
Γ carries the 2π-rotation

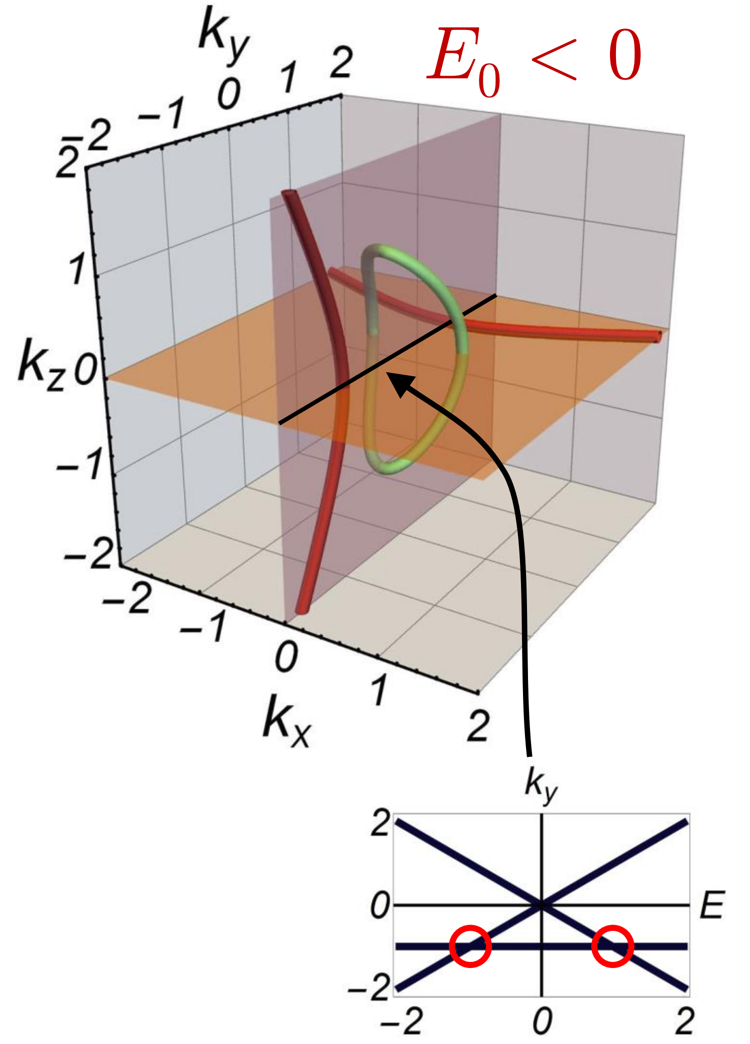
Q.S. Wu, A. A. Soluyanov, T. Bzdušek, Science **365**, 1273 (2019)

Nodal chains in three-band models



critical point





$$\mathcal{H}(\boldsymbol{k}; E_0) = \begin{pmatrix} E_0 & \frac{1}{2}k_x & \frac{1}{2}k_z \\ \frac{1}{2}k_x & k_y & k_x k_z \\ \frac{1}{2}k_z & k_x k_z & -k_y \end{pmatrix}$$

Q.S. Wu, A. A. Soluyanov, <u>T. Bzdušek</u>, Science **365**, 1273 (2019)

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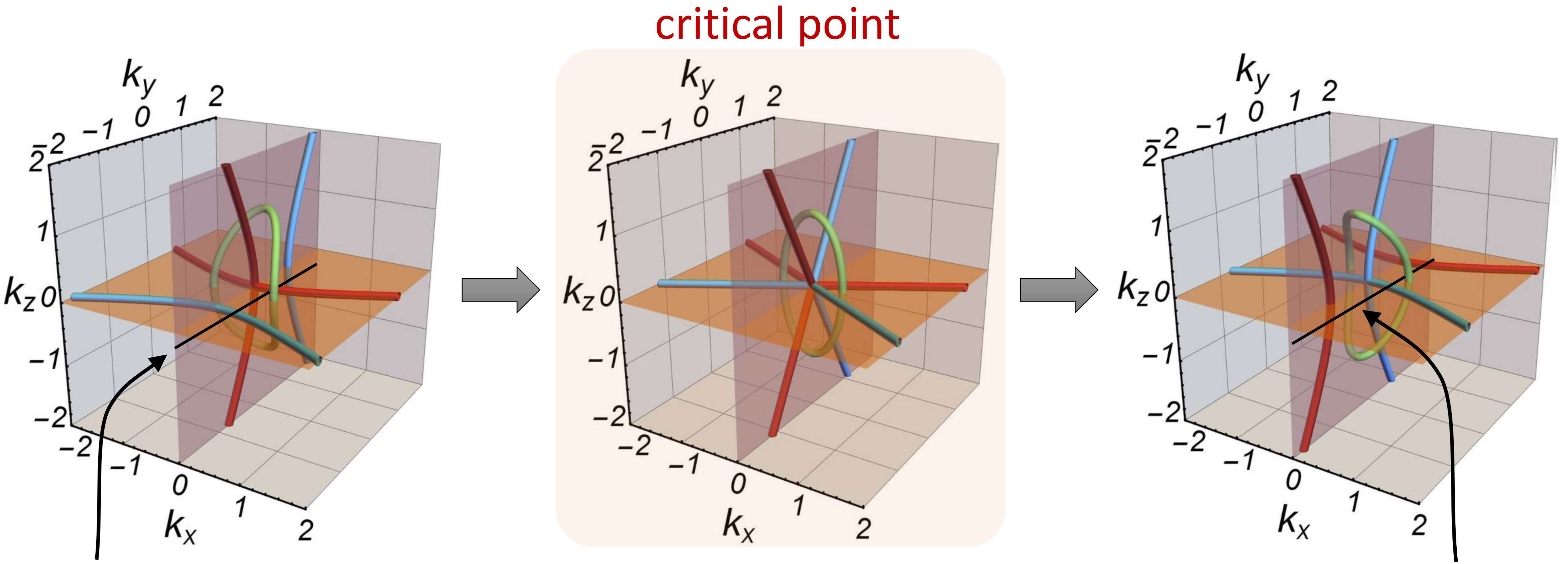
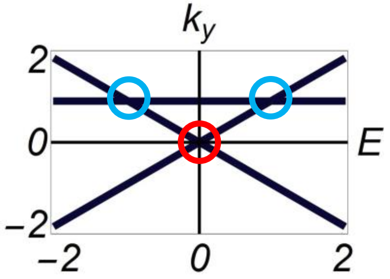
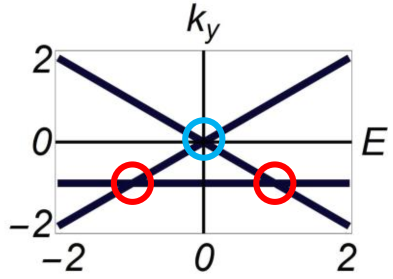




$$\mathcal{H}(\boldsymbol{k};E_0)=\begin{pmatrix} E_0 & \frac{1}{2}k_x & \frac{1}{2}k_z \\ \frac{1}{2}k_x & k_y & k_xk_z \\ \frac{1}{2}k_z & k_xk_z & -k_y \end{pmatrix}$$



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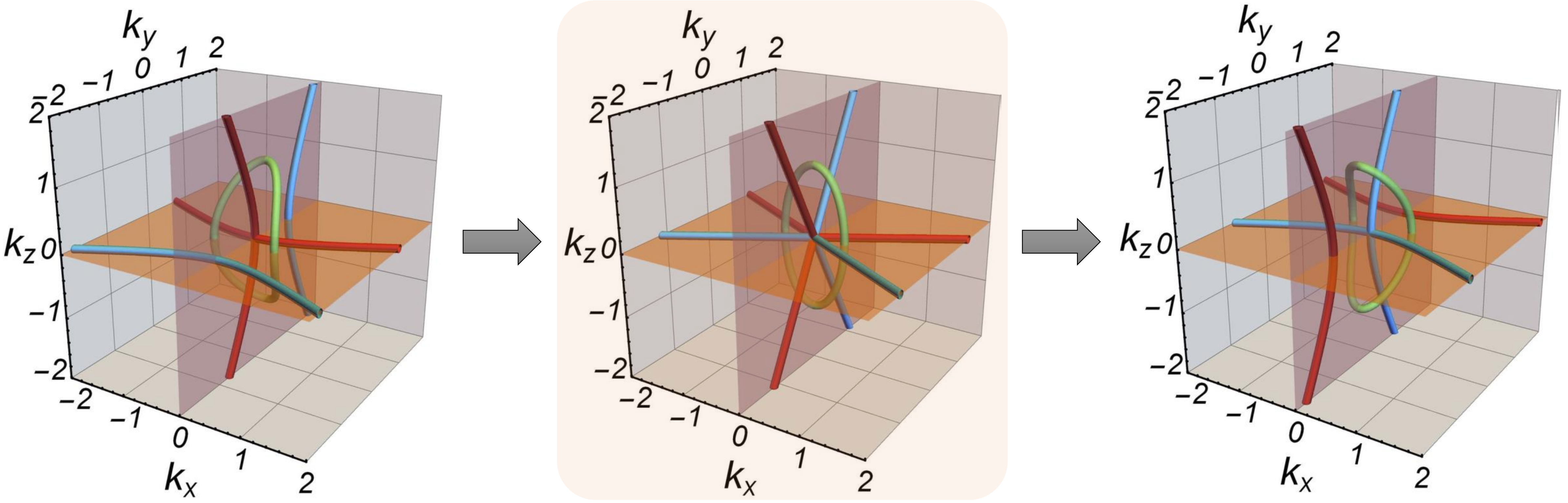
critical point

Reinterpret the 2π rotation
from being $(C_{2z})^2$ (on the left) as being $(C_{2x})^2$ (on the right)

Q.S. Wu, A. A. Soluyanov, T. Bzdušek, Science **365**, 1273 (2019)

Non-commutative
“frame-rotation charge”
(arbitrarily many bands)

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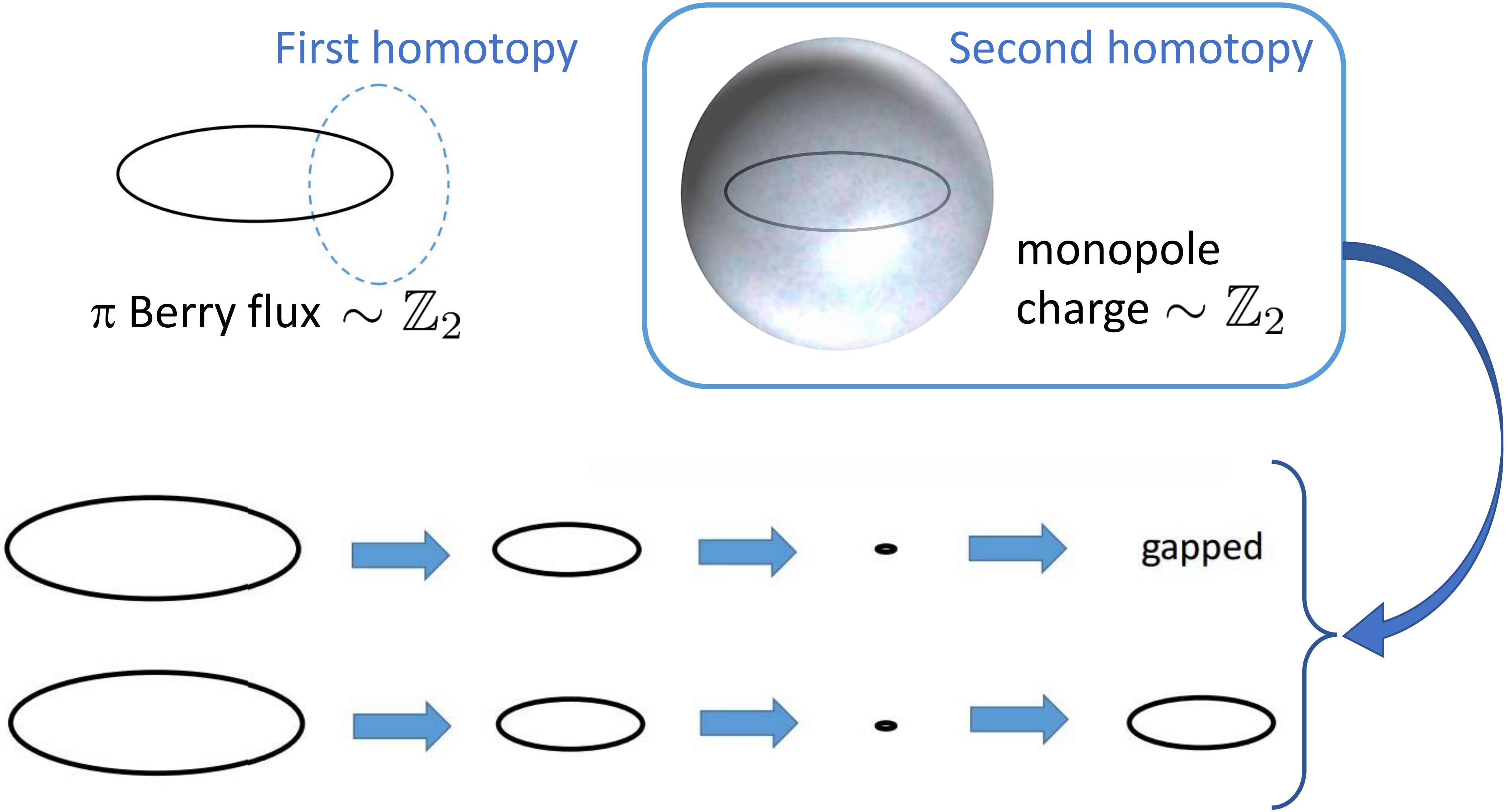
Nodal class with $(\mathcal{PT})^2 = +1$



First homotopy

π Berry flux $\sim \mathbb{Z}_2$

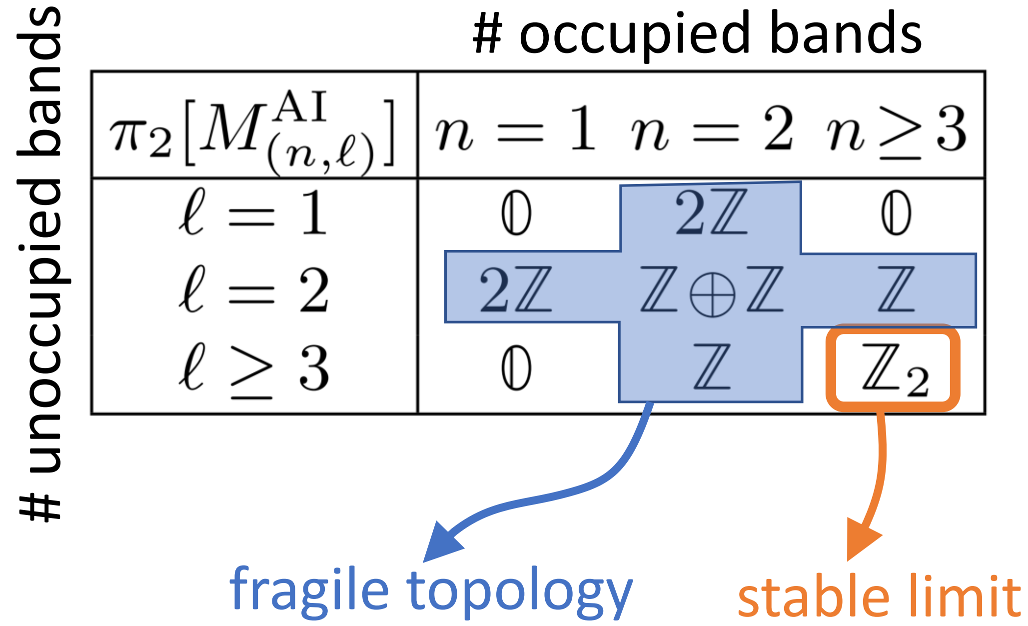
Second homotopy

monopole charge $\sim \mathbb{Z}_2$

gapped

C. Fang, Y. Chen, H.-Y. Kee, L. Fu, Phys. Rev B **92**, 081201(R) (2015)

Relates monopole charge to linking structure



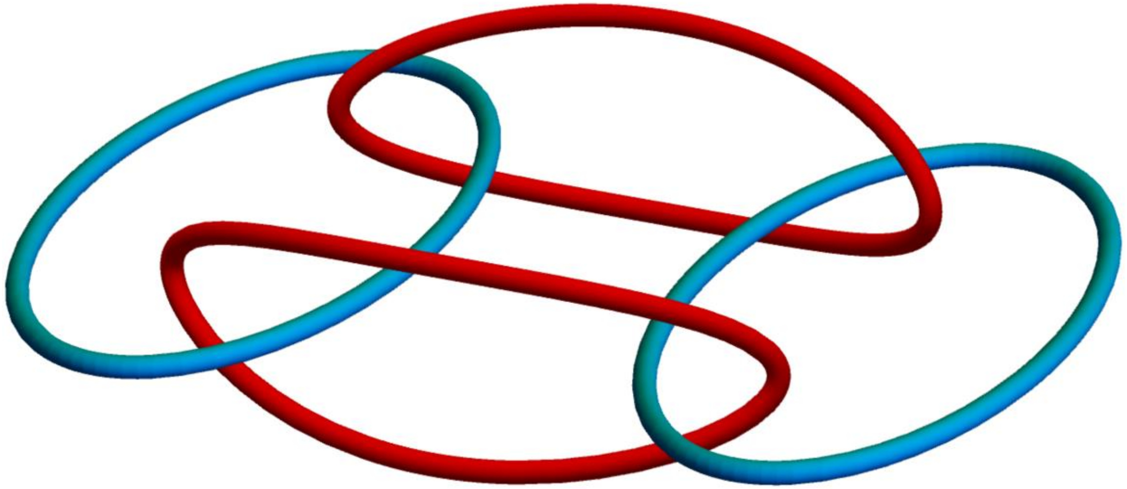
occupied bands

unoccupied bands

$\pi_2[M^{\mathrm{AI}}_{(n,\ell)}]$	$n=1$	$n=2$	$n\geq 3$
$\ell=1$	$\mathbb{0}$	$2\mathbb{Z}$	$\mathbb{0}$
$\ell=2$	$2\mathbb{Z}$	$\mathbb{Z}\oplus\mathbb{Z}$	$\mathbb{Z}$
$\ell\geq 3$	$\mathbb{0}$	$\mathbb{Z}$	$\mathbb{Z}_2$

fragile topology

stable limit



Monopole charge of a nodal-line ring in band gap “j”
counts the Gauss linking with nodal lines in band gaps “j - 1” resp. “$j+1$”

T. Bzdušek and M. Sigrist, Phys. Rev. B **96**, 155105 (2017)

J. Ahn, D. Kim, Y. Kim, and B.-J. Yang, Phys. Rev. Lett. **121**, 106403 (2018)

A. Tiwari and T. Bzdušek, arXiv:1903.0018 (2019)

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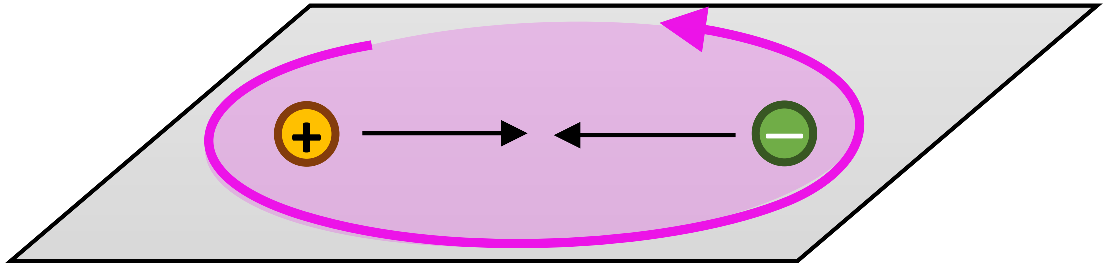
Interplay with crystalline symmetries in 3D

$\mathcal{C}_{2z}\mathcal{T}$ symmetry (no $\mathcal{PT}$ symmetry)

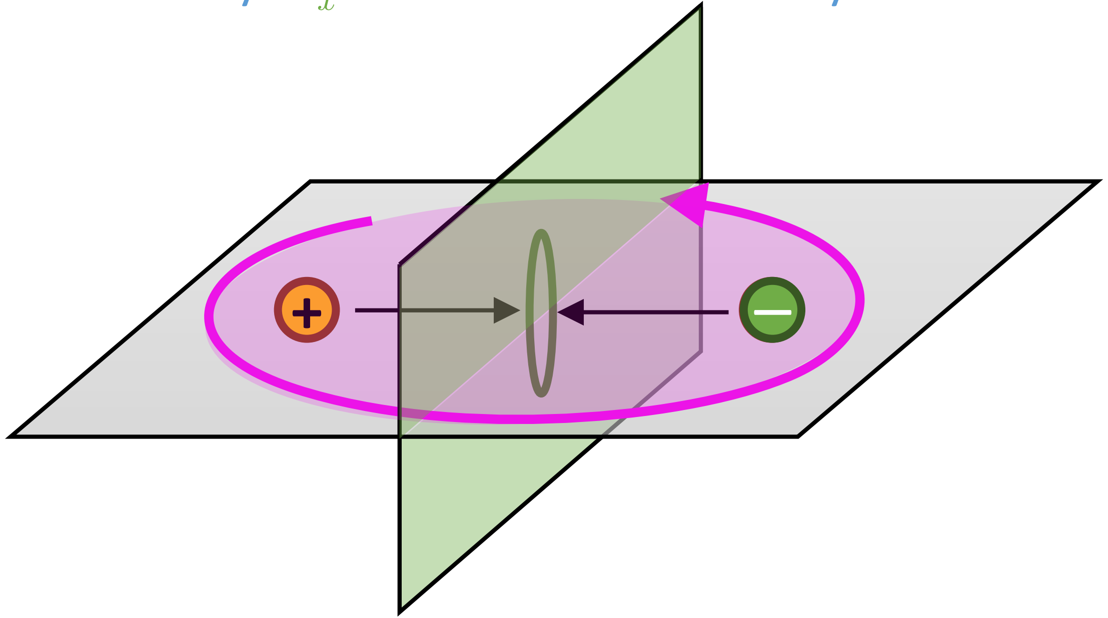
Two in-plane Weyl points of opposite chirality:



If 2π rotation they cannot annihilate, and remain stuck inside the plane.

$\mathcal{C}_{2z}\mathcal{T}$ + m_x symmetry (no $\mathcal{PT}$ symmetry)

Two in-plane Weyl points related by m_x have the same chirality:



If 2π rotation the two Weyl points convert into a mirror-protected nodal ring

R.-J. Slager, A. Bouhon, and T. Bzdušek, arXiv:1907:10611 (2019)
X.-Q. Sun, S.C. Zhang, and T. Bzdušek, Phys. Rev. Lett. **121**, 106402 (2018)

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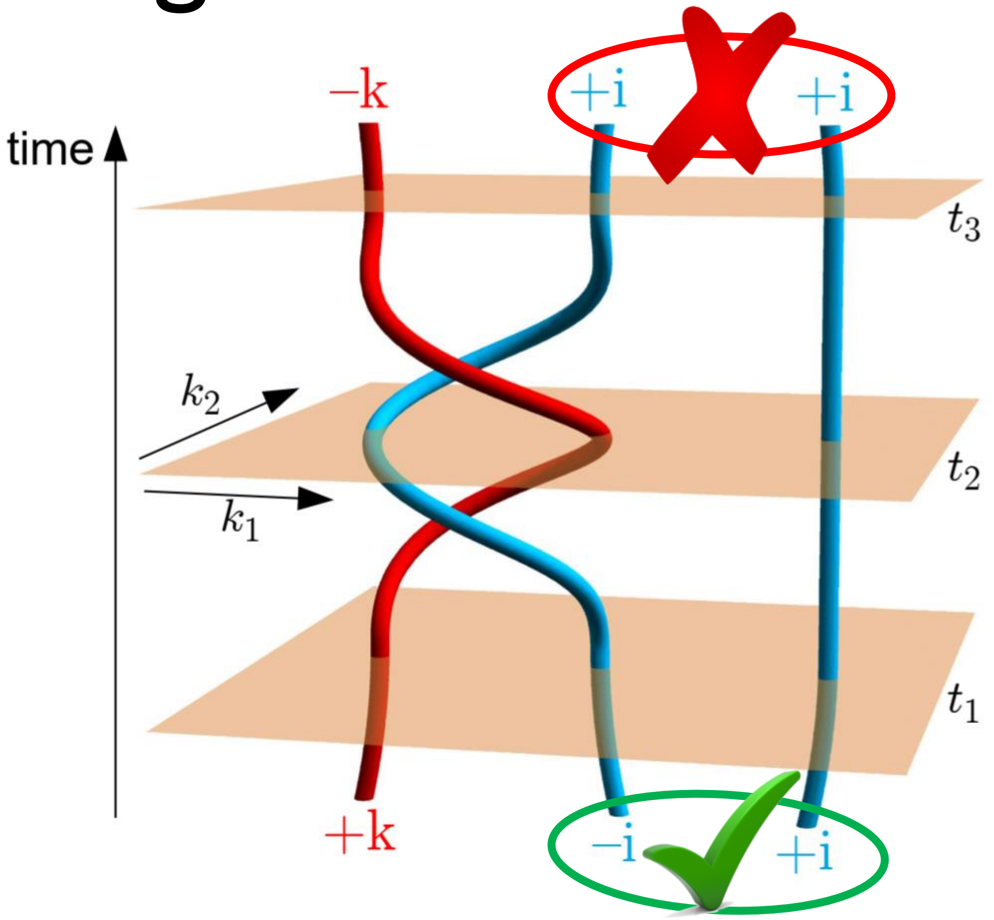


(k-space vs. time trajectories)

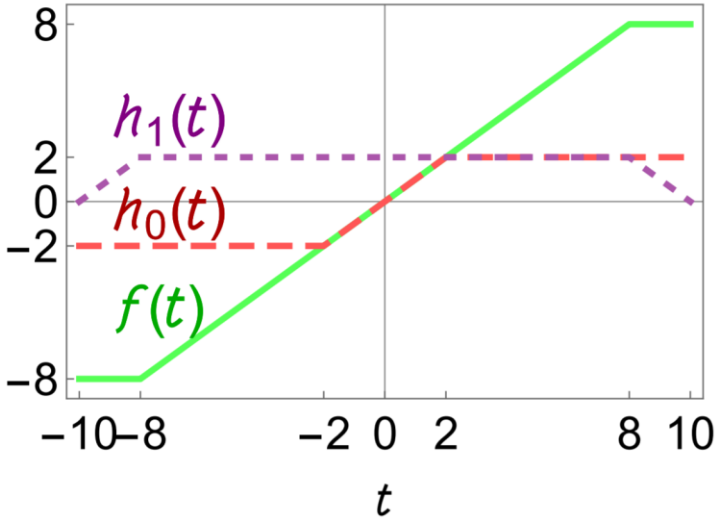
Q.S. Wu, A. A. Soluyanov, T. Bzdušek, Science **365**, 1273 (2019)

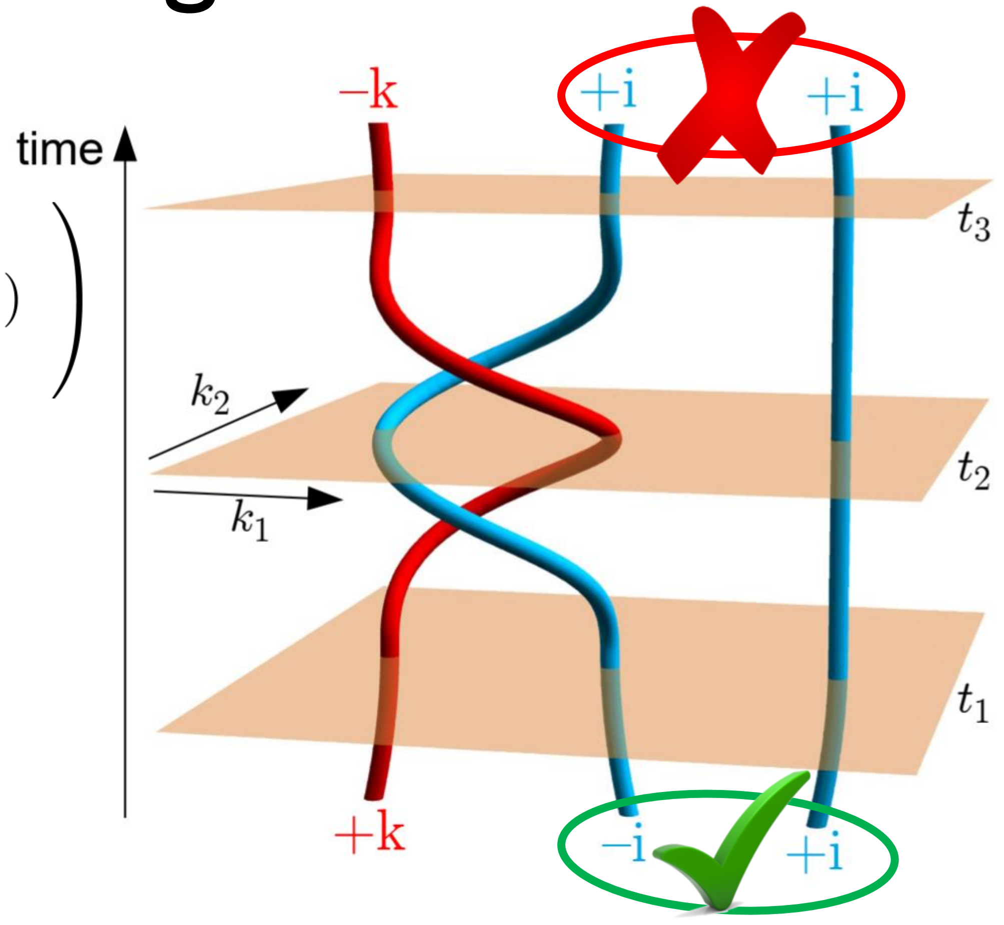
R.-J. Slager, A. Bouhon, and T. Bzdušek, arXiv:1907.10611 (2019)

Non-Abelian “reciprocal” braiding

$$\mathcal{H}(\boldsymbol{k};t) = \begin{pmatrix} f(t) & \alpha(\boldsymbol{k}) & \alpha^*(\boldsymbol{k}) \\ \alpha^*(\boldsymbol{k}) & 0 & h_0(t) + h_1(t)\beta(\boldsymbol{k}) \\ \alpha(\boldsymbol{k}) & h_0(t) + h_1(t)\beta^*(\boldsymbol{k}) & 0 \end{pmatrix}$$

$$\alpha(\boldsymbol{k}) = -\mathrm{i}\left(\mathrm{e}^{-\mathrm{i}k_1\pi} - \mathrm{e}^{-\mathrm{i}k_2\pi}\right) \qquad \beta(\boldsymbol{k}) = \mathrm{e}^{\mathrm{i}k_1\pi} + \mathrm{e}^{\mathrm{i}k_2\pi}$$





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R.-J. Slager, A. Bouhon, and T. Bzdušek, arXiv:1907.10611 (2019)

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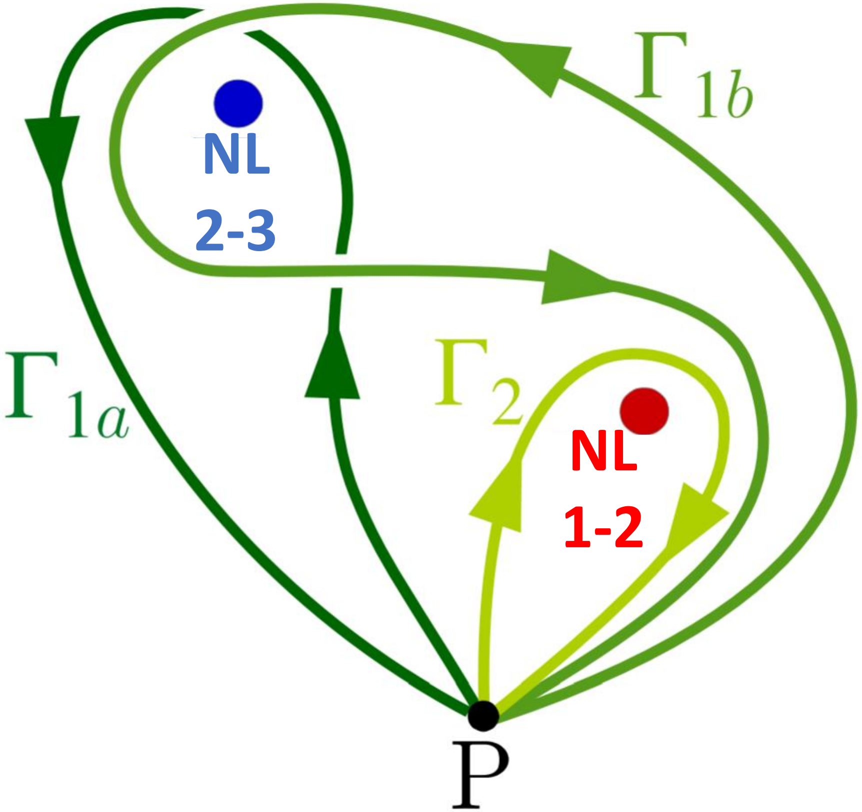
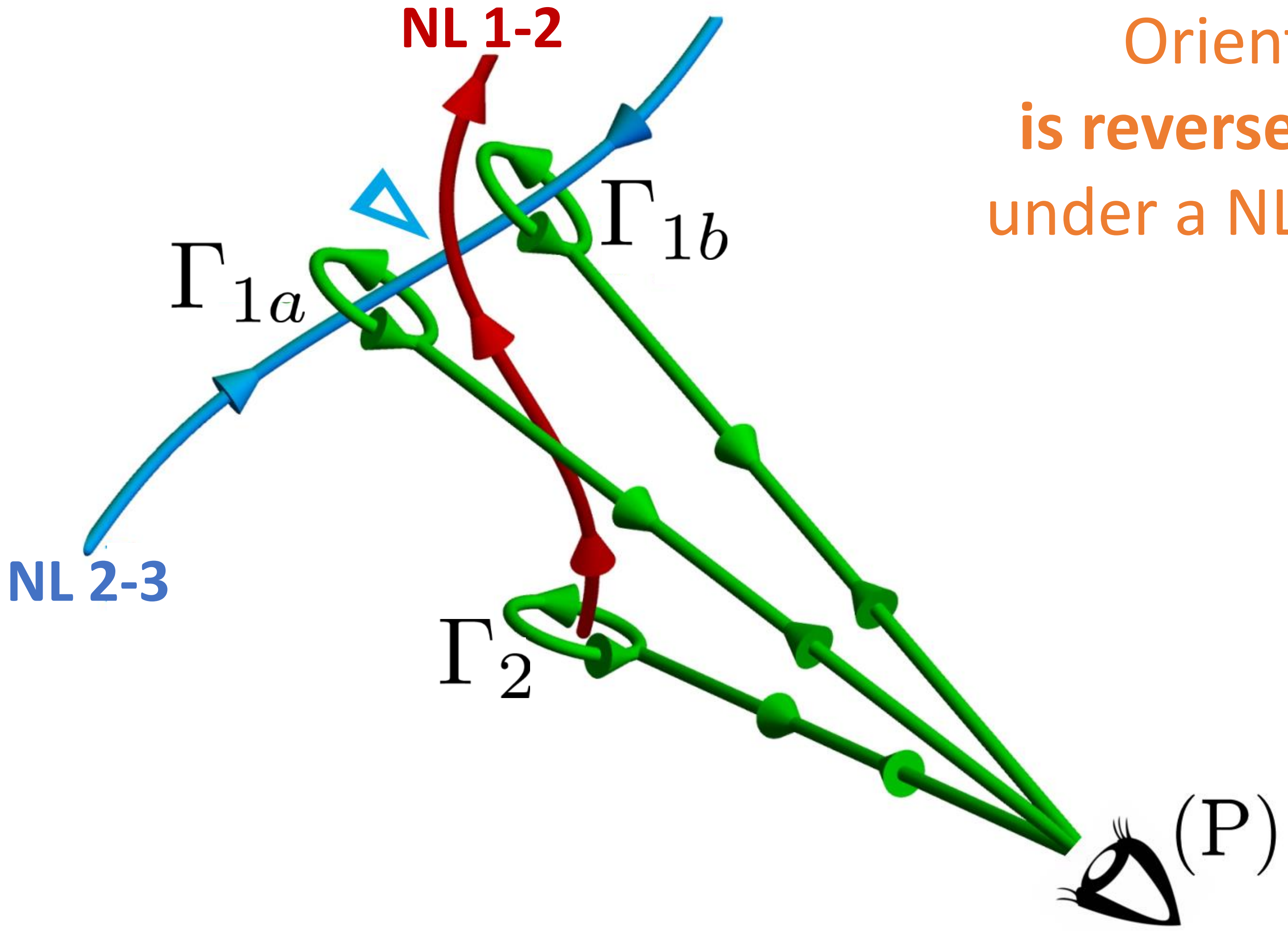


$$\Gamma_{1b} \sim \Gamma_2 \circ \Gamma_{1a} \circ \Gamma_2^{-1}$$

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

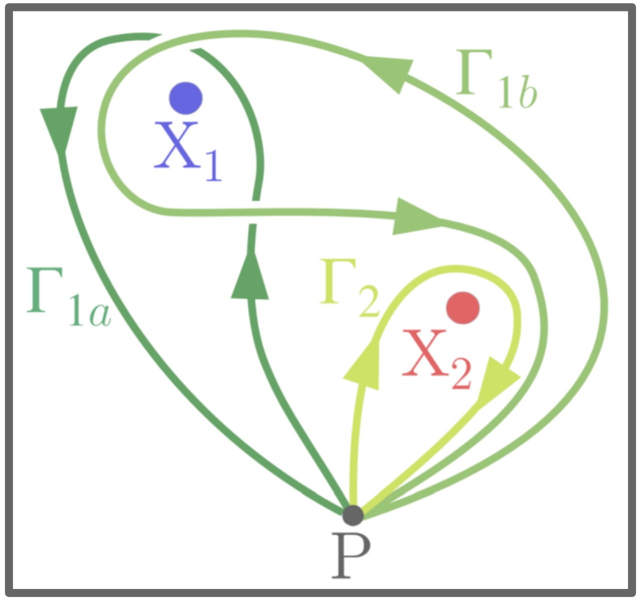
$$-\mathrm{i} = \mathrm{k} \cdot \mathrm{i} \cdot (-\mathrm{k})$$

Anticommuting charges = orientation reversals

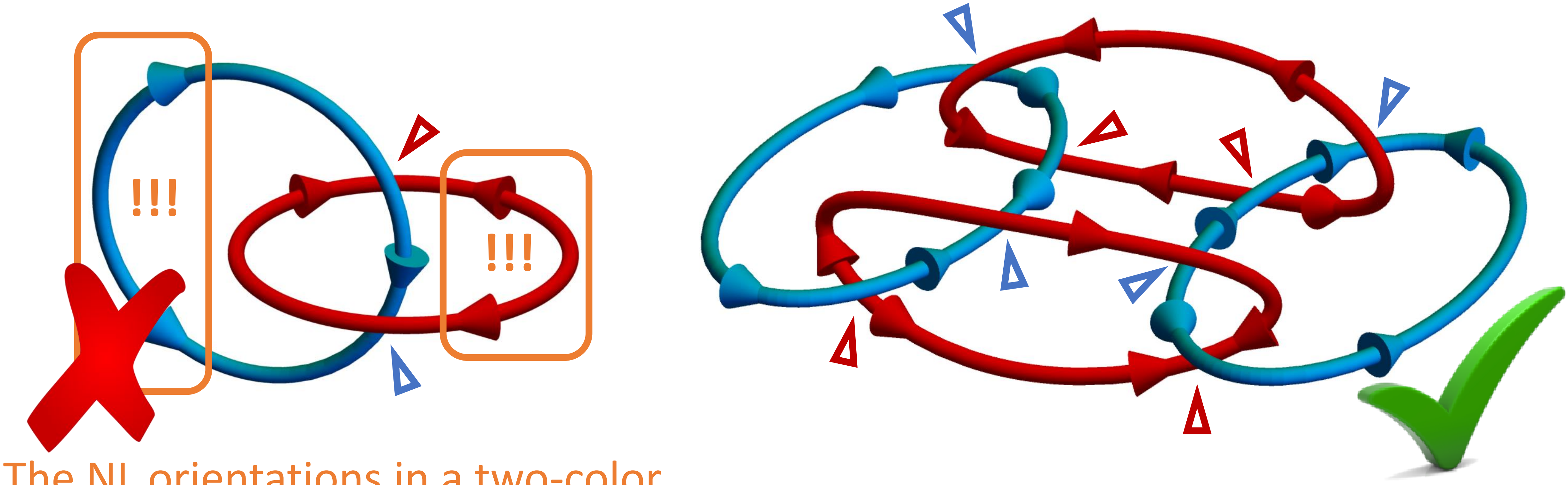


Orientation of a NL
is reversed when it passes
under a NL of the other color

Recall:



Constraints on “multi-gap” nodal-line compositions



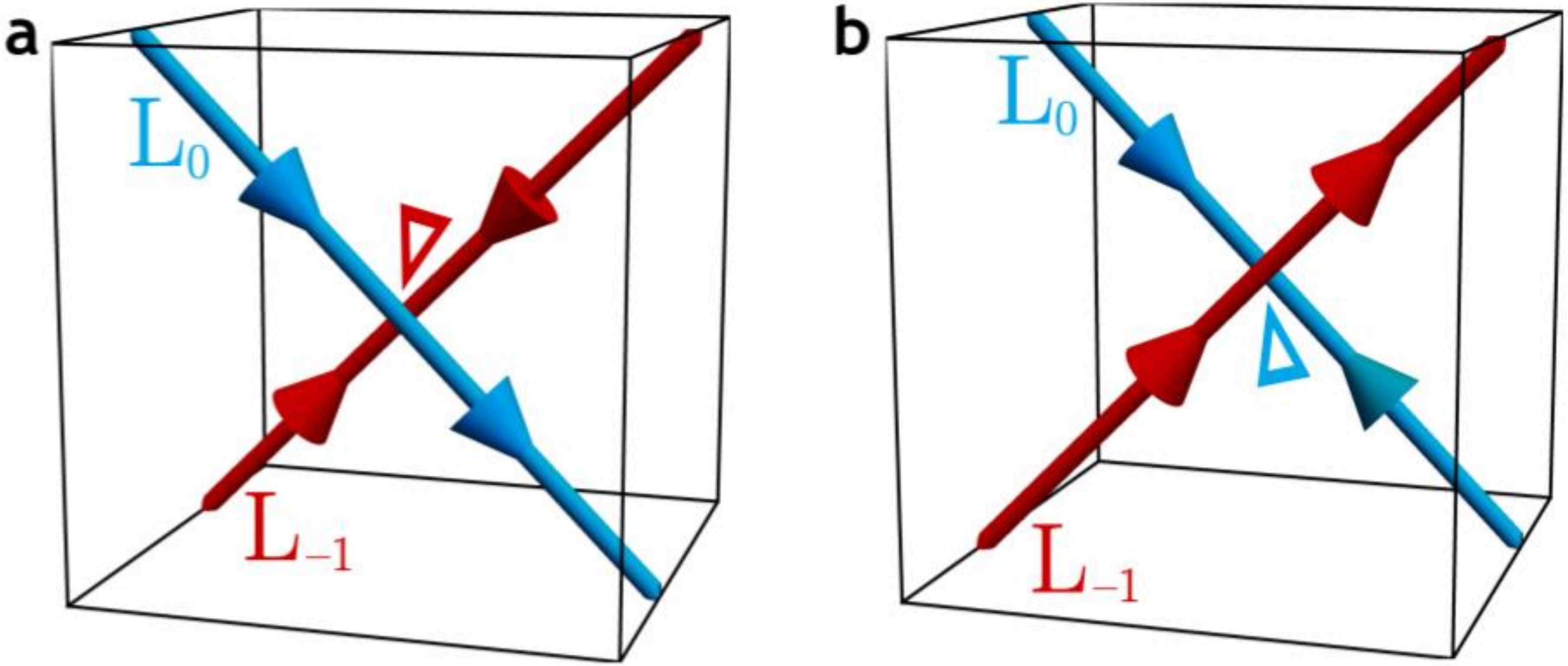
The NL orientations in a two-color Hopf link are **inconsistent**!

Red color = NL between bands 1–2 (at Fermi level)

Blue color = NL between bands 2–3 (“hidden”)

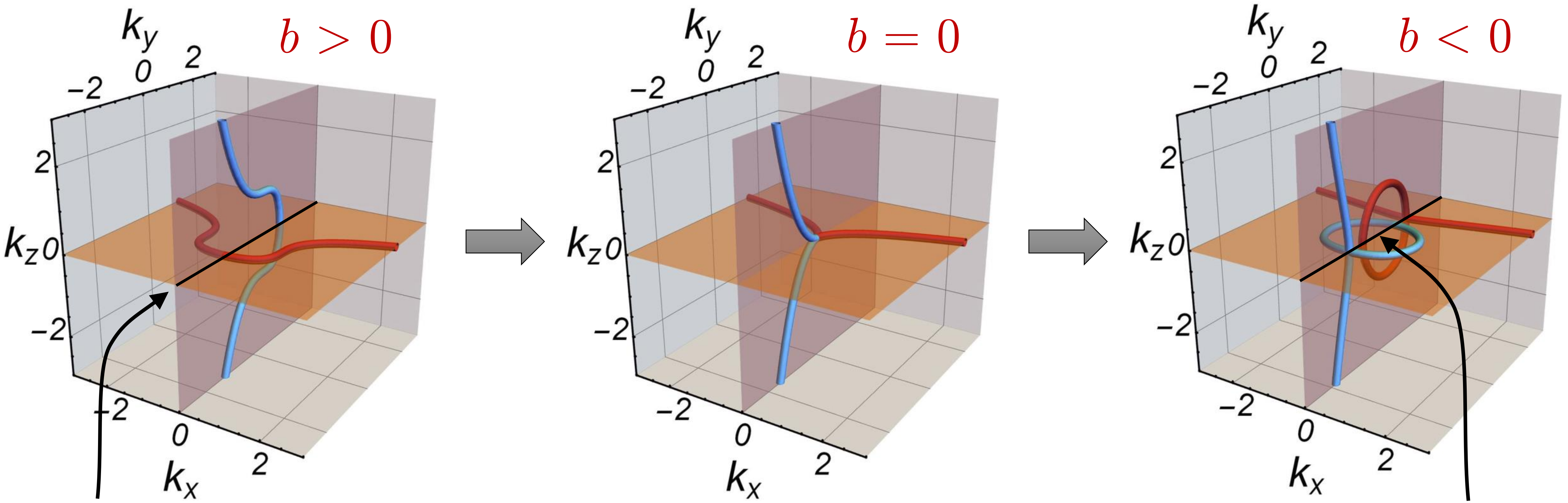
A. Tiwari and T. Bzdušek, arXiv:1903.0018 (2019)

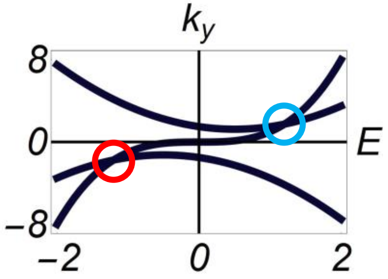
Anticommuting charges = orientation reversals



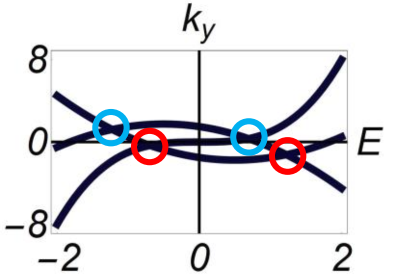
… therefore the “red” and “blue” nodal lines cannot move across one another.

Moving two nodal lines across one another





$$\mathcal{H}(\boldsymbol{k};b) = \begin{pmatrix} k_y^3 & 2k_x & 2k_y \\ 2k_x & -k_y + (b+k_y^2) & \frac{1}{4}k_xk_y \\ 2k_y & \frac{1}{4}k_xk_y & -k_y-(b+k_y^2) \end{pmatrix}$$



Non-commutative
“frame-rotation charge”
(arbitrarily many bands)

Generalizes Z_2 **Berry phase** + new 1D topological phases.

Explains the topological stability of **nodal chains**

Relates **monopole charge** (on S^2) to the linking structure

Governs **node conversions** between Weyl points and Nodal loops

Predicts **reciprocal braiding** (in k-space) of band nodes

Puts **constraints on** multi-gap **nodal line configurations**.

Relates **Euler class** and **second Stiefel-Whitney class**

Relation to Euler class

To predict whether two nodes in the same band gap annihilate (total charge +1) or not (total charge -1), **check whether the following integer is zero**:

$$\chi(\mathcal{D}) = \frac{1}{2\pi}\left[\int_{\mathcal{D}} \mathrm{Eu}(\boldsymbol{k})\,\mathrm{d}k_1\mathrm{d}k_2 - \oint_{\partial\mathcal{D}} \mathbf{a}(\boldsymbol{k})\cdot\mathrm{d}\boldsymbol{k}\right]$$

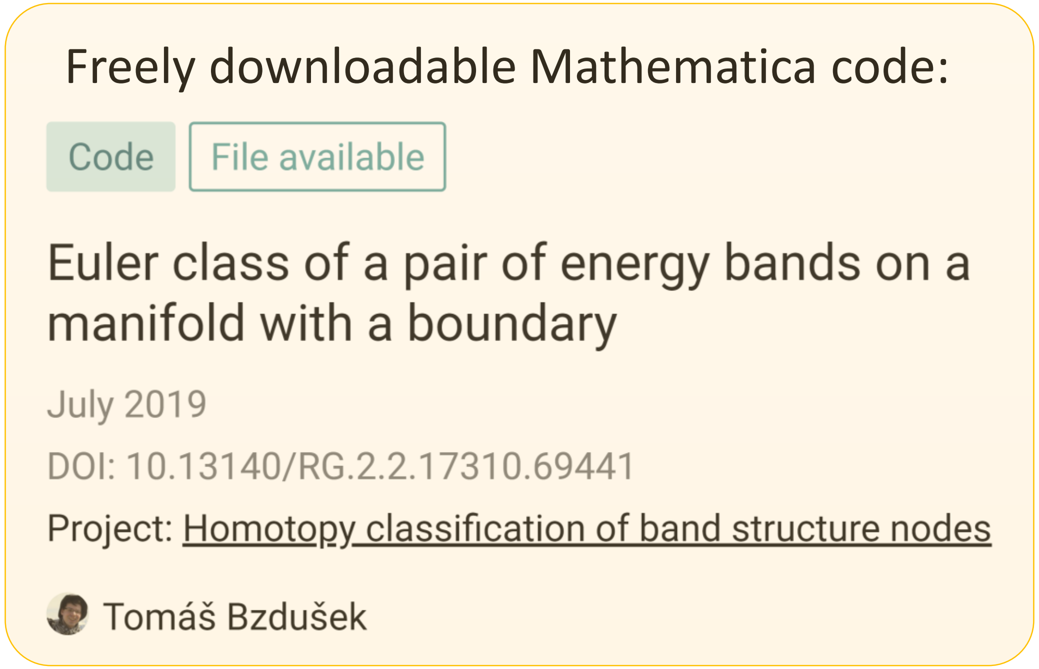
Euler (“Pfaffian”) curvature:

$$\mathrm{Eu}(\boldsymbol{k}) = \langle \boldsymbol{\nabla} u^1(\boldsymbol{k})| \times |\boldsymbol{\nabla} u^2(\boldsymbol{k})\rangle$$

Euler connection:

$$\mathbf{a}(\boldsymbol{k}) = \langle u^1(\boldsymbol{k})|\boldsymbol{\nabla} u^2(\boldsymbol{k})\rangle$$

Important to write the eigenstates in a real gauge that is continuous on the whole boundary!



Freely downloadable Mathematica code:

Euler class of a pair of energy bands on a manifold with a boundary

July 2019

DOI: 10.13140/RG.2.2.17310.69441

Project: Homotopy classification of band structure nodes

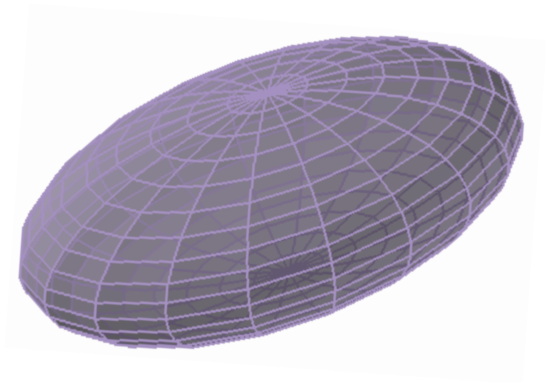
Tomáš Bzdušek

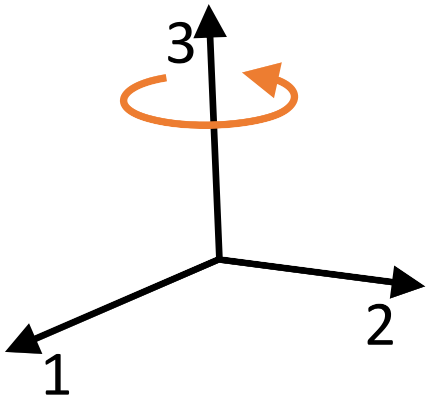
J. Ahn, S. Park, and B.-J. Yang, Phys. Rev. X **9**, 021013 (2019)

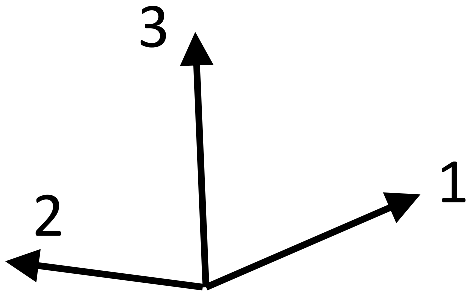
R.-J. Slager, A. Bouhon, and T. Bzdušek, arXiv:1907:10611

A few final remarks…

Mathematically equivalent to defects in biaxial nematics







$$\left.\begin{aligned} M = \mathsf{SO}(3)/\{1, C_{2x}, C_{2y}, C_{2z}\} = \mathsf{SU}(2)/\mathsf{Q} \\ \mathsf{Q} = \{\pm 1, \pm \mathrm{i}, \pm \mathrm{j}, \pm \mathrm{k}\} \end{aligned}\right\} \quad \pi_1(M) = \mathsf{Q}$$

M. Kléman, L. Michel, and G. Toulouse, J. Phys. Lett. 38, **195** (1977)

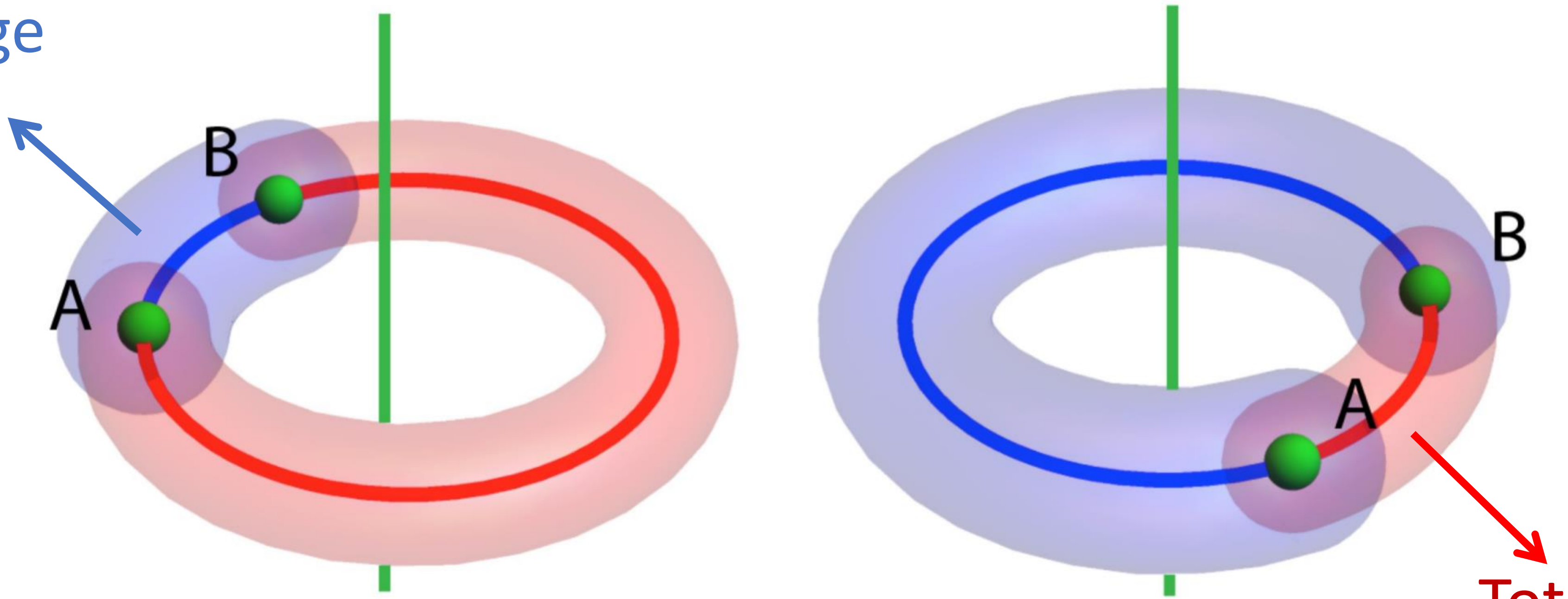
N. D. Mermin, Rev. Mod. Phys. **51**, 591 (1979)

Q.S. Wu, A. A. Soluyanov, T. Bzdušek, Science **365**, 1273 (2019)

Action of the first homotopy on higher ones

(Abe homotopy)

Total charge
1 + 1 = 2



Total charge
1 - 1 = 0

X.-Q. Sun, C. C. Wojcik, S. Fan, T. Bzdušek, arXiv:1905.04338 (2019)

G. E. Volovik and V. P. Mineev, Zh. Eksp. Teor. Fiz. **72**, 2256 (1977)

A. Tiwari and T. Bzdušek, arXiv:1903.0018 (2019) →→→ Non-trivial action of Berry phase on the monopole charge

Open questions about the non-Abelian topology

Signatures in surface states?

Signatures in transport?

Effects of interactions?

Generalized topological order in 1D?

Material examples?

Thank you for your attention!

Science

Cite as: Q. Wu *et al.*, *Science*
10.1126/science.aau8740 (2019).

Non-Abelian band topology in noninteracting metals

QuanSheng Wu[1,2], Alexey A. Soluyanov[3,4], Tomáš Bzdušek[5,6]*

Apoorv Tiwari and T. Bzdušek,
Non-Abelian topology of nodal-line rings in $\mathcal{PT}$-symmetric systems
arXiv:1903.00018 (Feb 2019)

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Non-Abelian Reciprocal Braiding of Weyl Nodes
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Tomáš Bzdušek, 30 September 2019, Mainz

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