NORDITA

UNIVERSITY OF CAMBRIDGE

Non-Abelian and Euler multi-gap topologies in crystalline materials

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May 2023, Abu Dhabi

Swedish Research Council

Horizon 2020 Programme

Quantum modeling of materials

Tight-binding model (sec. quant.):

$$\widehat{\mathcal{H}} = \sum_{ij,\alpha\beta} |w_\alpha, i\rangle t_{\alpha\beta}(\boldsymbol{R}_j - \boldsymbol{R}_i)\langle w_\beta, j|$$

translational symmetry

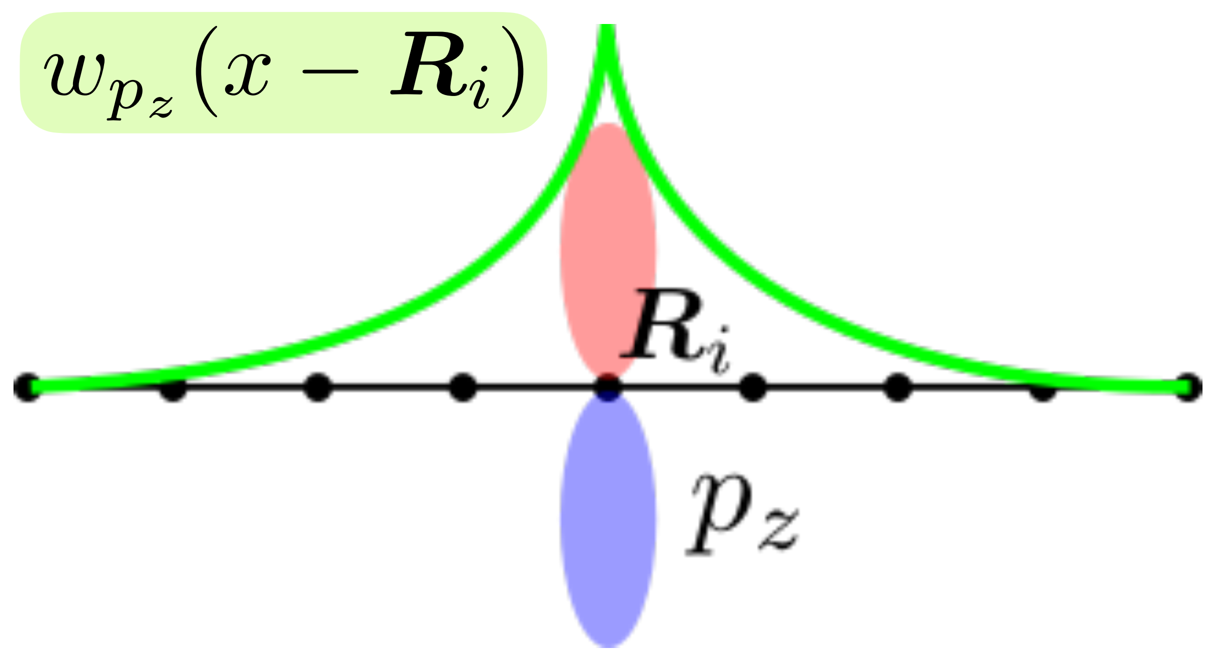
$$H_{\alpha\beta}(\boldsymbol{k}) = \sum_{\boldsymbol{R}_j} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_j}\ t_{\alpha\beta}(\boldsymbol{R}_j - \boldsymbol{0})$$

Bloch picture:

$$\widehat{\mathcal{H}} = \sum_{\boldsymbol{k}\in\mathrm{BZ},\alpha\beta} |\phi_\alpha, \boldsymbol{k}\rangle H_{\alpha\beta}(\boldsymbol{k})\langle\phi_\beta, \boldsymbol{k}|$$

$$|\phi_\alpha, \boldsymbol{k}\rangle = \frac{1}{\sqrt{N_\alpha}}\sum_{\boldsymbol{R}_i} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_i}|w_\alpha, i\rangle$$

Wannier functions



N degrees of freedom per unit cell:
Wyckoff positions, sub-lattice sites, electronic orbitals, spins

$$H(\boldsymbol{k}) \in \mathbb{C}^N \times \mathbb{C}^N$$

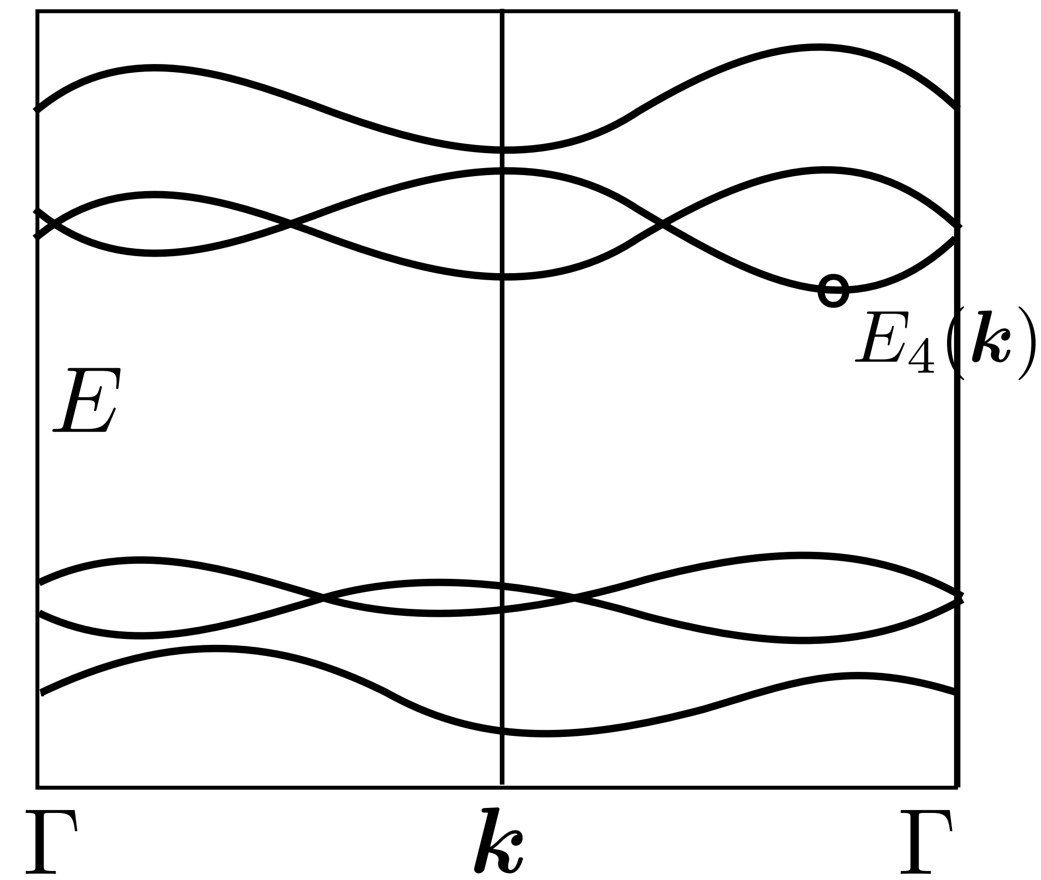
Grassmannian modeling of gapped band structures

Bloch Hamiltonian:

$$H(\boldsymbol{k}) = U(\boldsymbol{k})\mathcal{E}(\boldsymbol{k})U^\dagger(\boldsymbol{k})$$

$$\mathcal{E}(\boldsymbol{k}) = \mathrm{diag}[E_1(\boldsymbol{k}), \ldots, E_N(\boldsymbol{k})]$$

$$U(\boldsymbol{k}) \in \mathsf{U}(N)$$



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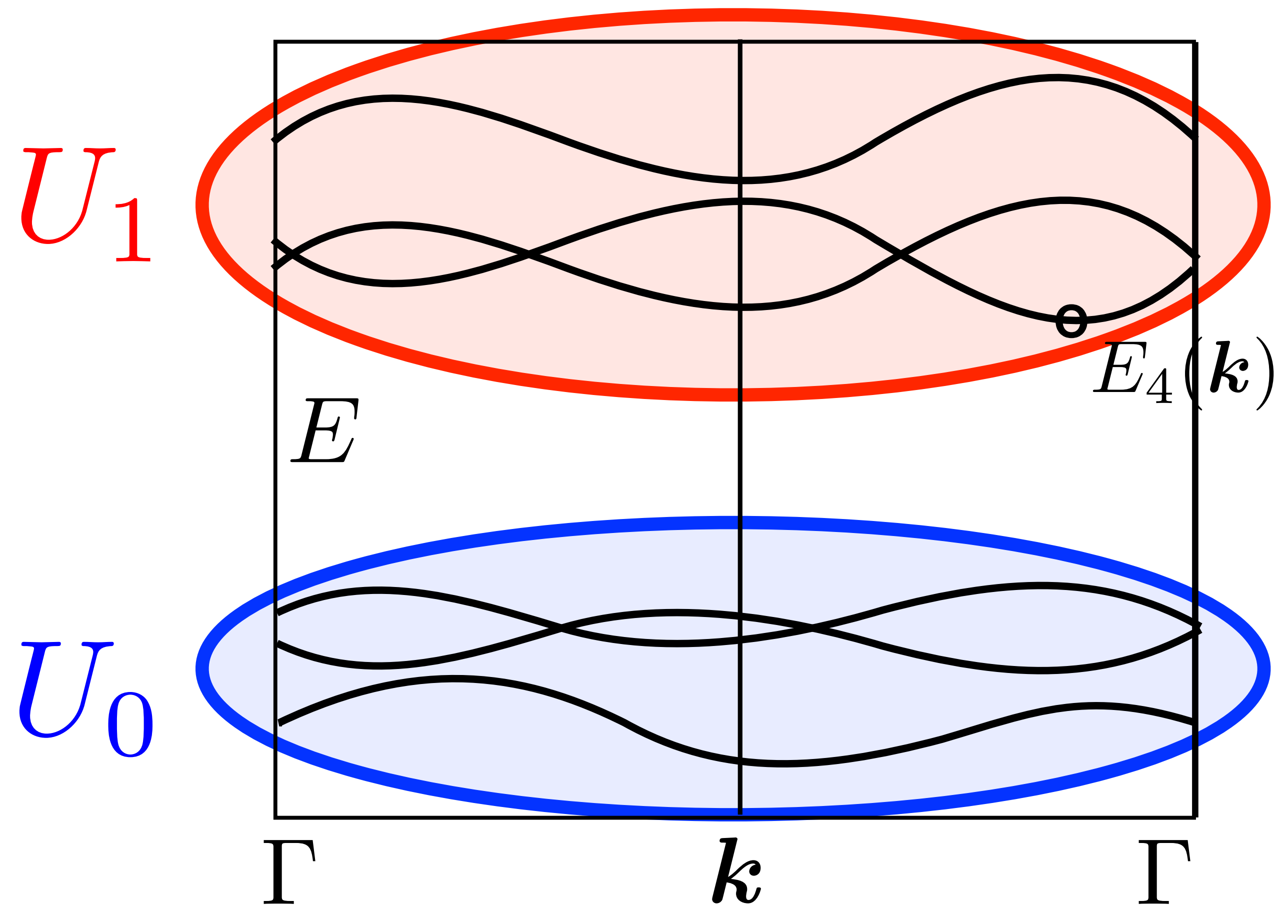

flattened Hamiltonian:

$$Q(\boldsymbol{k}) = (U_0(\boldsymbol{k})\ U_1(\boldsymbol{k})) \begin{bmatrix} -\mathbf{1} & 0 \\ 0 & \mathbf{1} \end{bmatrix} (U_0(\boldsymbol{k})\ U_1(\boldsymbol{k}))^\dagger$$

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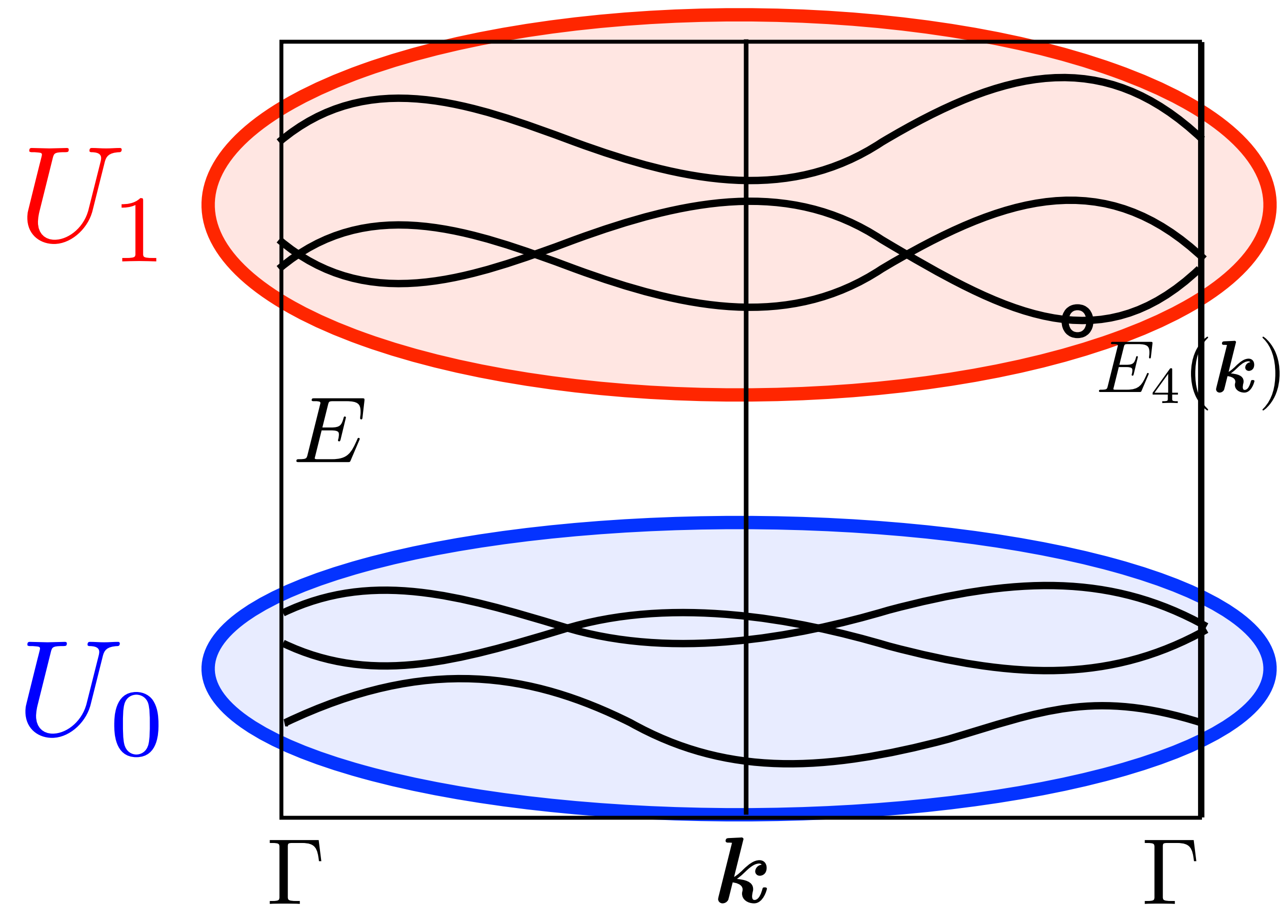

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gauge invariance of the flattened Hamiltonian:

$$(U_0(\boldsymbol{k})\ U_1(\boldsymbol{k})) \longrightarrow (U_0(\boldsymbol{k})\ U_1(\boldsymbol{k})) \cdot \begin{pmatrix} G_o(\boldsymbol{k}) & 0 \\ 0 & G_u(\boldsymbol{k}) \end{pmatrix}$$

$$\mathbb{T}^2 \to \mathrm{Gr}_{N_o}(\mathbb{C}^N) \cong U(N)/[U(N_o) \times U(N_u)]$$

Classifying space (gauge structure)

C_2T symmetry and reality condition

$$C_2(k_1, k_2, k_3) = (-k_1, -k_2, k_3)$$

$$C_2 I = \sigma_h(k_1, k_2, k_3) = (k_1, k_2, -k_3)$$

C_2T symmetry (spinful or spinless), spinless ***PT*** symmetry

$$\mathcal{A} = U\mathcal{K}$$

$$\mathcal{A}^2 = +\mathbf{1} \quad \longrightarrow$$ no Kramers degeneracies:

$$\mathcal{A} = D\mathcal{K}$$

$$D = \mathrm{diag}\{\mathrm{e}^{\mathrm{i}\varphi_j}\}_{j=1}^{N}$$

we rotate the orbitals basis by $W = \sqrt{D^*}$ and get $W\mathcal{A}W^\dagger = \mathcal{K}$

within the *C_2T* plane:

$$\sigma_h \boldsymbol{k} = \boldsymbol{k}$$

$$\mathbf{1} \cdot \widetilde{H}^*(\boldsymbol{k}) \cdot \mathbf{1} = \widetilde{H}(\boldsymbol{k})$$ **real and symmetric**

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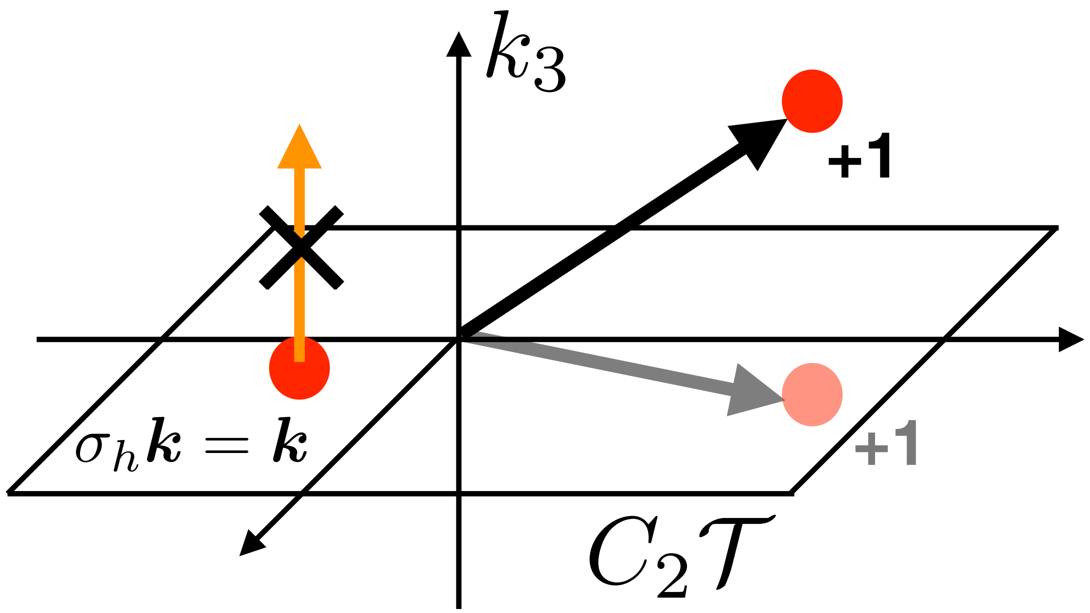

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"Real" topologies

$$\mathsf{Gr}^{\mathbb{R}}_{p,N} = \frac{\mathsf{O}(N)}{\mathsf{O}(p) \times \mathsf{O}(N-p)} = \frac{\mathsf{SO}(N)}{\mathsf{S}[\mathsf{O}(p) \times \mathsf{O}(N-p)]}$$

“Real” topologies

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$$\pi_1(\mathsf{Gr}^{\mathbb{R}}_{p,N})\Big|_{N\geq 3} = \mathbb{Z}_2$$

$$\pi_2(\mathsf{Gr}^{\mathbb{R}}_{2,N})\Big|_{N\neq 4} = \mathbb{Z} \qquad \pi_4(\mathsf{Gr}^{\mathbb{R}}_{4,N})\Big|_{N\neq 7,8} = \mathbb{Z}$$

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1D	spinful or spinless ***mT*** symmetry, ***C_2T, PT***	Graphene, SSH insulators
2D	spinful or spinless ***C_2T*** symmetry, ***PT***	Euler insulators
3D	spinless ***PT*** symmetry	Linked nodal rings
4D	spinless ***PT*** symmetry	Second Euler insulators

1.5D topology:
Non-Abelian braiding of Weyl nodes

1.5D topology of three-level system

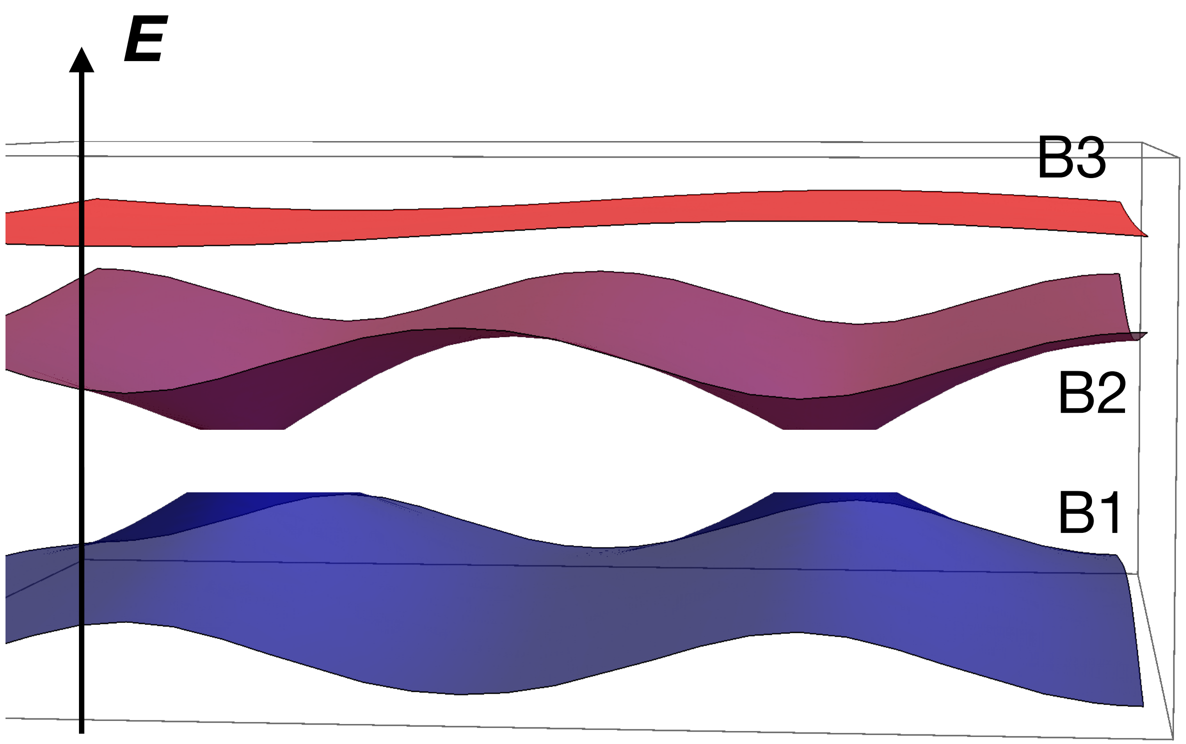
$$\widetilde{H}(\boldsymbol{k}) = R(\boldsymbol{k})\mathcal{E}(\boldsymbol{k})R^T(\boldsymbol{k})$$

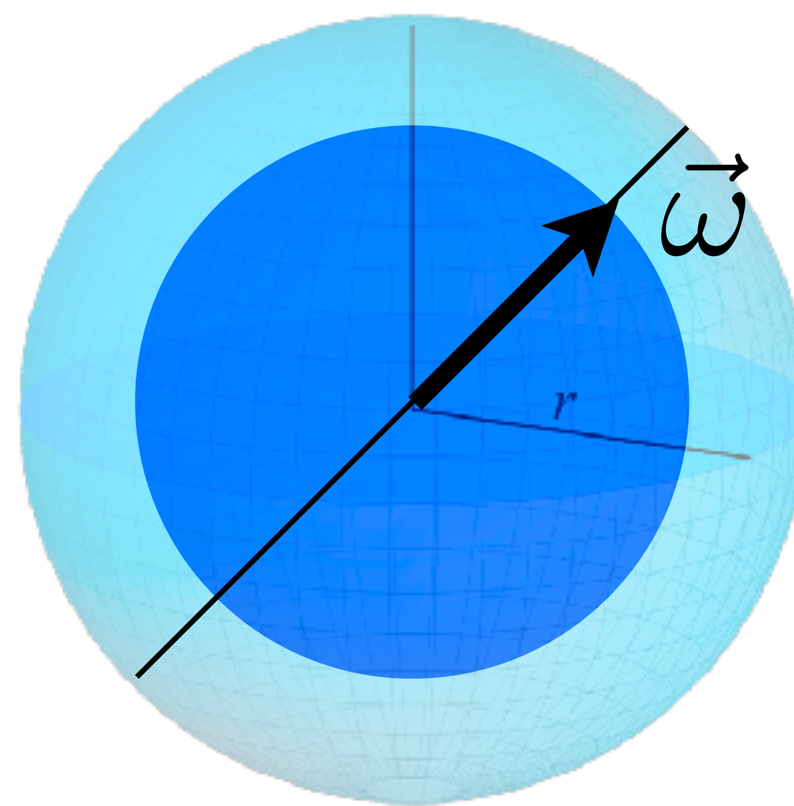
$$R(\boldsymbol{k}) = (\boldsymbol{e}_1 \ \boldsymbol{e}_2 \ \boldsymbol{e}_3)$$

$$\mathcal{E}(\boldsymbol{k}) = \begin{pmatrix} E_1(\boldsymbol{k}) & 0 & 0 \\ 0 & E_2(\boldsymbol{k}) & 0 \\ 0 & 0 & E_3(\boldsymbol{k}) \end{pmatrix}$$

Lie algebra representation:

$$R(\boldsymbol{k}) = e^{\vec{\omega}\cdot\vec{L}} \in \mathrm{SO}(3)$$





$$\vec{\omega} = \theta\hat{\omega}$$

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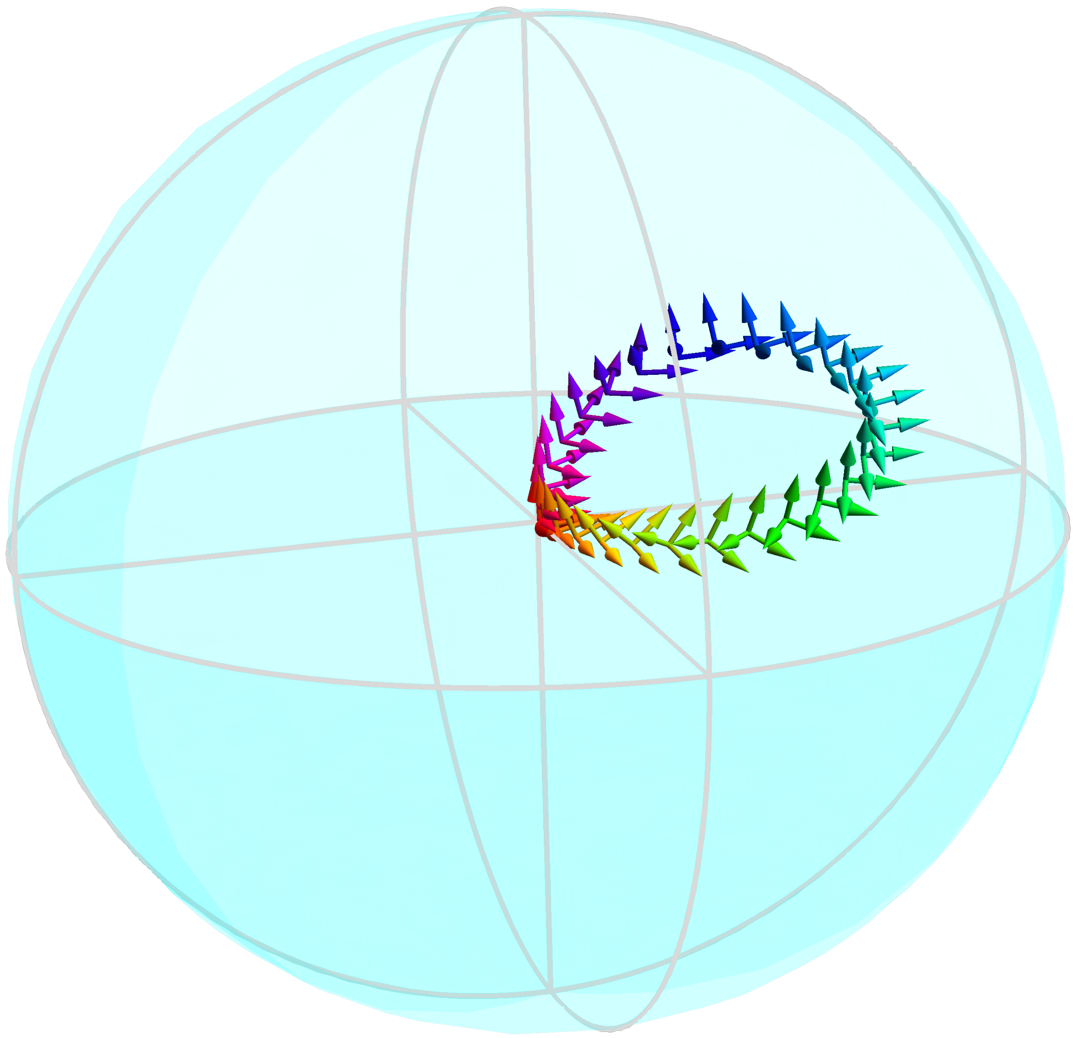
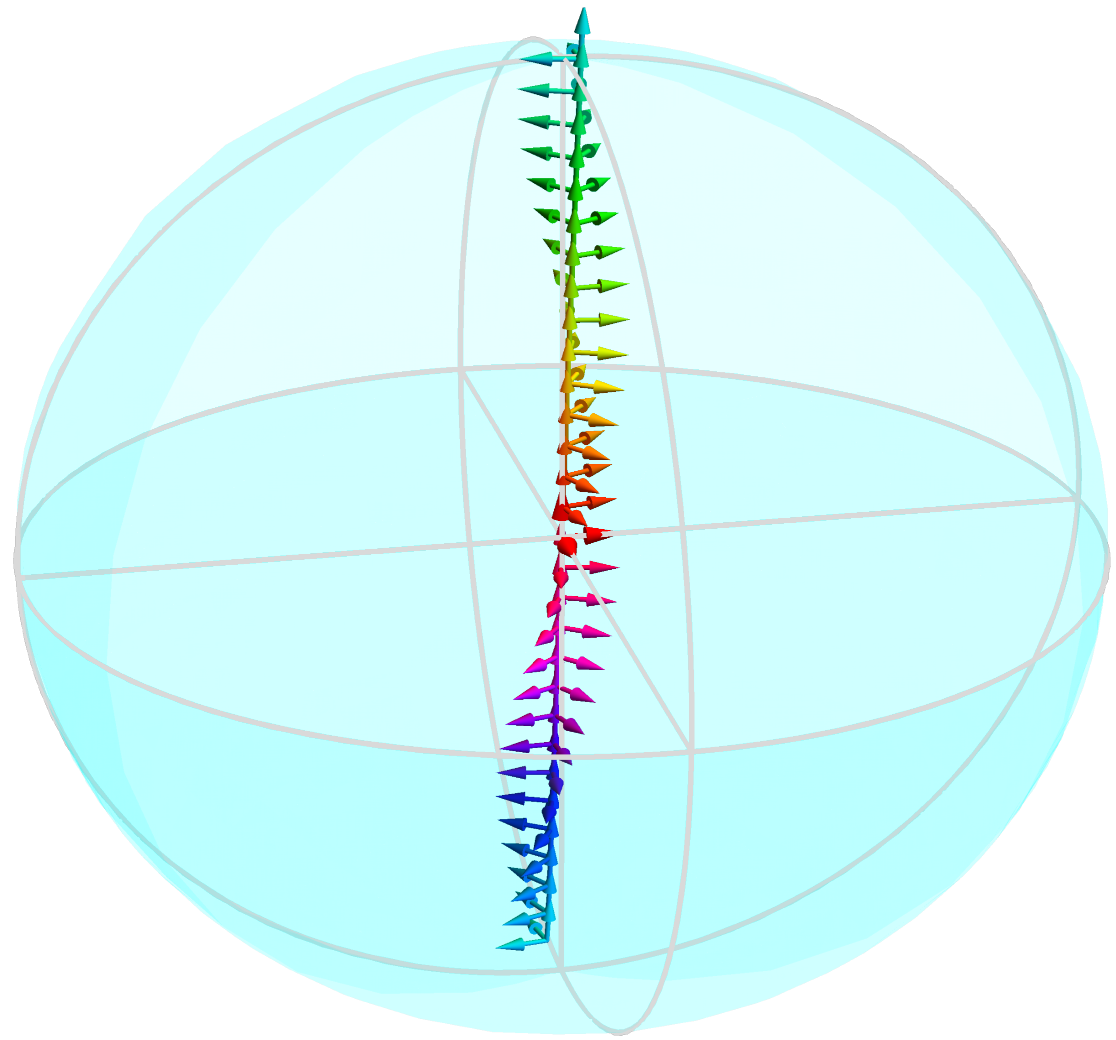
Topology over a loop in the BZ:

$$\pi_1\left(\mathsf{SO}(3)\right) = \mathbb{Z}_2$$

accumulated {0, 2π}-frame rotation,





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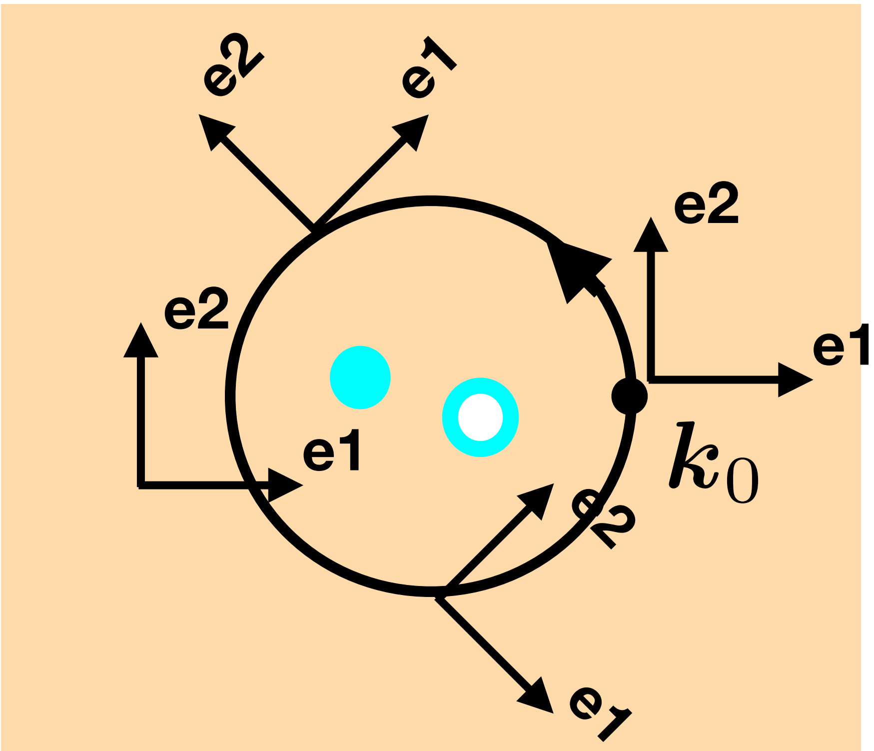
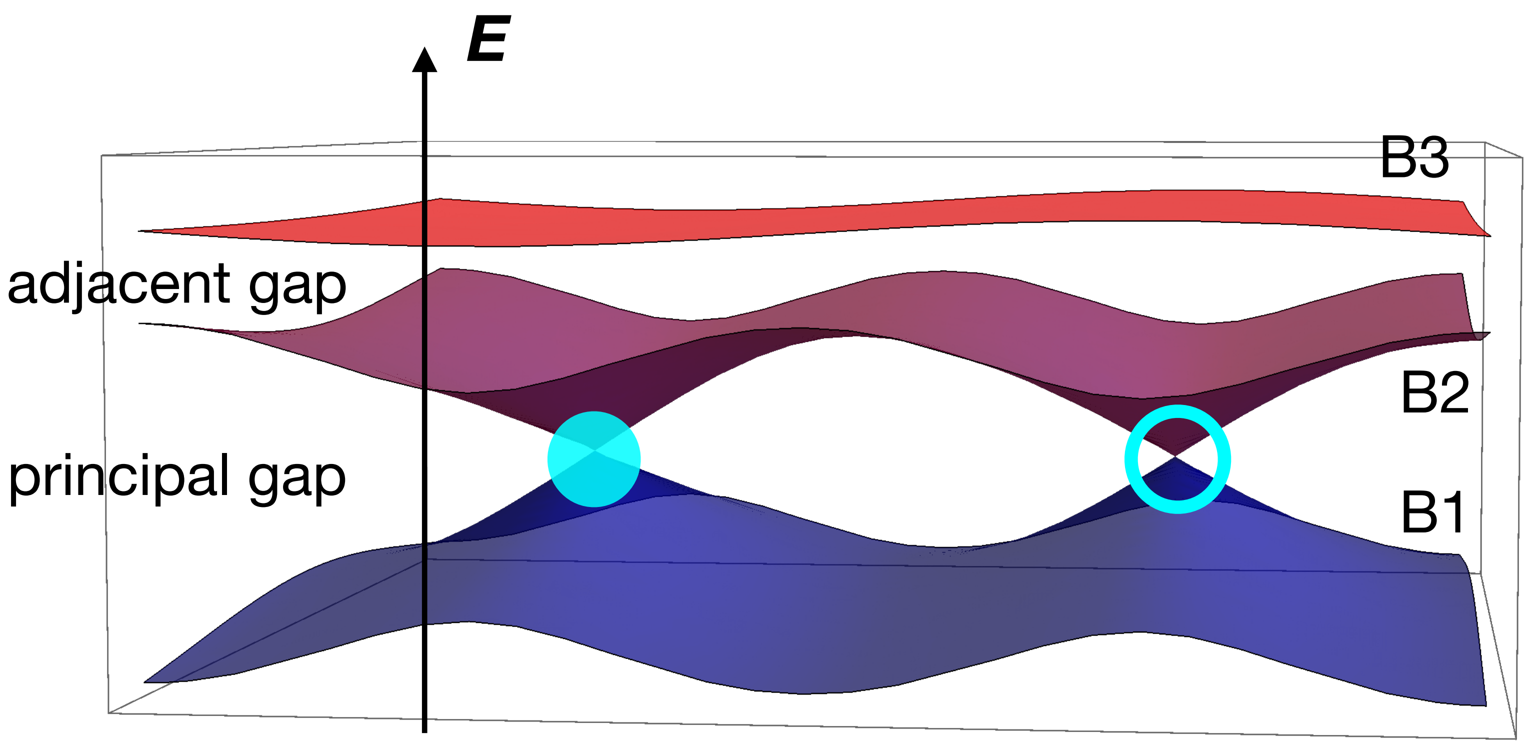
accumulated {0, 2π}-frame rotation,
stability of Nodal-Points pair

Nodal-Point charge has two signs!

0-frame rotation around e_3





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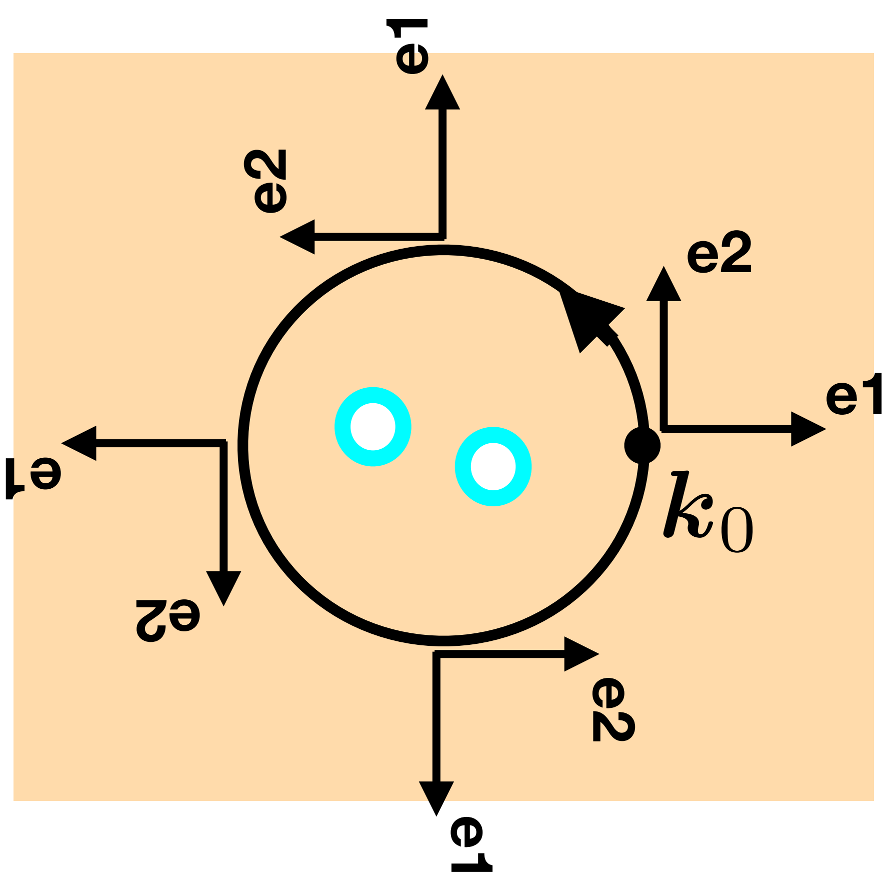
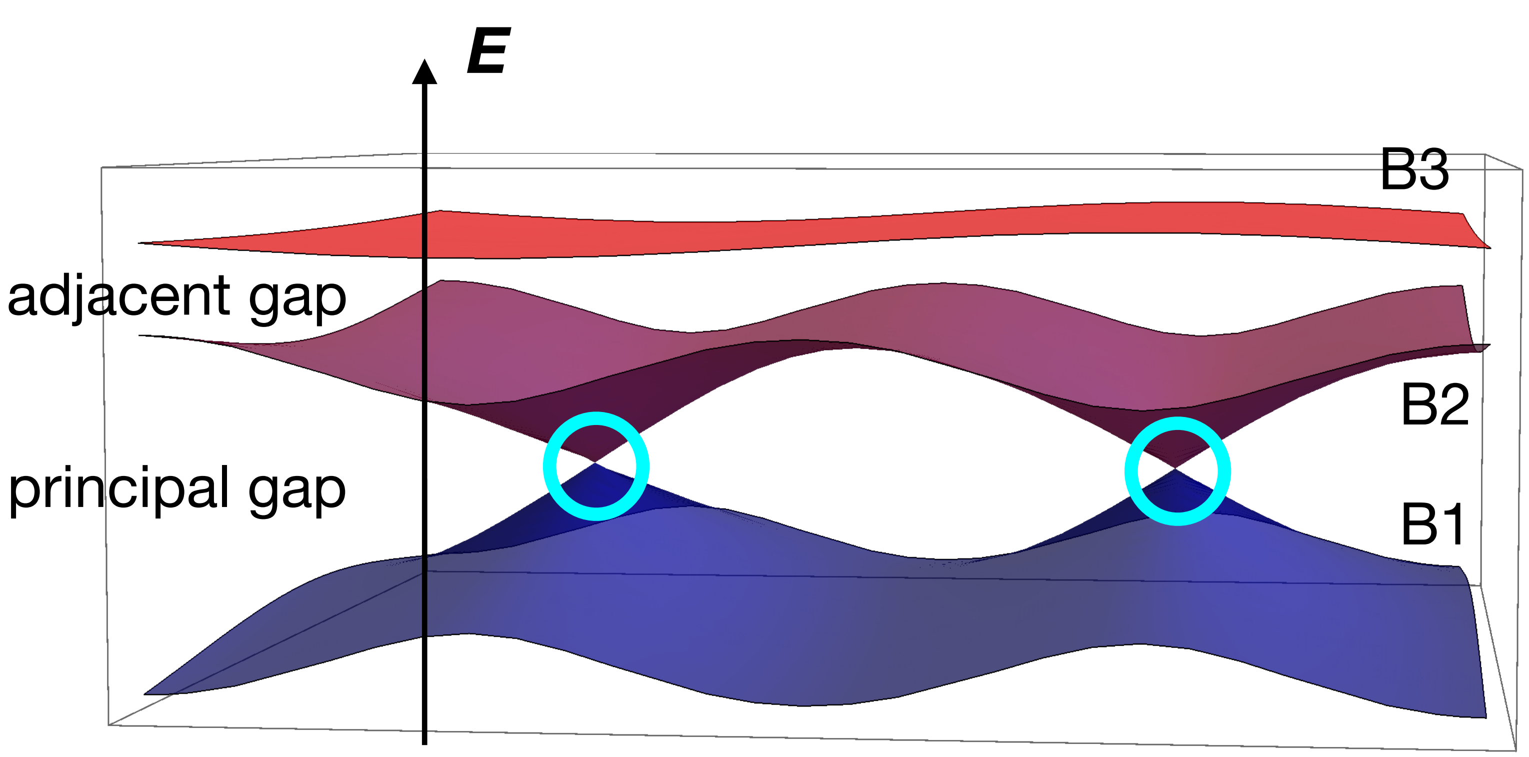
2π-frame rotation around e3





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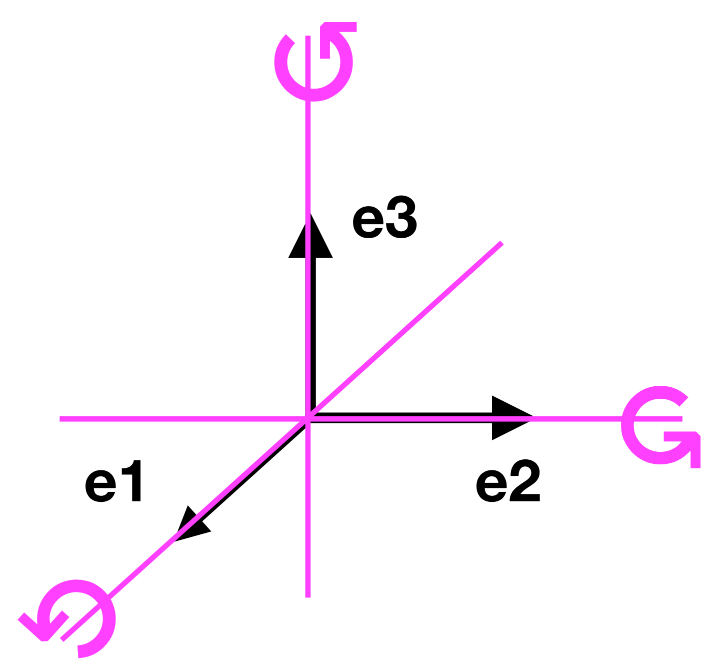
$$\widetilde{H}(\boldsymbol{k}) = R(\boldsymbol{k})\mathcal{E}(\boldsymbol{k})R^T(\boldsymbol{k}) \qquad R(\boldsymbol{k}) = (\boldsymbol{e}_1\ \boldsymbol{e}_2\ \boldsymbol{e}_3) \sim (\pm\boldsymbol{e}_1\ \pm\boldsymbol{e}_2\ \pm\boldsymbol{e}_3)$$

Group of gauge freedom: $\mathsf{O}(1)^3 = \mathsf{C}_i \times \mathsf{D}_2$

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

D_2 : **dihedral point group,**

π-frame rotation around e1, e2, e3



Bdzusek *et al*, Science (2019)

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Flag manifold

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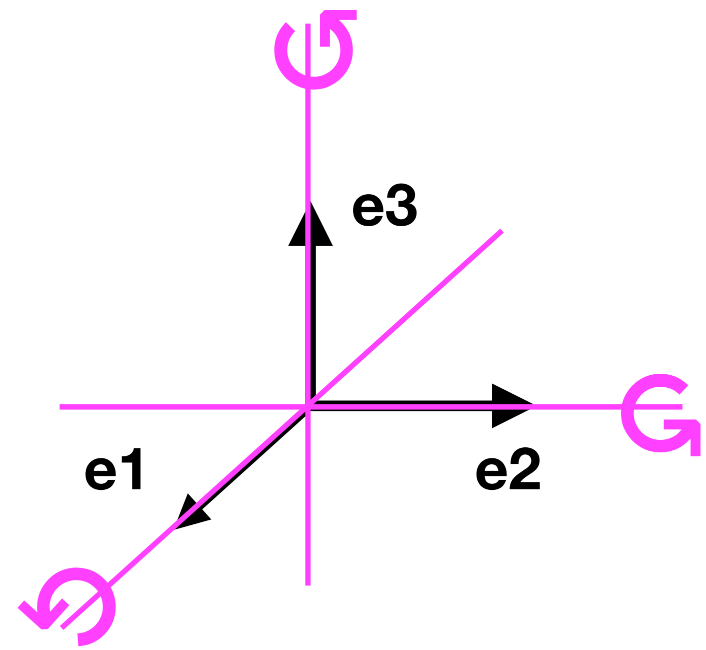

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Lie algebra representation

accumulated rotation of parallel transp. frame

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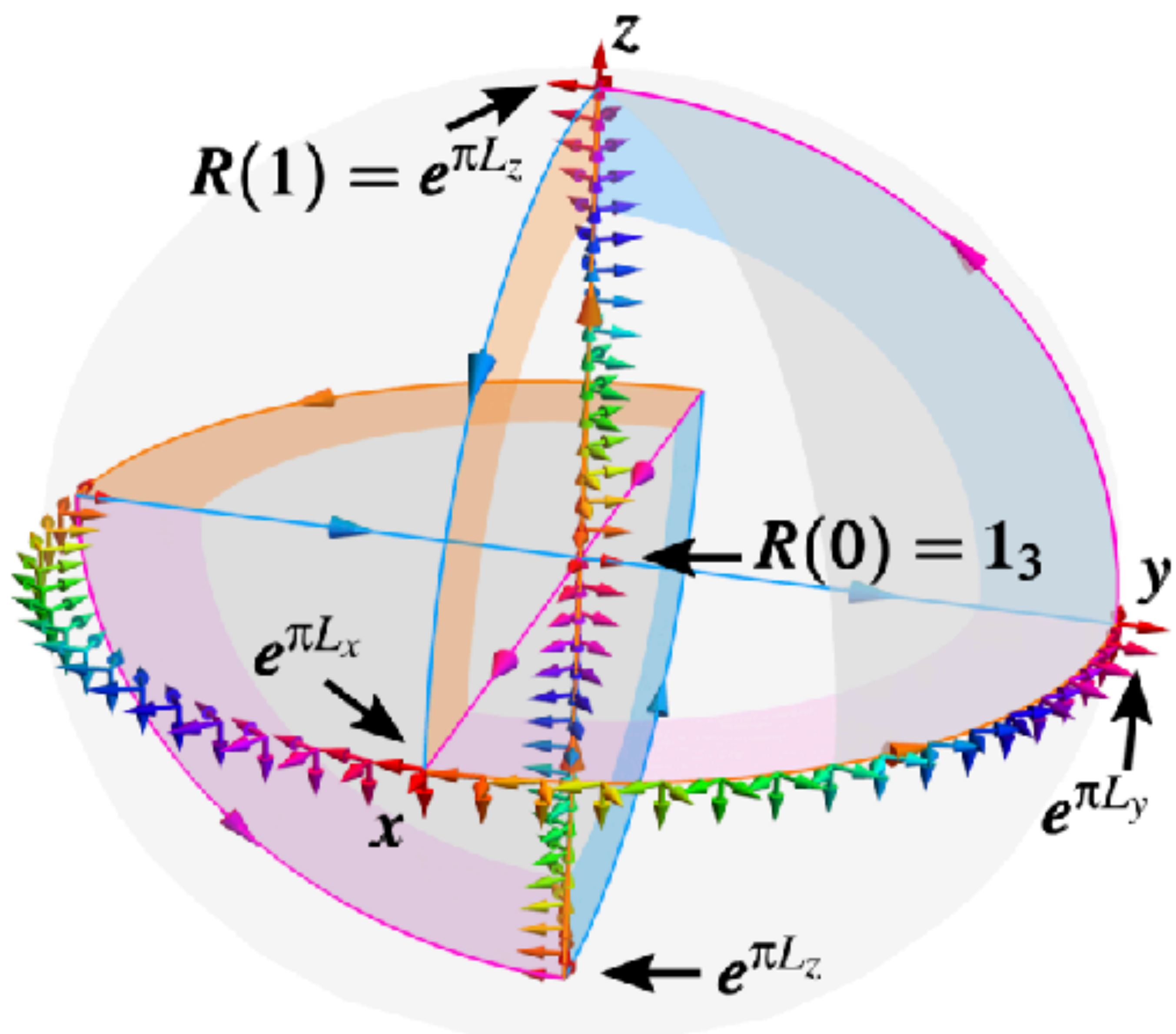
$$\pi_1\left(\mathsf{SO}(3)/\mathsf{D}_2\right) = \mathbb{Q} = \overline{\mathsf{D}}_2$$

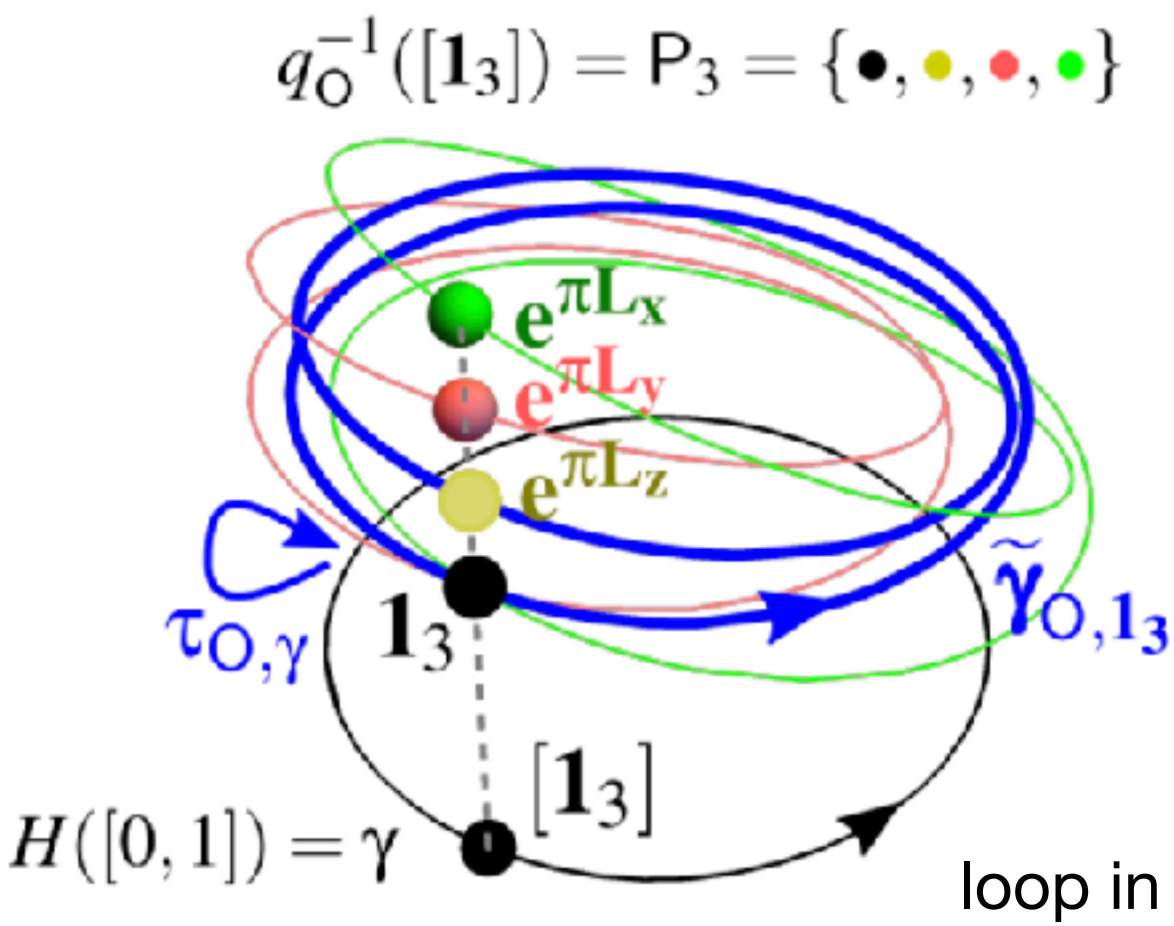
$$\mathbb{Q} = \{1, \pm i, \pm j, \pm k, -1\}$$



Ambiguity of the parallel transported SO(3)-frame

principal fiver bundle
with discrete structure group $\mathsf{D}_2 \hookrightarrow \mathsf{SO}(3) \to \mathsf{SO}(3)/\mathsf{D}_2$

SO(3)-monodromy representation of $\pi_1\left(\mathsf{SO}(3)/\mathsf{D}_2\right)$



loop in the flag

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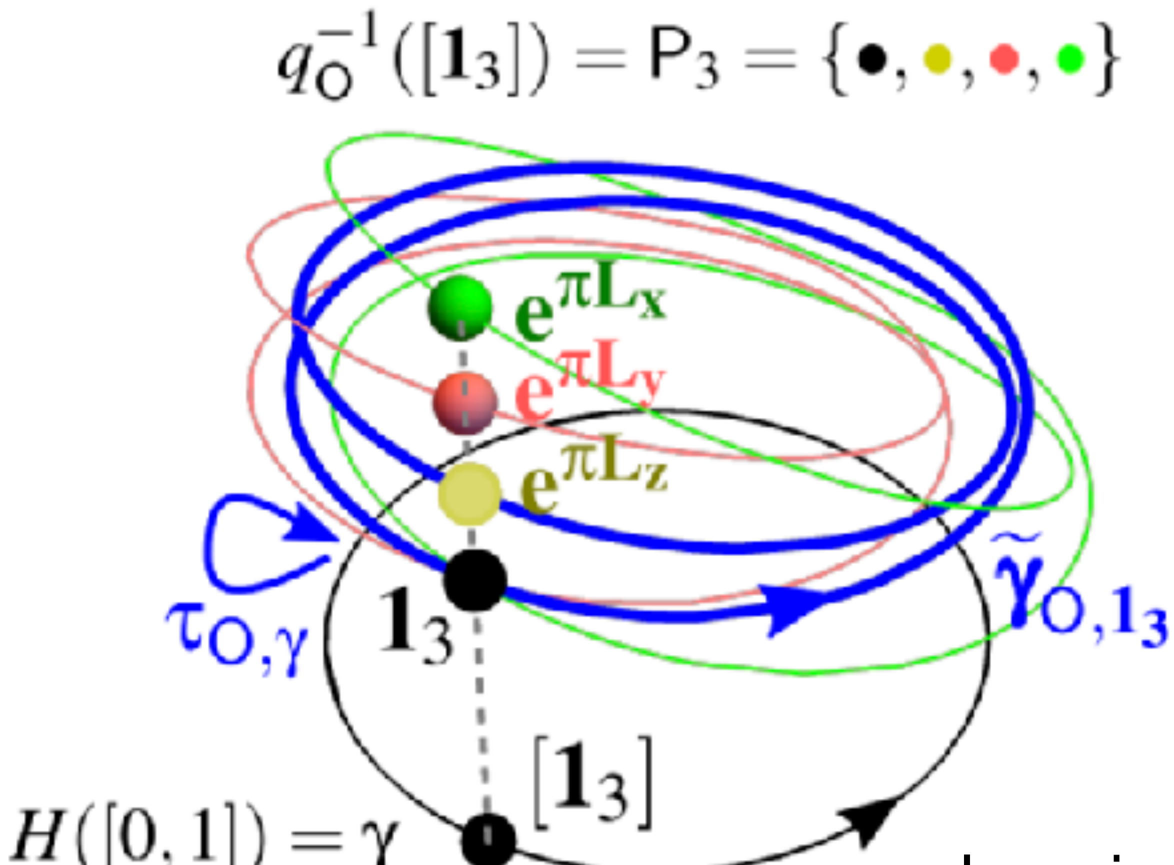


loop in the flag

It does not distinguishes a

π-rotation

from a

($-\pi$)-rotation around $\mathbf{e}_3$

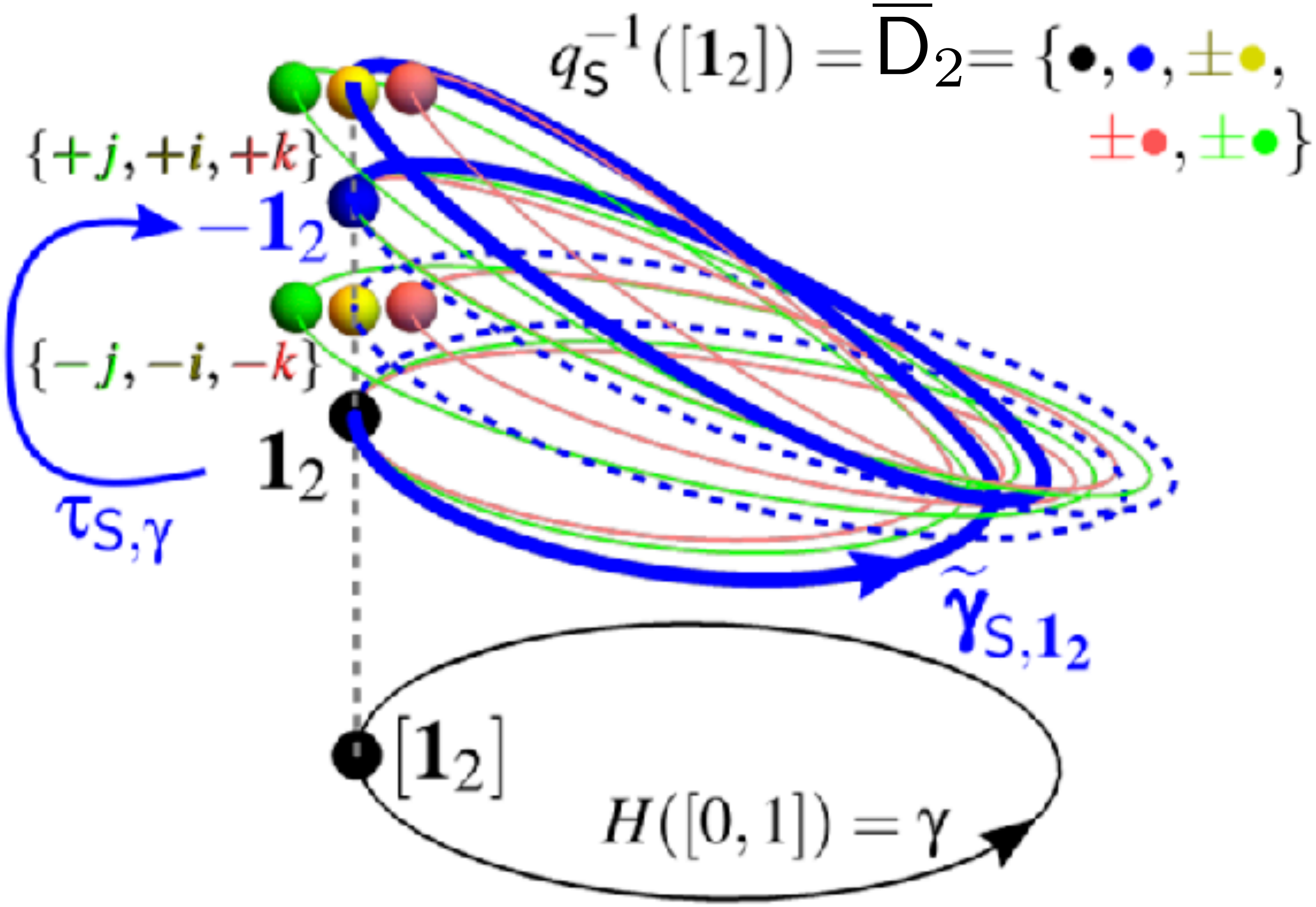
$$\frac{\mathsf{SO}(3)}{\mathsf{D}_2} = \frac{\mathsf{Spin}(3)}{\overline{\mathsf{D}}_2}$$

Ambiguity of the parallel transported SO(3)-frame
Lift to spin double cover

principal fiver bundle
with discrete structure group

$$\overline{\mathsf{D}}_2 \hookrightarrow \mathsf{Spin}(3) \to \mathsf{Spin}(3)/\overline{\mathsf{D}}_2$$

Spin(3)-monodromy representation of $\pi_1\left(\mathsf{SO}(3)/\mathsf{D}_2\right) = \overline{\mathsf{D}}_2$



π-rotation around $\mathbf{e}_3$ = i

and

($-\pi$)-rotation around $\mathbf{e}_3$ = -i

$$\frac{\mathsf{SO}(3)}{\mathsf{D}_2} = \frac{\mathsf{Spin}(3)}{\overline{\mathsf{D}}_2}$$

N-band generalization

Discrete group of all principal C_2 rotations of a rank-N frame:

$$\mathsf{P}_N \quad \subset \mathsf{SO}(N)$$

Classifying space: $$\frac{\mathsf{O}(N)}{\mathsf{P}_N} = \frac{\mathsf{Spin}(N)}{\overline{\mathsf{P}}_N}$$

$$\pi_1\left(\frac{\mathsf{Spin}(N)}{\overline{\mathsf{P}}_N}\right) = \overline{\mathsf{P}}_N$$ Non-Abelian Salingaros group

Bdzusek *et al*, Science (2019)

Computation of non-Abelian charges: lift diagram

monodromy representation = holonomy representation

Frame connection:

$$\mathcal{A} = R^{\top}(\boldsymbol{k}) \cdot dR(\boldsymbol{k})$$

Parallel transport:

$$F(\boldsymbol{k}) = \overline{\exp}\left\{\int_0^{\boldsymbol{k}} \mathcal{A}\right\} = e^{A(\boldsymbol{k})}$$

SO(N)-holonomy element:

$$F(\ell) = \overline{\exp}\left\{\int_{\ell} \mathcal{A}\right\} = e^{A(\ell)} \in P_N$$

Spin(N)-holonomy element:

$$\overline{F}(\ell) = \overline{\exp}\left\{\int_{\ell} \overline{\mathcal{A}}\right\} = e^{\overline{A}(\ell)} \in \overline{P}_N$$

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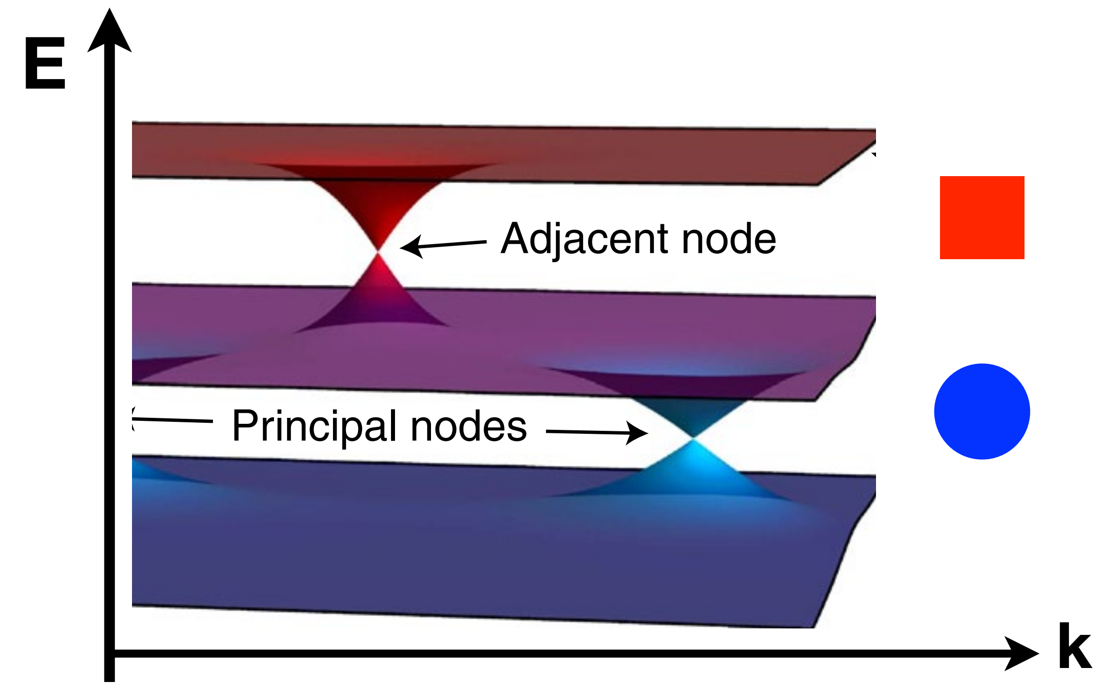

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quaternion group:

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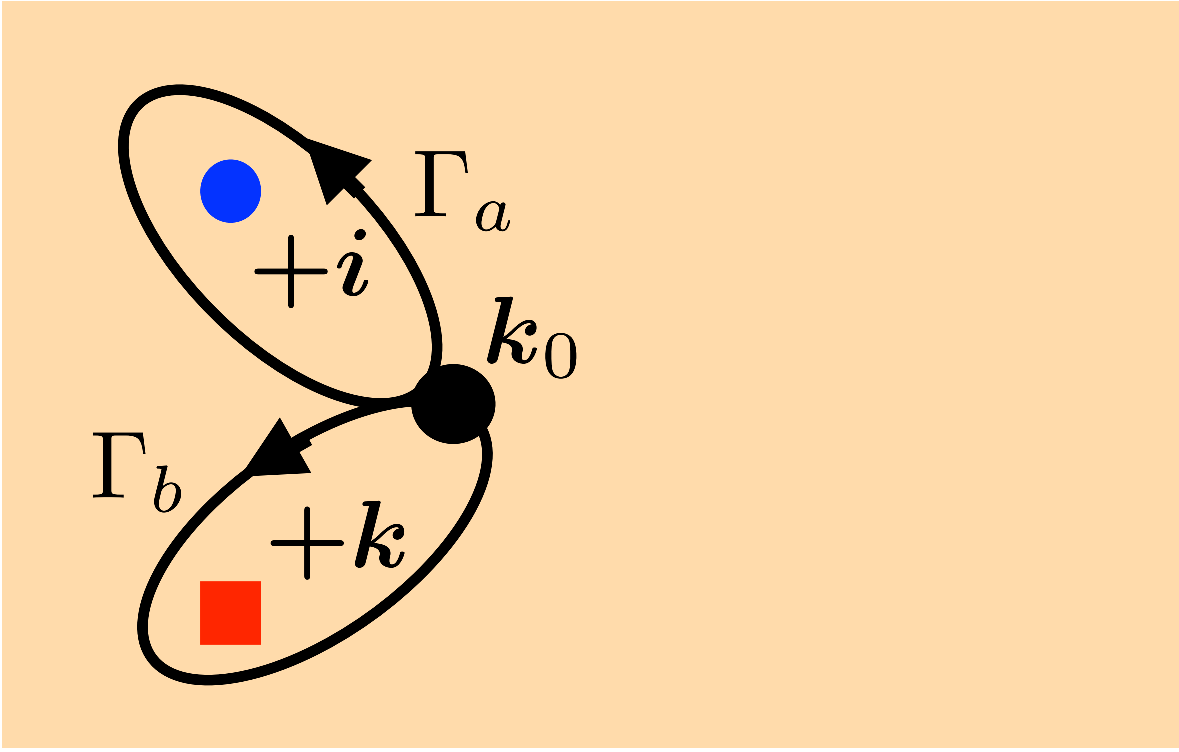
accumulated frame rotations around multi-gap nodes



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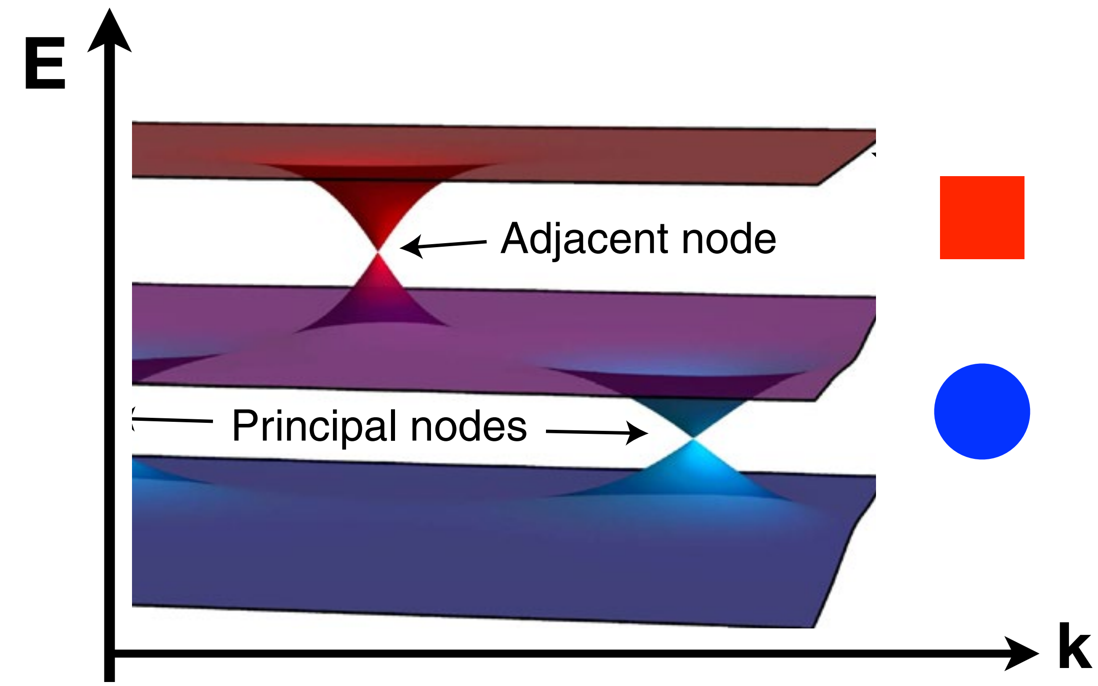

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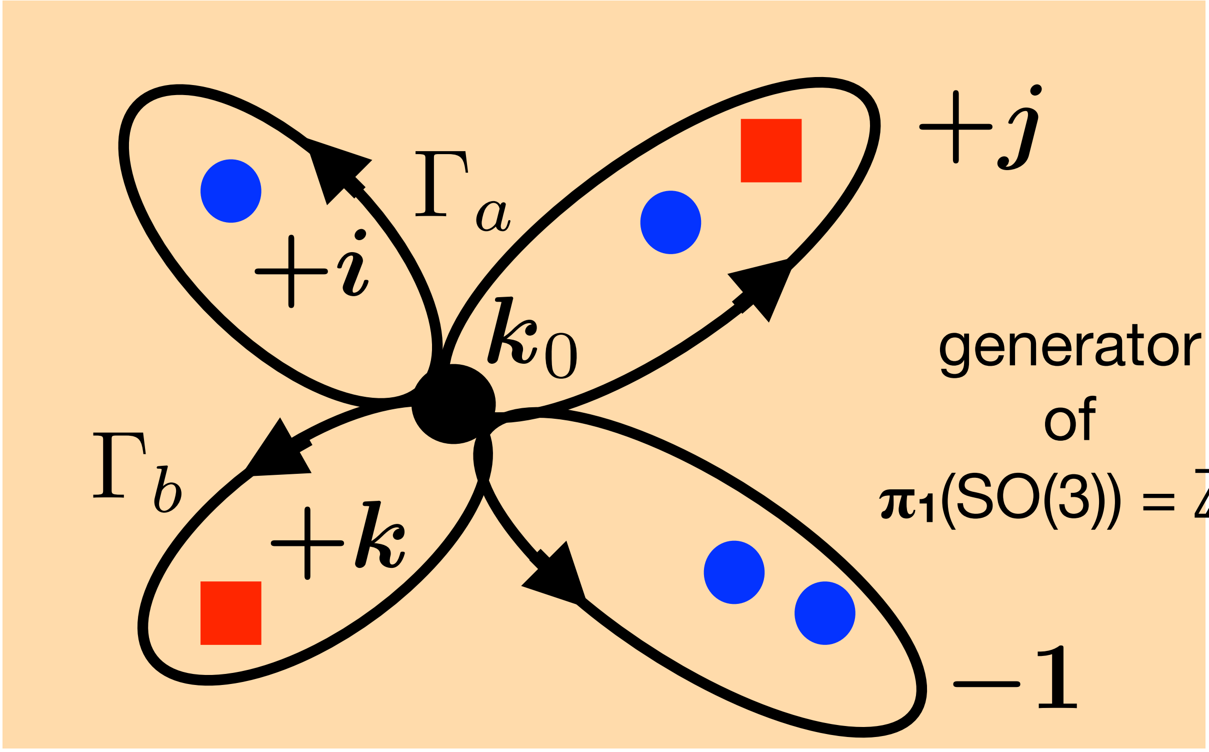
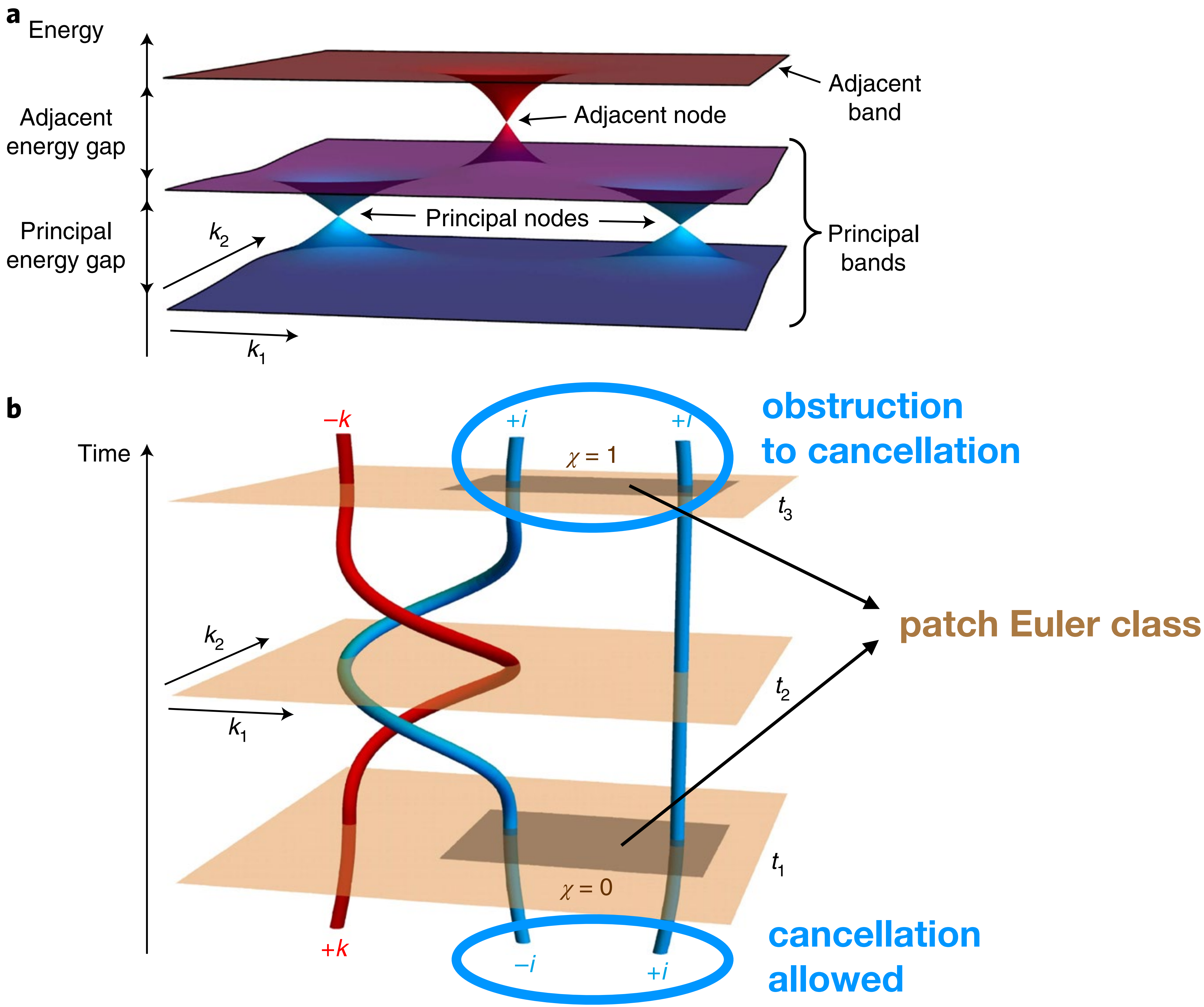


Bdzusek *et al*, Science (2019)

Reciprocal braiding of Weyl points in a C_2T-plane

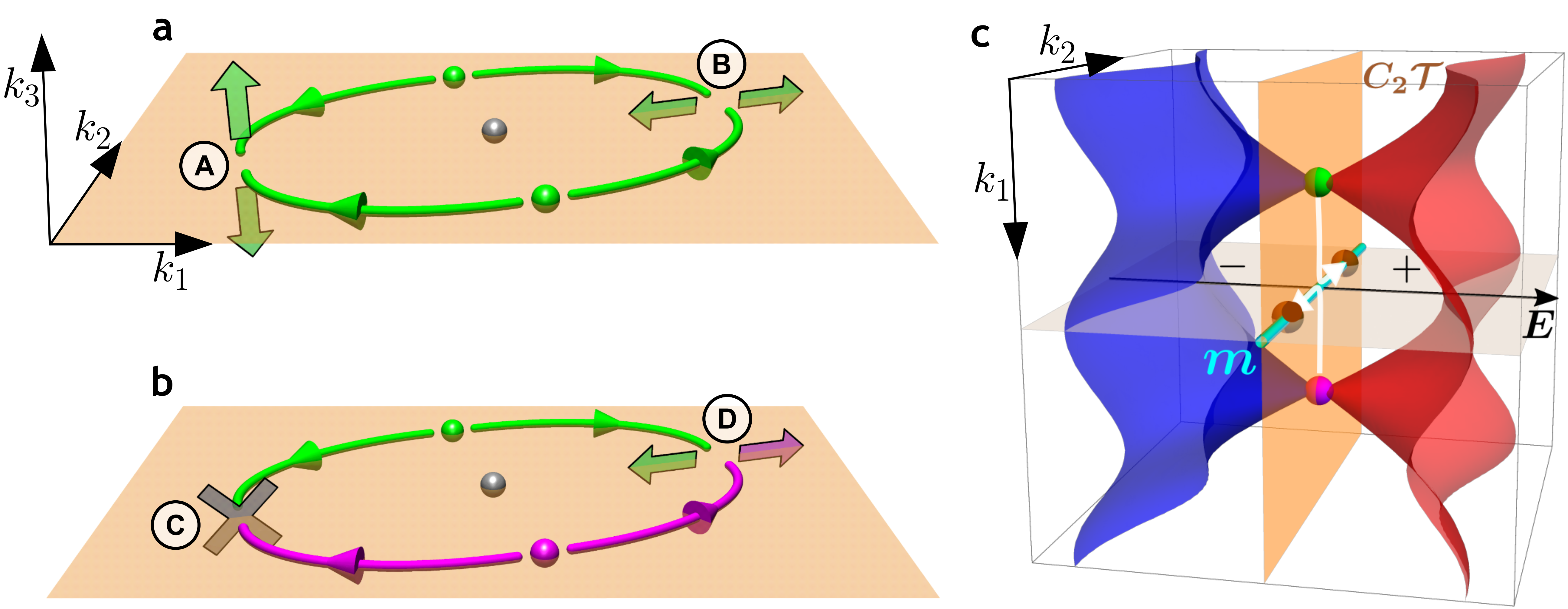


AB, et al Nature Physics 16, 1137 (2020)

Obstruction to annihilation of Weyl point-pairs

The non-Abelian charges are COMPLEMENTARY to the chirality of the Weyl points

C2T plane



AB, et al Nature Physics 16, 1137 (2020)

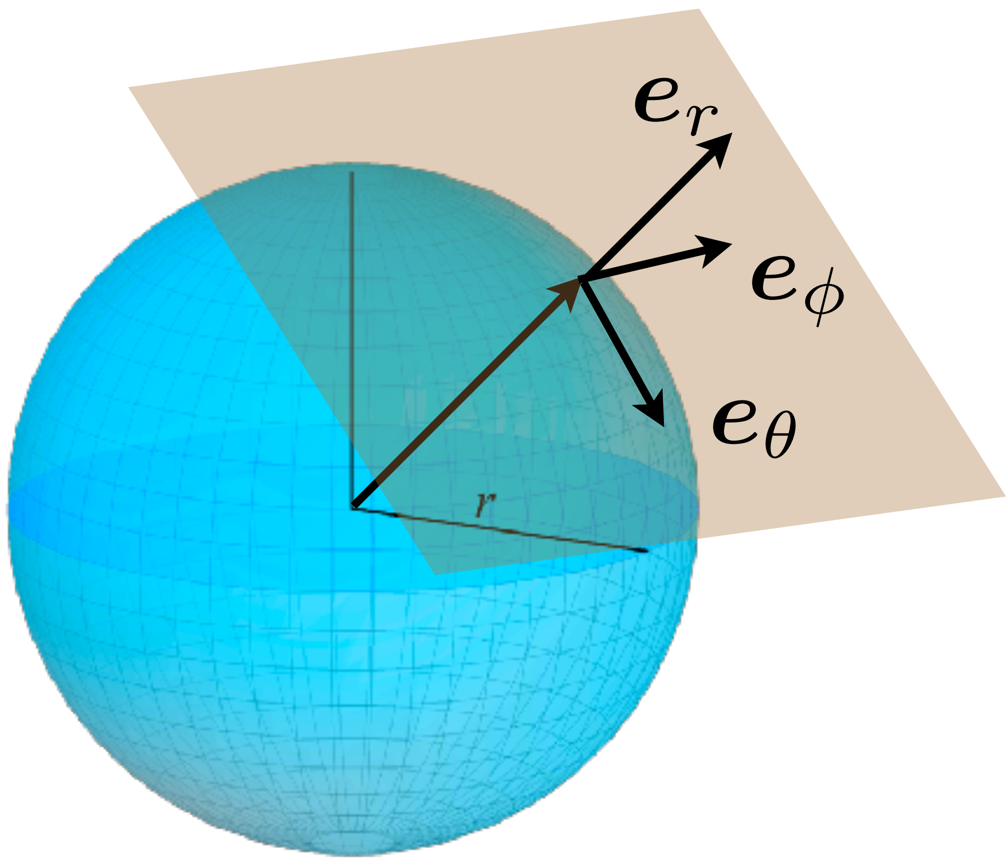
2D topology:
Euler insulators and Z accumulation of nodal points

Tangent bundle of the sphere

Hairy ball theorem:

combing a hairy ball lead to vortices!

$$T\mathbb{S}^2$$



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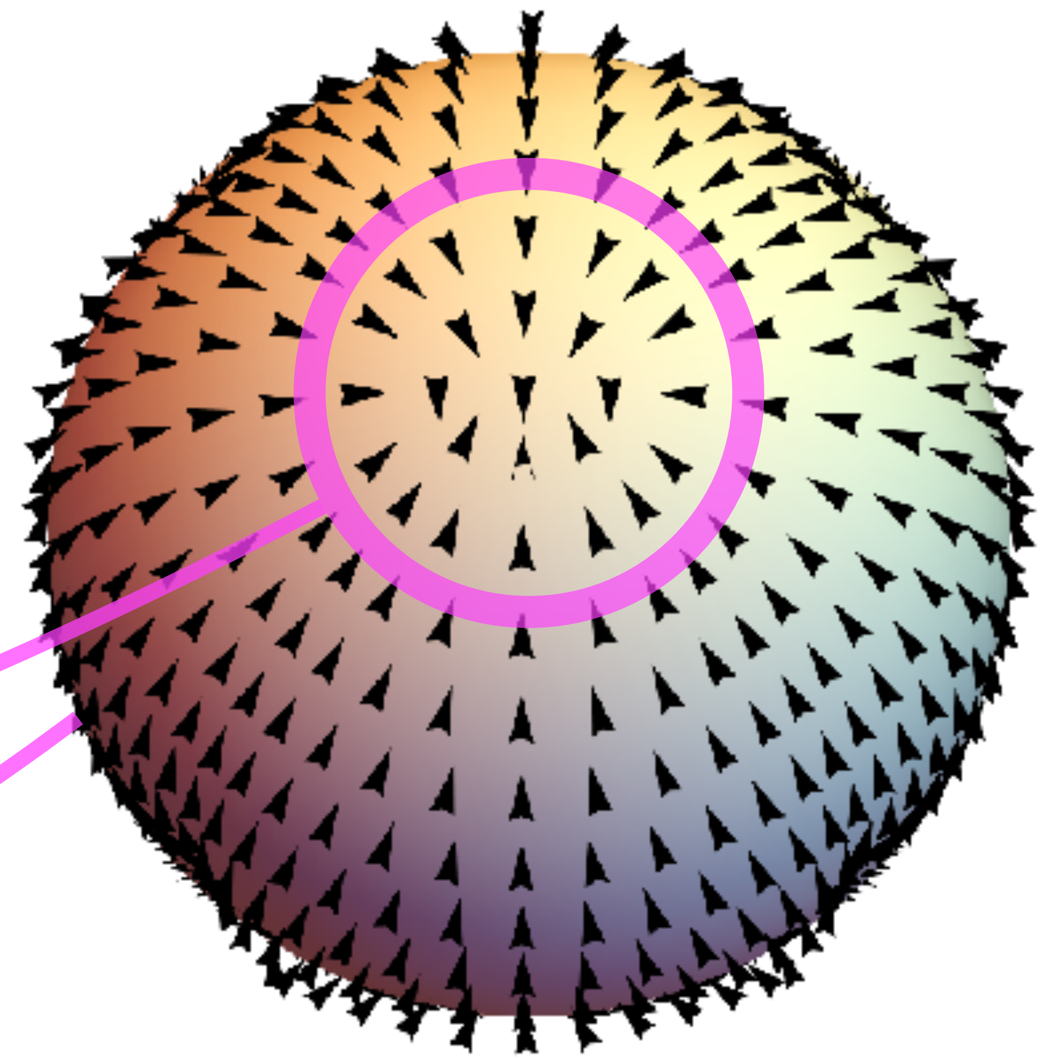


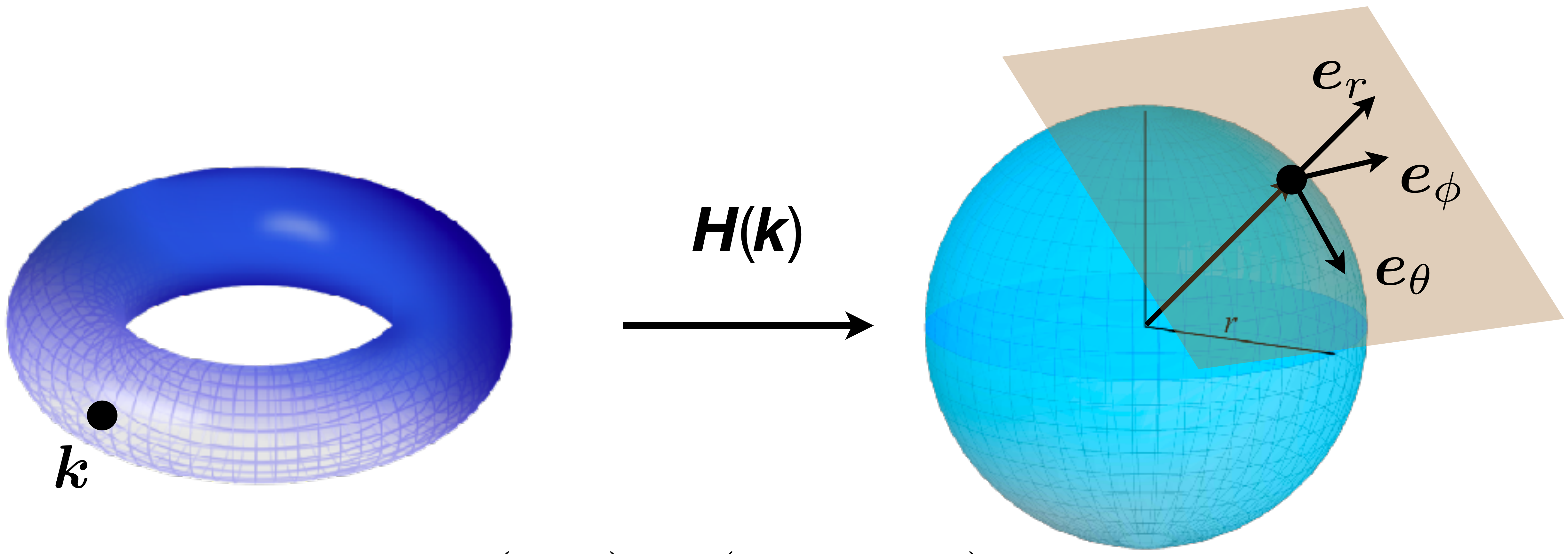
Poincaré-Hopf (Gauss-Bonnet) theorem:

$$\sum_j \mathrm{index}_{x_j}(v) = \chi[\mathbb{S}^2] = 2$$

vorticity of the tangent vector field

Euler characteristic of the sphere

Tangent bundle of the sphere *on a lattice*



$$R(\theta,\phi) = (\boldsymbol{e}_\theta \ \boldsymbol{e}_\phi \ \boldsymbol{e}_r)$$

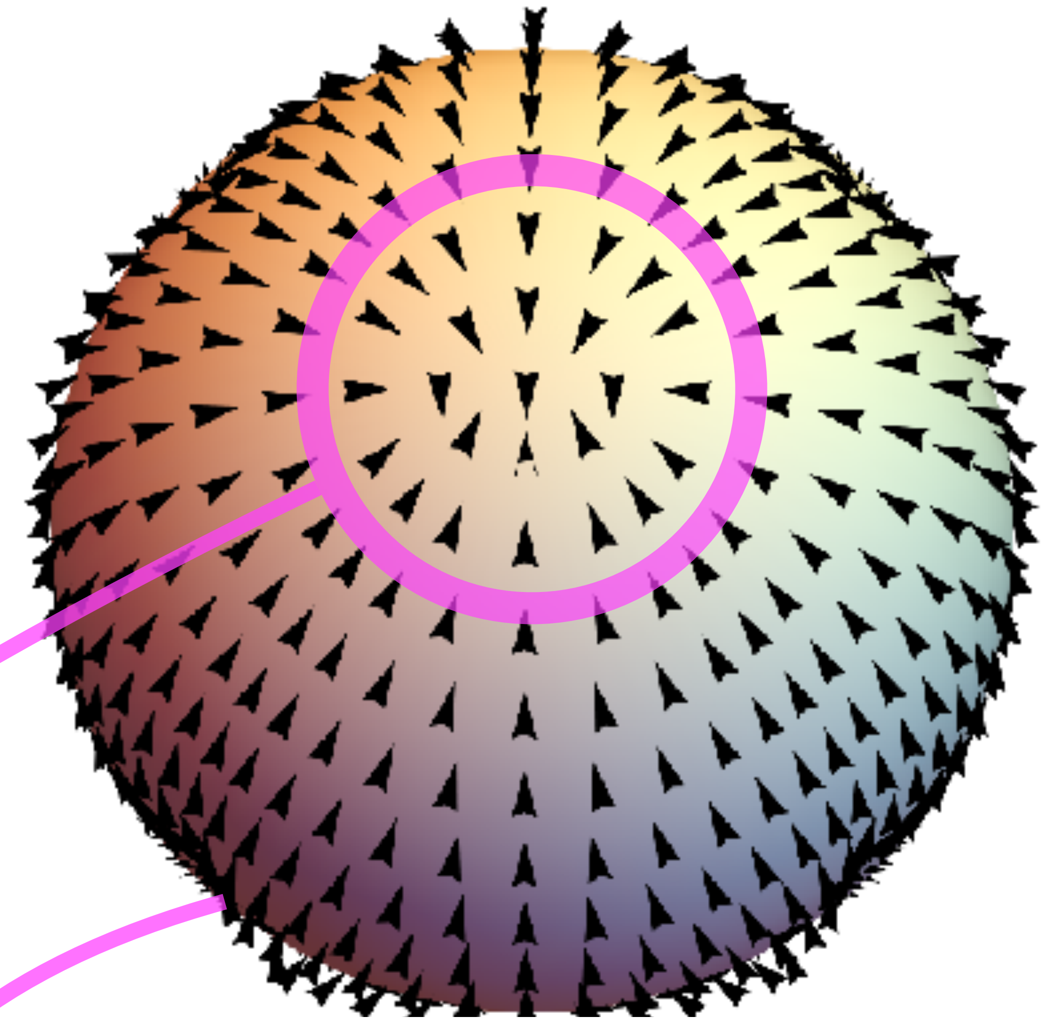
$$H(\theta,\phi) = R(\theta,\phi)\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} R(\theta,\phi)^T$$

Topological Euler insulator

AB, T. Bzdusek, RJ Slager, Phys. Rev. B **102**, 115135 (2020)

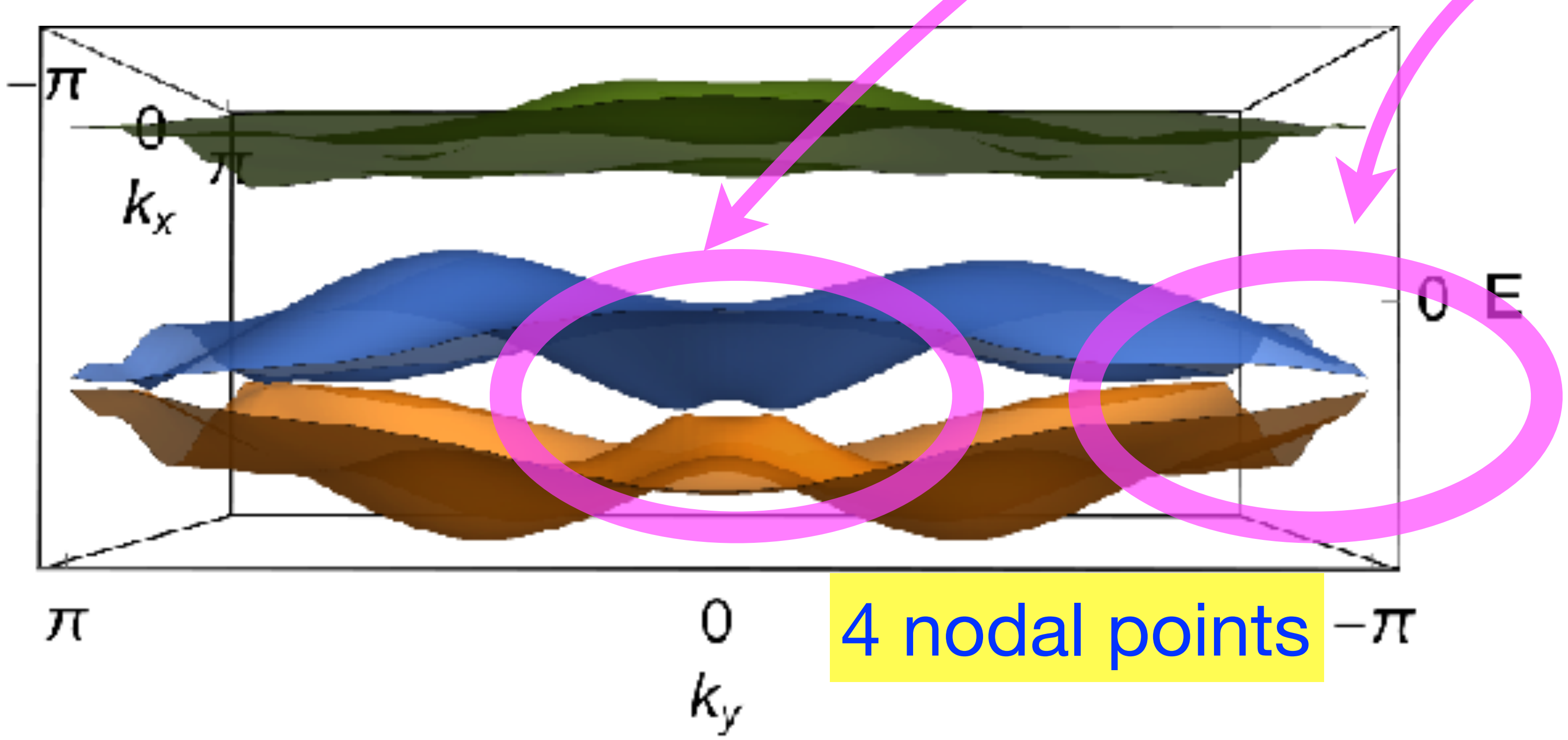
$$R(\boldsymbol{k}) = (u_1(\boldsymbol{k})\ u_2(\boldsymbol{k})\ \boldsymbol{n}(\boldsymbol{k}))$$

with $\boldsymbol{n}(\boldsymbol{k})$ covering the sphere one time

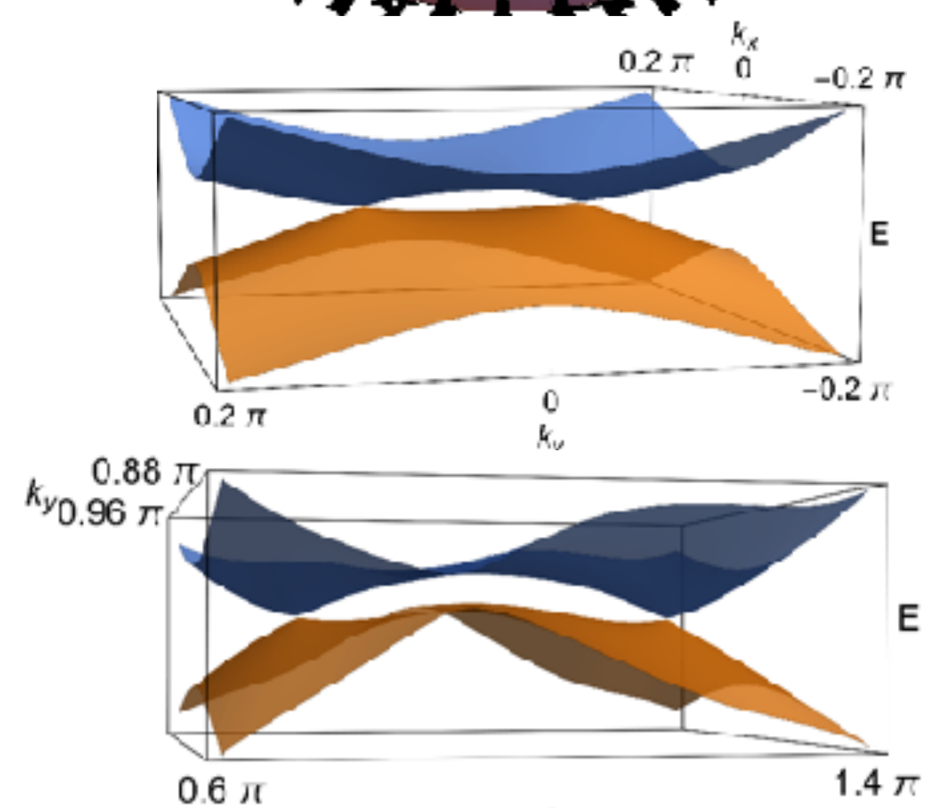


vortices of the vector field

nodal points between bands 1 and 2



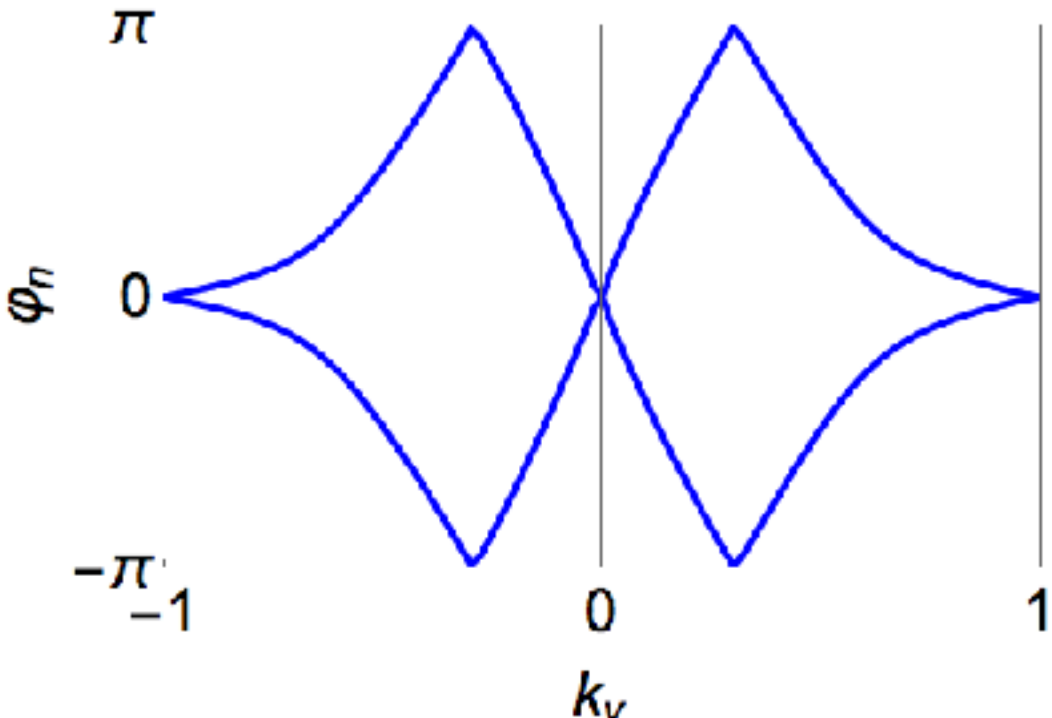
4 nodal points

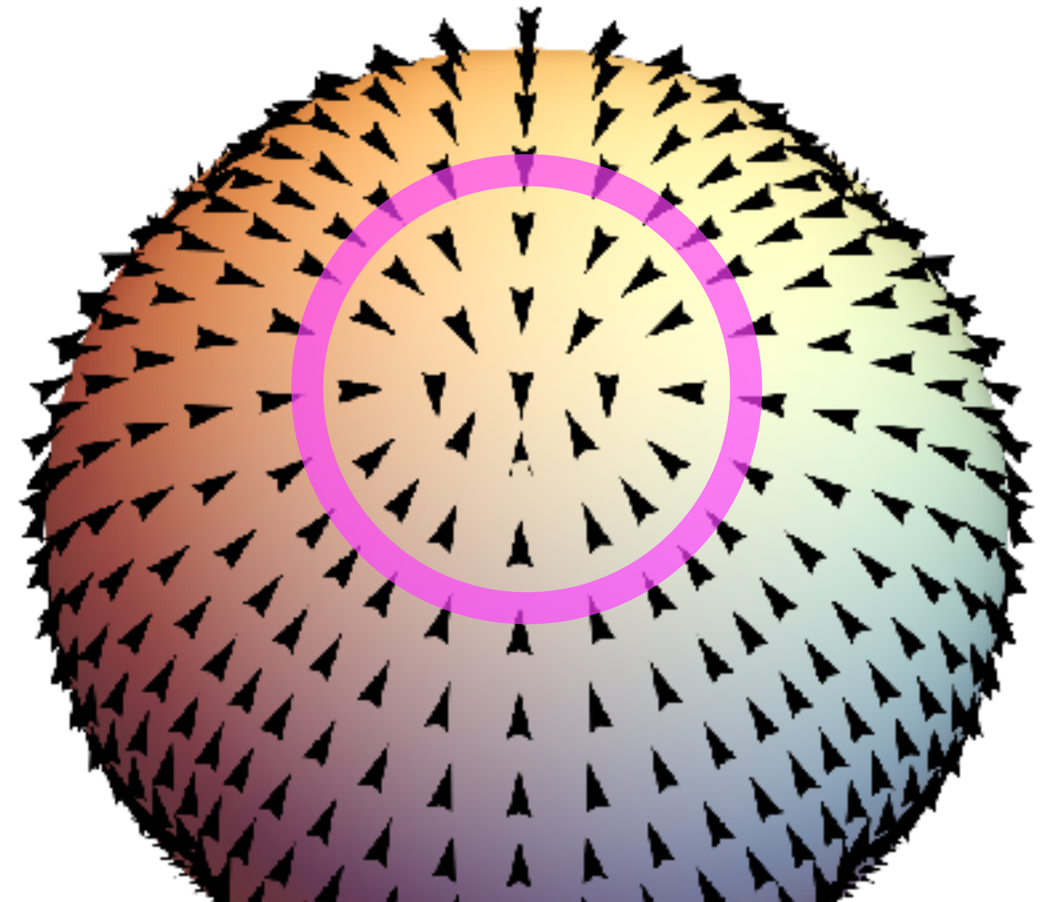


Topological Euler insulator

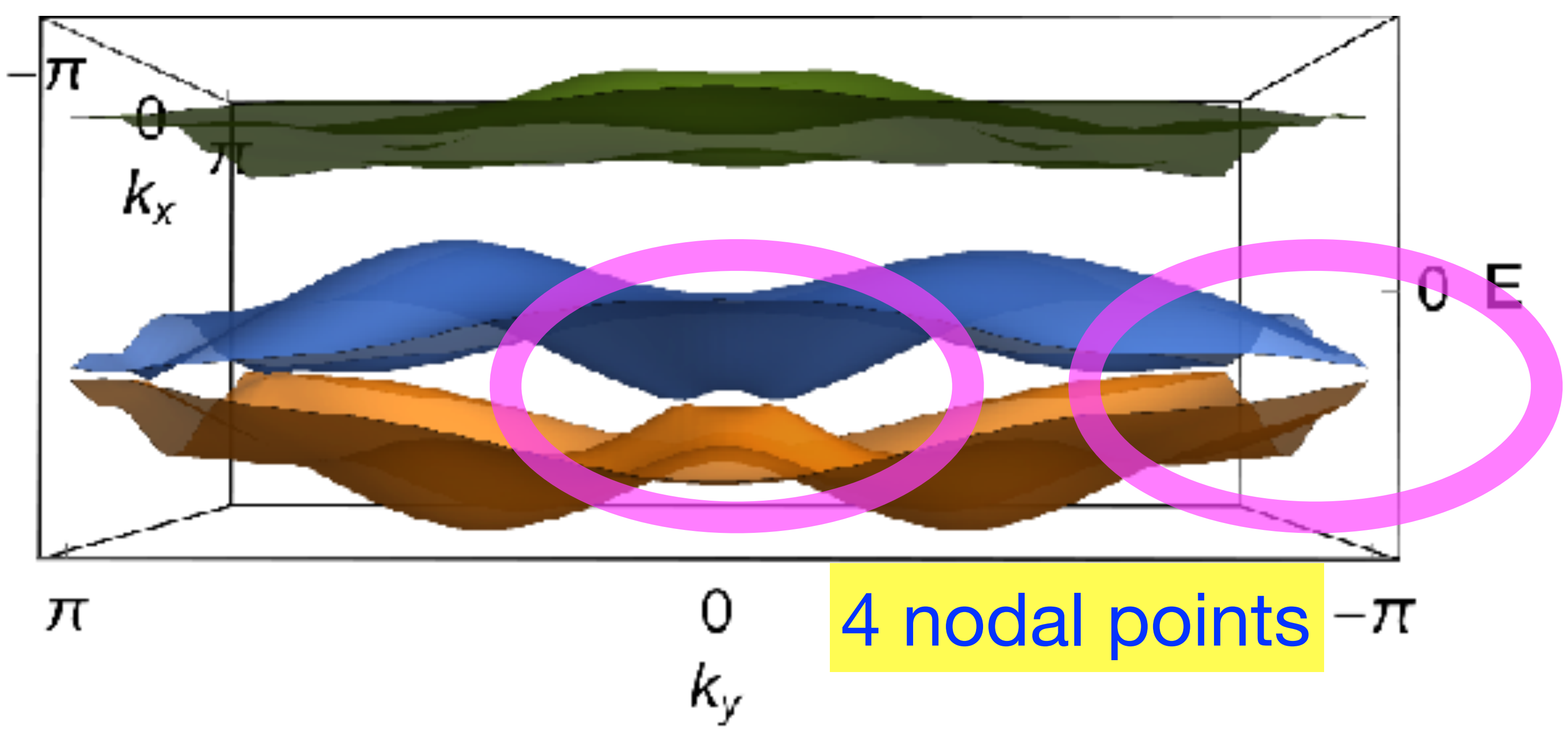
AB, T. Bzdusek, RJ Slager, Phys. Rev. B **102**, 115135 (2020)

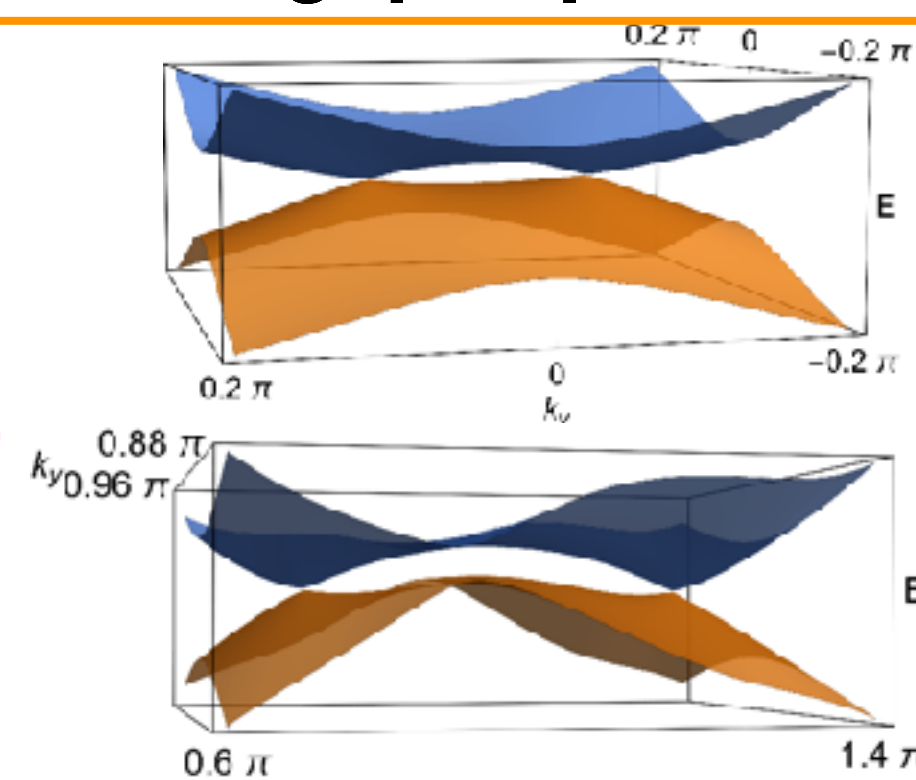
Wilson loop winding $\chi = 2$



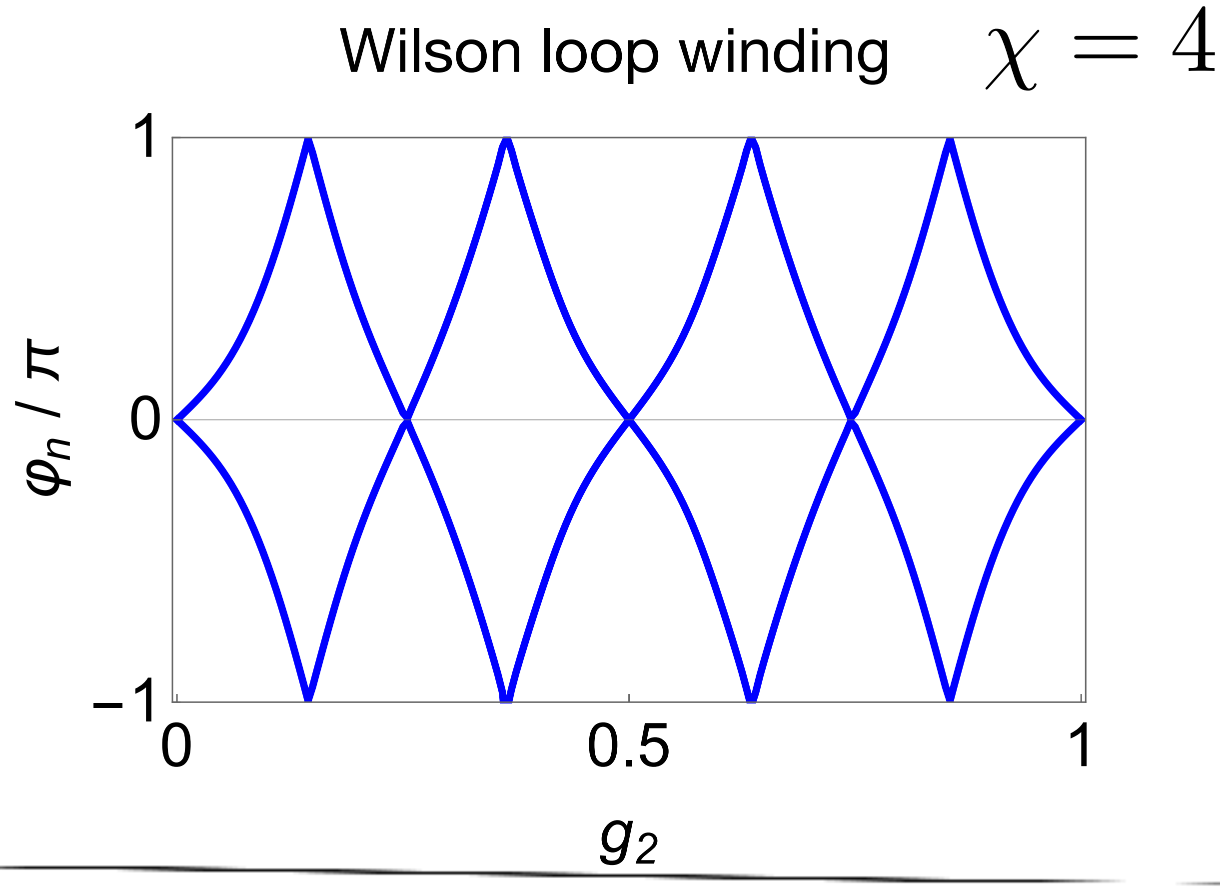


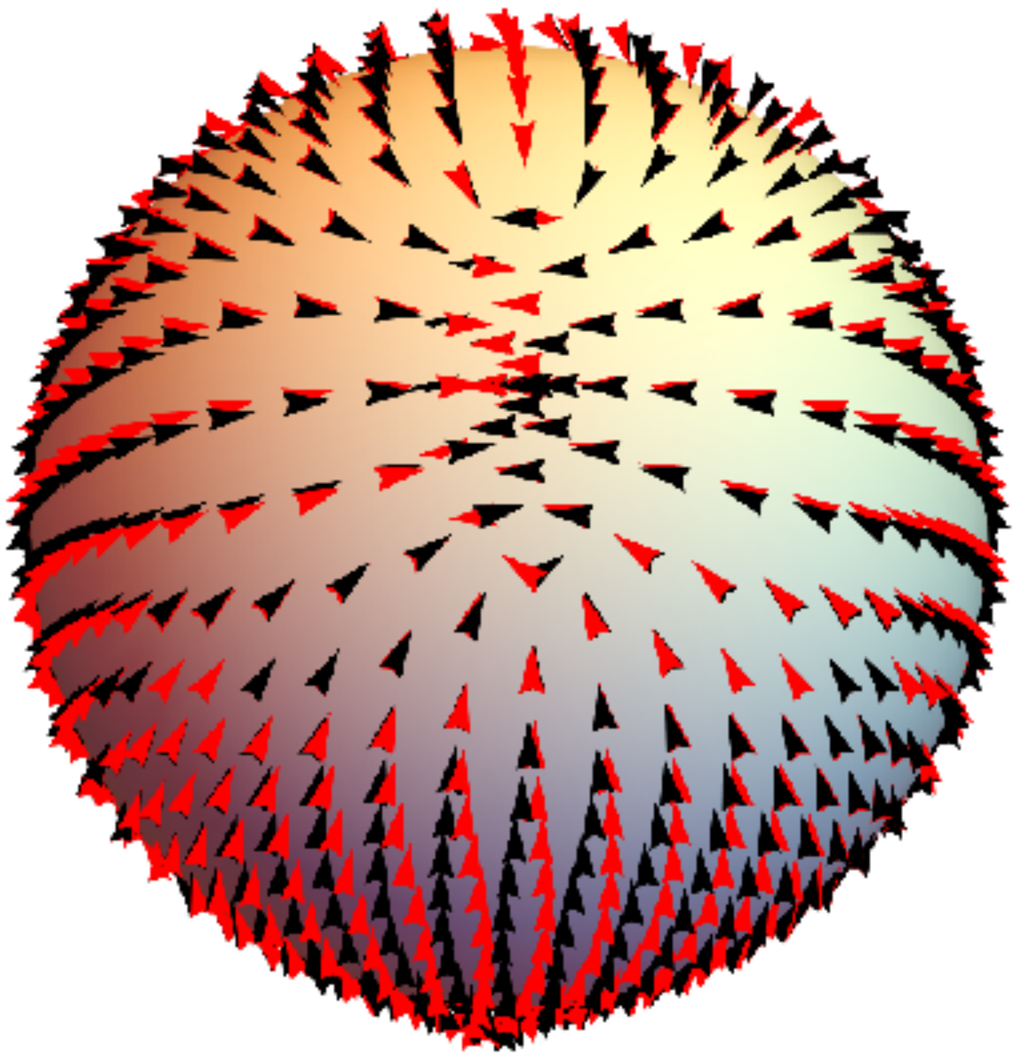
the 4 nodes are unremovable as long as the gap is preserved!

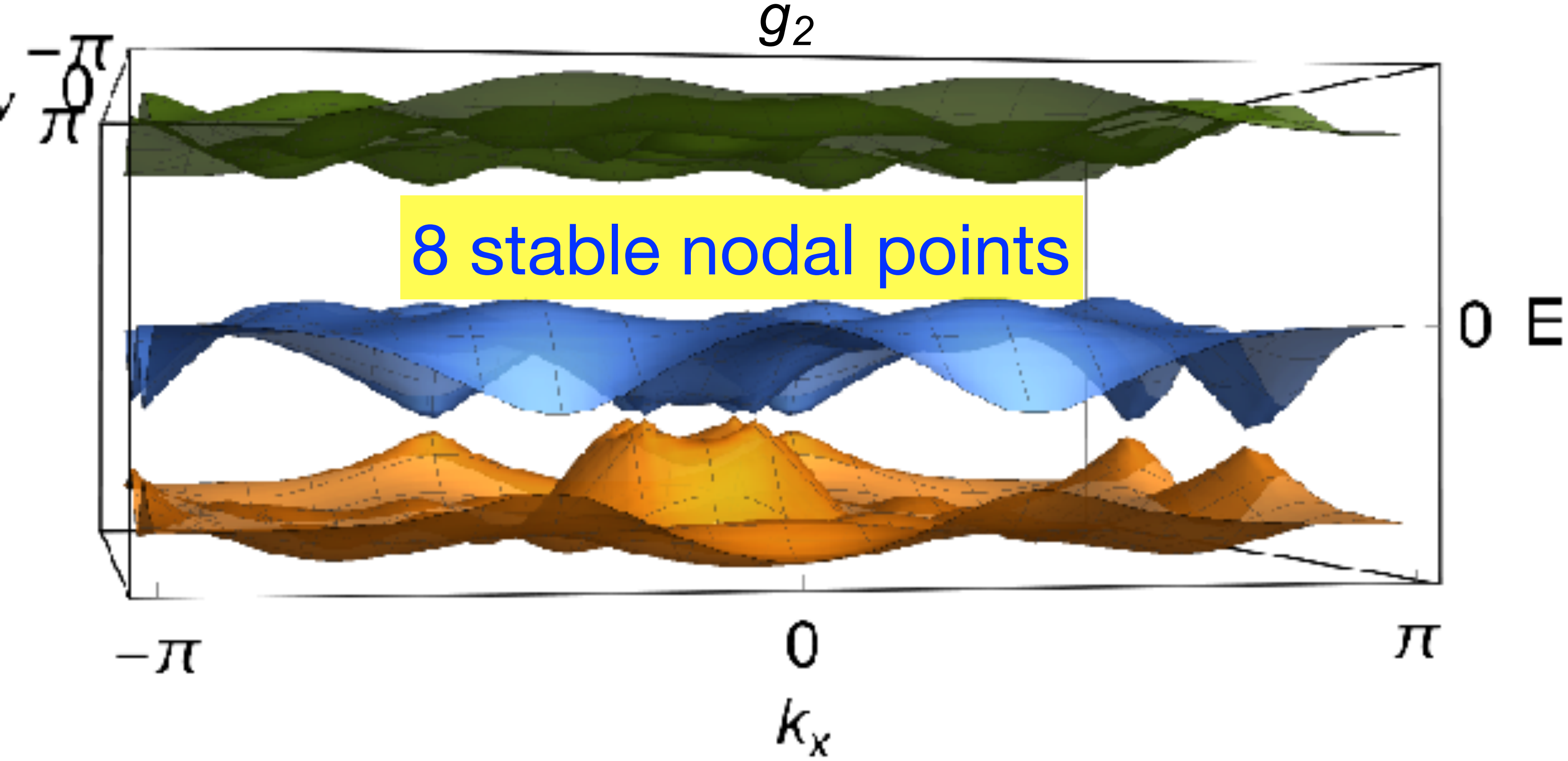




Topological Euler insulator







Total number of stable Nodal Points:

$$\#\mathrm{NP} = 2|\chi|$$

AB, T. Bzdusek, RJ Slager, PRB **102**, 115135 (2020)

Euler number of “real” 2D insulating phases

$$\widetilde{H}(\boldsymbol{k}) = R(\boldsymbol{k})\mathcal{E}(\boldsymbol{k})R^T(\boldsymbol{k})\ , \quad R(\boldsymbol{k}) \in SO(3)$$

$\widetilde{\mathcal{A}} = \mathcal{U}^\dagger d\mathcal{U} = \widetilde{A}_i dk^i$ is a 1-form in $\mathfrak{so}(N_o)$, i.e. $\widetilde{A}_i$ are skew-symmetric matrices

Euler connection: $\mathrm{a} = \mathrm{Pf}(A_i)dk^i$ (for a two-band subspace)

Euler form: $\mathrm{Eu} = d\mathrm{a}$

Euler class: $\chi(\mathcal{E}_v) = \frac{1}{2\pi}\oint_B \mathrm{Eu} \in \mathbb{Z}$ (if *B* and *E*$_v$ are orientable)

Patch Euler number (gauge invariance of nodal points)

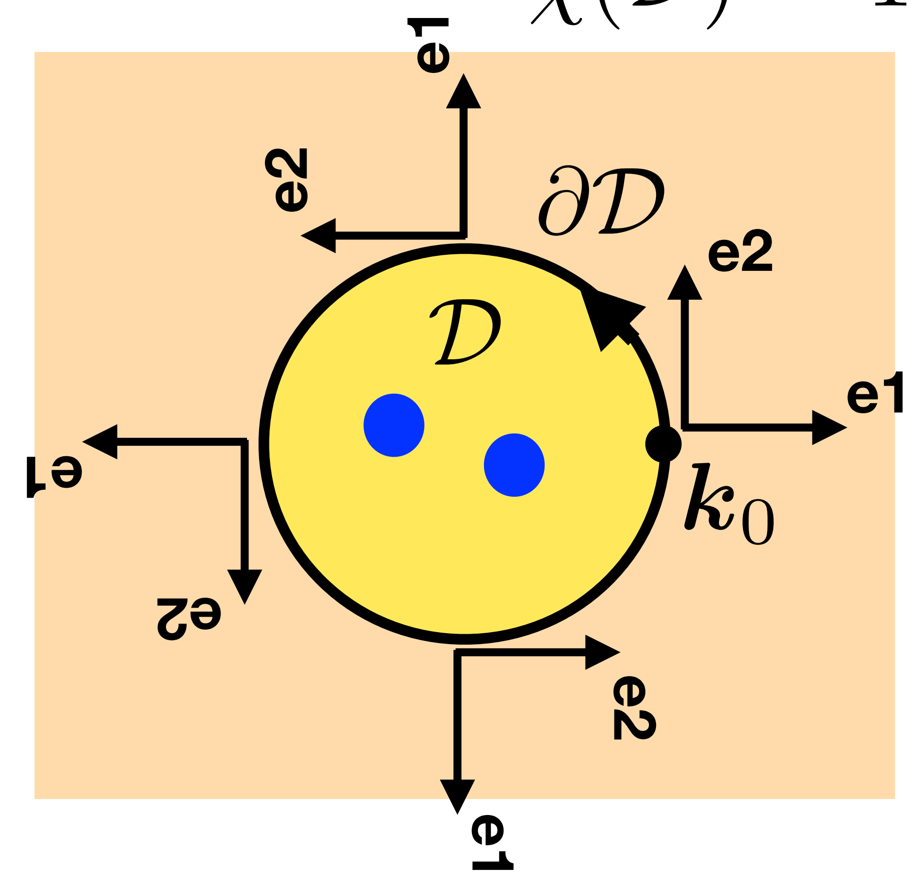
Euler number:

$$\chi(\mathcal{D}) = \frac{1}{\pi}\left[\int_{\mathcal{D}} \mathrm{Eu} - \oint_{\partial\mathcal{D}} \mathrm{a}\right]$$

$$= \frac{1}{\pi}\sum_n \left[\int_{\mathcal{D}_n^\epsilon} \mathrm{Eu} - \oint_{\partial\mathcal{D}_n^\epsilon} \mathrm{a}\right]$$

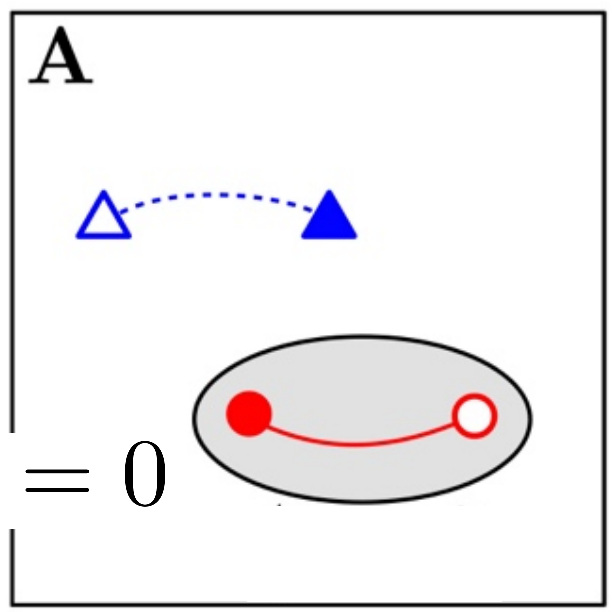
$$= \sum_n W_n \in \mathbb{Z}$$

$\chi(\mathcal{D}) = 1$



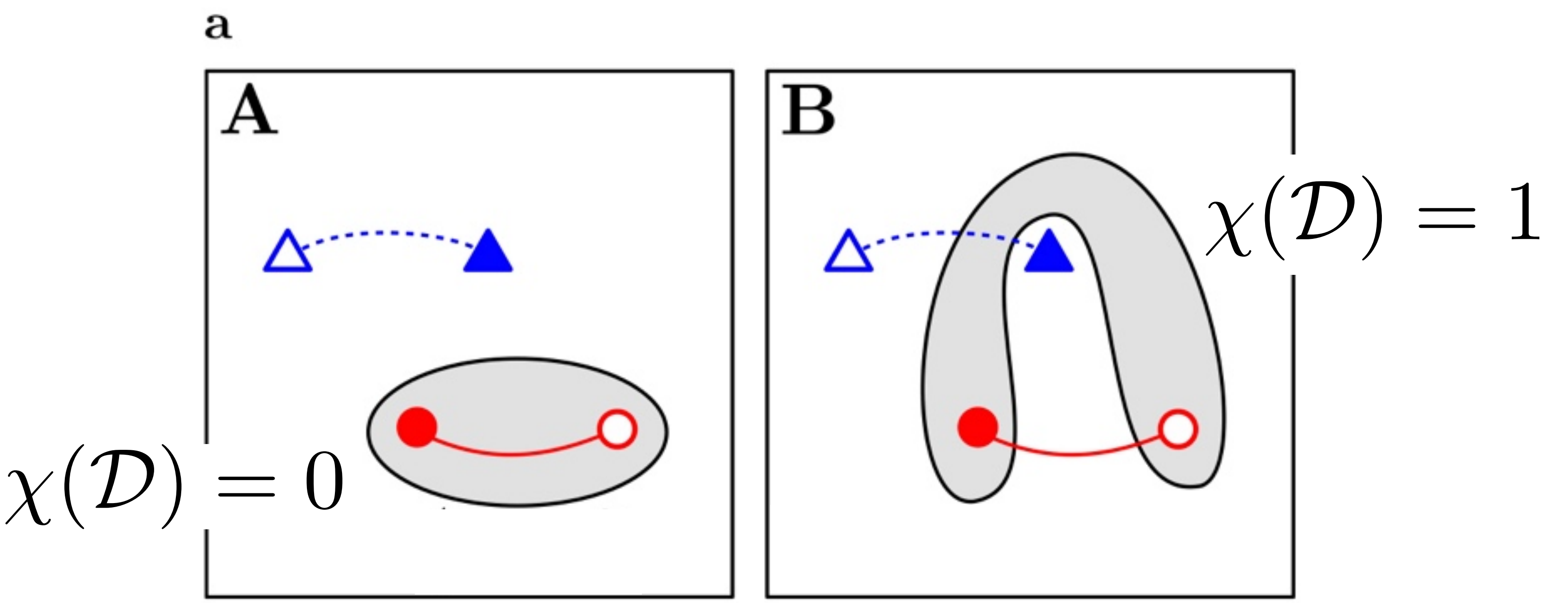
Braiding rules in terms of Dirac string and patch Euler class

a

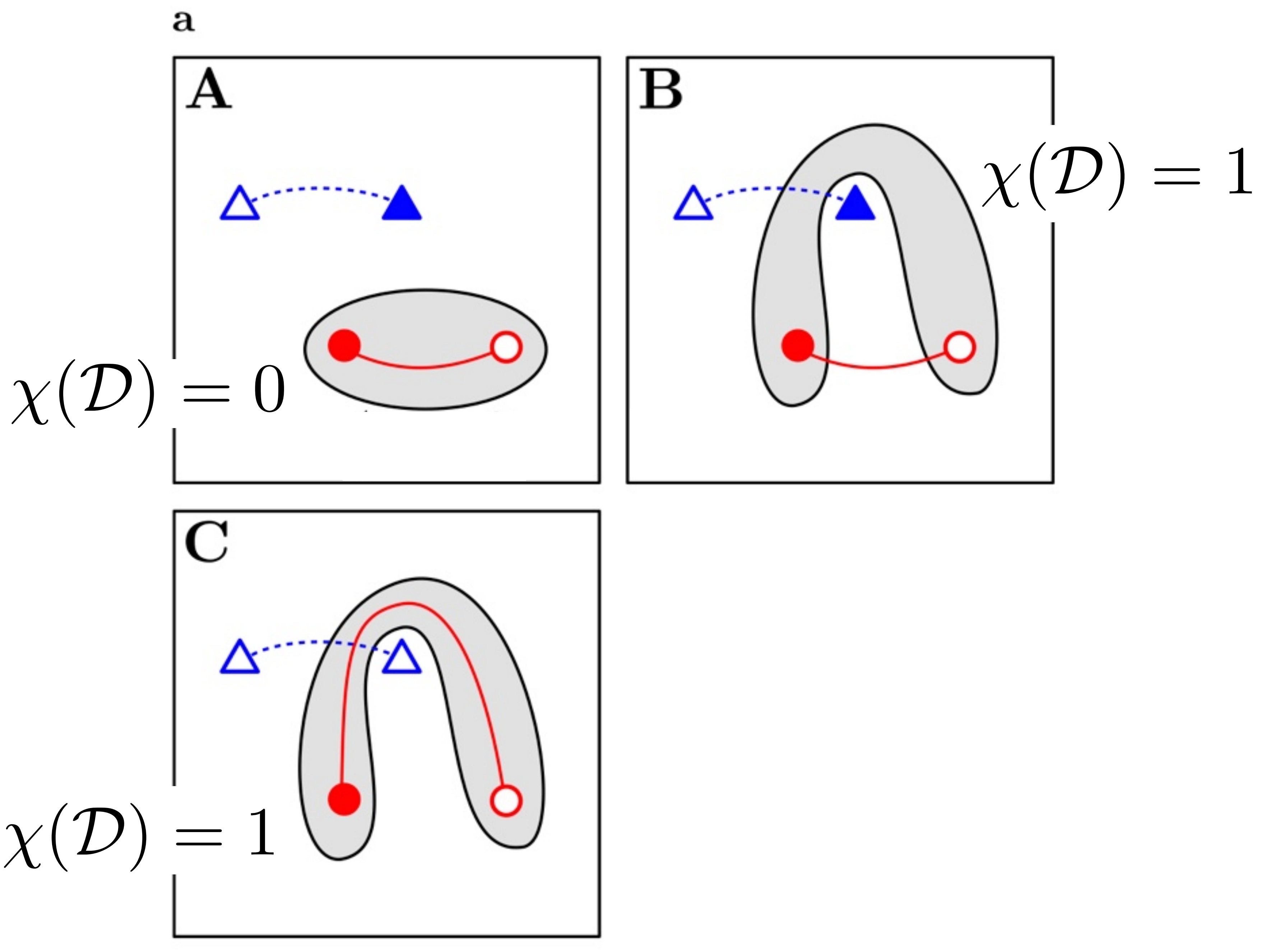


$$\chi(\mathcal{D}) = 0$$

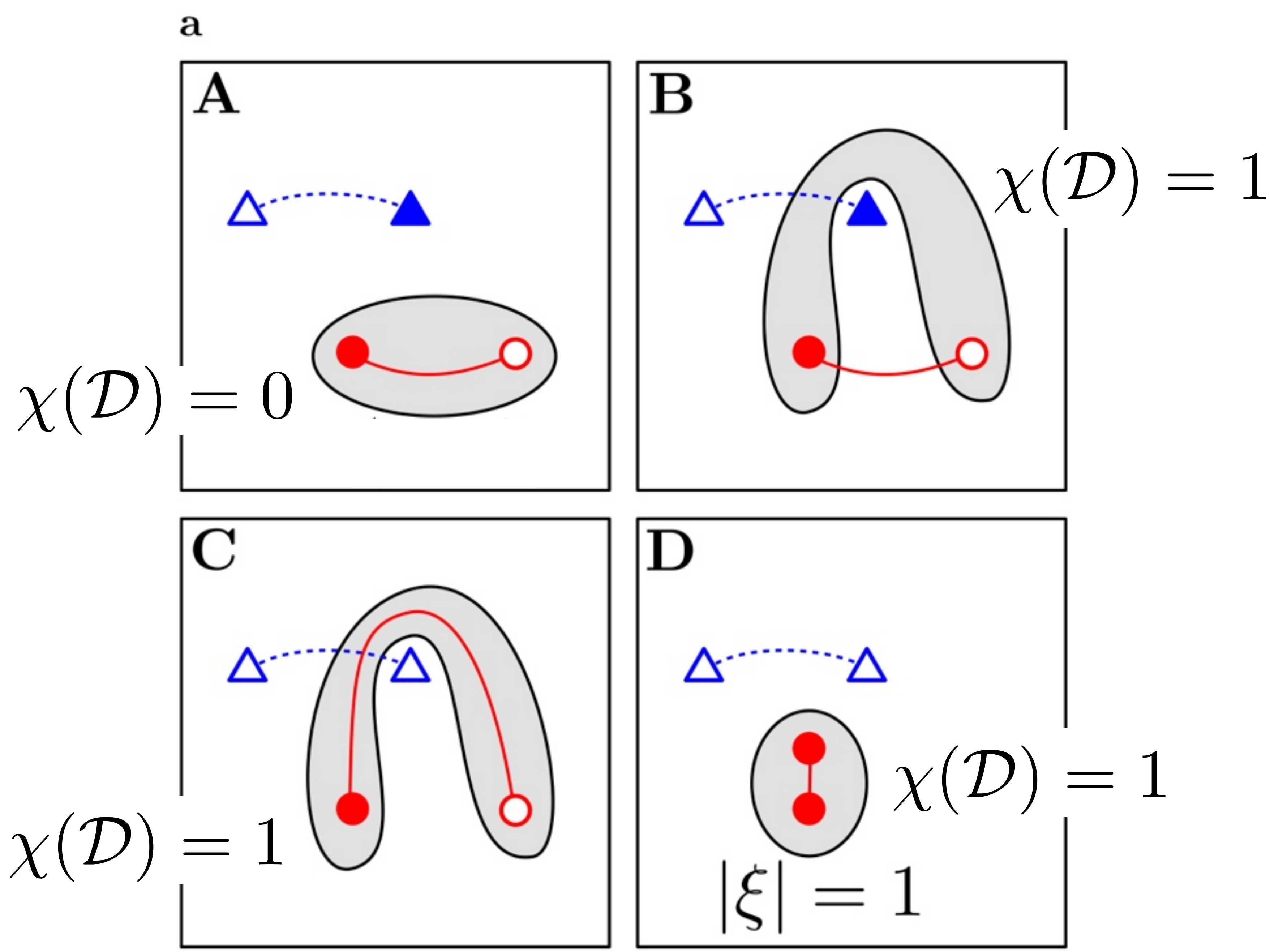
Braiding rules in terms of Dirac string and patch Euler class



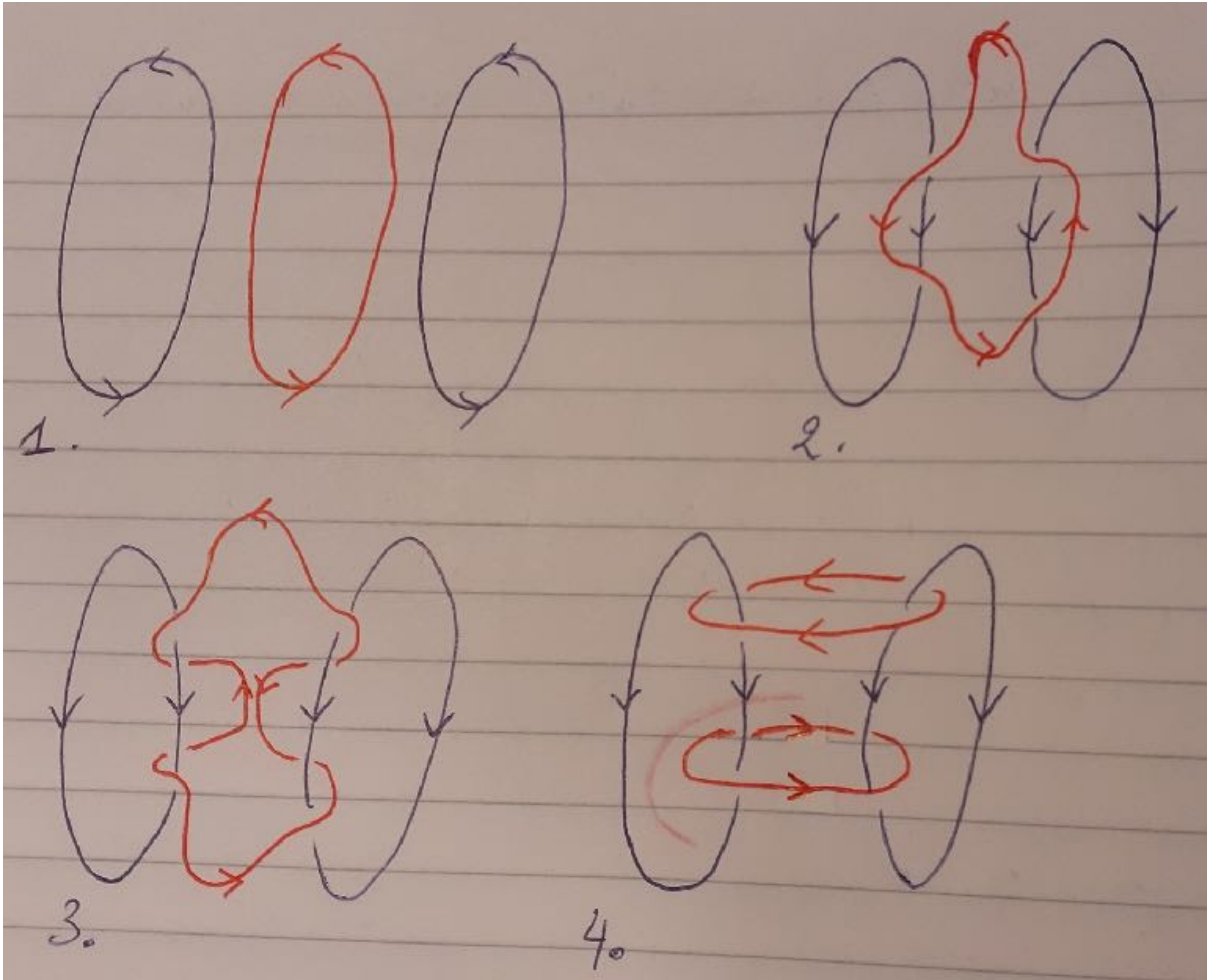
Braiding rules in terms of Dirac string and patch Euler class



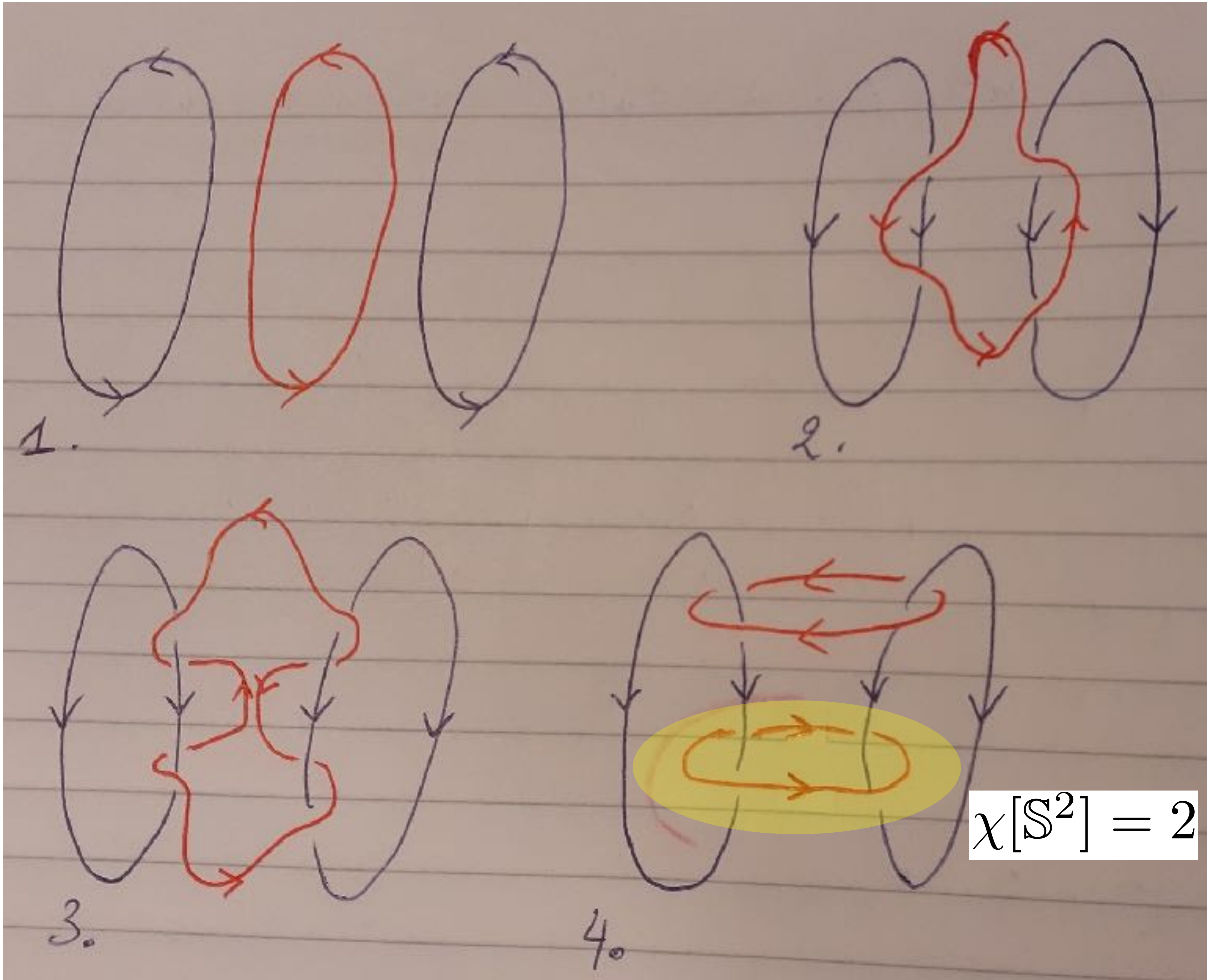
Braiding rules in terms of Dirac string and patch Euler class



Braiding of nodal rings in 3D PT phases

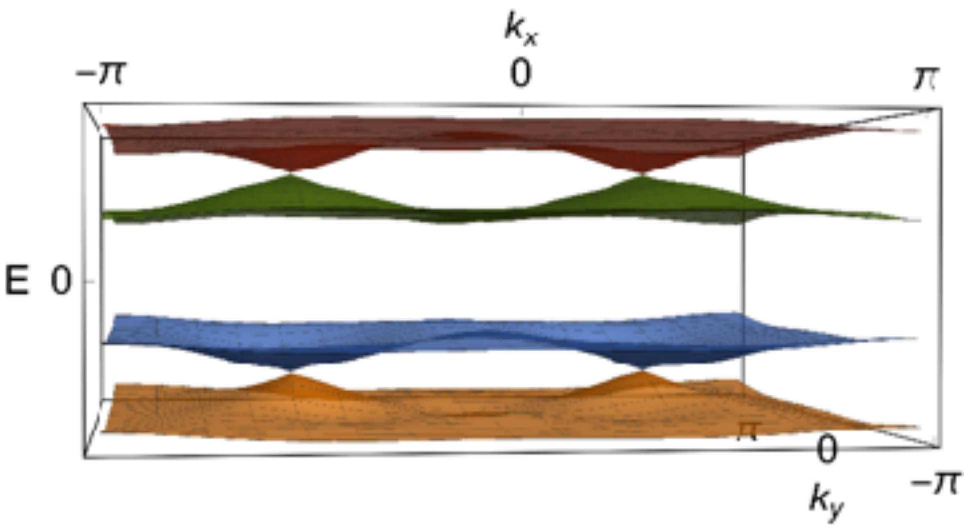


Braiding of nodal rings in 3D PT phases

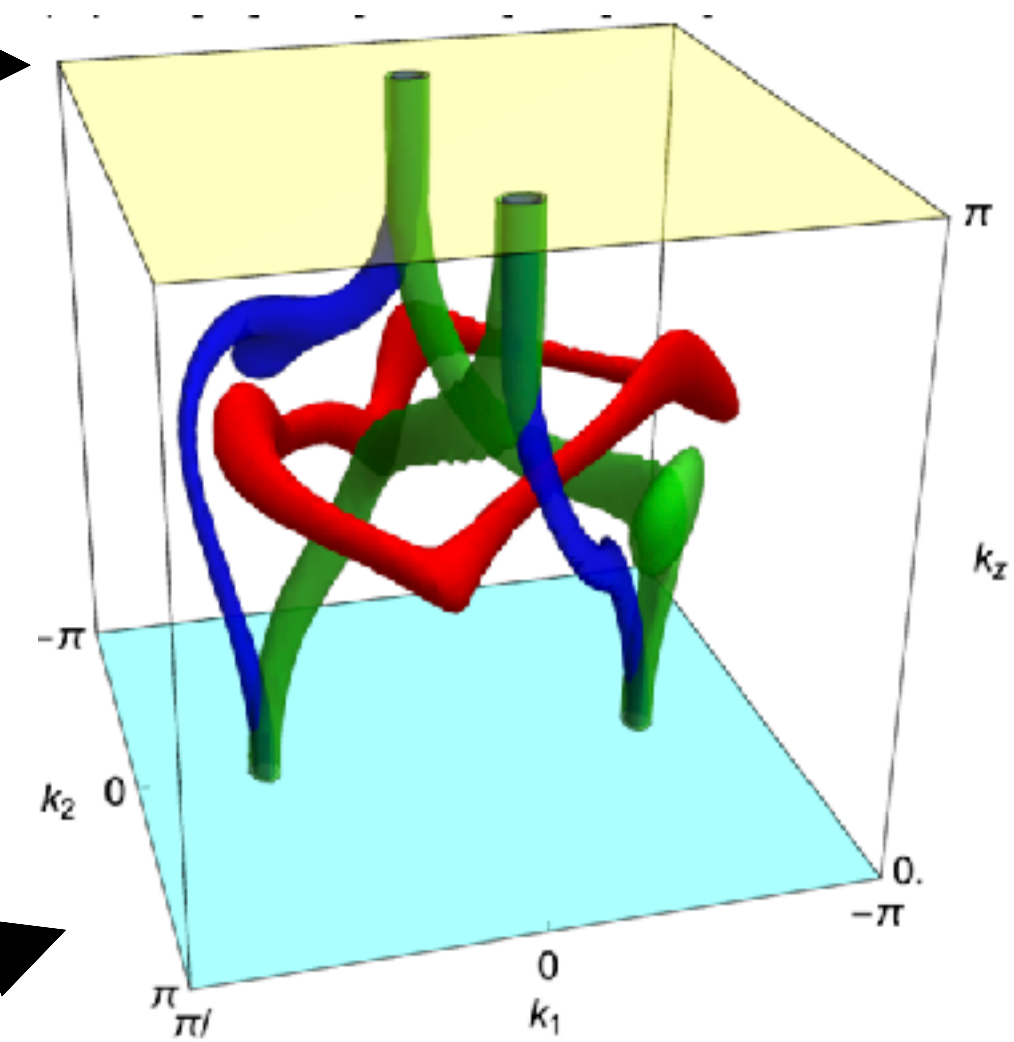


Euler number conversion via braiding of Weyl points

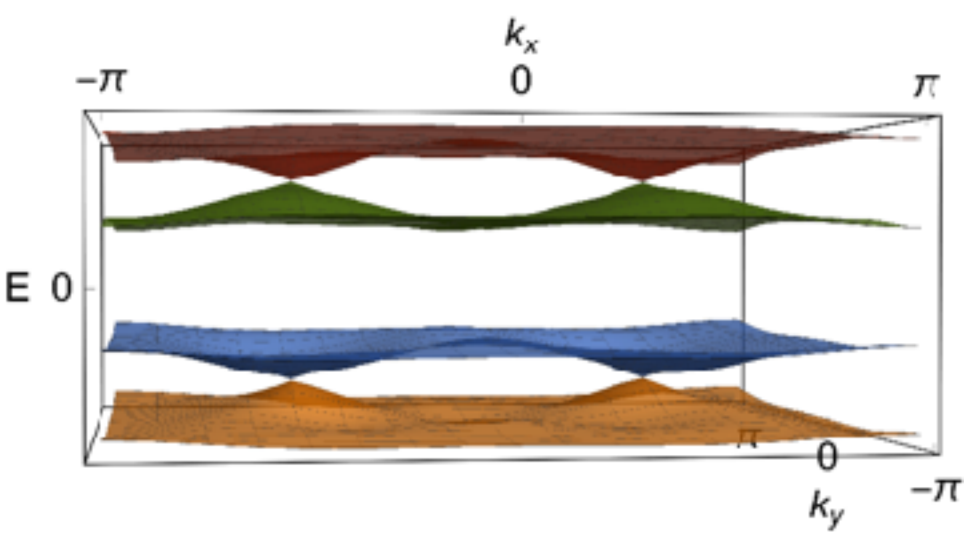
$$(\chi_I, \chi_{II}) = (1, 1)$$



Linked nodal rings = braiding trajectories of NP



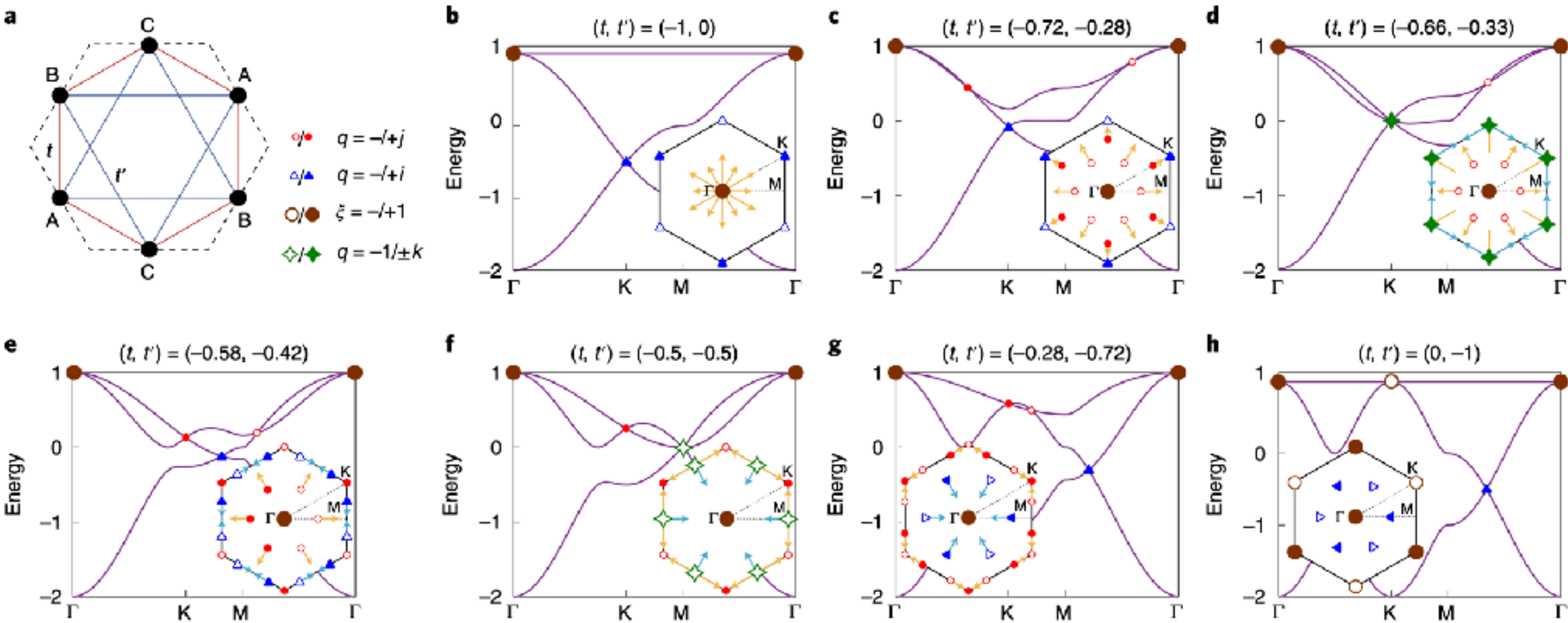
$$(\chi_I, \chi_{II}) = (1, -1)$$



AB, RJ Slager, arxiv:2203.16741

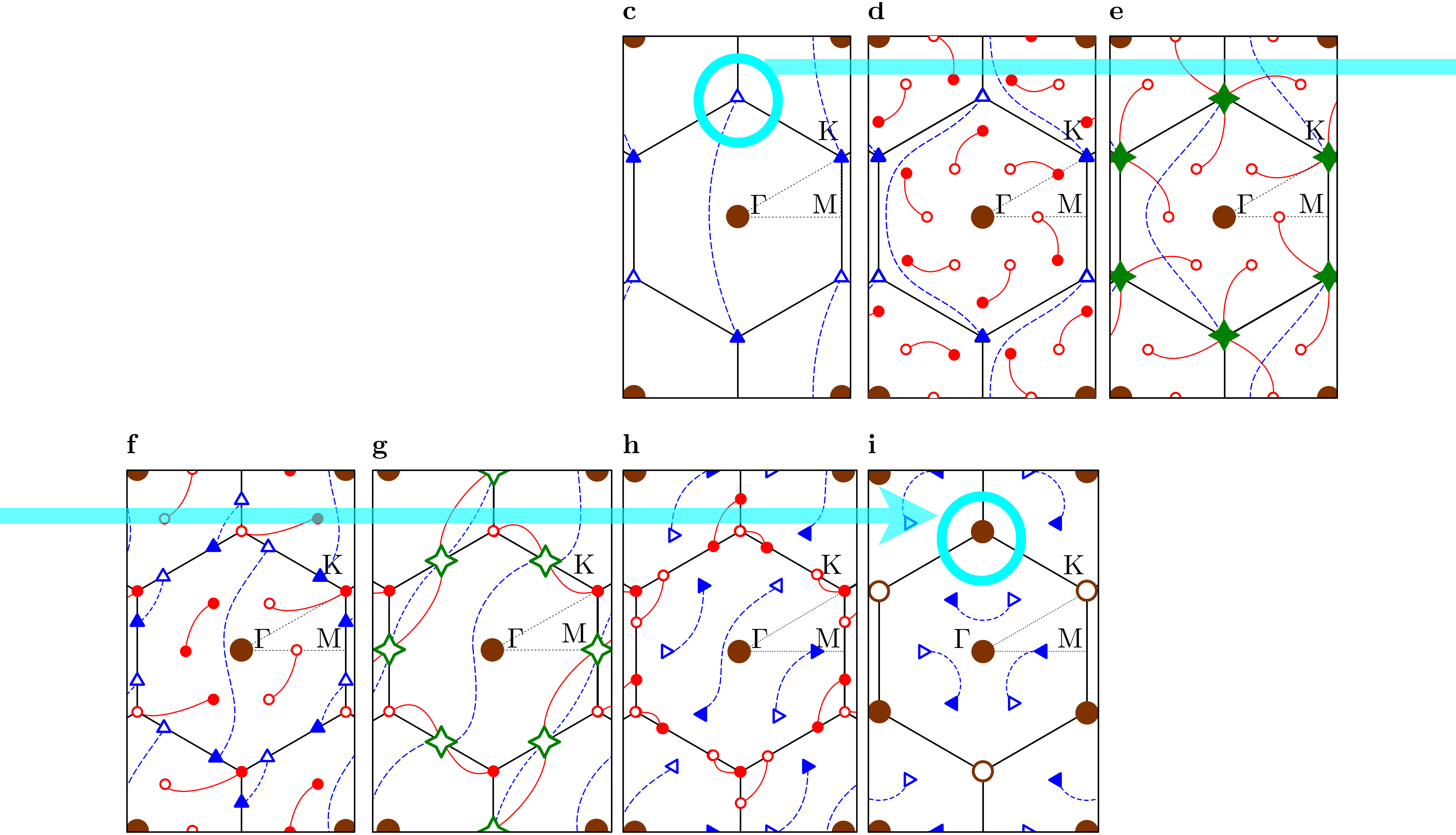
Metamaterial realizations
and
material candidates

Experimental observation of Euler class transition through non-Abelian braiding of nodal points in the kagome lattice



AB, et al Nat. Phys. (2021)

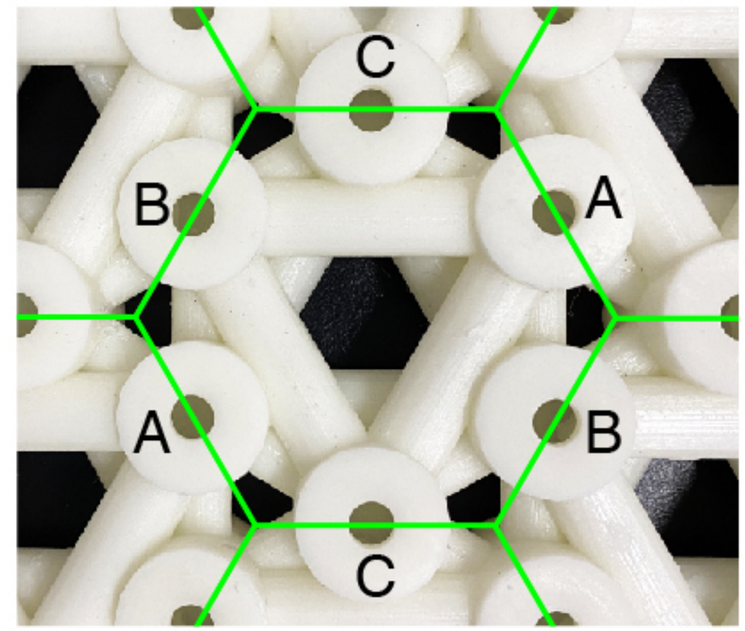
Experimental observation of Euler class transition through non-Abelian braiding of nodal points in the kagome lattice

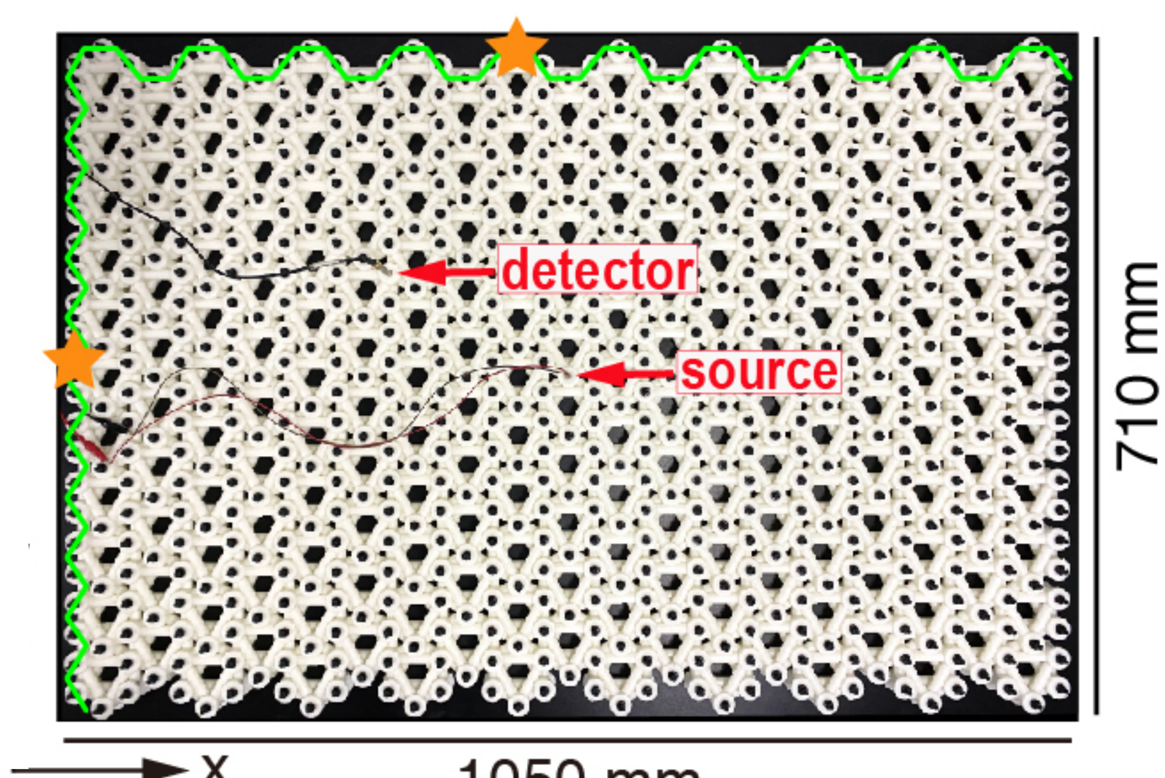


AB, et al Nat. Phys. (2021)

Experimental observation of Euler class transition through non-Abelian braiding of nodal points in the kagome lattice

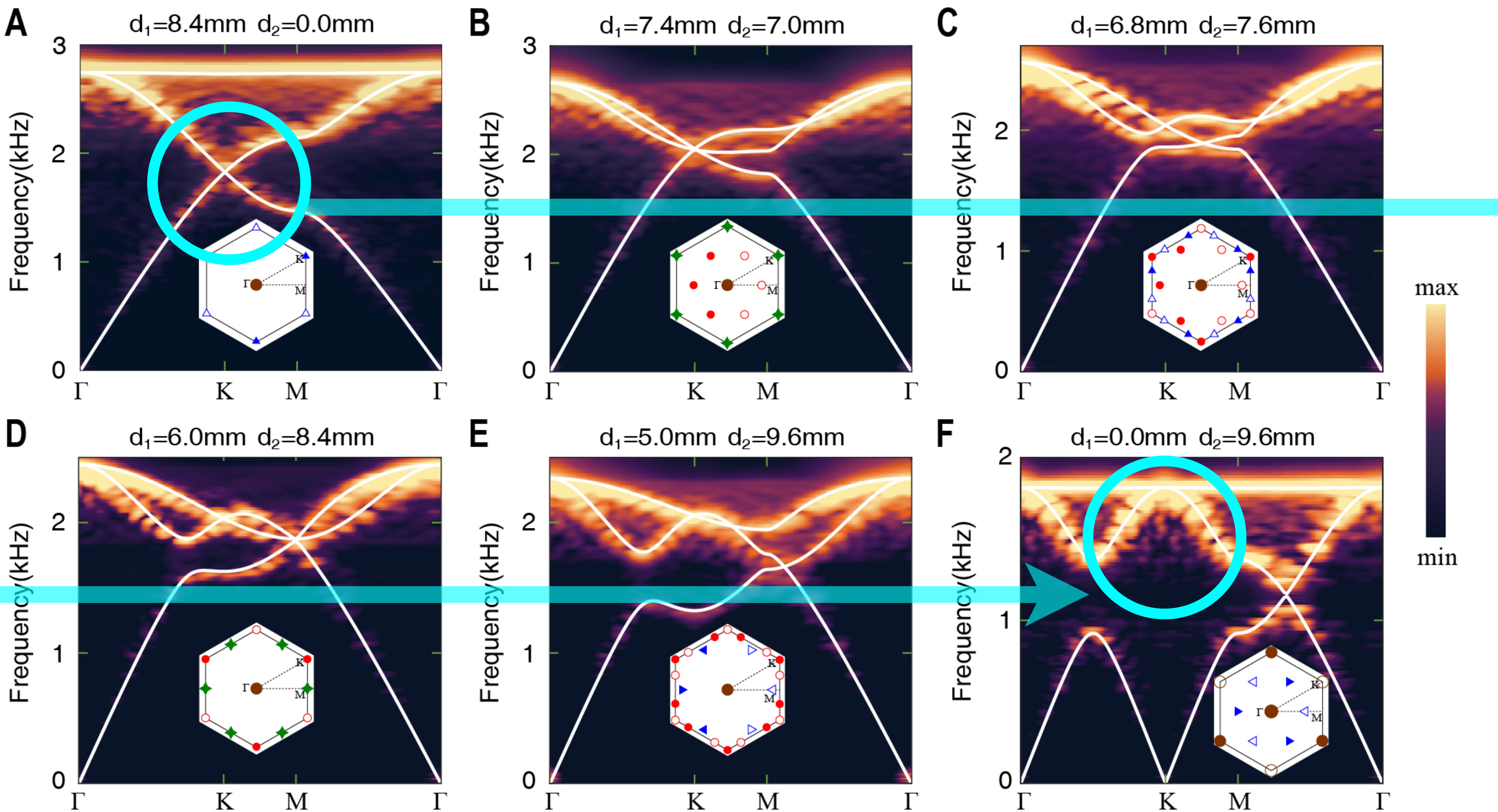
Acoustic metamaterial:





AB, et al Nat. Phys. (2021)

Experimental observation of Euler class transition through non-Abelian braiding of nodal points in the kagome lattice



AB, et al Nat. Phys. (2021)

Real topologies in materials

Monolayer silicate Si_2O_3 under strain and varying eternal electric field

nature COMMUNICATIONS

ARTICLE

Check for updates

https://doi.org/10.1038/s41467-022-28046-9 OPEN

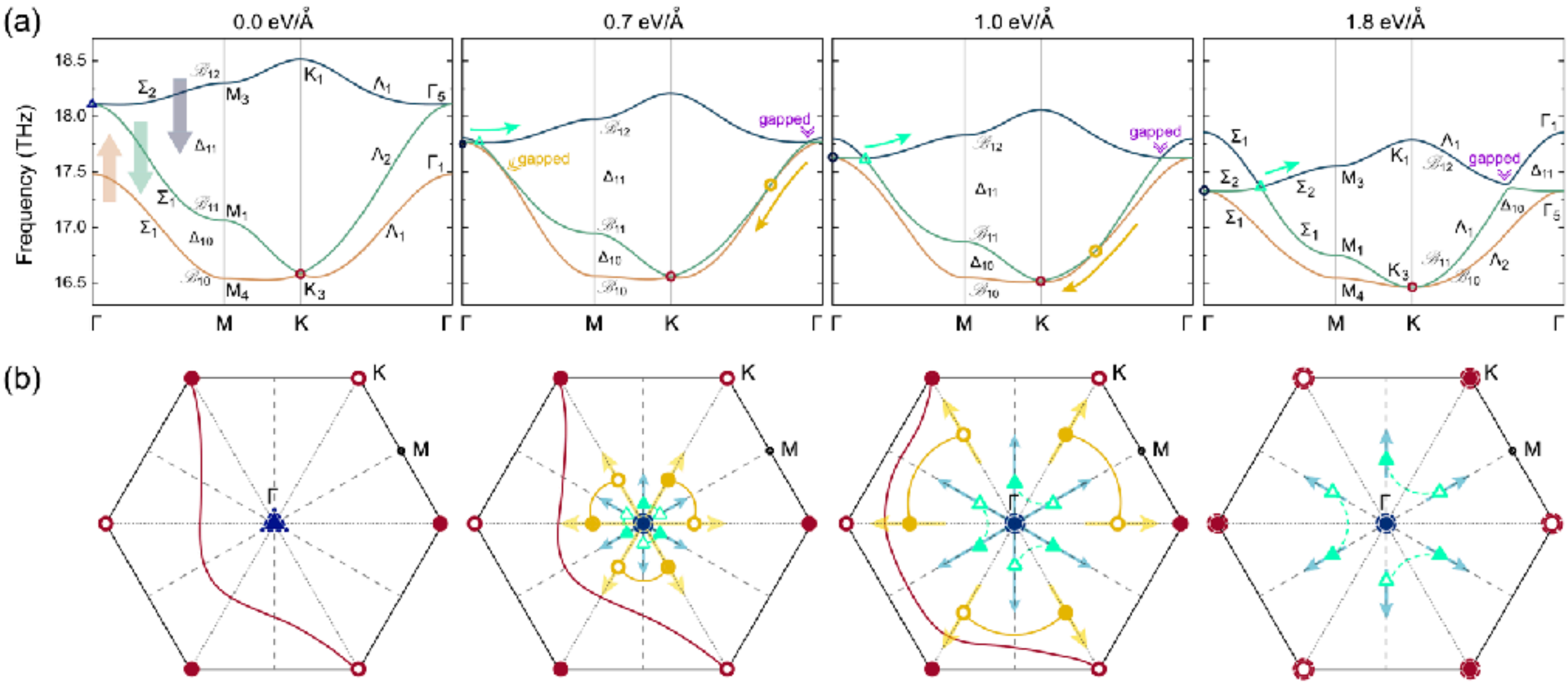
Phonons as a platform for non-Abelian braiding and its manifestation in layered silicates

Bo Peng[1,4]✉, Adrien Bouhon[2,4]✉, Bartomeu Monserrat[1,3,4]✉ & Robert-Jan Slager[1,4]✉

Peng, AB, et al, Nat. Com.

Real topologies in materials

Monolayer silicate Si_2O_3 under strain and varying eternal electric field

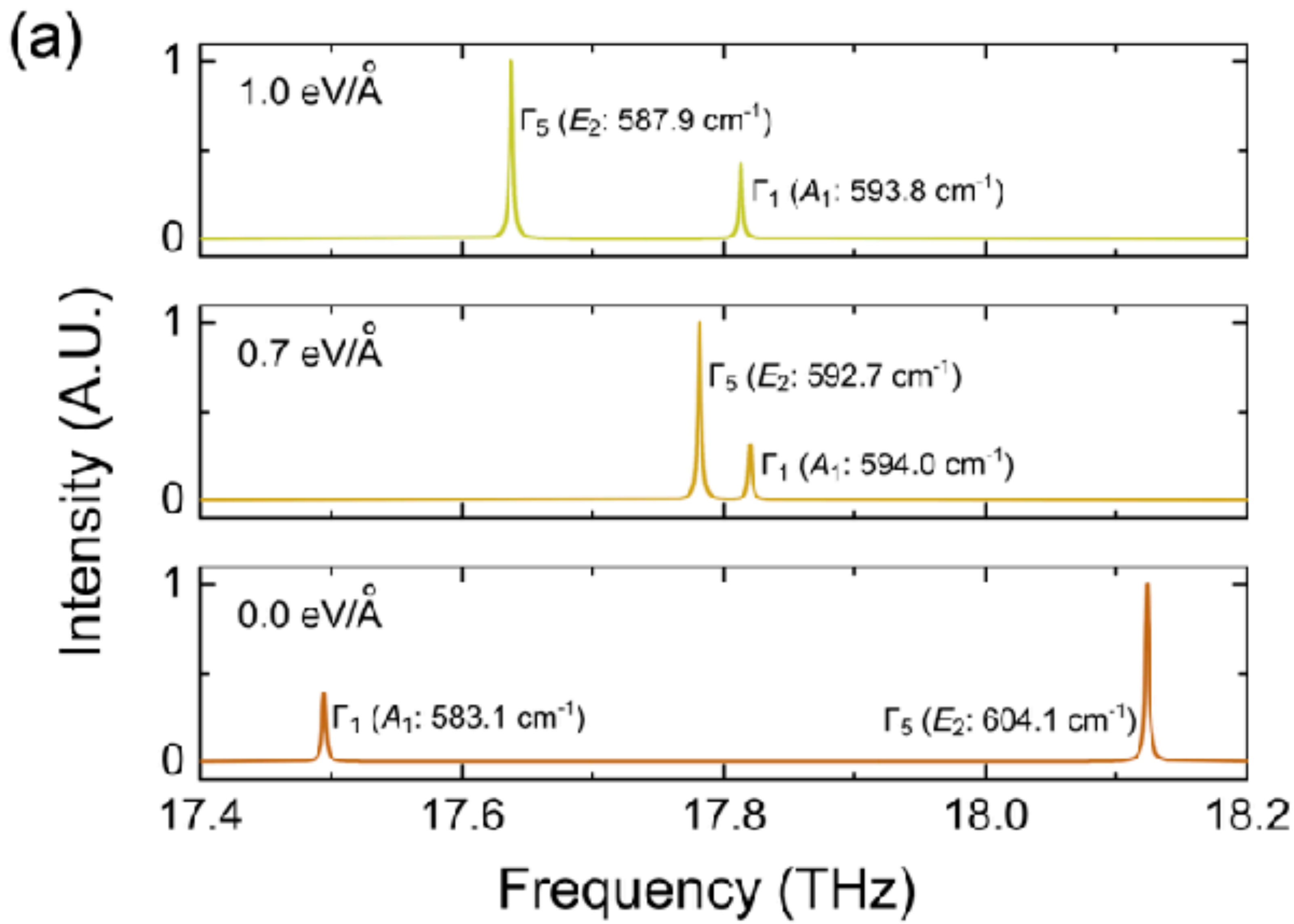


Peng, AB, et al, Nat. Com.

Real topologies in materials

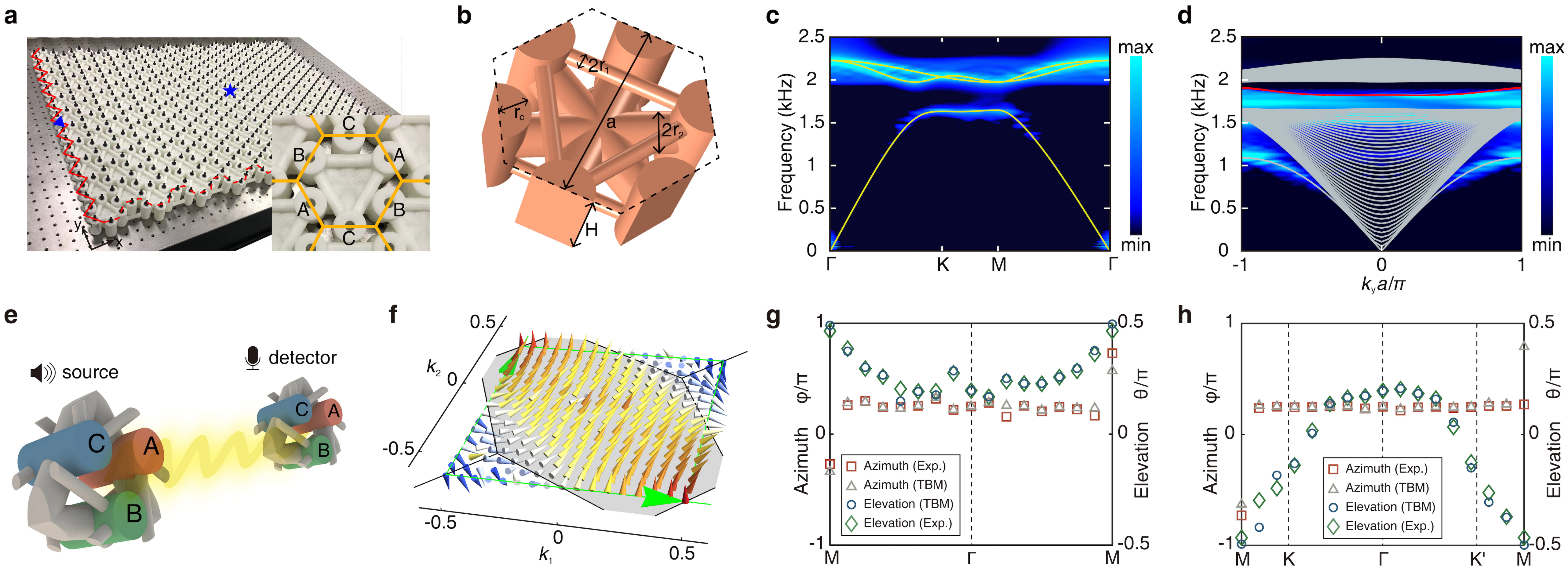
Monolayer silicate Si_2O_3 under strain and varying eternal electric field

Raman scattering spectrum



Peng, AB, et al, Nat. Com.

Gapped kagome phase: meronic Euler insulators



AB, RJ Slager, arxiv:2205.03429

Real topologies in materials

$Cd_2Re_2O_7$
temperature driven
structural phase transition

PHYSICAL REVIEW B **105**, L081117 (2022)

Letter

Non-Abelian braiding of Weyl nodes via symmetry-constrained phase transitions

Siyu Chen,[1,*] Adrien Bouhon,[2,†] Robert-Jan Slager,[1,‡] and Bartomeu Monserrat[1,3,§]

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[2] *Nordic Institute for Theoretical Physics (Nordita), Stockholm University and KTH Royal Institute of Technology, Hannes Alfvéns väg 12, Stockholm SE-106 91, Sweden*

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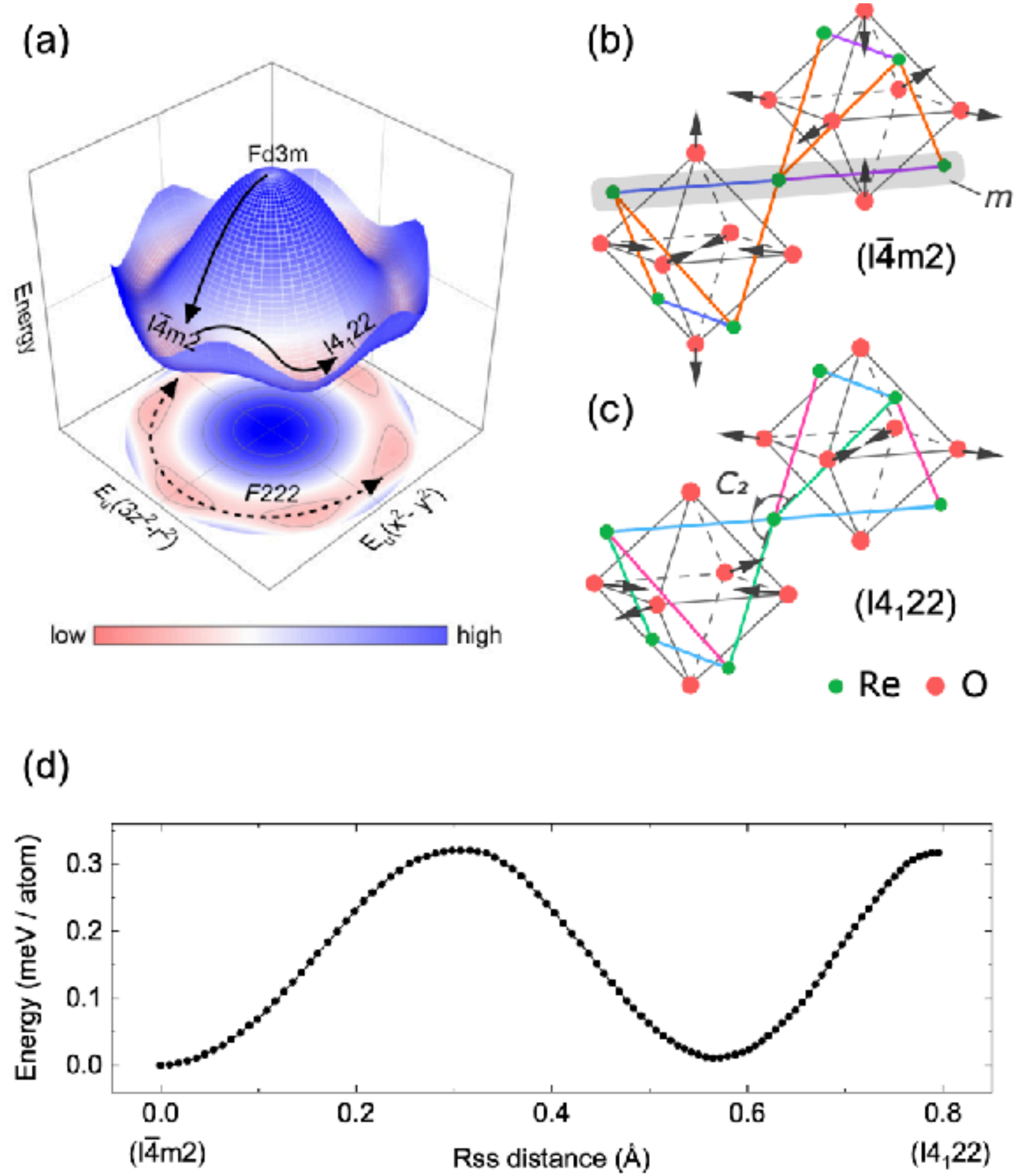
(Received 2 September 2021; accepted 14 February 2022; published 28 February 2022)

Siyu, AB, RJ Slager et al, PRB **105**, L081117

Real topologies in materials

$Cd_2Re_2O_7$
temperature driven
structural phase transition

$$D_{2d} \rightarrow D_4$$

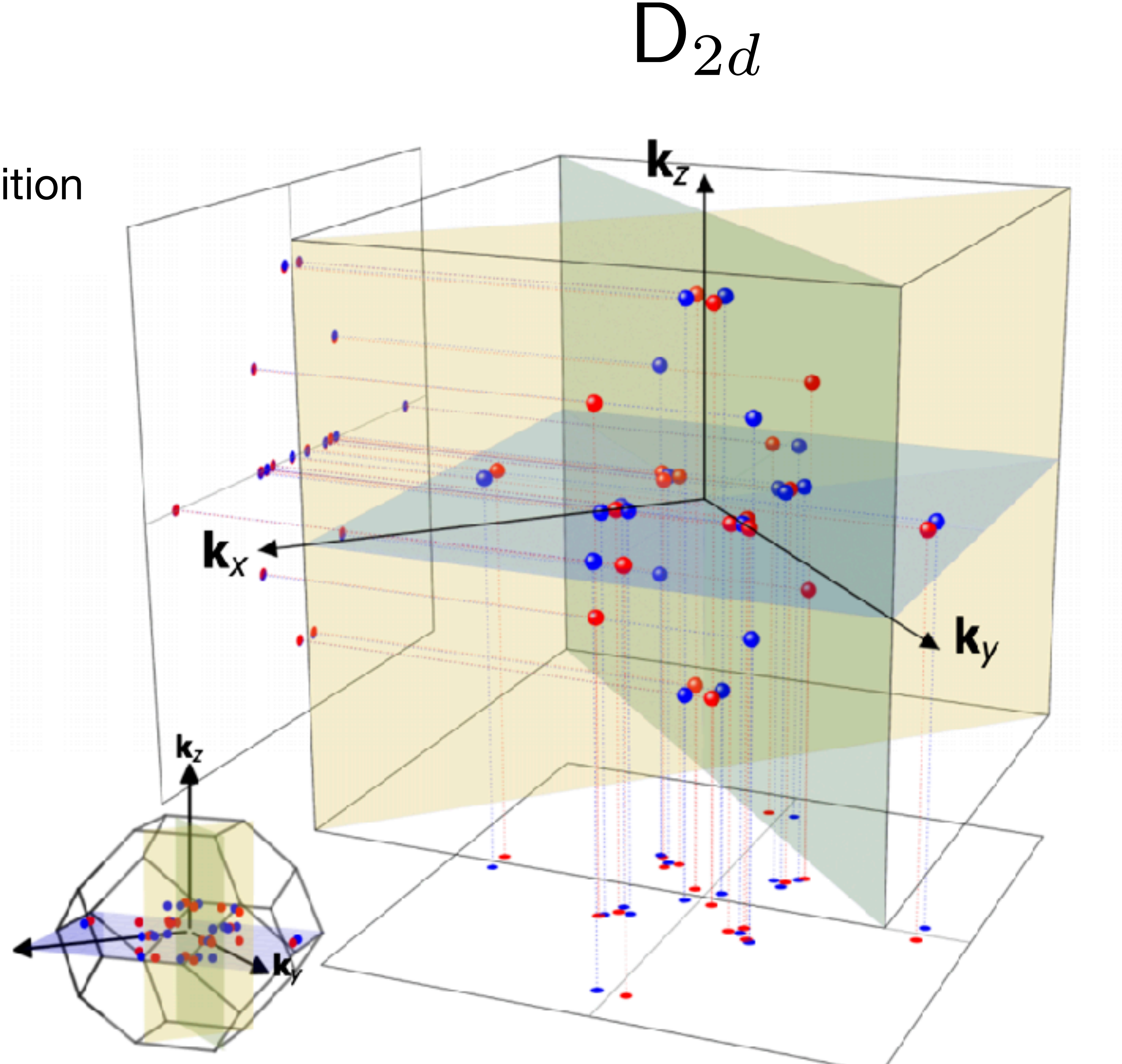


Siyu, AB, RJ Slager et al,

PRB **105**, L081117

Real topologies in materials

$Cd_2Re_2O_7$
temperature driven
structural phase transition



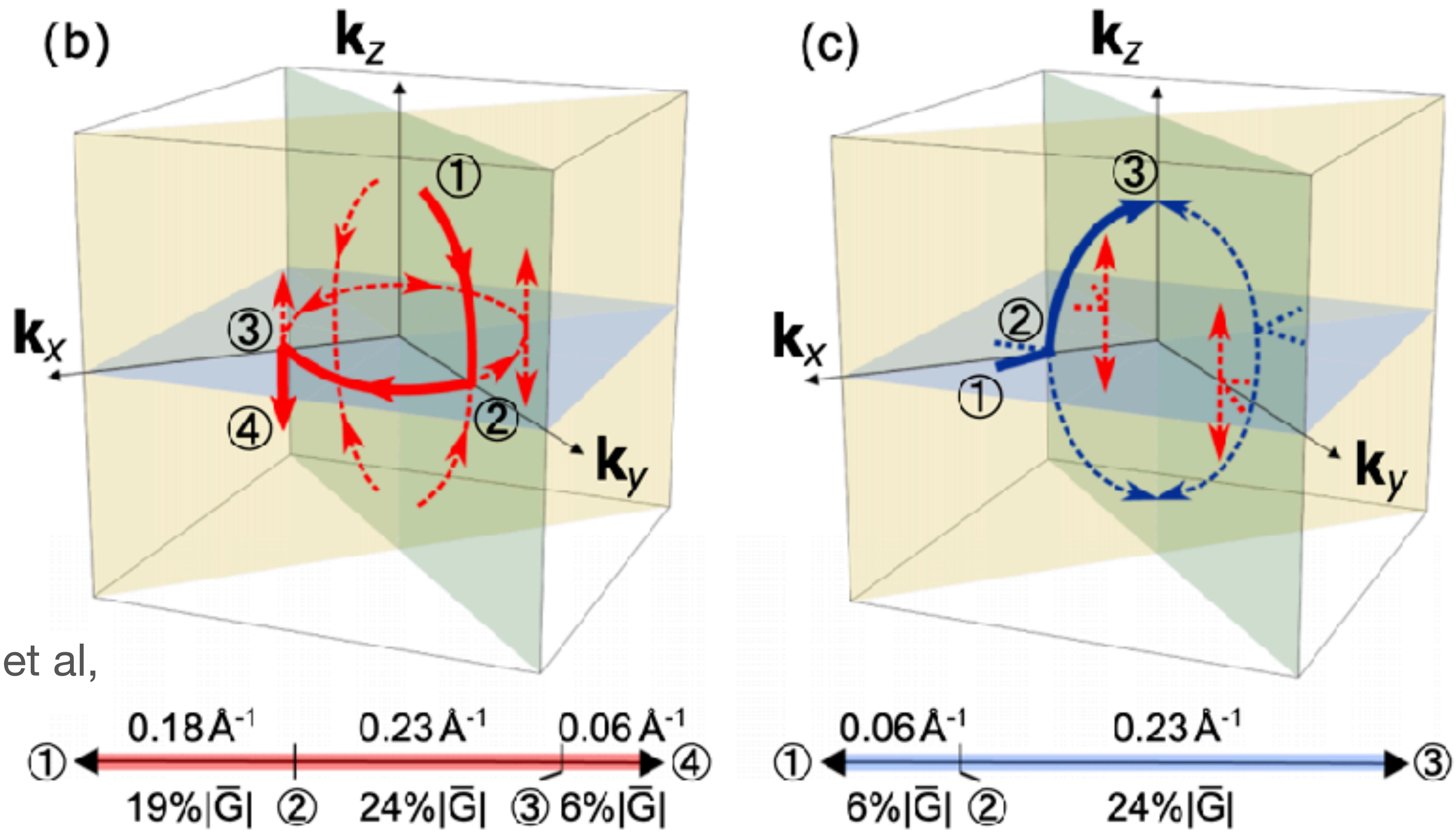
Siyu, AB, RJ Slager et al,

PRB **105**, L081117

Real topologies in materials

$Cd_2Re_2O_7$
temperature driven
structural phase transition

$$D_{2d} \rightarrow D_4$$



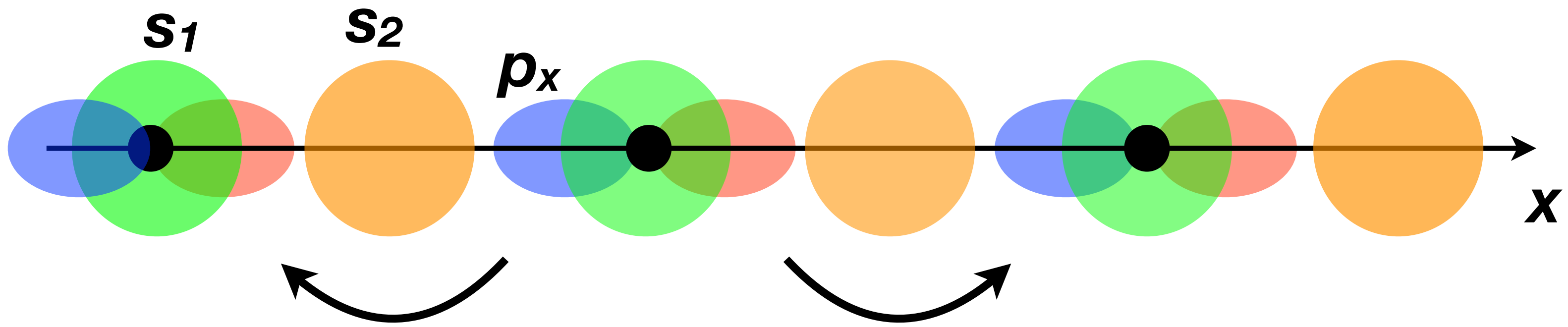
Siyu, AB, RJ Slager et al,

PRB **105**, L081117

Non-Ablian topological gapped phases: intrinsic 1D systems and sub-dimensional contexts

Intrinsic or projected 1D topology

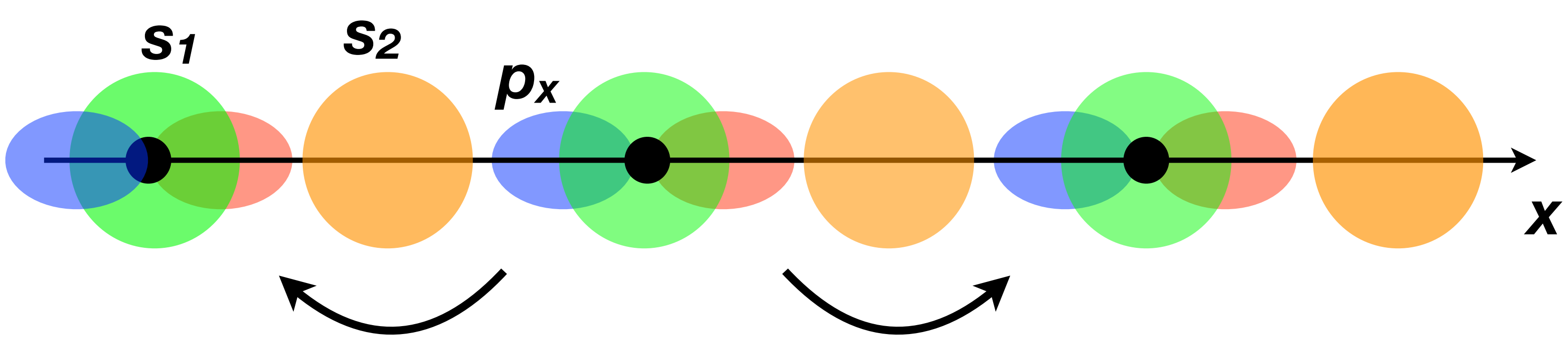
intrinsic: atomic-like orbitals
projected: hybrid Wannier functions



In C_2T (mT, PT) only the unitary part acts on the position operator!

Intrinsic or projected 1D topology

intrinsic: atomic-like orbitals
projected: hybrid Wannier functions



In C_2T (mT, PT) only the unitary part acts on the position operator!

There is a {0,1/2}-quantization of the sub-lattice sites due to C_2T (mT, PT) symmetry

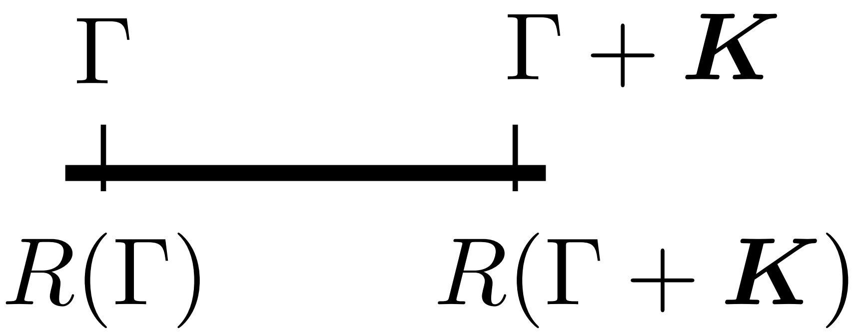
even though C_2 (m,P) is not a symmetry of the Bloch Hamiltonian

This matches the $\{0,\pi\}$-quantization of Zak phase

Only two Wyckoff positons: 1a = center of the 1D unit cell
1b = boundary of the 1D u.c.

Intrinsic or projected 1D topology

Cyclic path in the Brillouin zone



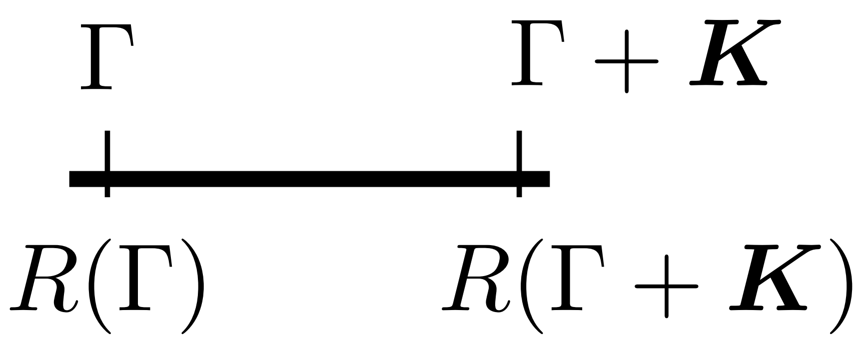
$$\begin{aligned} V(\boldsymbol{K}) &= \mathrm{diag}\left(e^{i\boldsymbol{r}_1\cdot\boldsymbol{K}},\ e^{i\boldsymbol{r}_2\cdot\boldsymbol{K}},\ \cdots\right) \\ &= \mathrm{diag}\left(\pm 1, \pm 1, \cdots\right) \end{aligned}$$

translation sym:

$$V(\boldsymbol{R})H(\boldsymbol{k}+\boldsymbol{K})V(\boldsymbol{K})^{\top} = H(\boldsymbol{k})$$

Intrinsic or projected 1D topology

Cyclic path in the Brillouin zone



$$V(\boldsymbol{K}) = \mathrm{diag}\left(e^{i\boldsymbol{r}_1 \cdot \boldsymbol{K}},\ e^{i\boldsymbol{r}_2 \cdot \boldsymbol{K}},\ \cdots\right) = \mathrm{diag}\left(\pm 1, \pm 1, \cdots\right)$$

translation sym:

$$V(\boldsymbol{R}) H(\boldsymbol{k} + \boldsymbol{K}) V(\boldsymbol{K})^\top = H(\boldsymbol{k})$$

general boundary condition
parallel-transported frame:

$$R_n(\boldsymbol{k} + \boldsymbol{K}) = V(\boldsymbol{K})^\top R_n(\boldsymbol{k}) g_{\boldsymbol{K},nn}$$

parallel-transported
sign flip of the n-th band:

$$g_{\boldsymbol{K},nn} \in \mathsf{O}(1) = \{+1, -1\}$$

Intrinsic or projected 1D topology

Discrete group of all principal C_2 rotations of a rank-N frame:

$$g_{\boldsymbol{K}} = \begin{pmatrix} g_{\boldsymbol{K},11} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & g_{\boldsymbol{K},NN} \end{pmatrix} \in \mathsf{P}_N \quad \subset \mathsf{SO}(N)$$

$g_{\boldsymbol{K},11} \in \pm 1$, $g_{\boldsymbol{K},NN} \in \pm 1$

Classifying space: $\dfrac{\mathsf{O}(N)}{\mathsf{P}_N} = \dfrac{\mathsf{Spin}(N)}{\overline{\mathsf{P}}_N}$ spin double cover

$$\pi_1\left(\mathsf{Fl}_N^{\mathbb{R}}\right) = \overline{\mathsf{P}}_N \quad \subset \mathsf{Spin}(N)$$

Non-Abelian Salingaros group

Intrinsic 1D topology: class of periodic Bloch Hamiltonian

Condition for the quantization of non-Abelian charges:

Existence of a gauge with periodic Bloch Hamiltonian

$$\widetilde{V}(\boldsymbol{K}) \propto \mathbf{1}_N \quad \longrightarrow \quad \widetilde{H}(\boldsymbol{k}+\boldsymbol{K}) = \widetilde{H}(\boldsymbol{k})$$

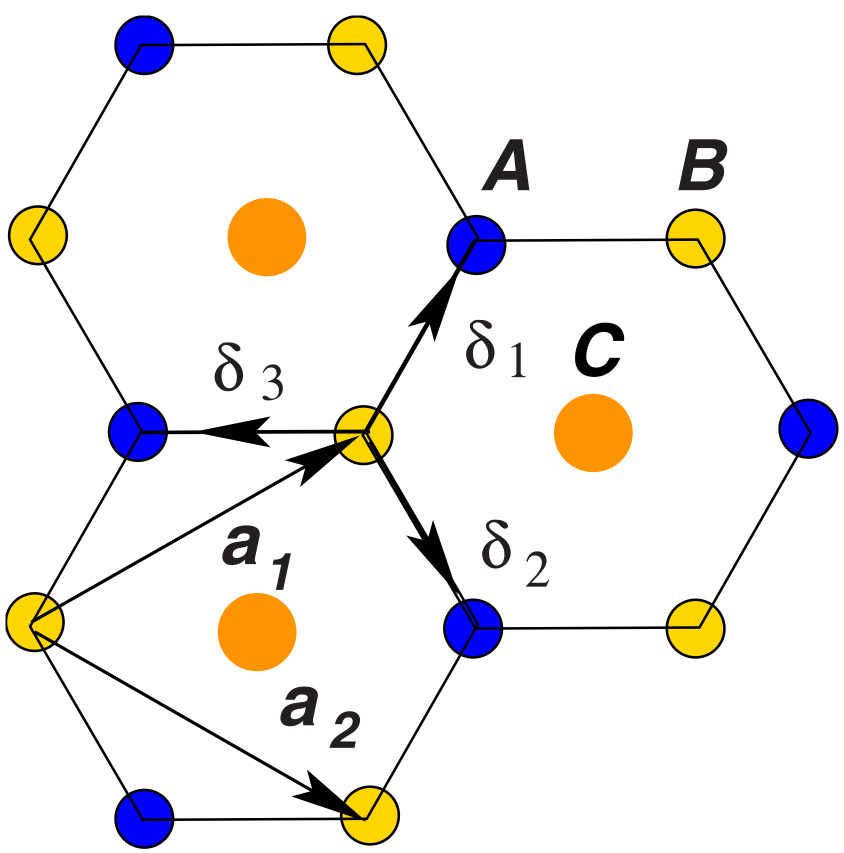
For any pair of orbitals located away from the Brillouin zone center and that are mapped onto-each other under C_2, we do change of gauge:

$$|\phi_a, \boldsymbol{k}\rangle \rightarrow e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_a}|\phi_a \boldsymbol{k}\rangle \qquad a = 1, 2$$

One can readily catalogue all the elementary band representations corresponding to the periodic class

Embedded 1D non-Abelian topology

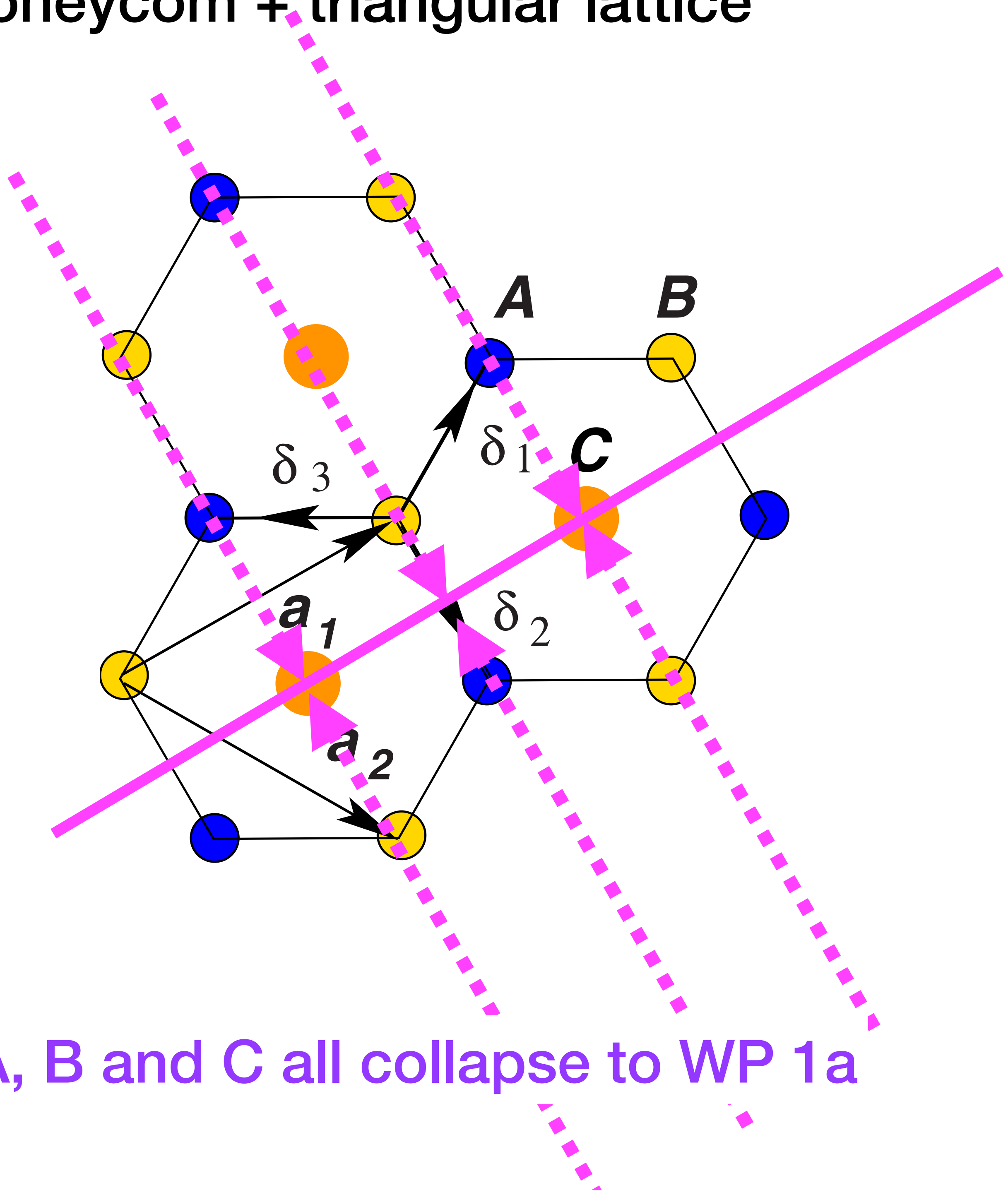
Honeycom + triangular lattice



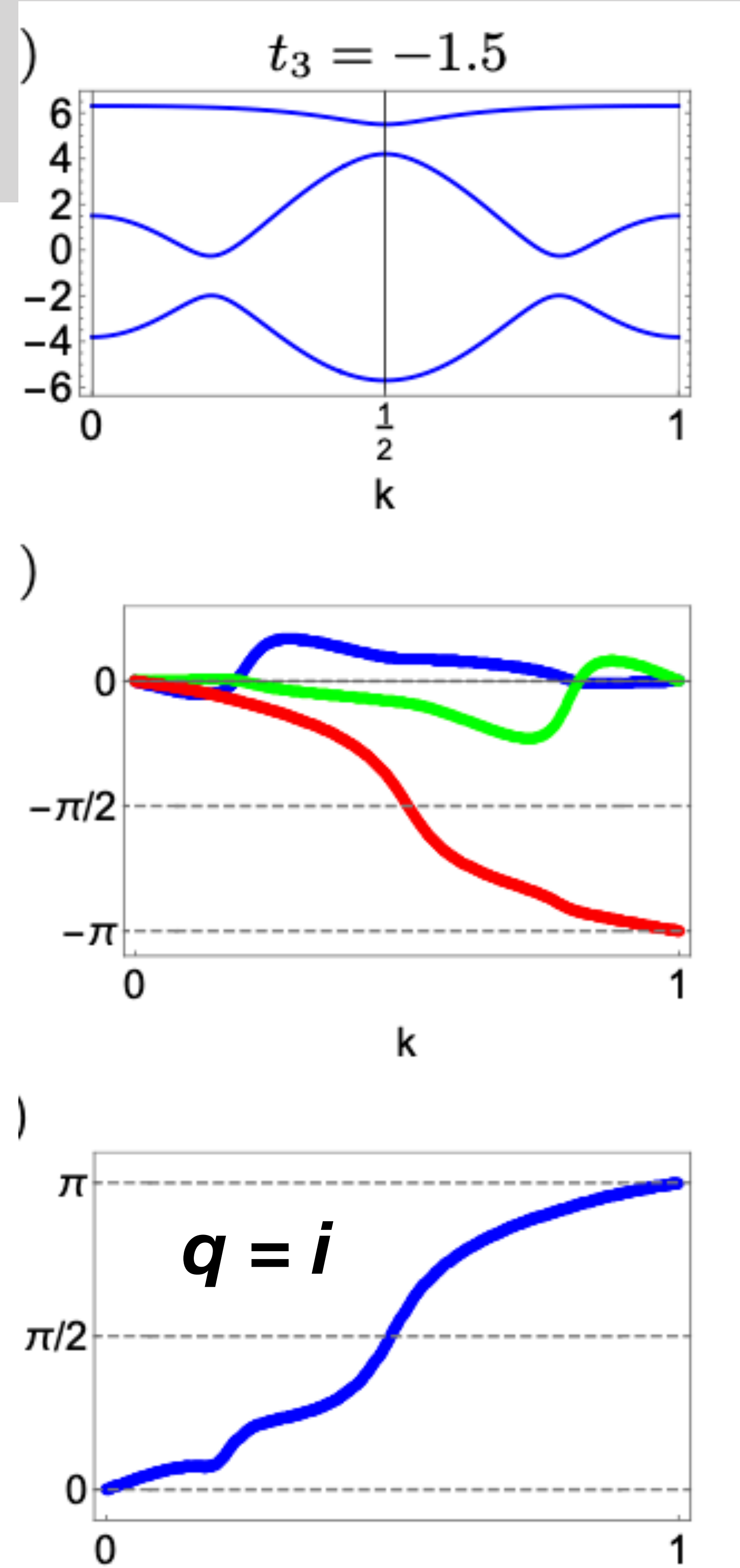
honeycomb sites (***A***,***B***): Wyckoff's position *2b*
triangular sites (***C***): Wyckoff's position *1a*

Embedded 1D non-Abelian topology

Honeycom + triangular lattice

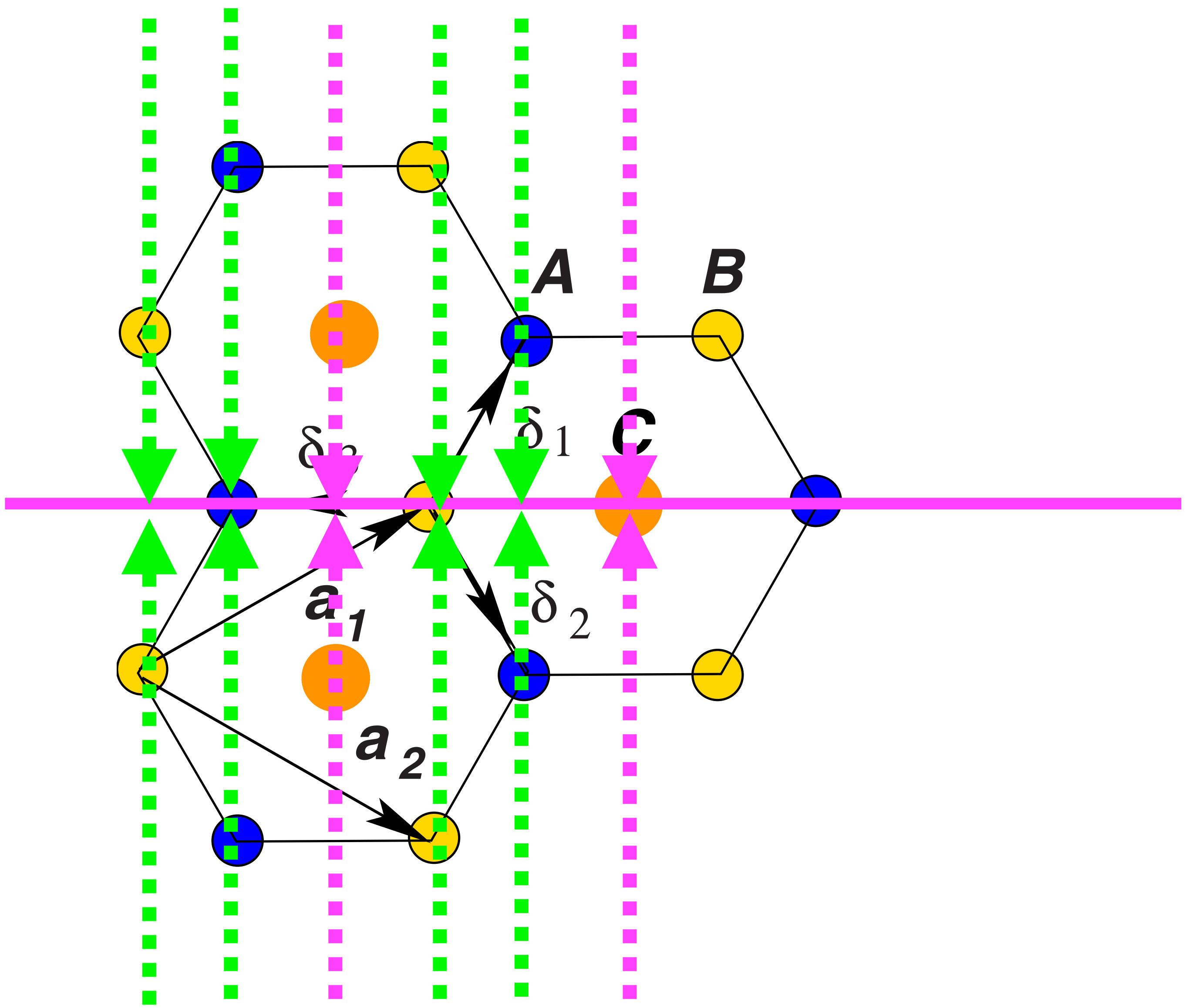


A, B and C all collapse to WP 1a

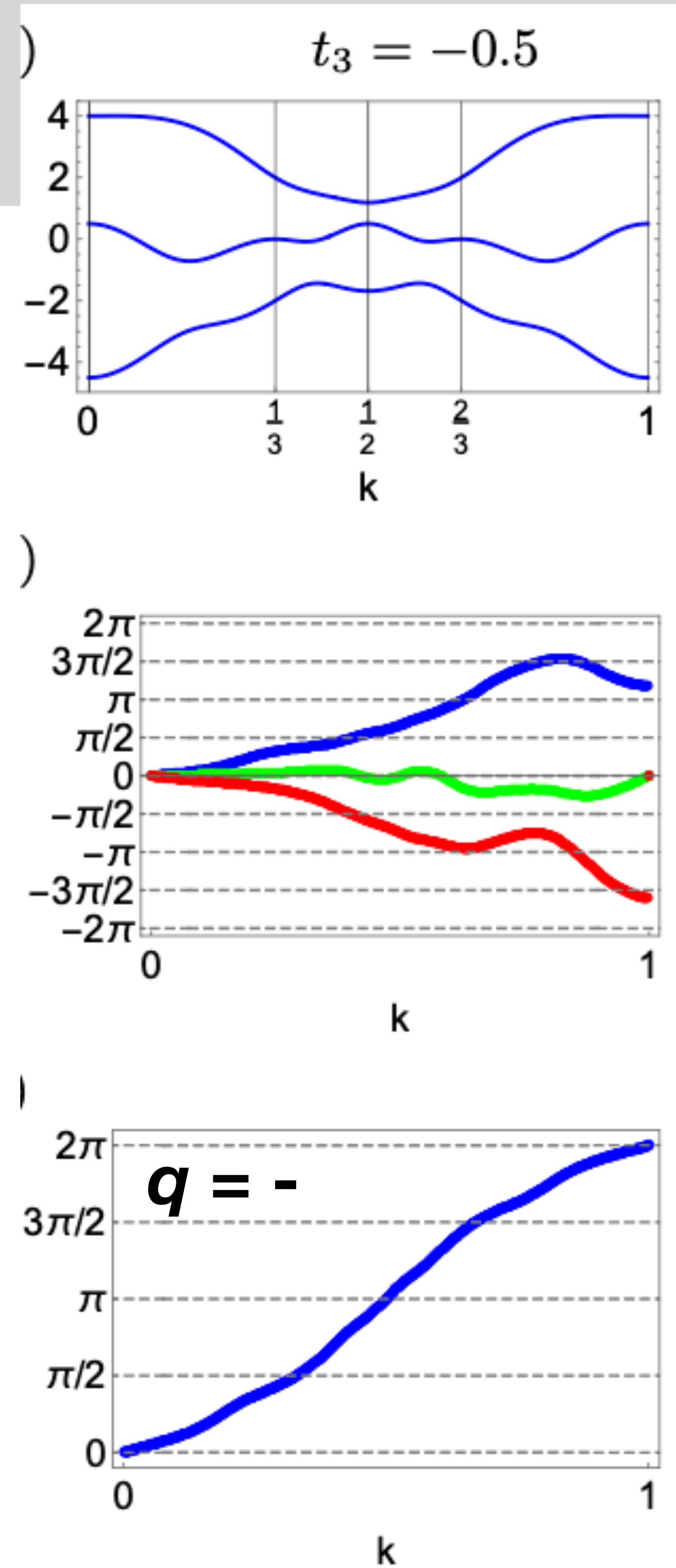


Embedded 1D non-Abelian topology

Honeycom + triangular lattice

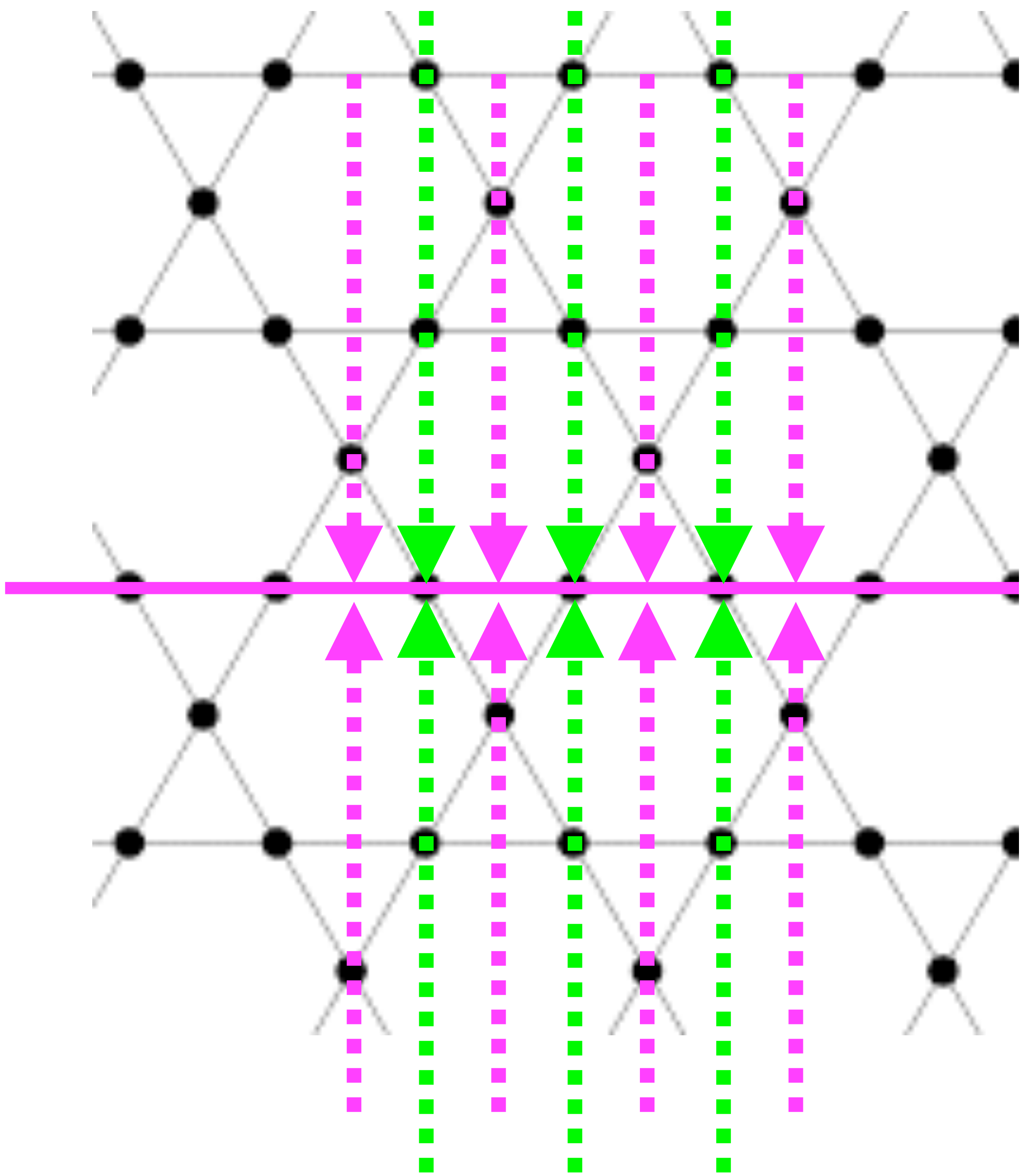


A image of B under C_2

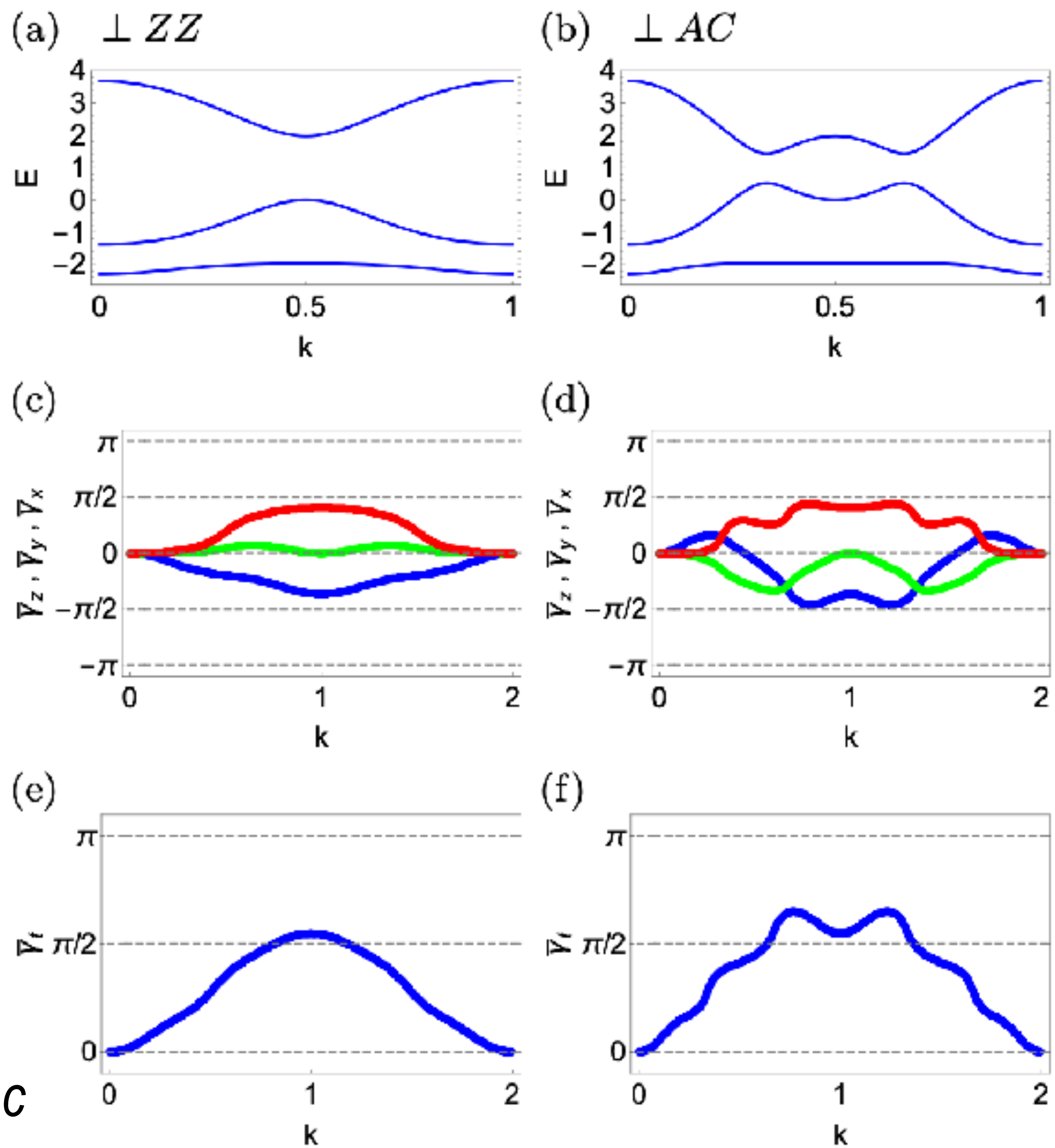


Embedded 1D non-Abelian topology

Kagome lattice

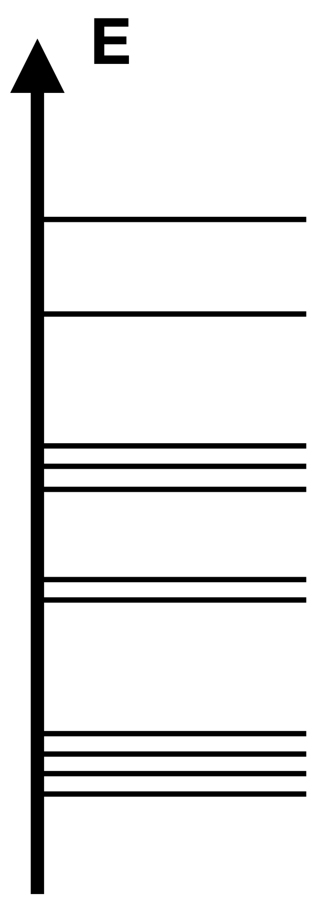


kagome sites: Wyckoff's position 3*c*



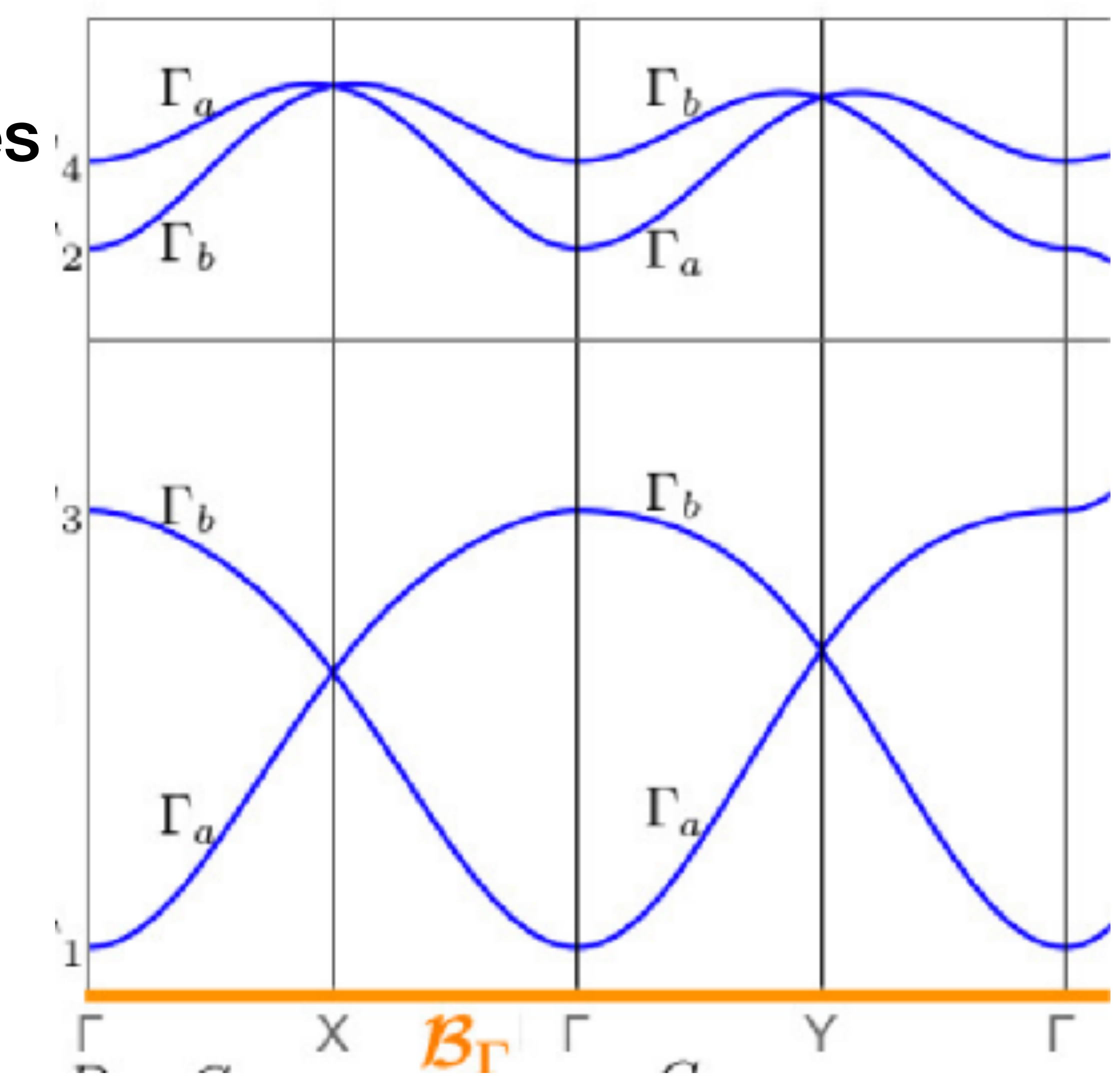
To come

Homotopy theory for generalized flag variety + crystalline symmetries



non-Abelian frame charges

through unfolding bands



Complete catalogue of elementary band representations supporting subdimensional non-Abelian topologies

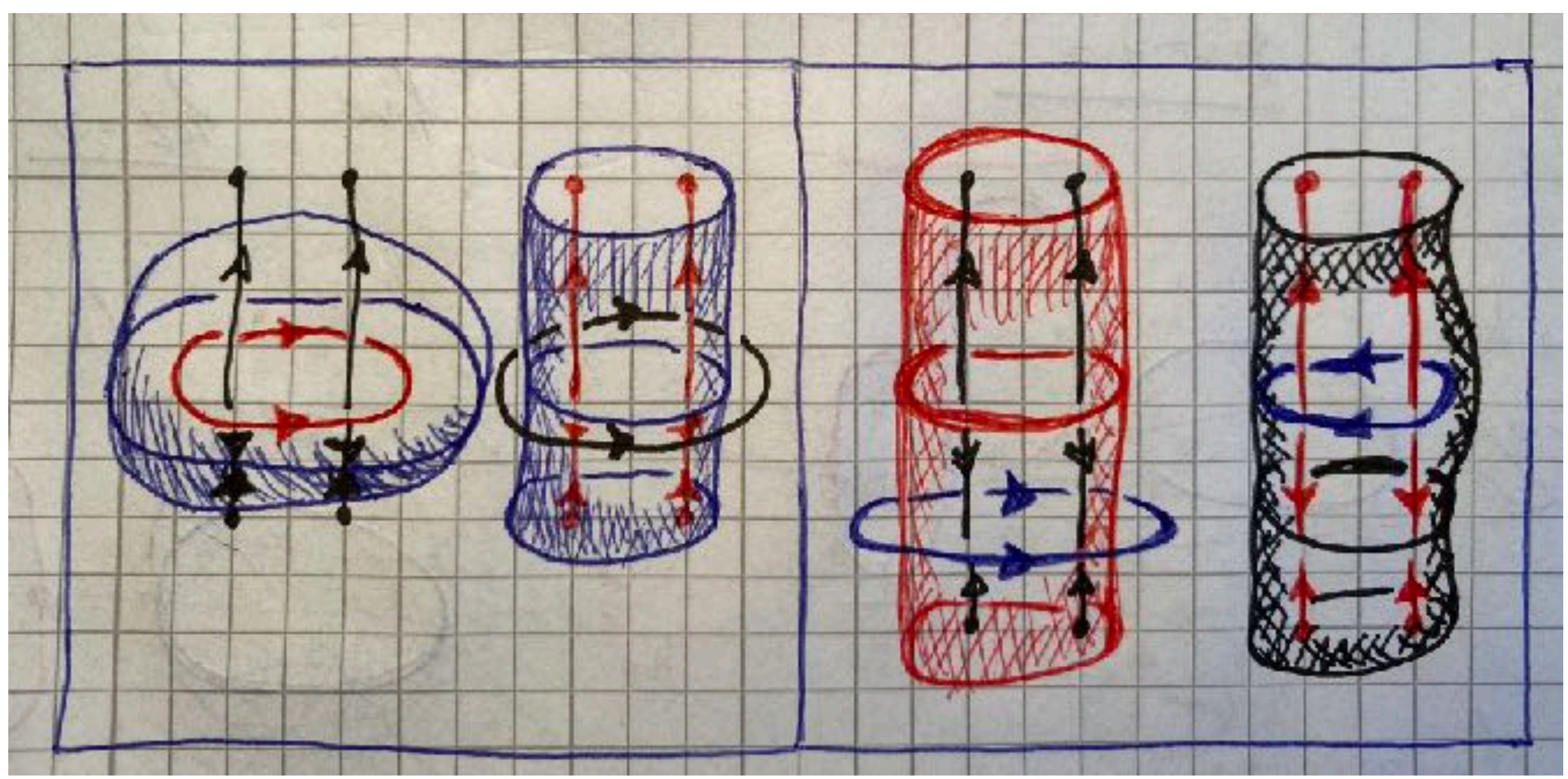
The story goes on…

From gapped Euler phases to stable nodal structures:

- 2D topology: **first** Euler class characterizes
  stable **nodal points** between two bands

- 4D topology: **second** Euler class characterizes
  stable **linked nodal surfaces** between four bands !

Hyperspherical realization of the tangent bundle of the four-sphere:



arxiv:2301.08827

The story goes on…

Nodal rings in 3D PT-symmetric phases:

- Generalized many-band Morse theory for creation/reconnection/annihilation of adjacent topological nodal rings [two-band limit: Murakami]

- Deterministic algorithm for the design of many-band **knotted** nodal rings [two-band limit:]

My collaborators:

Robert-Jan Slager
University of Cambridge

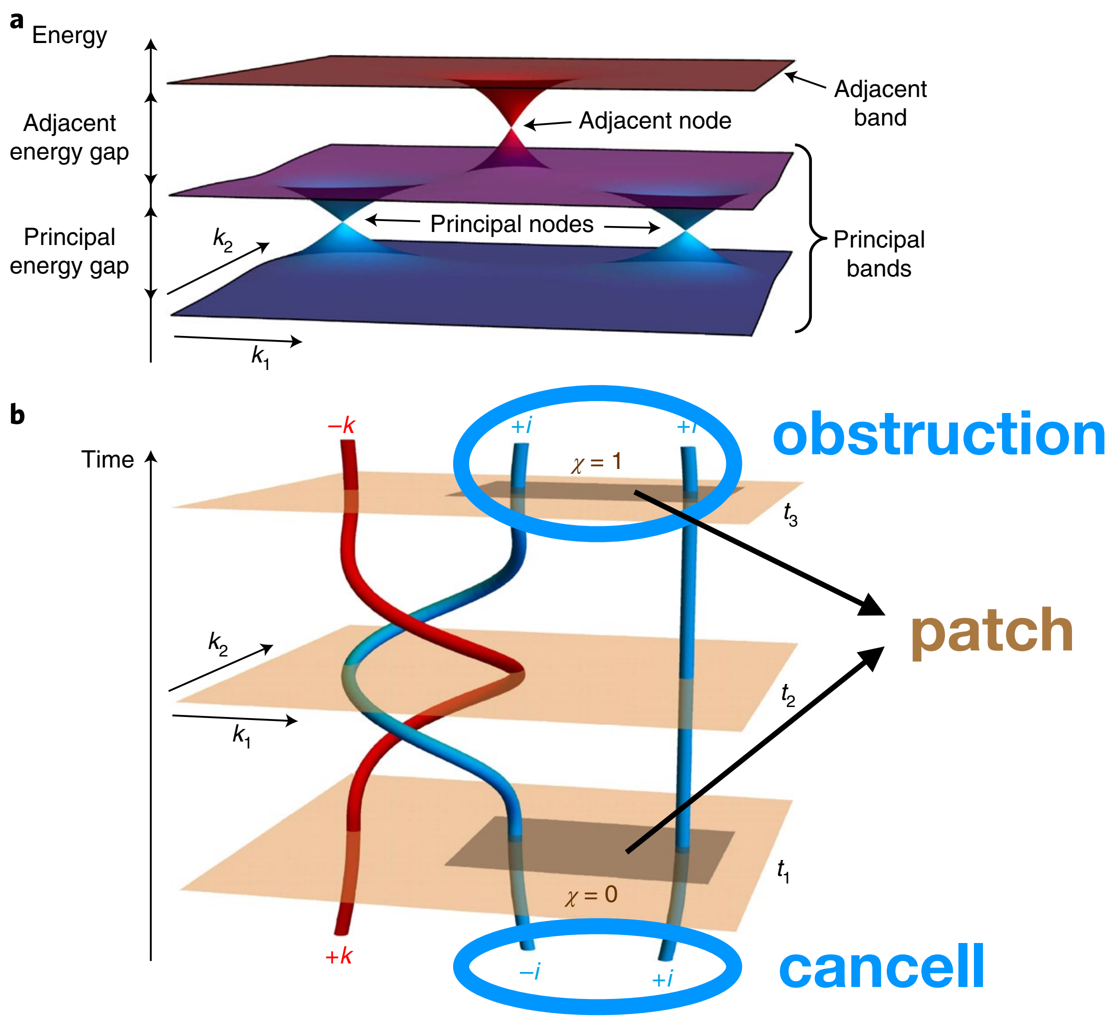
Tomas Bzdusek
University of Zurich

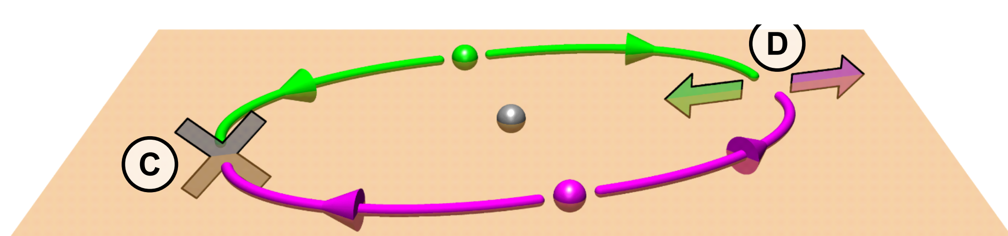
Jian-Hua Jiang
Suzhou University

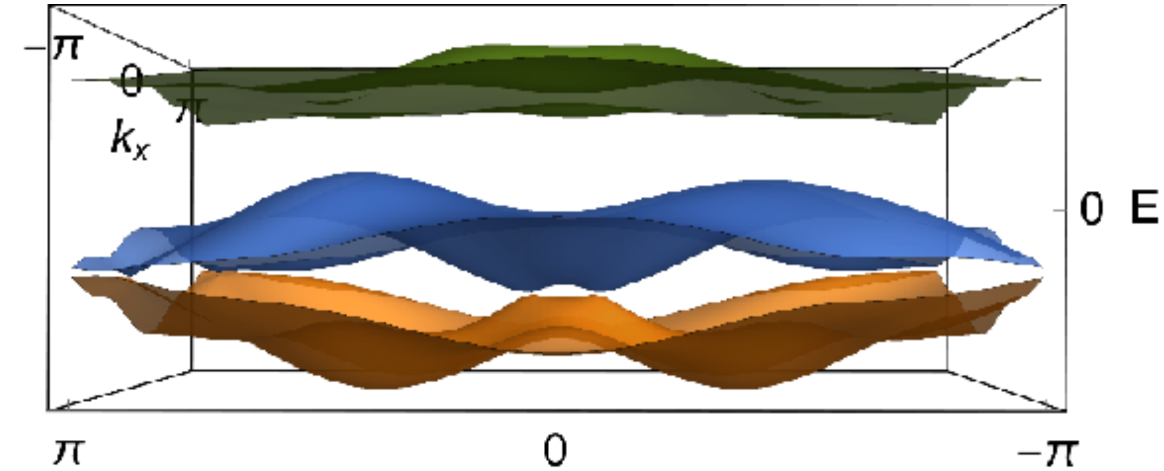
Nur Unal
University of Cambridge

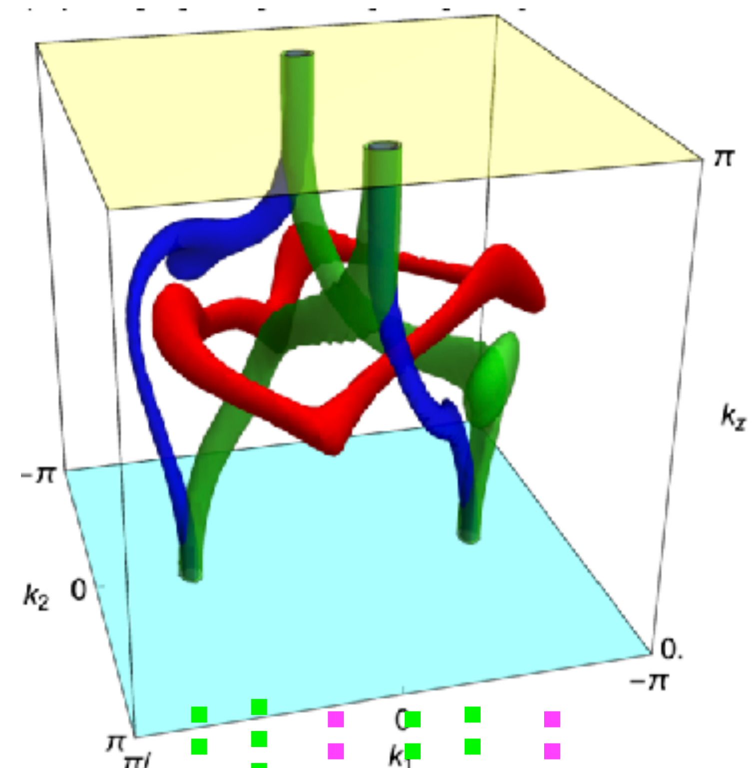
Bartomeu Monserrat
University of Cambridge

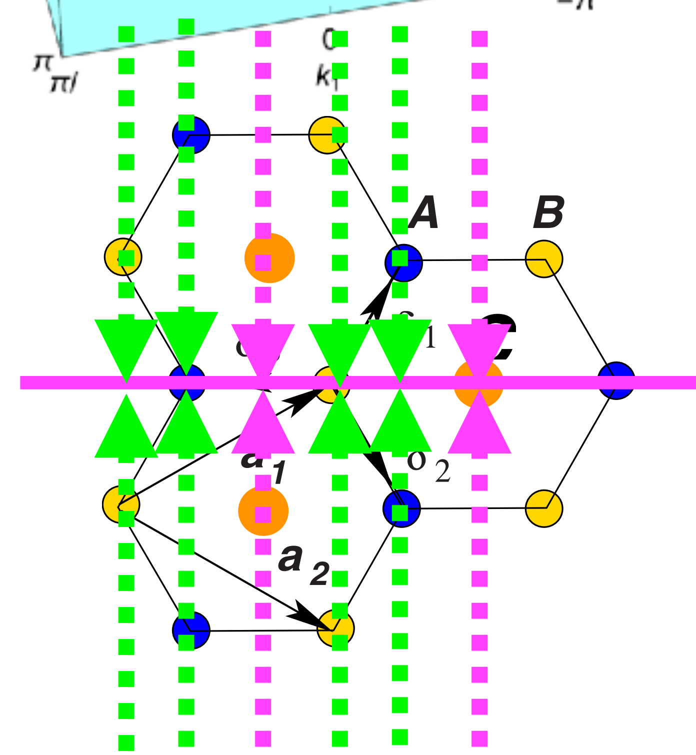
Overview

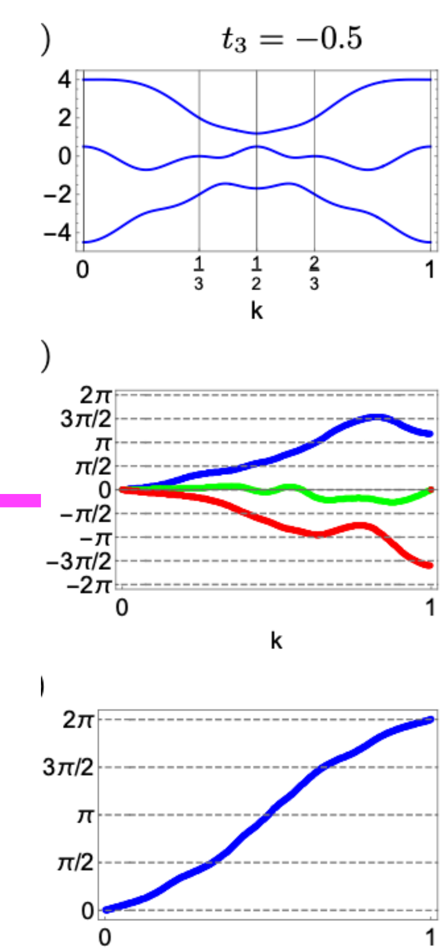

a
Energy
Adjacent energy gap
Principal energy gap
Adjacent node
Adjacent band
Principal nodes
Principal bands
k_1
k_2
b
Time
$-k$
$+k$
$+i$
$-i$
$\chi = 1$
$\chi = 0$
t_1
t_2
t_3
obstruction
patch
cancell


C
D


$-\pi$
0
k_x
0 E
π
0
$-\pi$


π
k_z
$-\pi$
k_2
0
$-\pi$
k_1


A
B
a_1
a_2


$t_3 = -0.5$
4
2
0
-2
-4
k
2π
$3\pi/2$
π
$\pi/2$
0
$-\pi/2$
$-\pi$
$-3\pi/2$
-2π
k

Real topologies

Anti-unitary symmetry $\mathcal{A} = U\mathcal{K}$ such that $\mathcal{A}^2 = +\mathbf{1}$

and $\mathcal{A}\,\bar{\boldsymbol{k}} = \bar{\boldsymbol{k}}$

there exists a gauge with $H(\bar{\boldsymbol{k}}) \to \widetilde{H}(\bar{\boldsymbol{k}})^* = \widetilde{H}(\bar{\boldsymbol{k}})$

3D	spinless ***PT*** symmetry	Linked nodal rings
2D	spinful or spinless $\boldsymbol{C_2T}$ symmetry, ***PT***	Euler insulators
1D	spinful or spinless ***mT*** symmetry, $\boldsymbol{C_2T}$, ***PT***	Non-Abelian top
4D	spinless ***PT*** symmetry	Second Euler insulators

1.5D and 2D multi-gap topology:

Non-Abelian braiding of Weyl nodes, Euler insulators

1.5D topology of three-level system

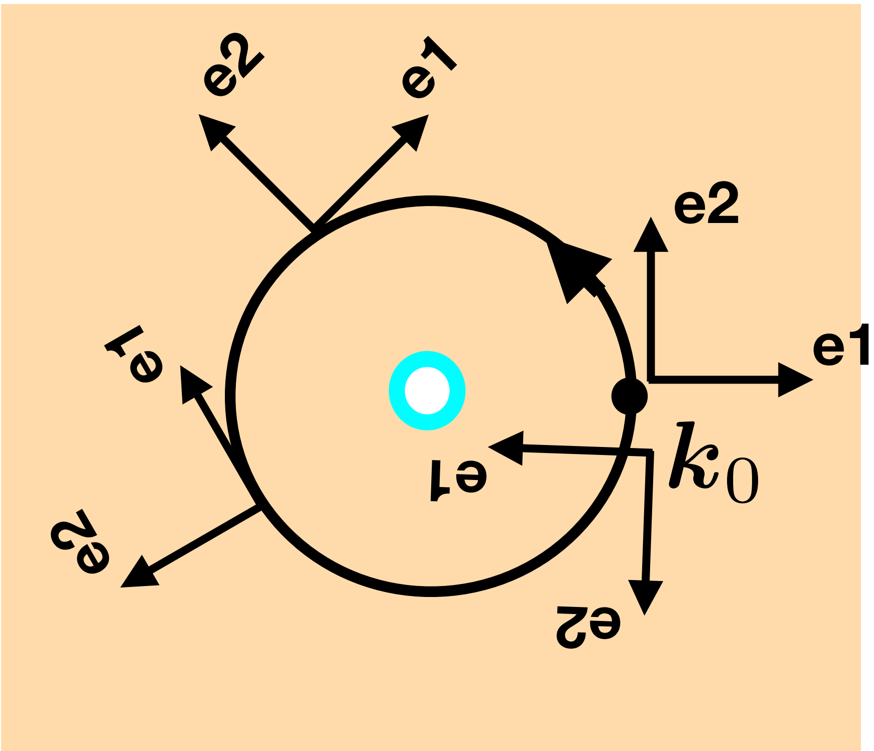
$$\widetilde{H}(\boldsymbol{k}) = R(\boldsymbol{k})\mathcal{E}(\boldsymbol{k})R^T(\boldsymbol{k}) \qquad R(\boldsymbol{k}) = (\boldsymbol{e}_1\ \boldsymbol{e}_2\ \boldsymbol{e}_3)$$

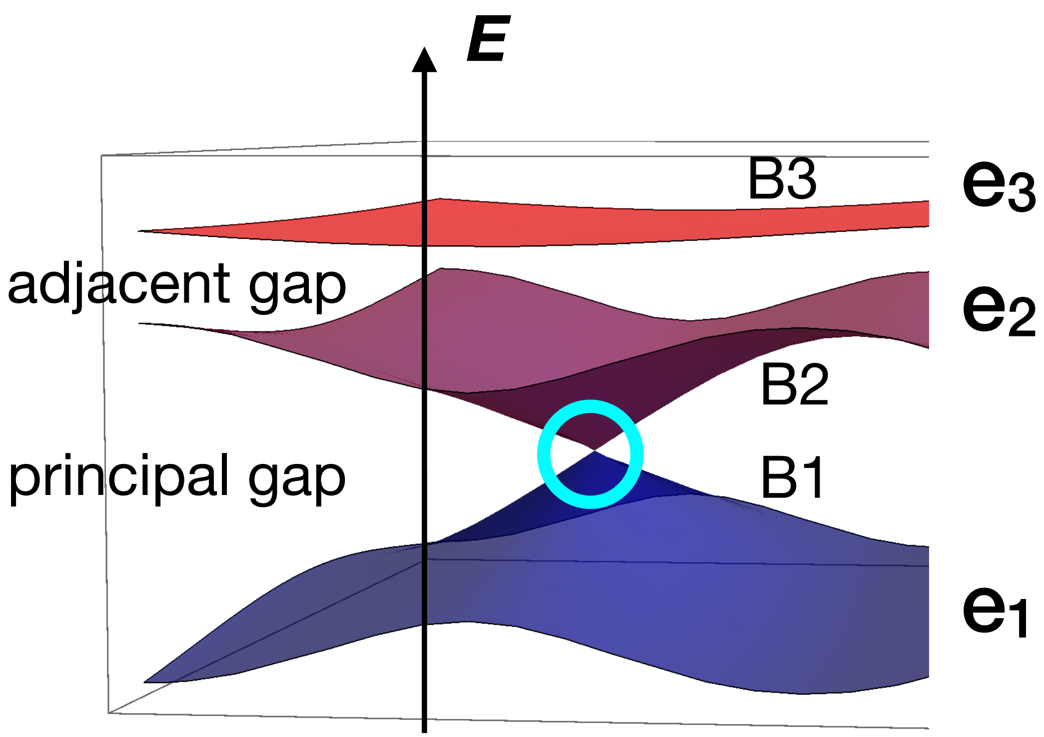
$$\pi_1\left(\frac{\mathsf{SO}(3)}{\{e, C_{2z}\}}\right) = \mathbb{Z}_2$$

{0,π}-Berry phase,

presence of a single NP

π-frame rotation around e3





Ambiguity of the parallel transported SO(N)-frame
Lift to spin double cover

$$\mathsf{D}_2 \hookrightarrow \mathsf{SO}(3) \to \mathsf{SO}(3)/\mathsf{D}_2$$

Frame connection: $\mathcal{A} = R^\top(\boldsymbol{k}) \cdot dR(\boldsymbol{k})$

Holonomy element: $F(\boldsymbol{k}) = \overline{\exp}\left\{\int_0^{\boldsymbol{k}} \mathcal{A}\right\} = e^{A(\boldsymbol{k})}$

$$F(\ell) = \overline{\exp}\left\{\int_\ell \mathcal{A}\right\} = e^{\overline{A}(\ell)} \in P_N$$

$$\overline{F}(\ell) = \overline{\exp}\left\{\int_\ell \overline{\mathcal{A}}\right\} = e^{\overline{A}(\ell)} \in \overline{P}$$

$$\overline{\mathsf{D}}_2 \hookrightarrow \mathsf{Spin}(3) \to \mathsf{Spin}(3)/\overline{\mathsf{D}}_2$$

2D multi-gap topology:

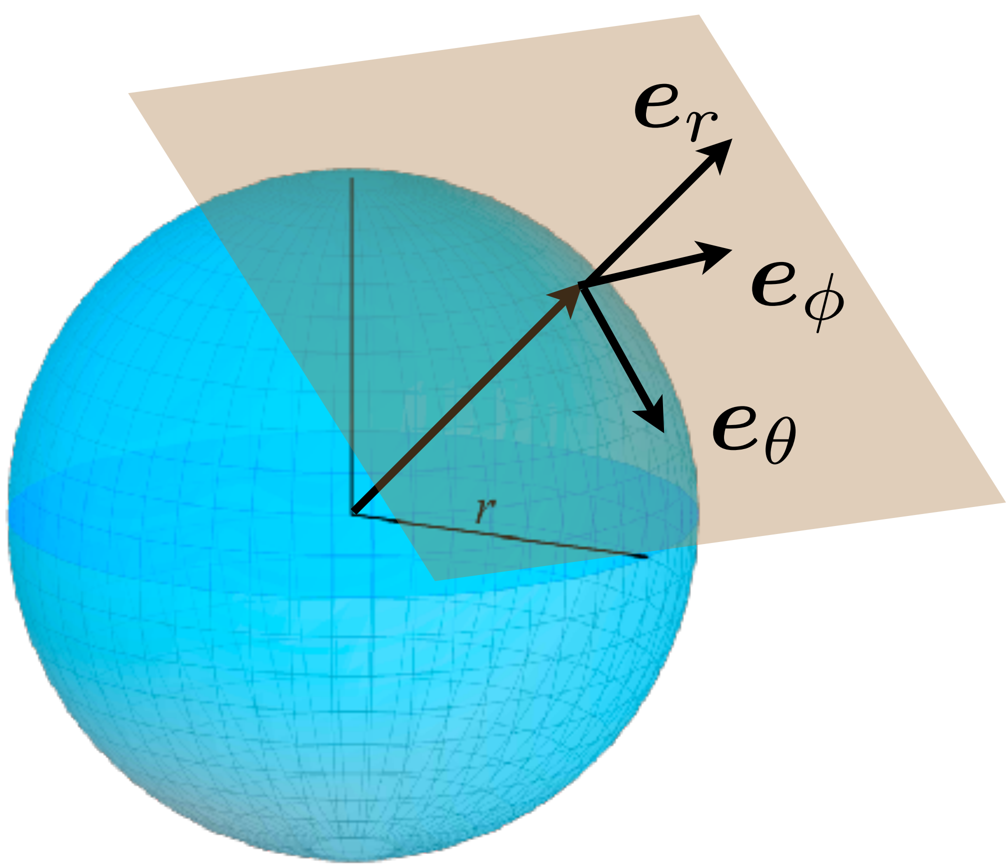
two-band Euler class and stable nodes

Tangent bundle of the sphere

Hairy ball theorem:

combing a hairy ball lead to vortices!

$$T\mathbb{S}^2$$



Tangent bundle of the sphere

Hairy ball theorem:

combing a hairy ball lead to vortices!

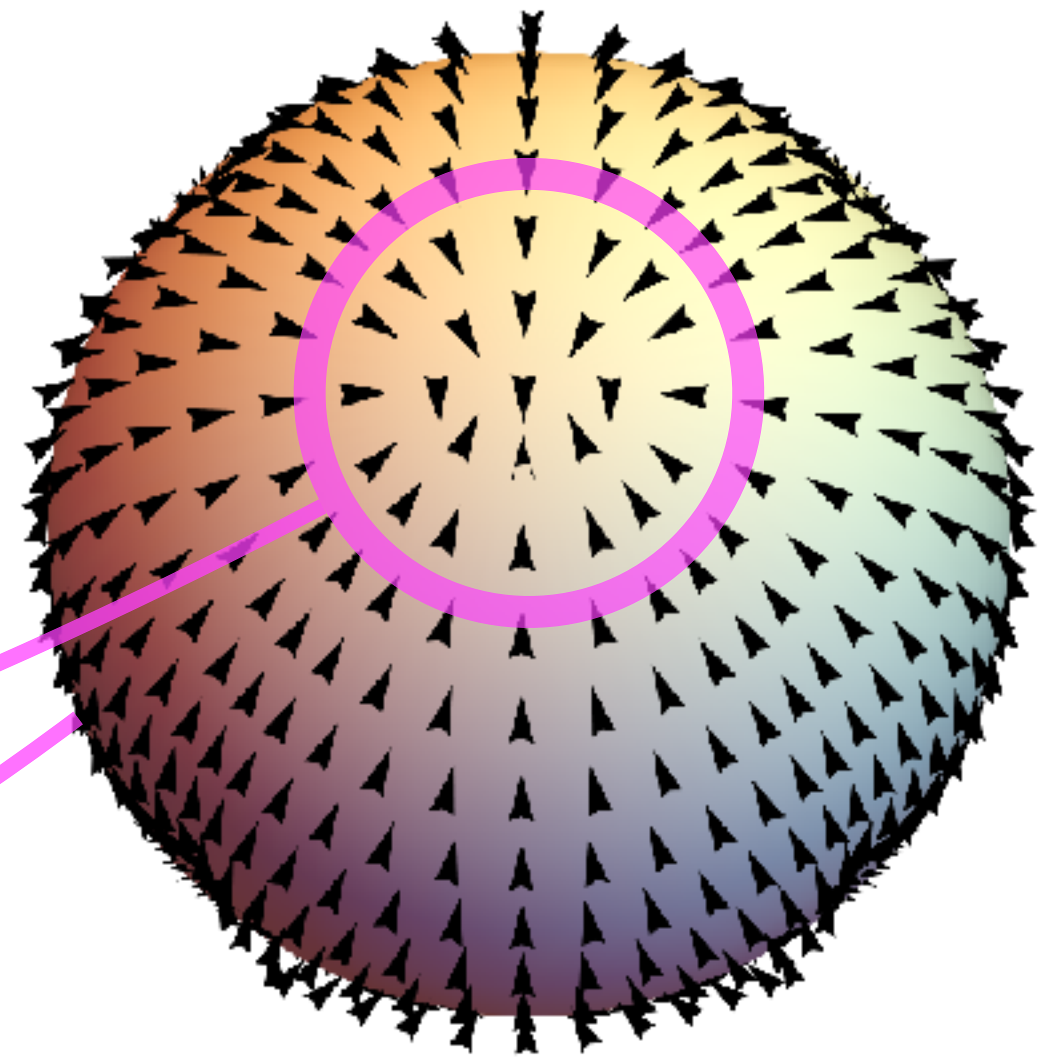
$$T\mathbb{S}^2$$

Poincaré-Hopf (Gauss-Bonnet) theorem:

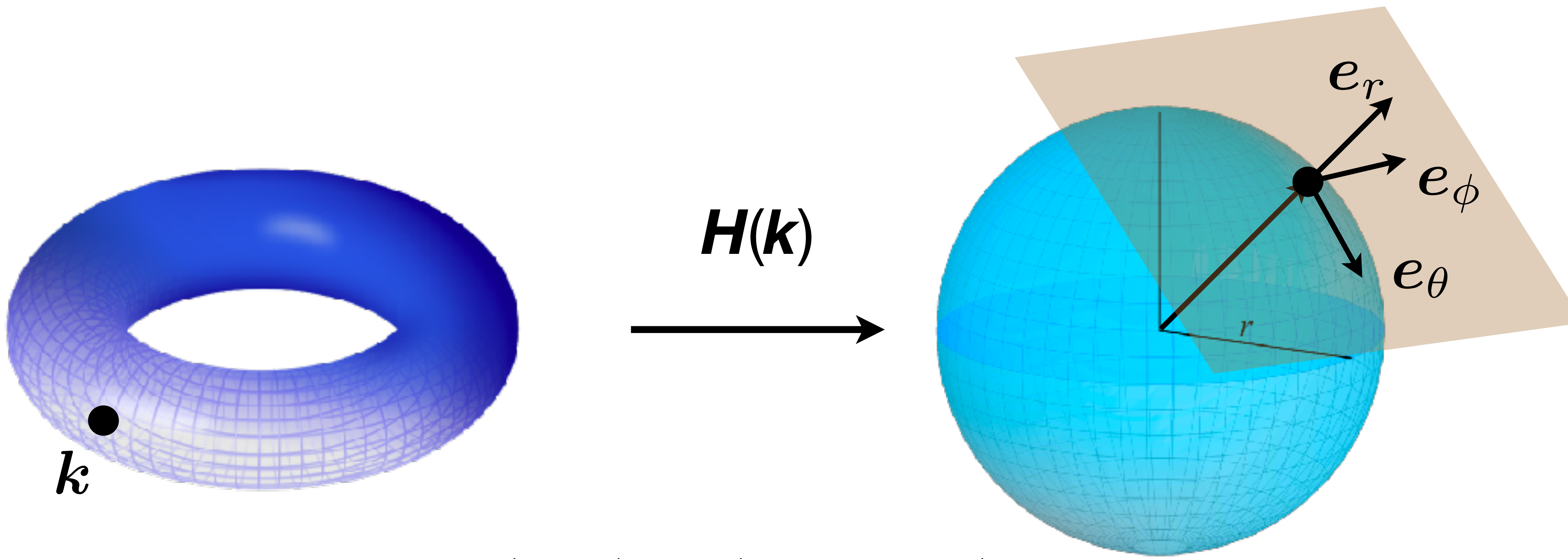
$$\sum_j \mathrm{index}_{x_j}(v) = \chi[\mathbb{S}^2] = 2$$

vorticity of the tangent vector field

Euler characteristic of the sphere



Tangent bundle of the sphere *on a lattice*



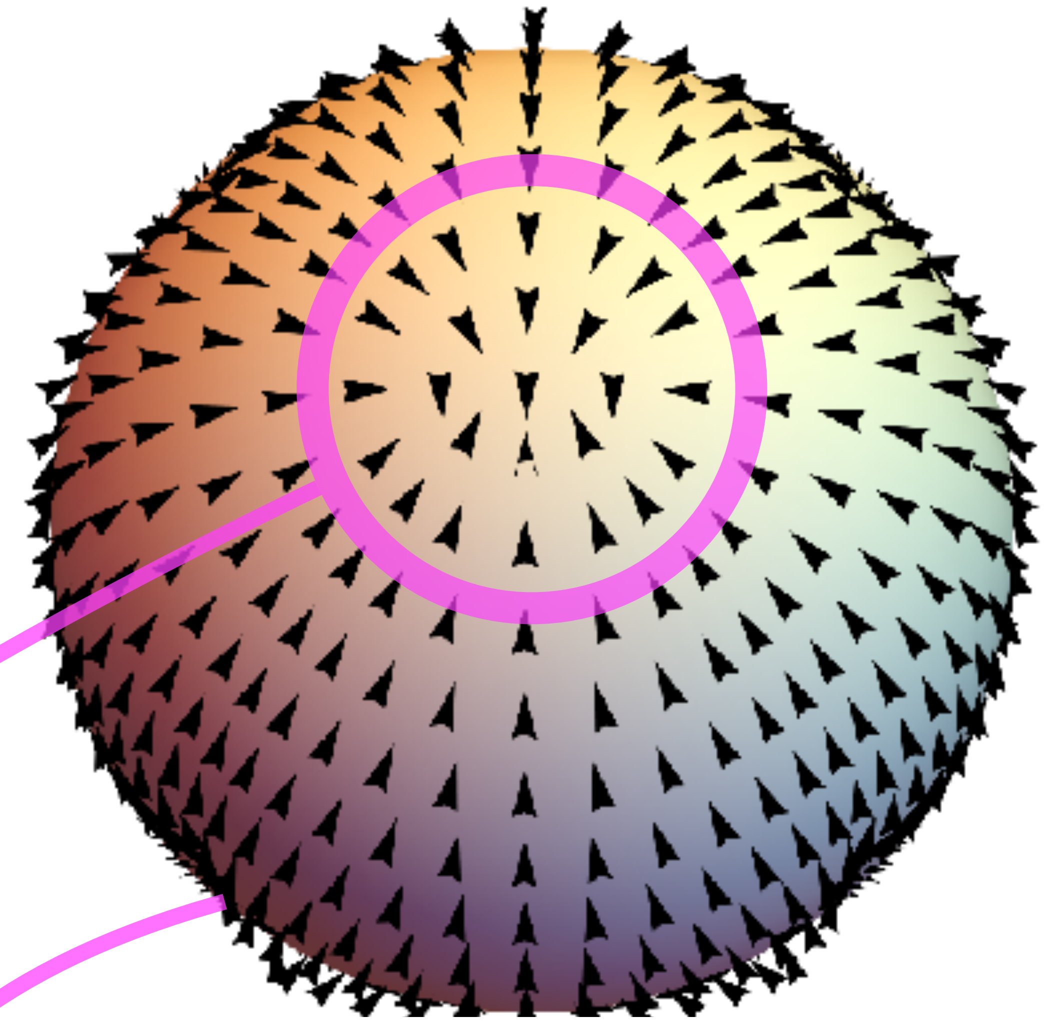
$$R(\theta,\phi) = (\boldsymbol{e}_\theta \ \boldsymbol{e}_\phi \ \boldsymbol{e}_r)$$

$$H(\theta,\phi) = R(\theta,\phi)\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} R(\theta,\phi)^T$$

Topological Euler insulator

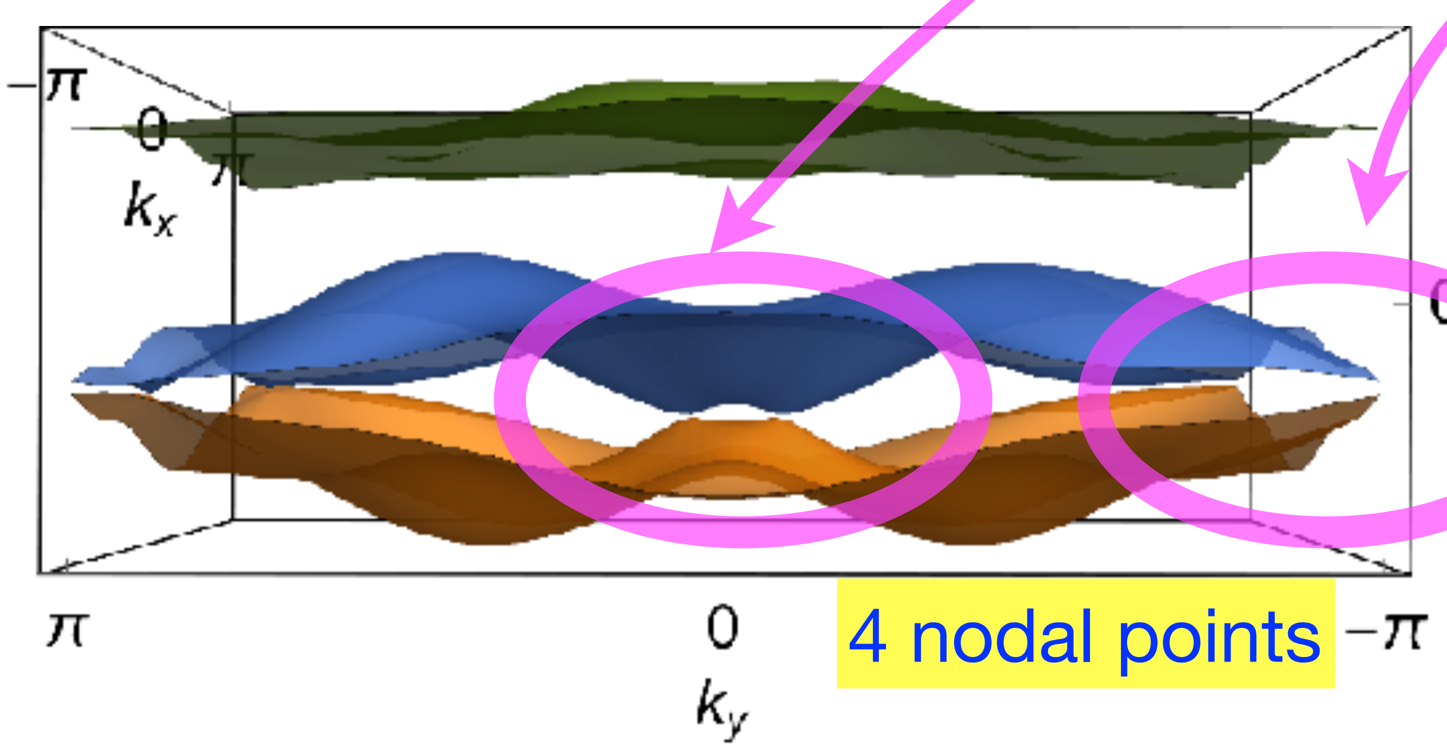
$$R(\boldsymbol{k}) = (u_1(\boldsymbol{k})\ u_2(\boldsymbol{k})\ \boldsymbol{n}(\boldsymbol{k}))$$

with $\boldsymbol{n}(\boldsymbol{k})$ covering the sphere one time

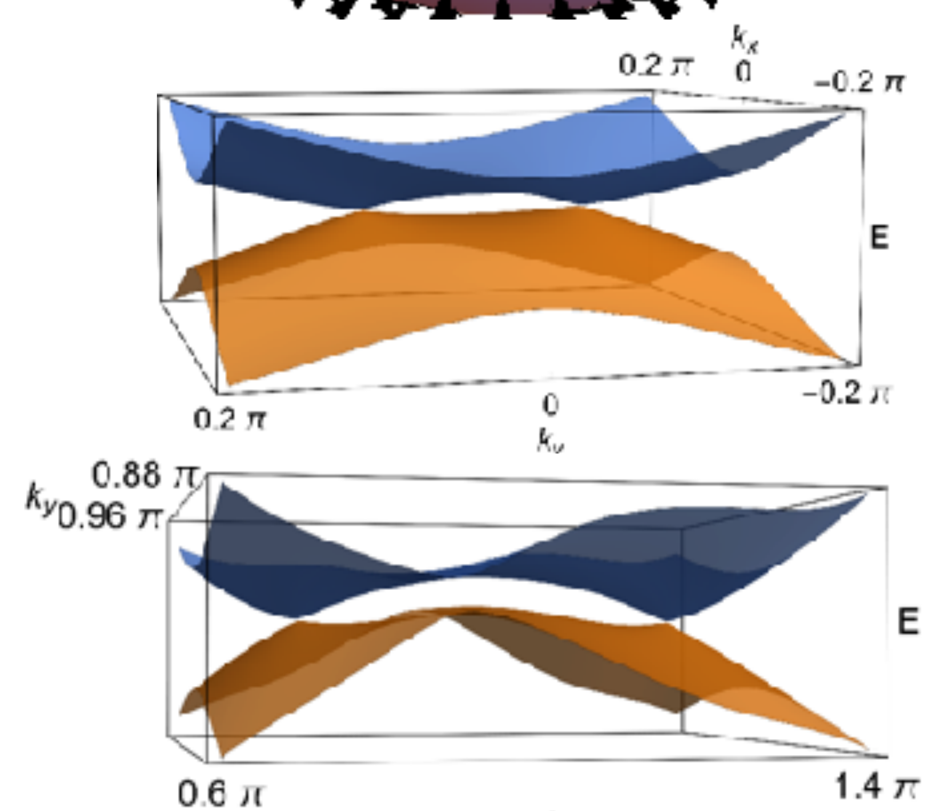


vortices of the vector field

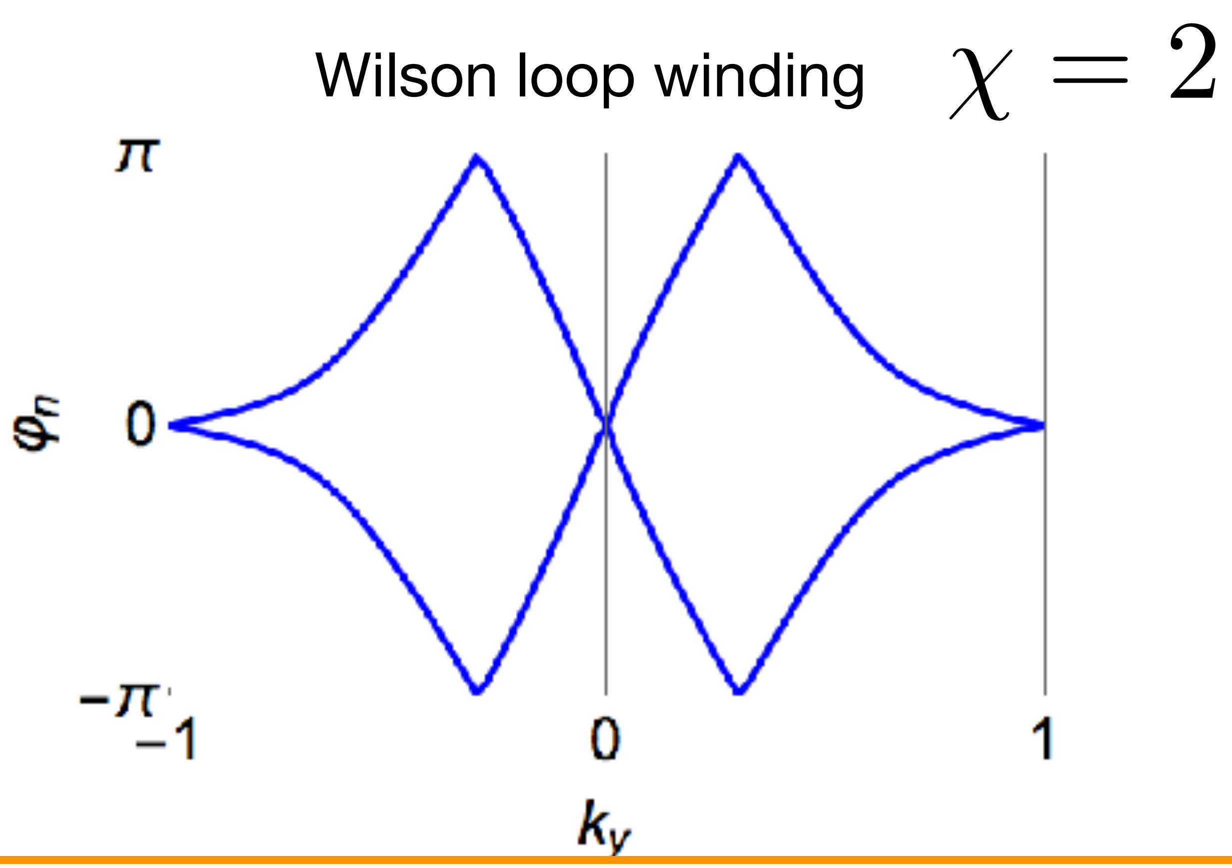
nodal points between bands 1 and 2

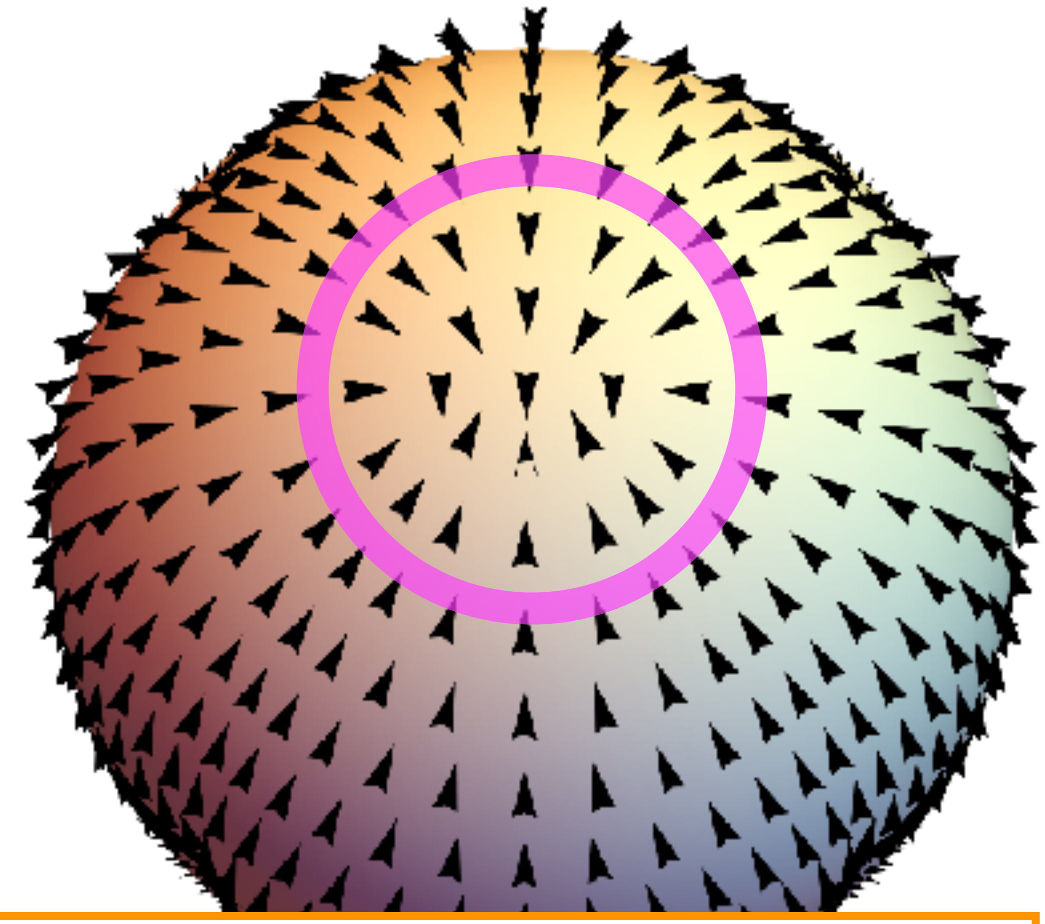


4 nodal points

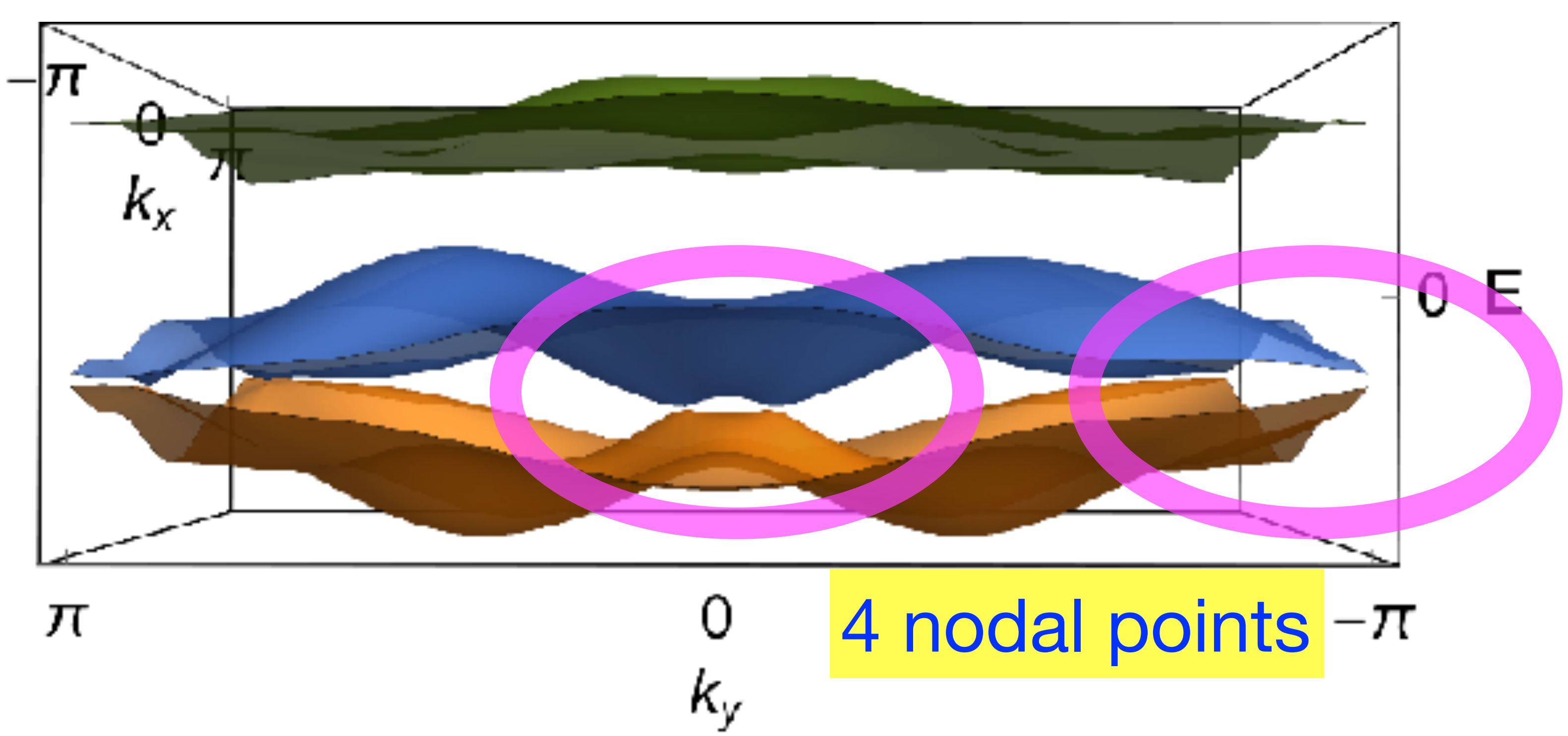


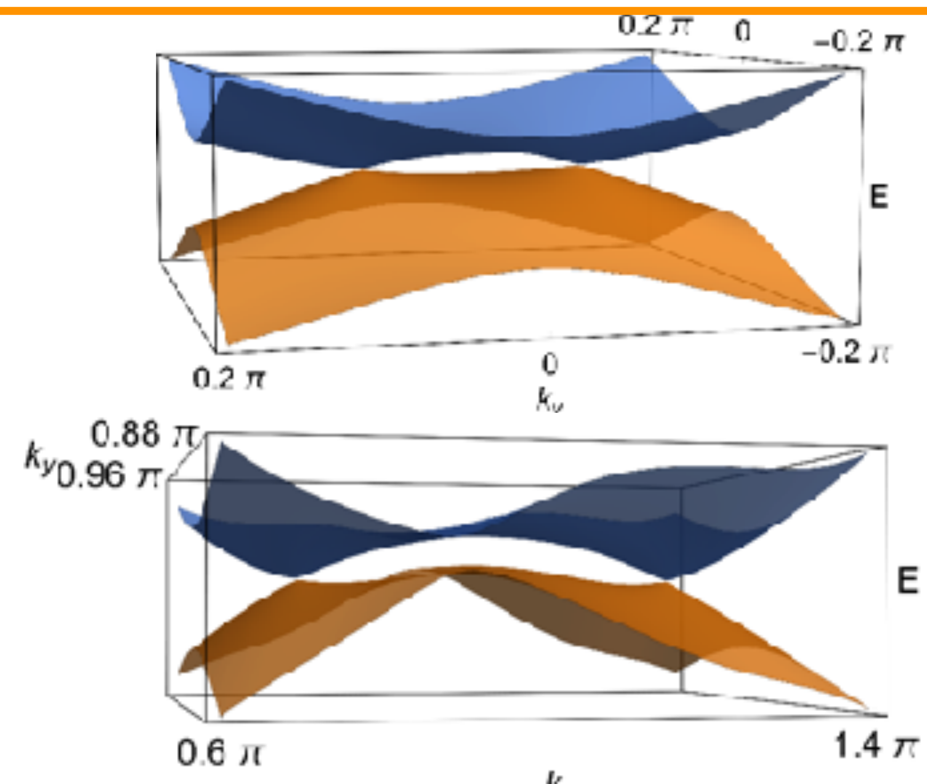
Topological Euler insulator





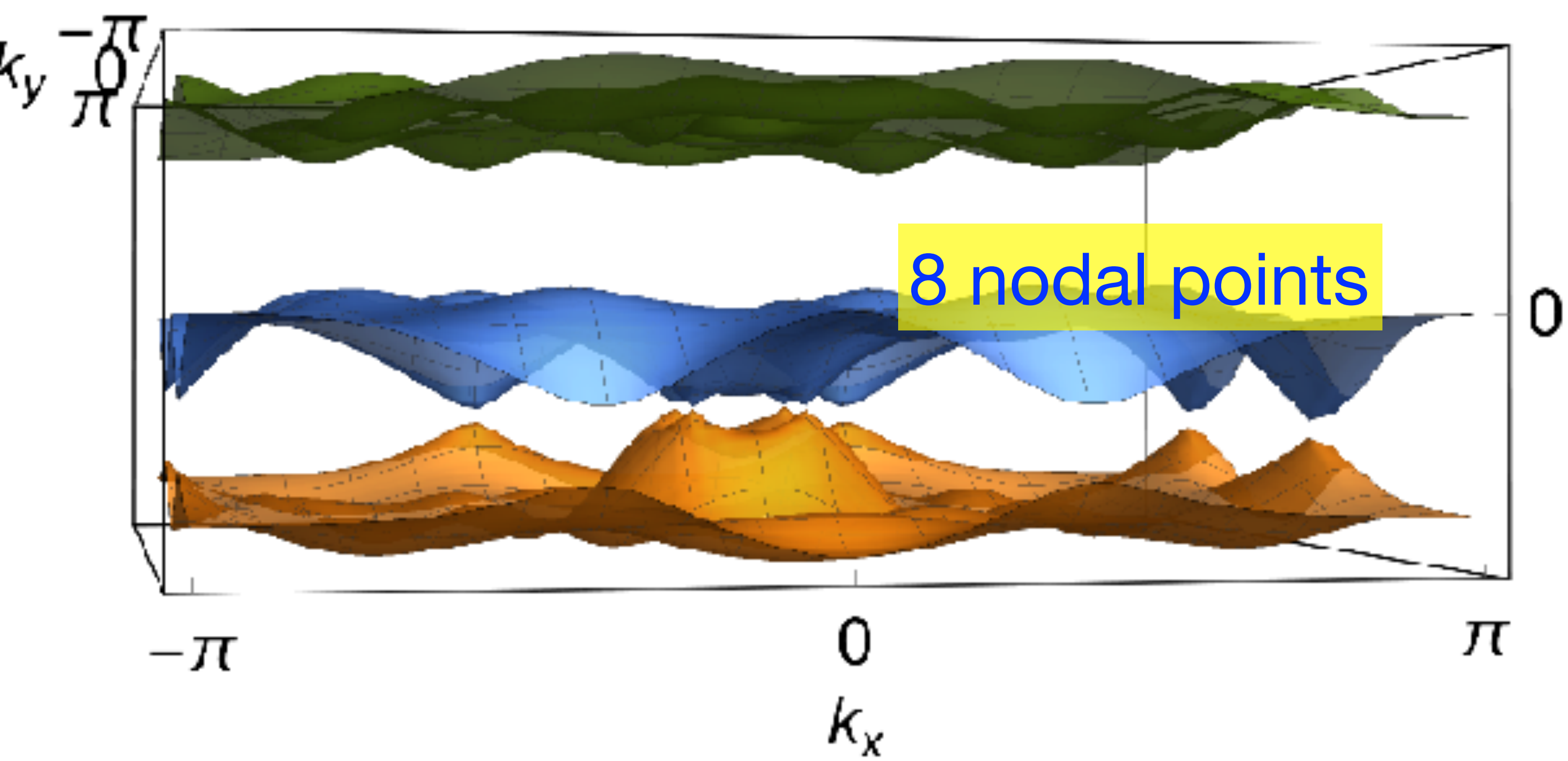
the 4 nodes are unremovable as long as the gap is preserved!

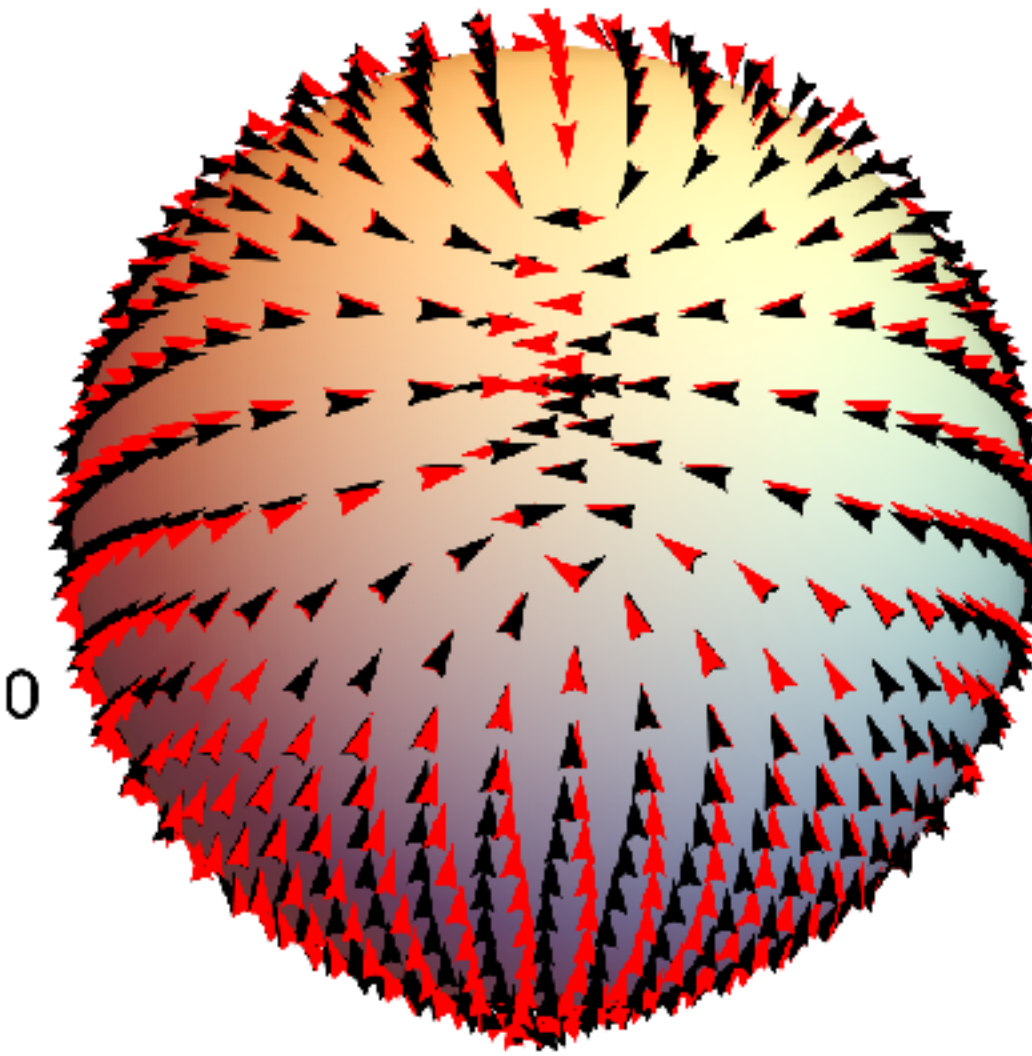




Topological Euler insulator

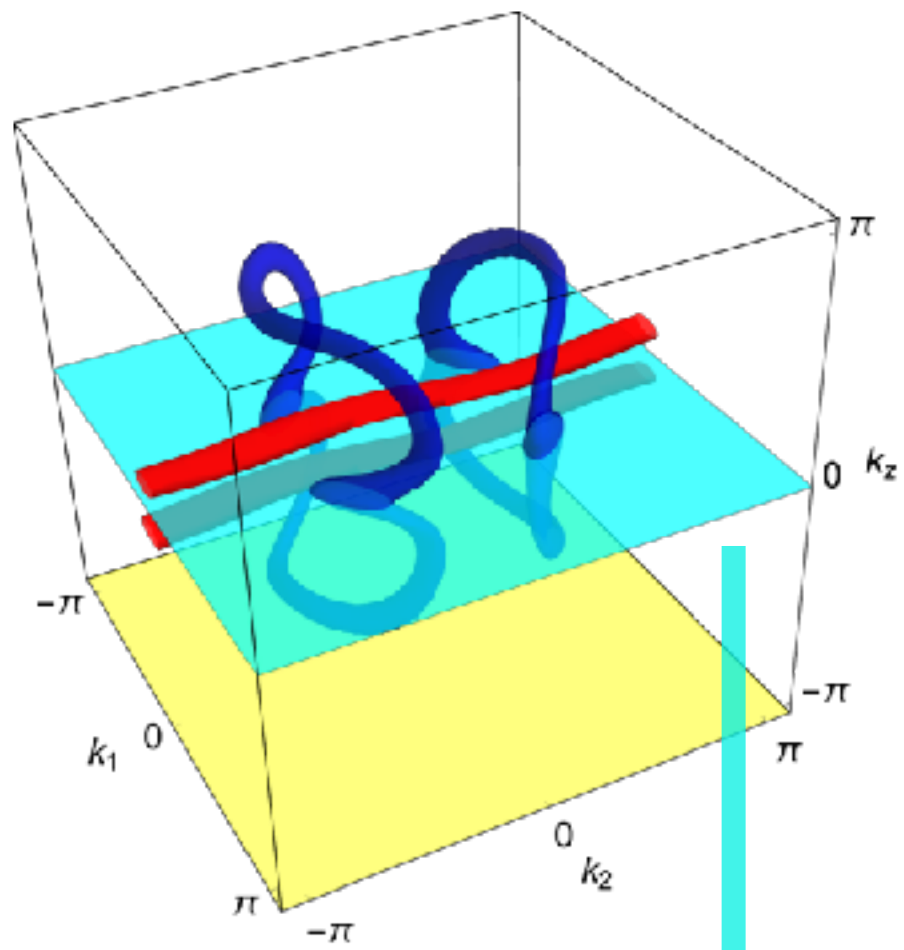
$$\chi = 4$$

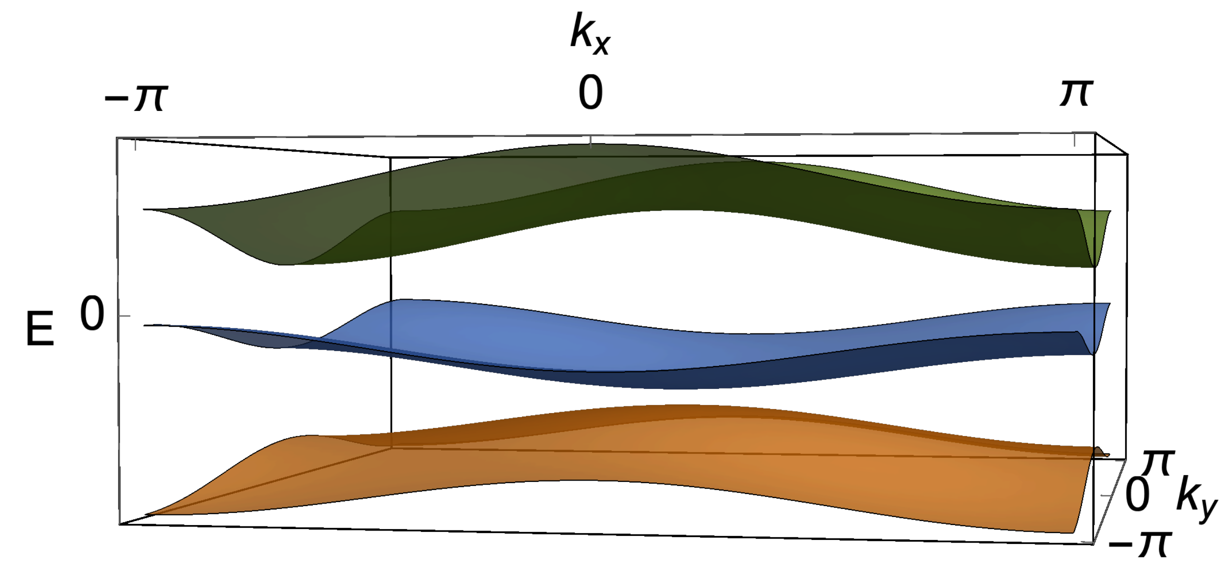


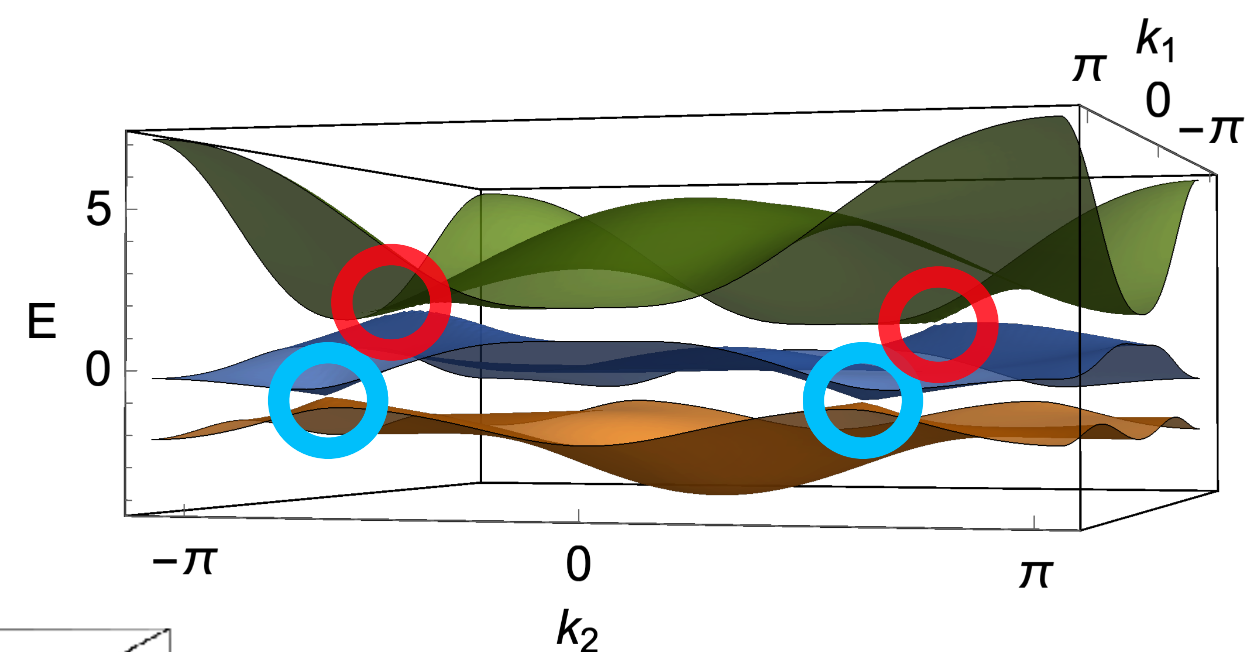


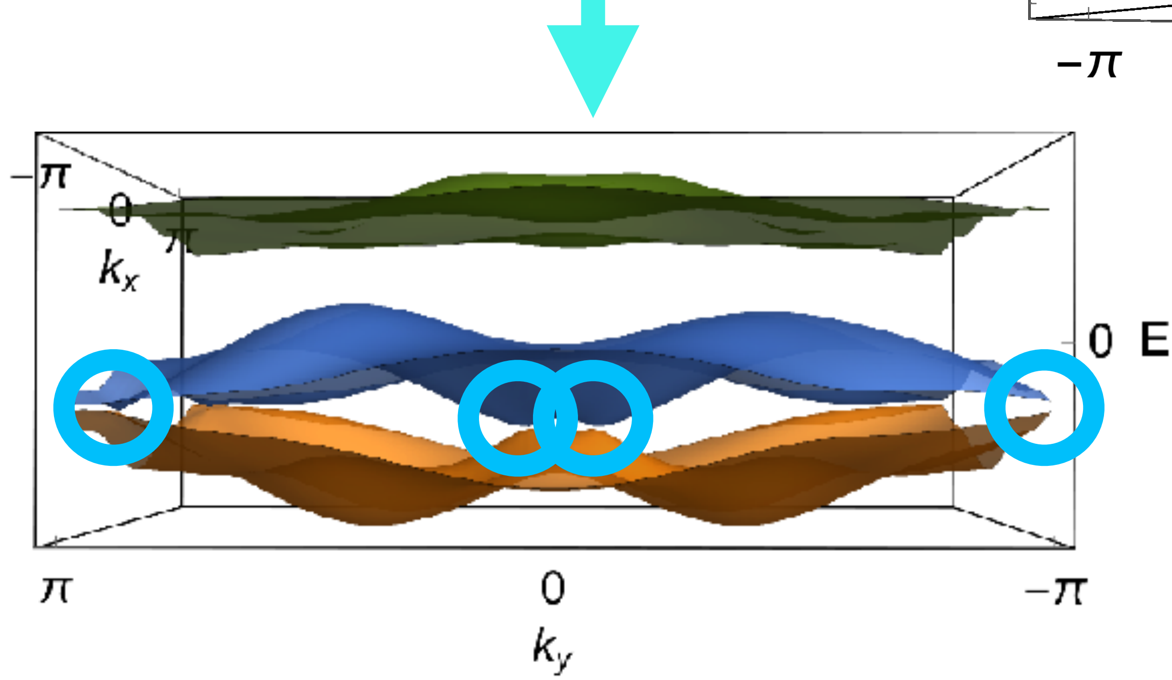
Total number of stable Nodal Points: $\#\mathrm{NP} = 2|\chi|$

Euler number conversion via braiding of Weyl points







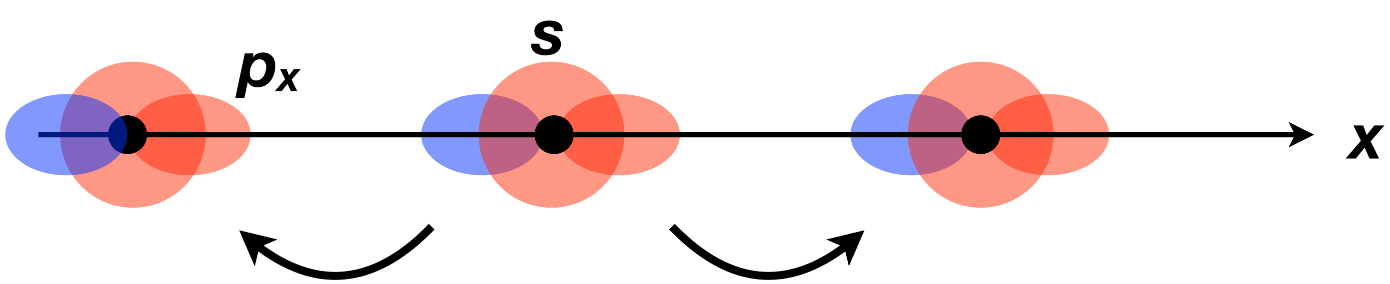


1D topology:
Möbius strip and orientability

Möbius bundle

SSH model:

$$H(k_x) = \begin{pmatrix} \Delta + \cos k_x & \sin k_x \\ \sin k_x & -\Delta - \cos k_x \end{pmatrix} = \underbrace{(\Delta + \cos k_x)}_{h_z}\sigma_z + \underbrace{\sin k_x}_{h_x}\sigma_x$$



t_{sp} = -1 t_{sp} = 1

t_{pp} = -1 t_{pp} = -1

t_{ss} = 1 t_{ss} = 1

$$\Delta = \epsilon_s - \epsilon_p$$

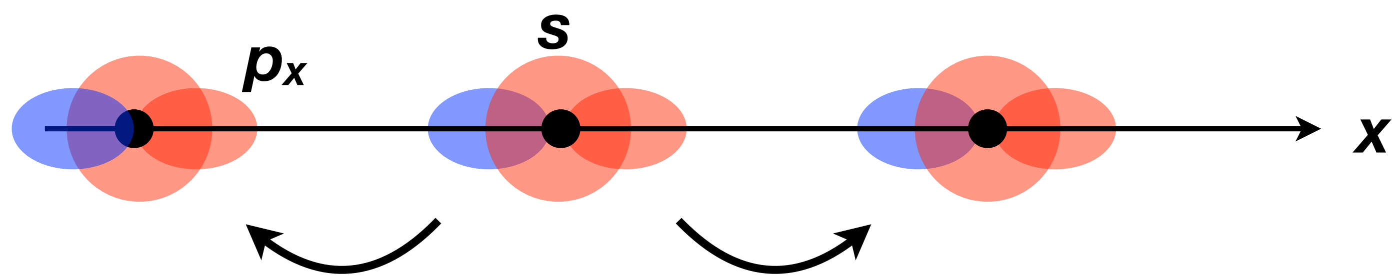
1D Brillouin zone:

$$\mathrm{BZ} \cong \mathbb{T}^1 = \mathbb{S}^1$$

Möbius bundle

SSH model:

$$H(k_x) = \begin{pmatrix} \Delta + \cos k_x & \sin k_x \\ \sin k_x & -\Delta - \cos k_x \end{pmatrix} = \underbrace{(\Delta + \cos k_x)}_{h_z}\sigma_z + \underbrace{\sin k_x}_{h_x}\sigma_x$$



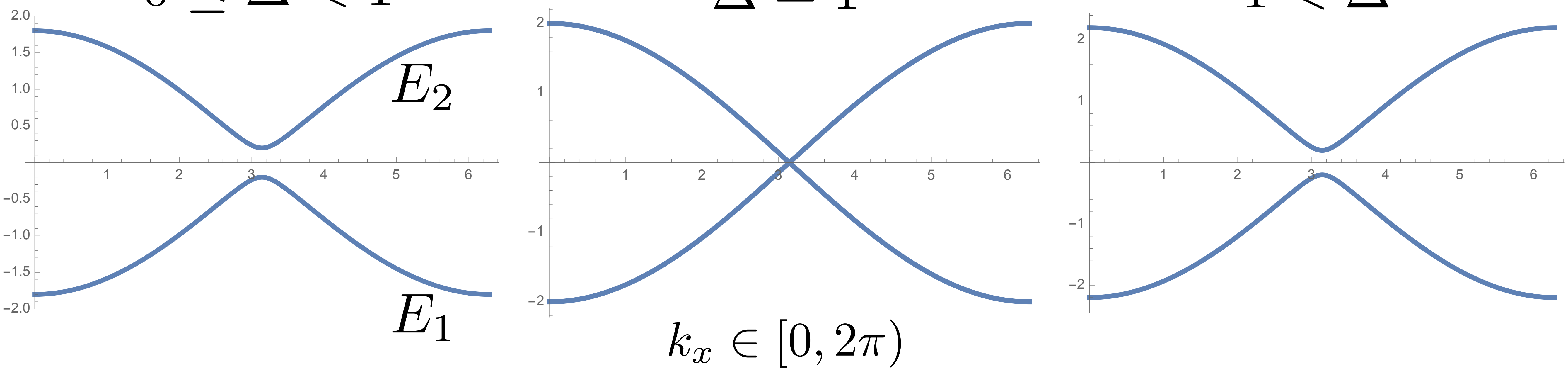
t_{sp} = -1	t_{sp} = 1
t_{pp} = -1	t_{pp} = -1
t_{ss} = 1	t_{ss} = 1

$$\Delta = \epsilon_s - \epsilon_p$$

1D Brillouin zone:

$$\mathrm{BZ} \cong \mathbb{T}^1 = \mathbb{S}^1$$

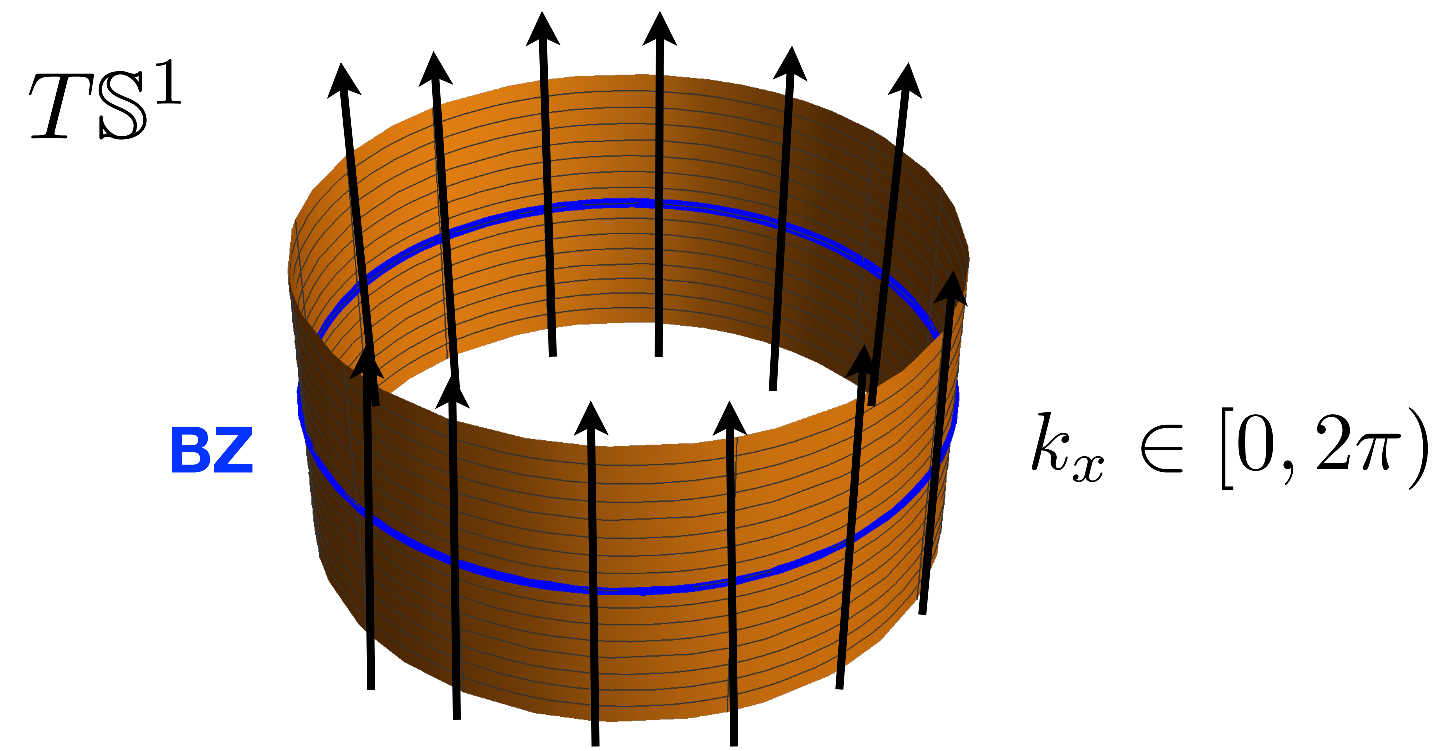
$$0 \leq \Delta < 1 \qquad \Delta = 1 \qquad 1 < \Delta$$



Möbius bundle (strip)

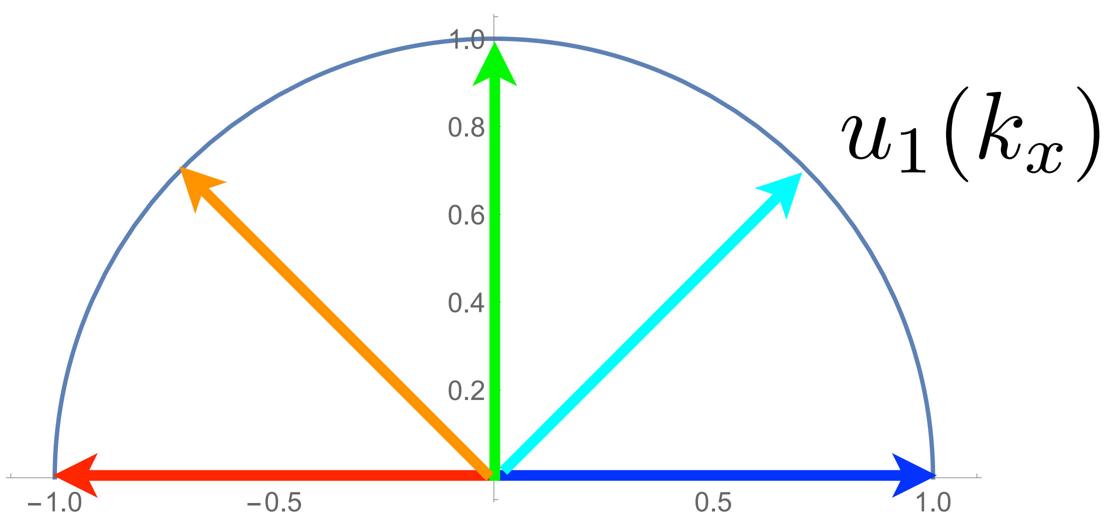
$1 < \Delta$ trivial bundle

"orientable"

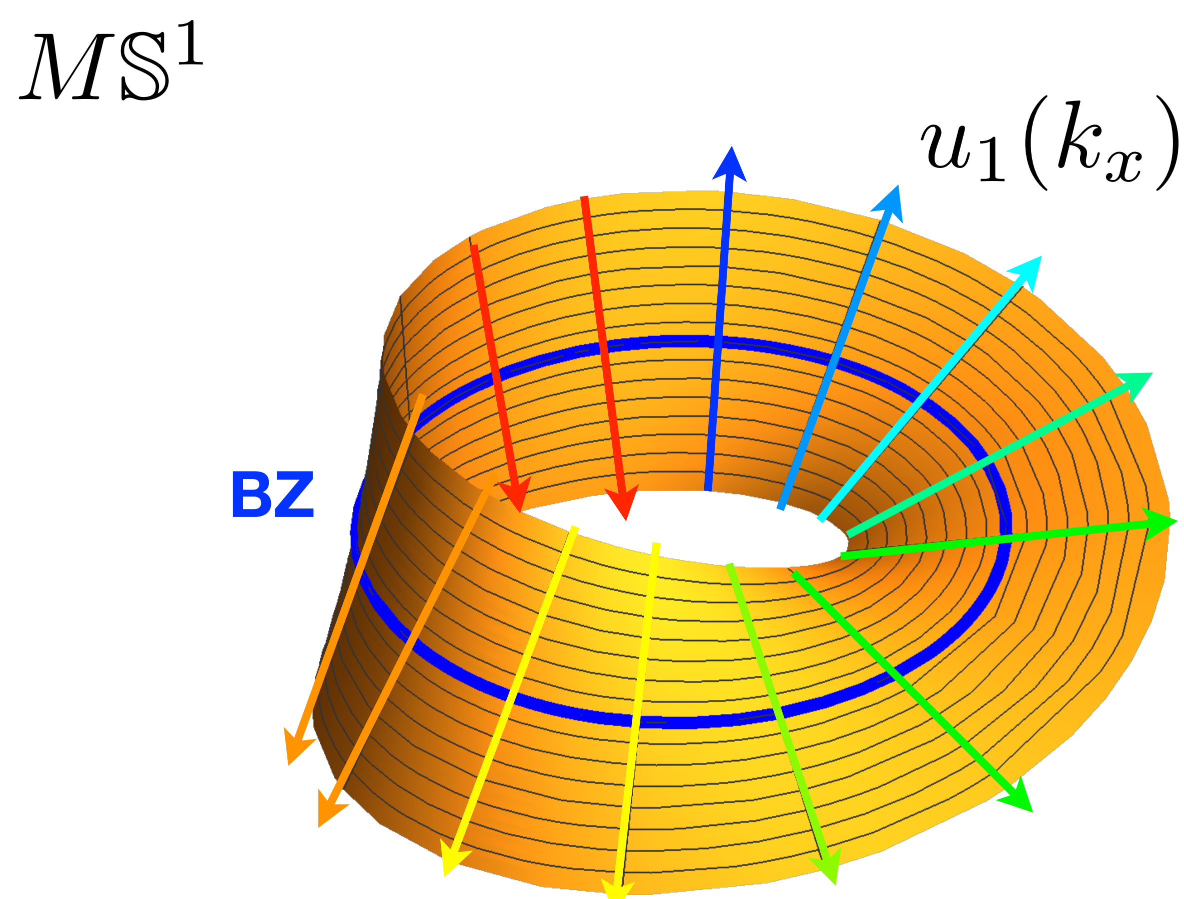


$0 \leq \Delta < 1$ nontrivial bundle

"non-orientable"



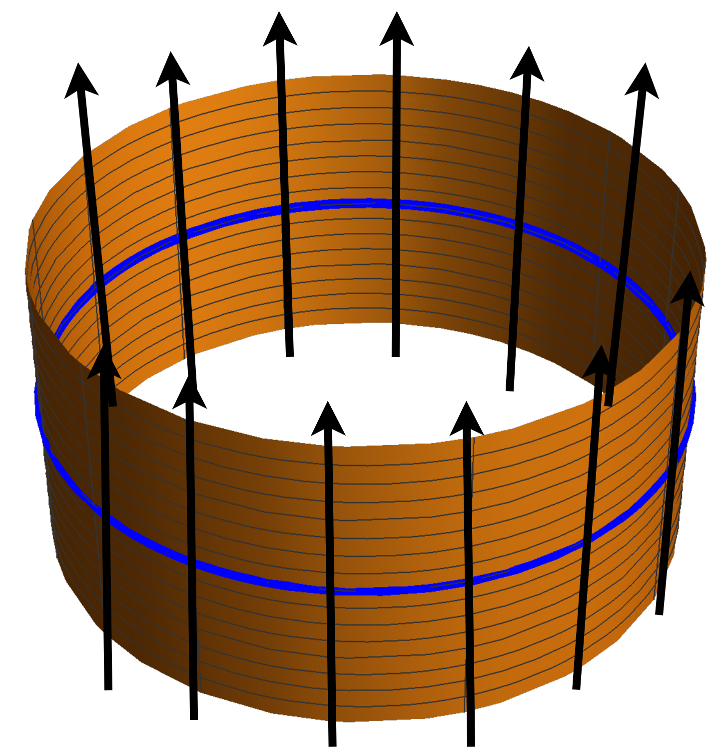
$u_1(2\pi) = \begin{bmatrix} -1 \\ 0 \end{bmatrix}$ $u_1(0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

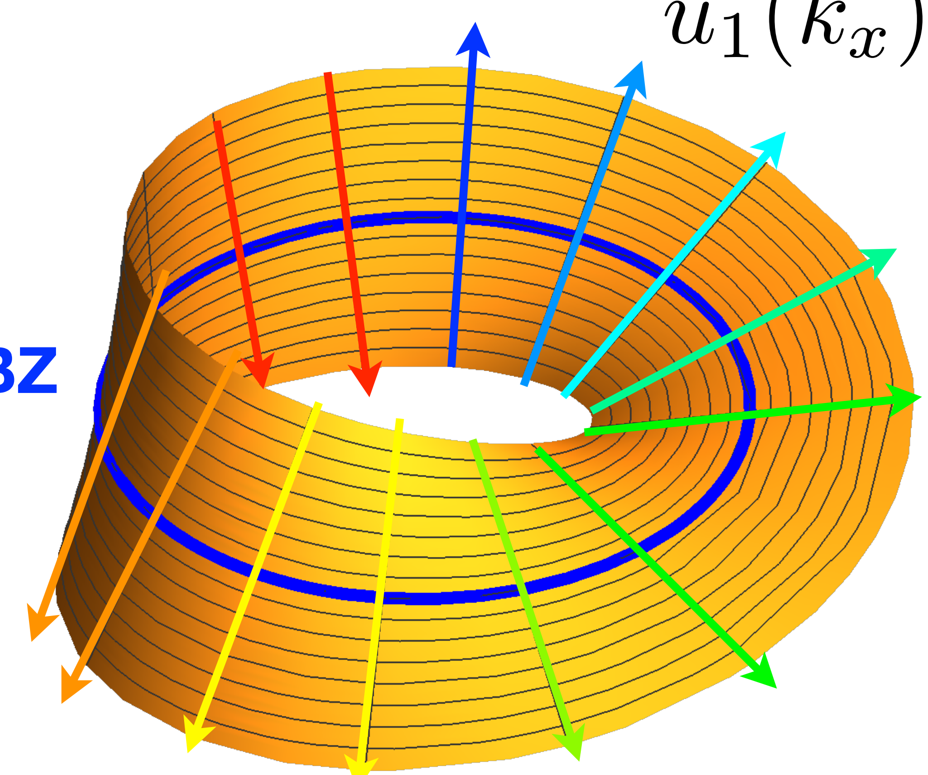


Möbius bundle (strip)

$$\pi_1[T\mathbb{S}^1] = \pi_1[M\mathbb{S}^1]$$

not enough to distinguish them!





Möbius bundle

Space of Hamiltonian: $U(k_x) = [u_1(k_x)\ u_2(k_x)] \in \mathsf{O}(2)$

Gap condition: $E_1 < E_2$

$$H(k_x) = [u_1(k_x)\ u_2(k_x)] \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} u_1(k_x)^T \\ u_2(k_x)^T \end{bmatrix}$$

Gauge symmetry of the gaped Hamiltonian:

$$[u_1(k_x)\ u_2(k_x)] \longrightarrow [u_1(k_x)\ u_2(k_x)] \begin{bmatrix} \pm 1 & 0 \\ 0 & \pm 1 \end{bmatrix}$$

Classifying space $\mathsf{O}(2)/[\mathsf{O}(1) \times \mathsf{O}(1)] = \mathrm{Gr}_1(\mathbb{R}^2) \cong \mathbb{R}P^1 \cong \mathbb{S}^1$

homotopy classification of gaped band structures: $\pi_1[\mathbb{S}^1] = \mathbb{Z}$

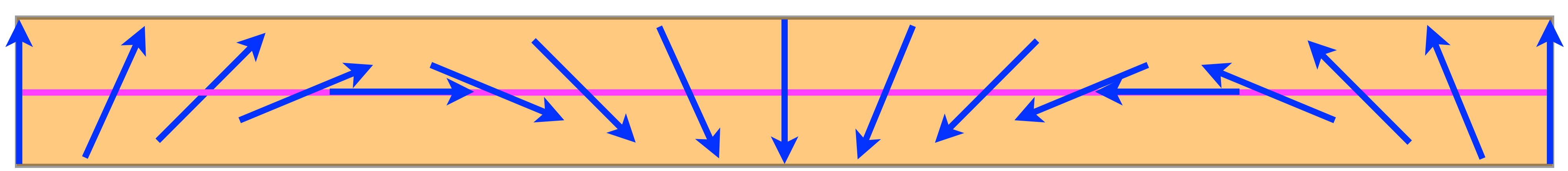
Möbius bundle

$$\pi_1[\mathbb{S}^1] = \mathbb{Z}$$

Computed as the winding number of

$$\hat{\boldsymbol{h}} = (h_x, h_z)/|\boldsymbol{h}| \in \mathbb{S}^1$$

This holds only when the Möbius bundle is restricted to the plane ! $u_1(k_x) \in \mathbb{R}^2$



Möbius bundle

$$\pi_1[\mathbb{S}^1] = \mathbb{Z}$$

Computed as the winding number of

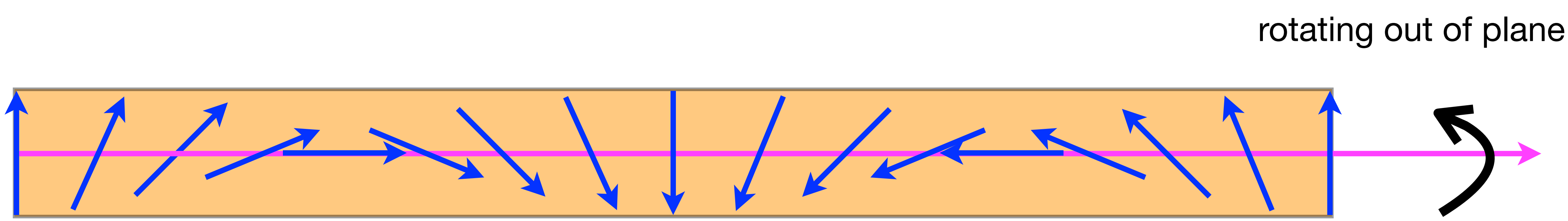
$$\hat{\boldsymbol{h}} = (h_x, h_z)/|\boldsymbol{h}| \in \mathbb{S}^1$$

This holds only when the Möbius bundle is restricted to the plane ! $u_1(k_x) \in \mathbb{R}^2$

If we embed the Möbius bundle in $\mathbb{R}^3$ $u_1(k_x) \in \mathbb{R}^3$

we effectively add one extra band: $\pi_1[\mathrm{Gr}_1(\mathbb{R}^3)] = \mathbb{Z}_2$

bundles with even twists can be untwisted !



Möbius bundle

$$\pi_1[\mathbb{S}^1] = \mathbb{Z}$$

Computed as the winding number of

$$\hat{\boldsymbol{h}} = (h_x, h_z)/|\boldsymbol{h}| \in \mathbb{S}^1$$

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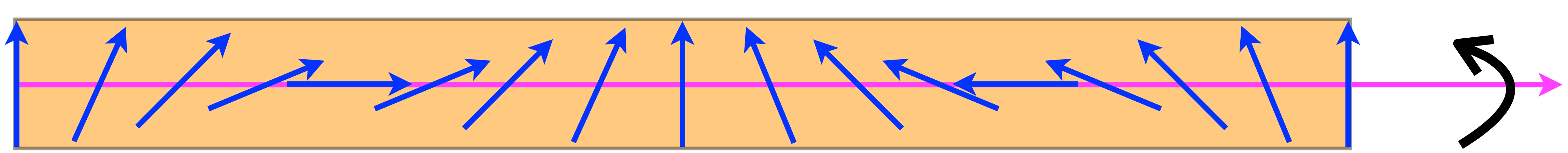


Möbius bundle

The first homotopy invariant is computed by the Berry phase factor

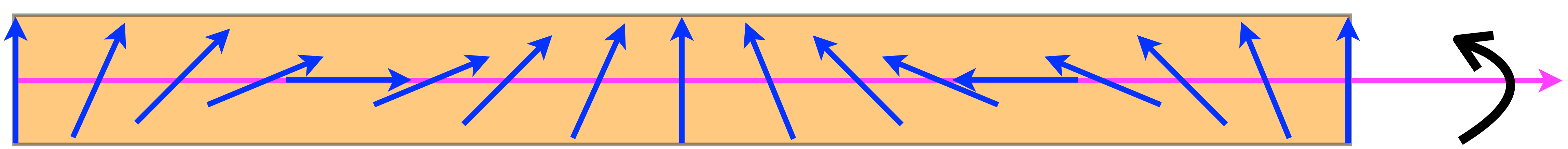
$$e^{i\gamma[l]} \in \{+1, -1\}$$

A π-Berry phase indicates a **non-orientable** occupied subspace (first Stiefel-Whitney class)

If we embed the Möbius bundle in $\mathbb{R}^3$ $\quad u_1(k_x) \in \mathbb{R}^3$

we effectively add one extra band: $\quad \pi_1[\mathrm{Gr}_1(\mathbb{R}^3)] = \mathbb{Z}_2$

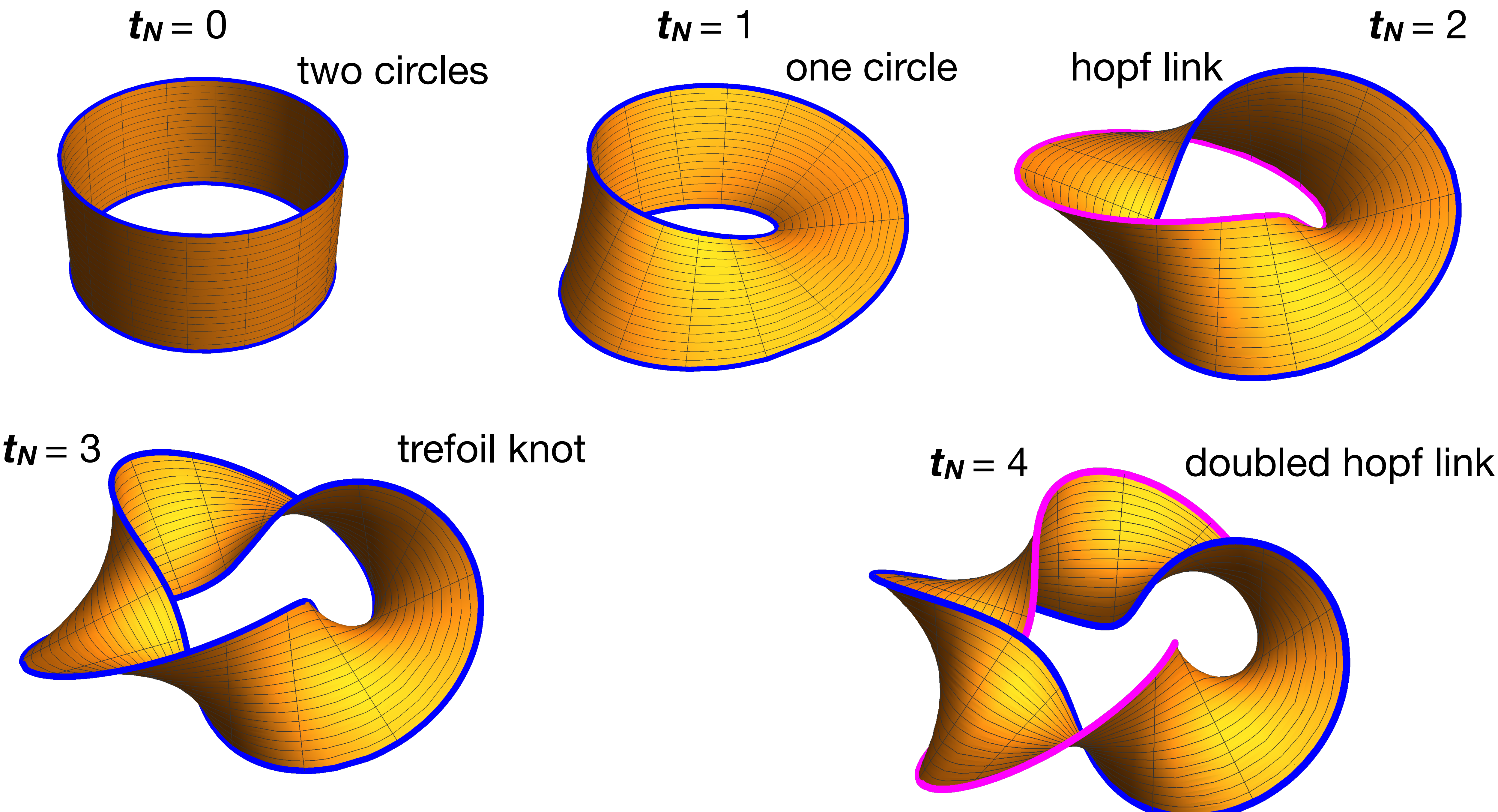
bundles with even twists can be untwisted !



Möbius strip

(t_N = twist number)

The topology of the *physical* twisted strip is characterized by the boundary knot



Correspondence between knots-links (in $\mathbb{R}^3$) and real 1D 2-band gapped phases (in $\mathbb{R}^2$)

2D topology:
projective plane, Euler class, fragile topology,
Weyl nodes accumulation

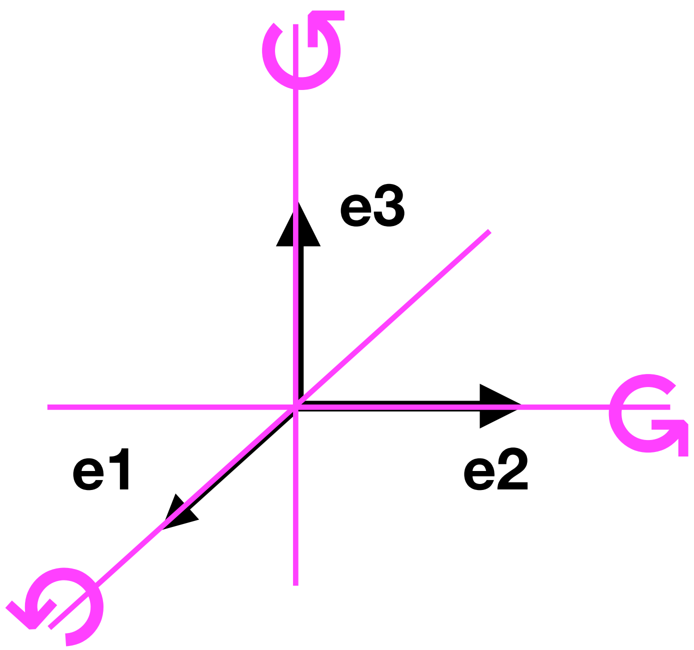
Three-level system

$$\widetilde{H}(\boldsymbol{k}) = R(\boldsymbol{k})\mathcal{E}(\boldsymbol{k})R^T(\boldsymbol{k}) \ , \quad R(\boldsymbol{k}) \in SO(3)$$

(global sign of R is a gauge freedom)

eigenvectors = right-handed orthonormal frame { $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ }

gauge freedom for each pair of eigenvectors ($\mathbf{e}_j$,$\mathbf{e}_k$) → -($\mathbf{e}_j$,$\mathbf{e}_k$)



classifying space is of nematics!

Classifying space for two-occupied bands and one unoccupied band:

$$\mathrm{Gr}_2(\mathbb{R}^3) = \frac{\mathsf{SO}(3)}{\mathsf{S}[\mathsf{O}(2)\times\mathsf{O}(1)]} = \mathbb{R}\mathrm{P}^2 = \mathbb{S}^2/\{x \sim -x\}$$

projective plane
(sphere with antipodal points identified)

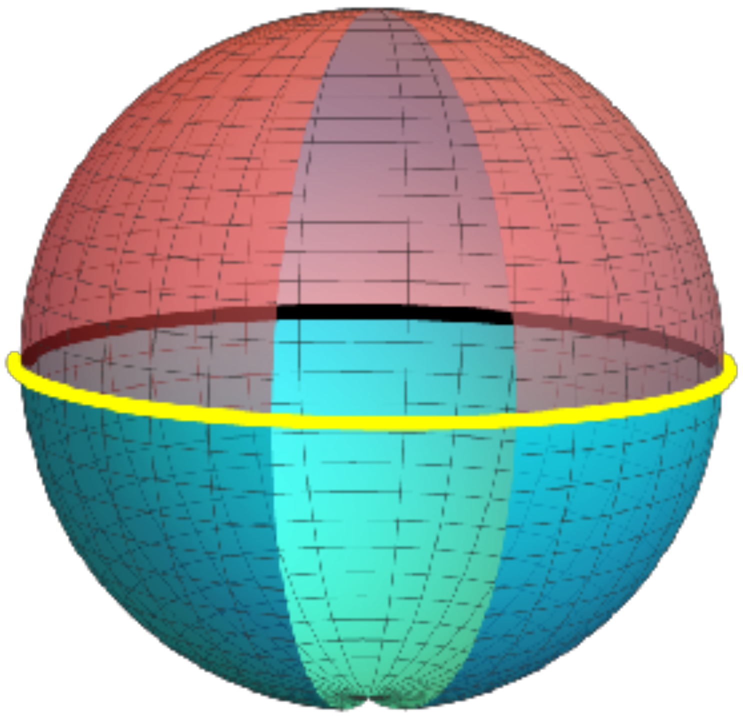
the orientation of subframes is a gauge freedom ! **“unoriented” surface**

($\mathbf{e}_1$, $\mathbf{e}_2$) , $\mathbf{e}_3$ ~ ($\mathbf{e}_1$, -$\mathbf{e}_2$) , -$\mathbf{e}_3$

Oriented double covering

$$\mathbb{RP}^2 = \mathbb{S}^2/\{x \sim -x\}$$

orientable

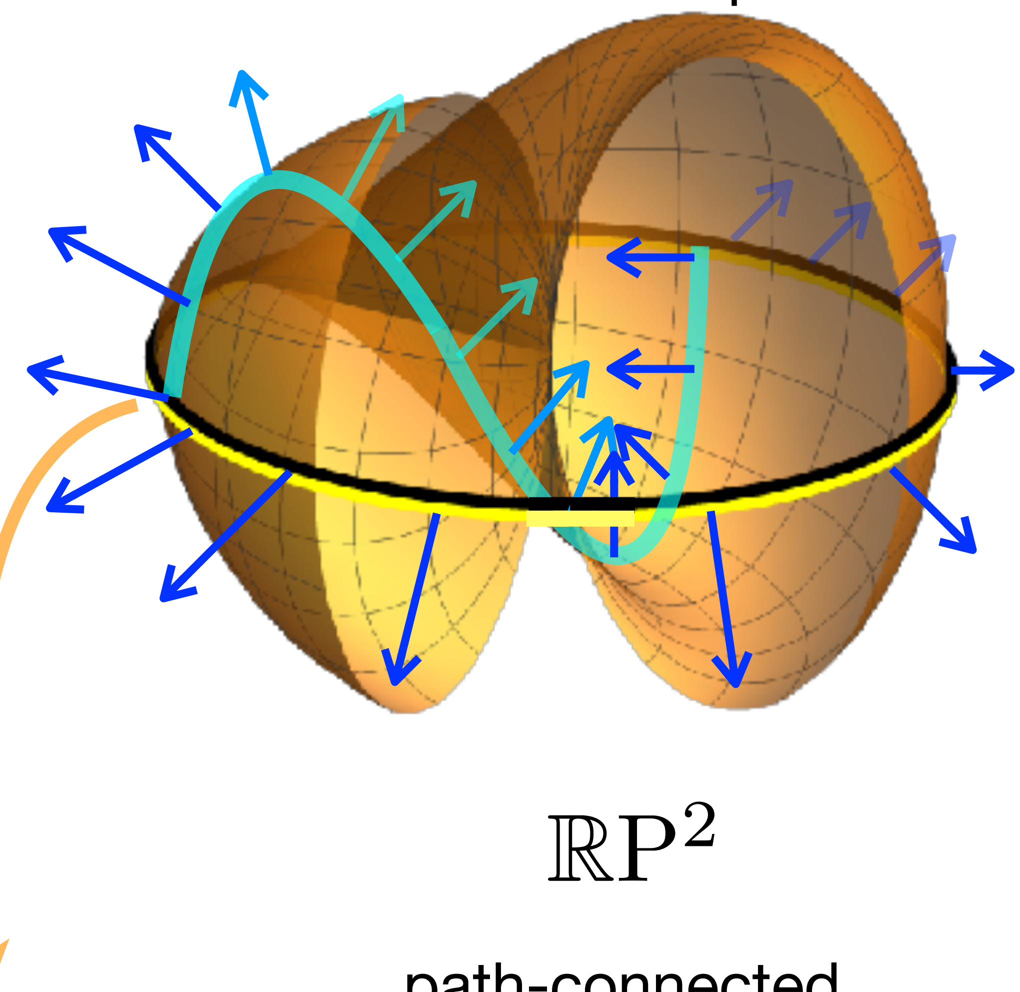


$\mathbb{S}^2$

path-connected
simply connected

non-orientable

"cross-cap"



non-contractible loop

$\mathbb{RP}^2$

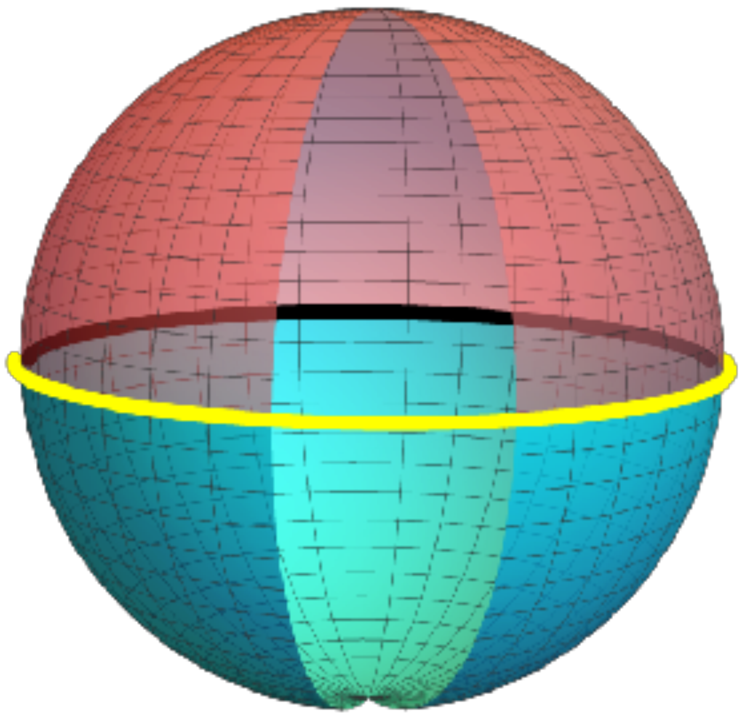
path-connected

$\pi_1[\mathbb{RP}^2] = \mathbb{Z}_2$

Oriented double covering

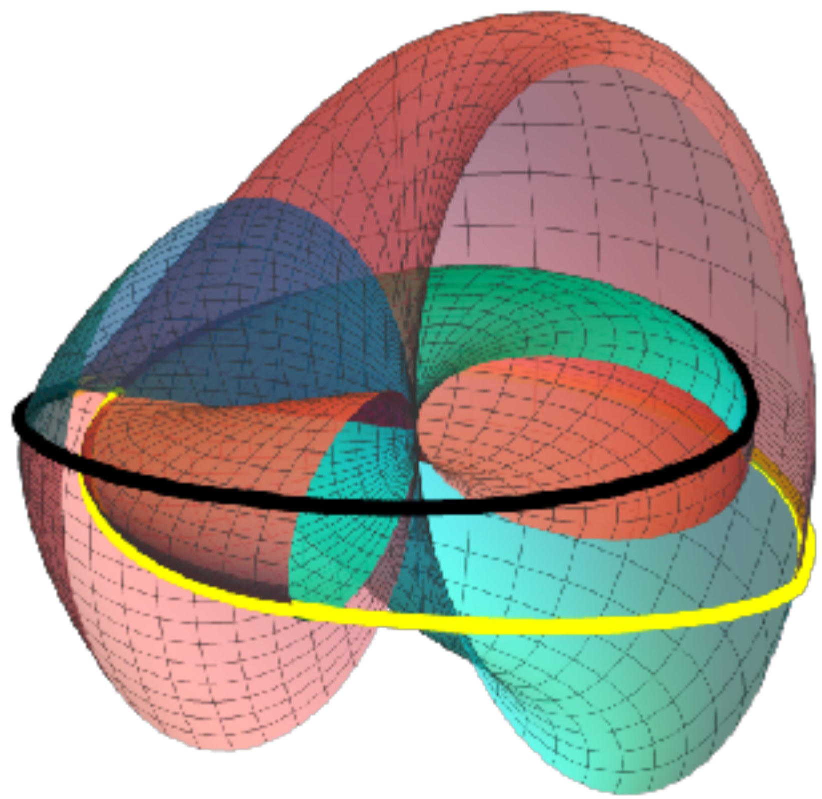
$$\mathbb{RP}^2 = \mathbb{S}^2/\{x \sim -x\}$$

orientable



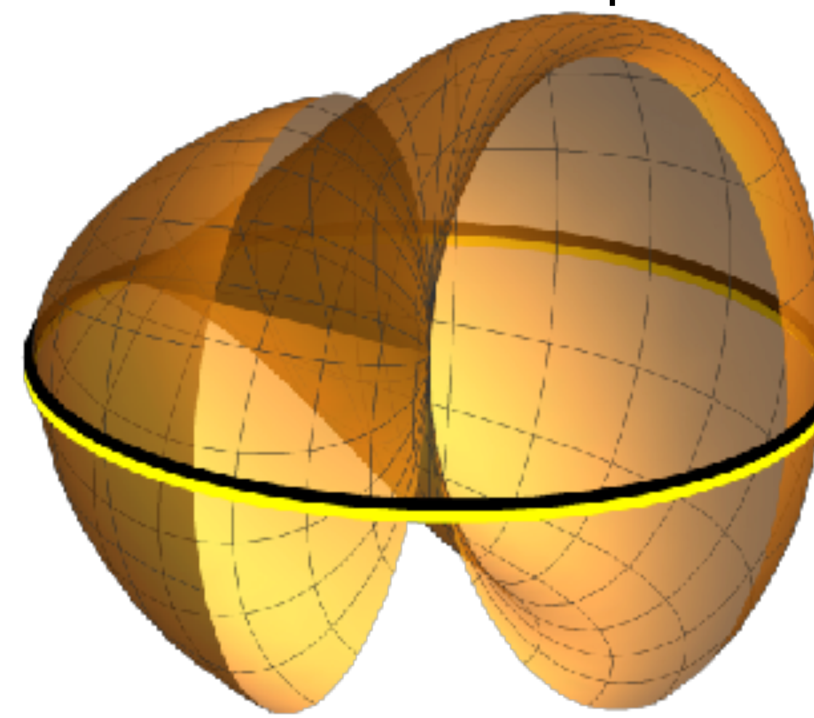
$\mathbb{S}^2$

path-connected
simply connected



$\mathbb{S}^2 \to \mathbb{RP}^2$

non-orientable
“cross-cap”



$\mathbb{RP}^2$

path-connected
$\pi_1[\mathbb{RP}^2] = \mathbb{Z}_2$

$$\pi_2[\mathbb{S}^2] = \mathbb{Z} \cong \pi_2[\mathbb{RP}^2] = 2\mathbb{Z}$$

1.5D topology of three-level system

$$\widetilde{H}(\boldsymbol{k}) = R(\boldsymbol{k})\mathcal{E}(\boldsymbol{k})R^T(\boldsymbol{k})$$

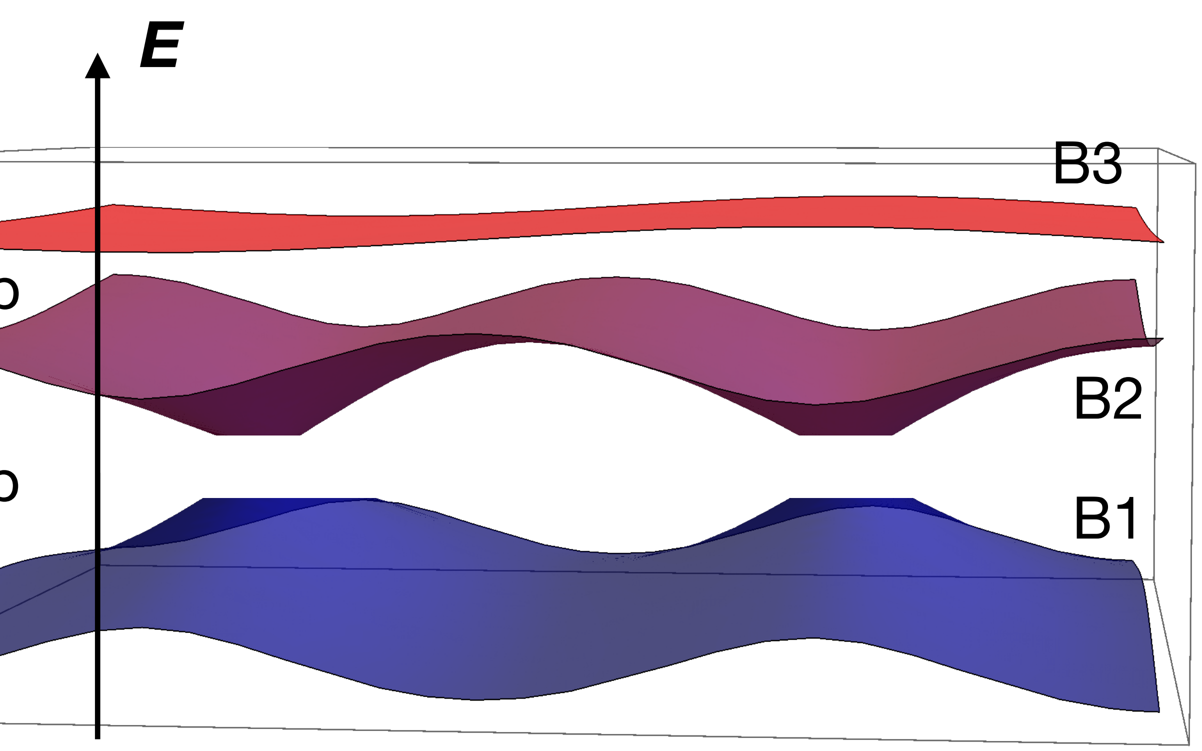
$$R(\boldsymbol{k}) = (\boldsymbol{e}_1 \ \boldsymbol{e}_2 \ \boldsymbol{e}_3)$$

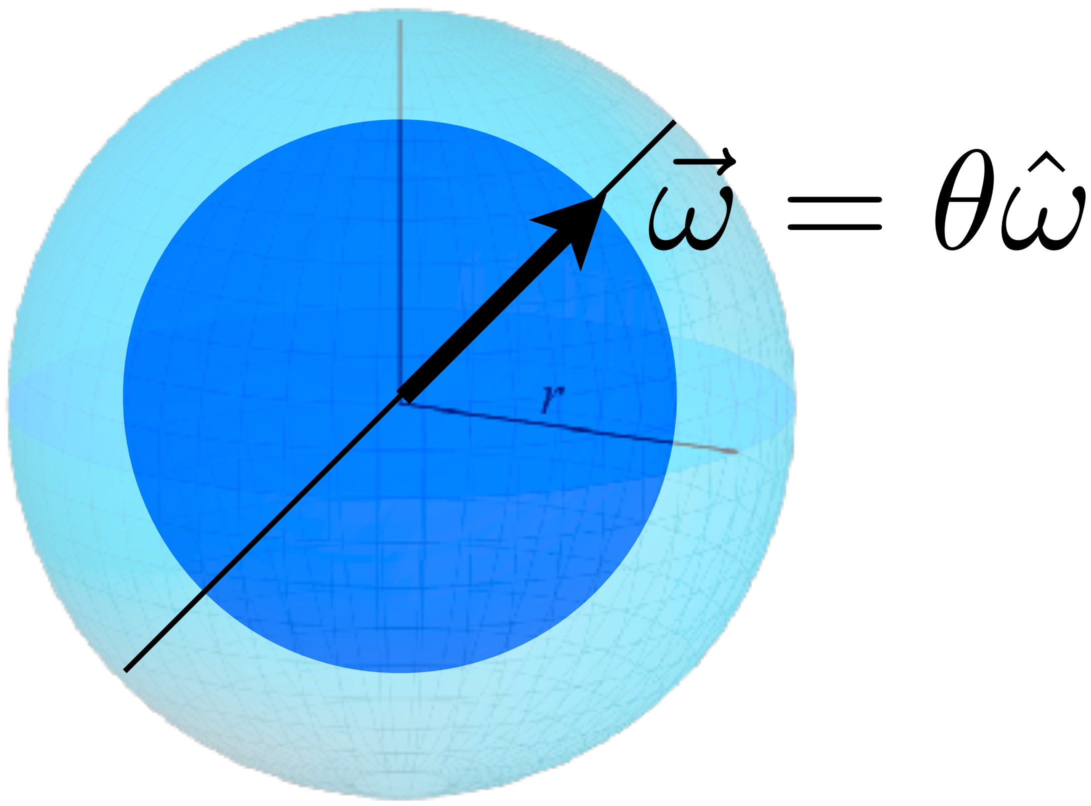
Topology over a loop of the BZ:

$$\pi_1\left(\mathsf{SO}(3)\right) = \mathbb{Z}_2$$

Lie algebra representation:

$$R(\boldsymbol{k}) = e^{\vec{\omega}\cdot\vec{L}} \in \mathsf{SO}(3)$$



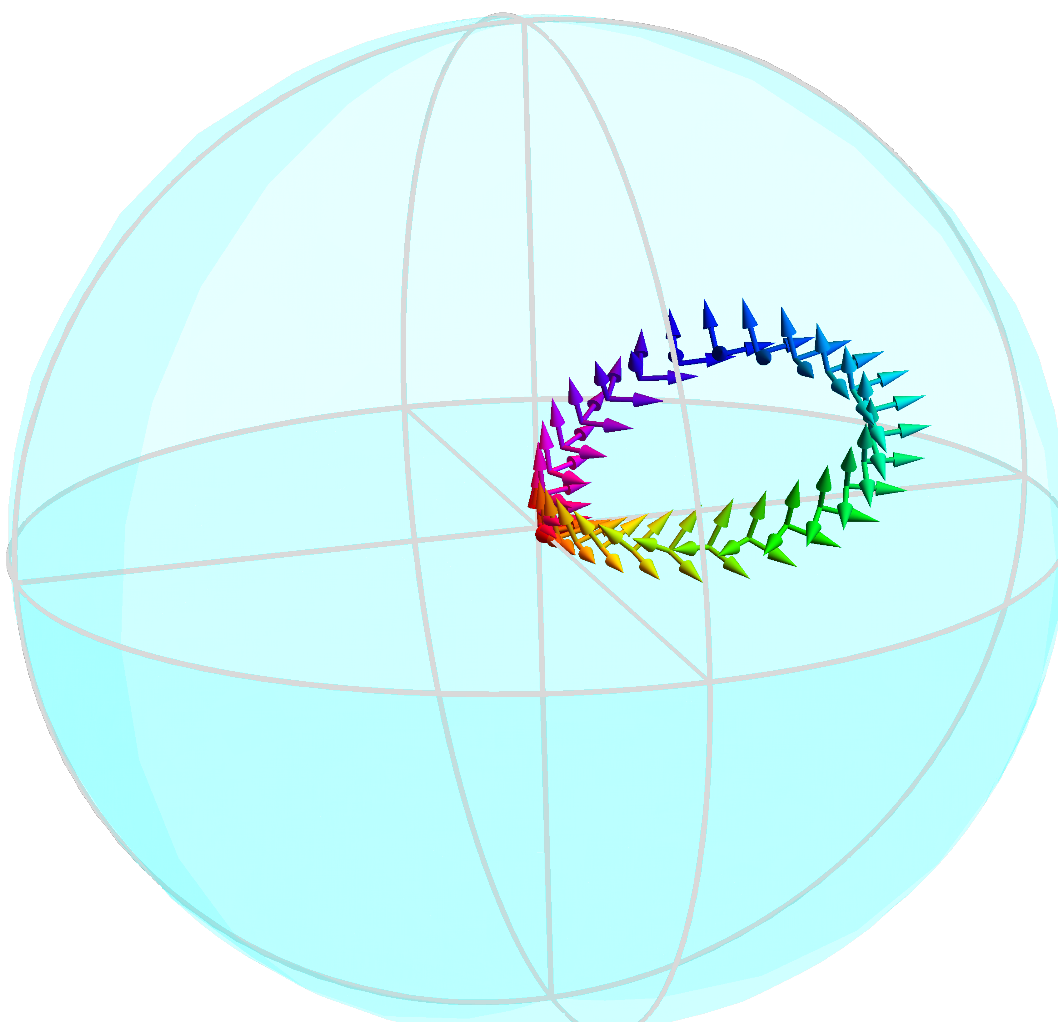


1.5D topology of three-level system

$$\widetilde{H}(\boldsymbol{k}) = R(\boldsymbol{k})\mathcal{E}(\boldsymbol{k})R^T(\boldsymbol{k}) \qquad R(\boldsymbol{k}) = (\boldsymbol{e}_1 \ \boldsymbol{e}_2 \ \boldsymbol{e}_3)$$

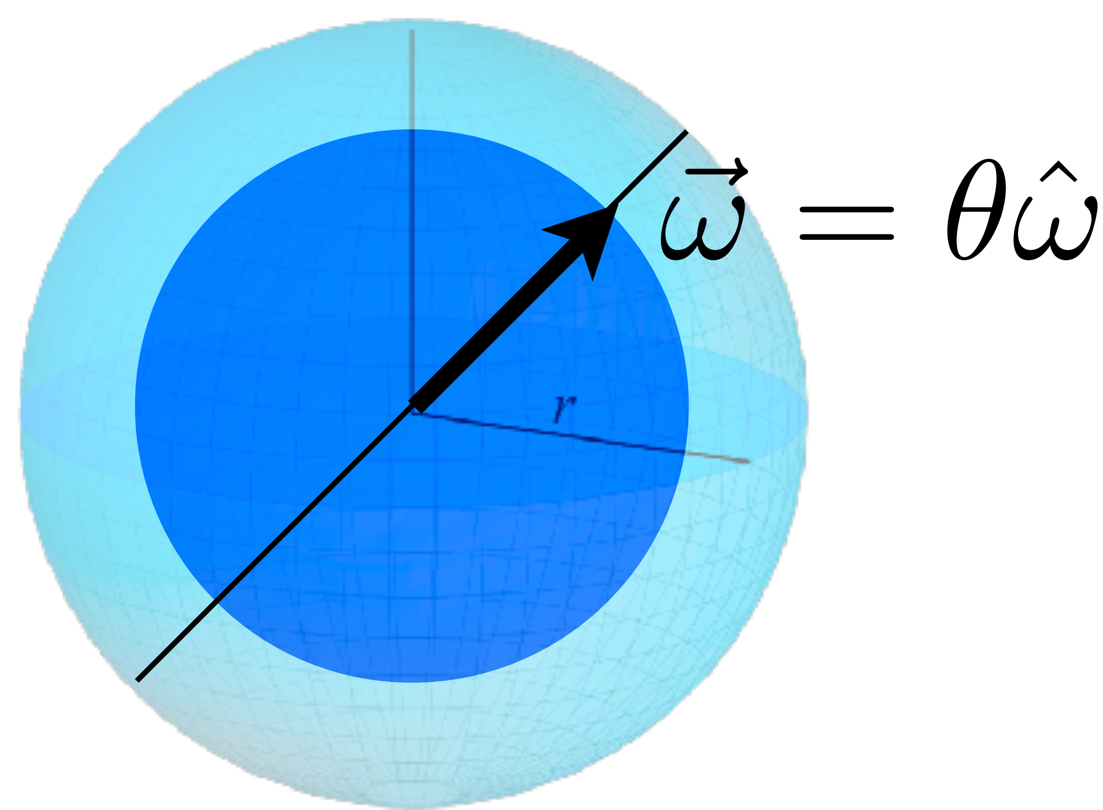
Topology over a loop of the BZ:

$$\pi_1\left(\mathrm{SO}(3)\right) = \mathbb{Z}_2$$

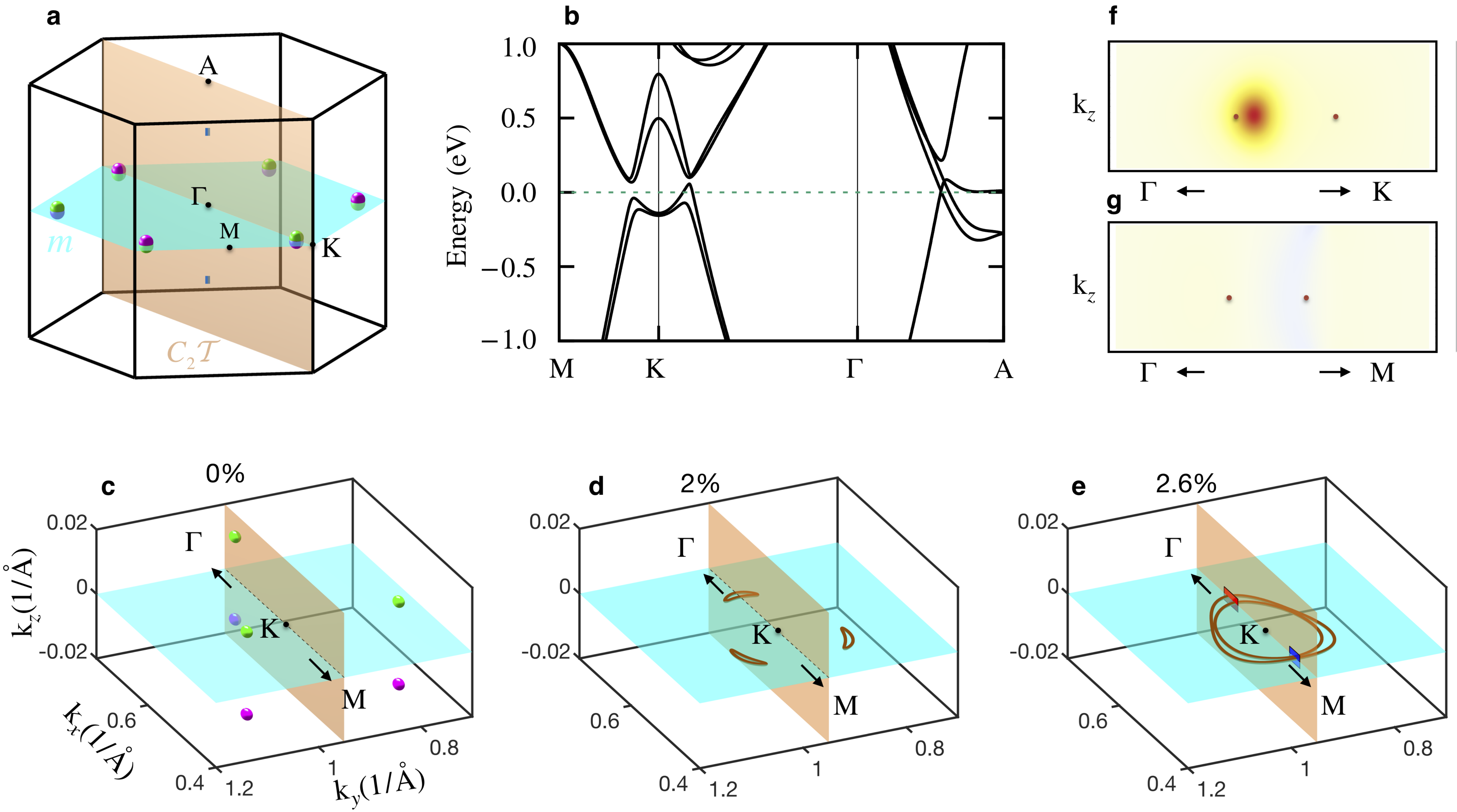


Lie algebra representation:

$$R(\boldsymbol{k}) = e^{\vec{\omega}\cdot\vec{L}} \in \mathrm{SO}(3)$$



Weyl nodes to nodal lines conversion rule for ZrTe



predictions of WPs with non-trivial Euler class in MoP, NbS, and TaAs

Nature Physics 16, 1137 (2020)

1D topology:
Möbius strip and orientability

1D topology:
Möbius strip and orientability

2D topology:
projective plane, Euler class, fragile topology,
Weyl nodes accumulation

“Real” topologies

Anti-unitary symmetry $\mathcal{A} = U\mathcal{K}$

such that $\mathcal{A}^2 = +\mathbf{1}$ and $\mathcal{A}\,\bar{\boldsymbol{k}} = \bar{\boldsymbol{k}}$

there exists a gauge with $H(\bar{\boldsymbol{k}}) \to \widetilde{H}(\bar{\boldsymbol{k}})^* = \widetilde{H}(\bar{\boldsymbol{k}})$

1D	spinful or spinless ***mT*** symmetry, ***C_2T, PT***	Non-Abelian topology
2D	spinful or spinless ***C_2T*** symmetry, ***PT***	Euler insulators
3D	spinless ***PT*** symmetry	Linked nodal rings
4D	spinless ***PT*** symmetry	Second Euler insulators

Berry curvature and Euler form

Chern class (complex case)

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

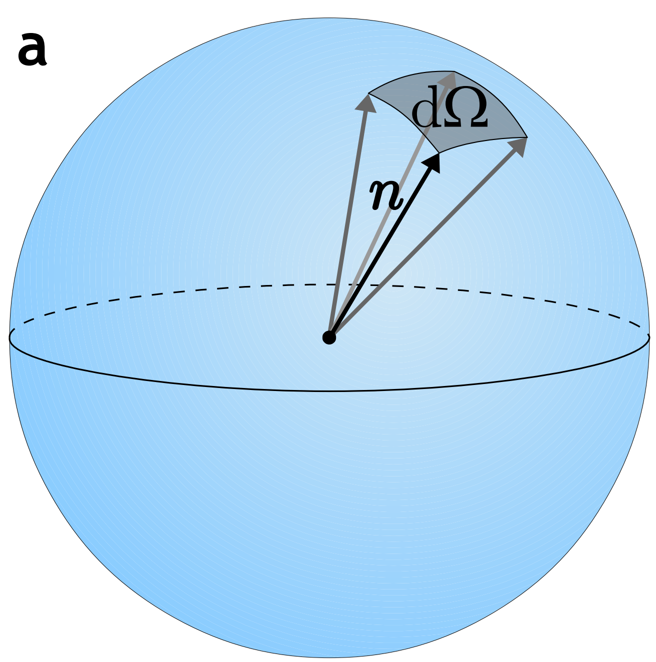
$$\boldsymbol{n} = \boldsymbol{h}/|\boldsymbol{h}| \in S^2$$

$$\mathrm{F}_{ij} = \tfrac{1}{2}\boldsymbol{n} \cdot (\partial_i \boldsymbol{n} \times \partial_j \boldsymbol{n})$$

$$d\Omega = \mathrm{F}_{ij} dk_i dk_j$$

$$c_1 \in \mathbb{Z}$$

a



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$$d\Omega = \mathrm{F}_{ij} dk_i dk_j$$

$$c_1 \in \mathbb{Z}$$

Euler class (real case, $(C_2T)^2 = +1$)

$$R(\boldsymbol{k}) = (u_1(\boldsymbol{k})\ u_2(\boldsymbol{k})\ \boldsymbol{n}(\boldsymbol{k}))$$

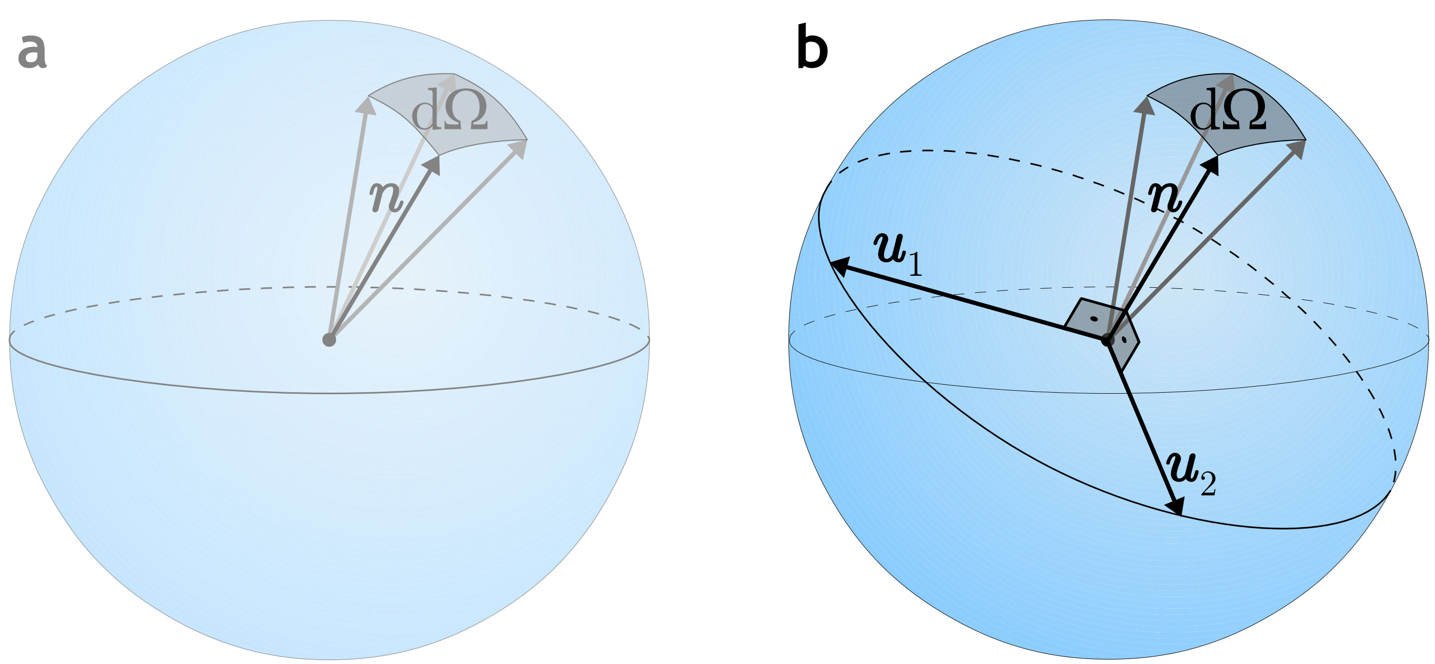
$$H(\boldsymbol{k}) = 2\boldsymbol{n} \cdot \boldsymbol{n}^T - \mathbf{1}$$ (flattened)

$$\boldsymbol{n}(\boldsymbol{k}) = \boldsymbol{u}_1(\boldsymbol{k}) \times \boldsymbol{u}_2(\boldsymbol{k}) \in S^2$$

$$\mathrm{Eu}_{ij} = \boldsymbol{n} \cdot (\partial_i \boldsymbol{n} \times \partial_j \boldsymbol{n})$$

$$d\Omega = \mathrm{Eu}_{ij} dk_i dk_j$$

$$\chi \in 2\mathbb{Z}$$



Three-level system

$$\widetilde{H}(\boldsymbol{k}) = R(\boldsymbol{k})\mathcal{E}(\boldsymbol{k})R^T(\boldsymbol{k}) \ , \quad R(\boldsymbol{k}) \in SO(3)$$

(global sign of R is a gauge freedom)

(e_1 , e_2 , e_3) ~ (-e_1 , e_2 , -e_3) : the rotation of subframes is a gauge freedom !

Classifying space for two-occupied bands and one unoccupied band:

$$\mathrm{Gr}_2(\mathbb{R}^3) = \frac{\mathsf{SO}(3)}{\mathsf{S}[\mathsf{O}(2) \times \mathsf{O}(1)]} = \mathbb{R}\mathrm{P}^2 = \mathbb{S}^2/\{x \sim -x\}$$

projective plane
(sphere with antipodal points identified)

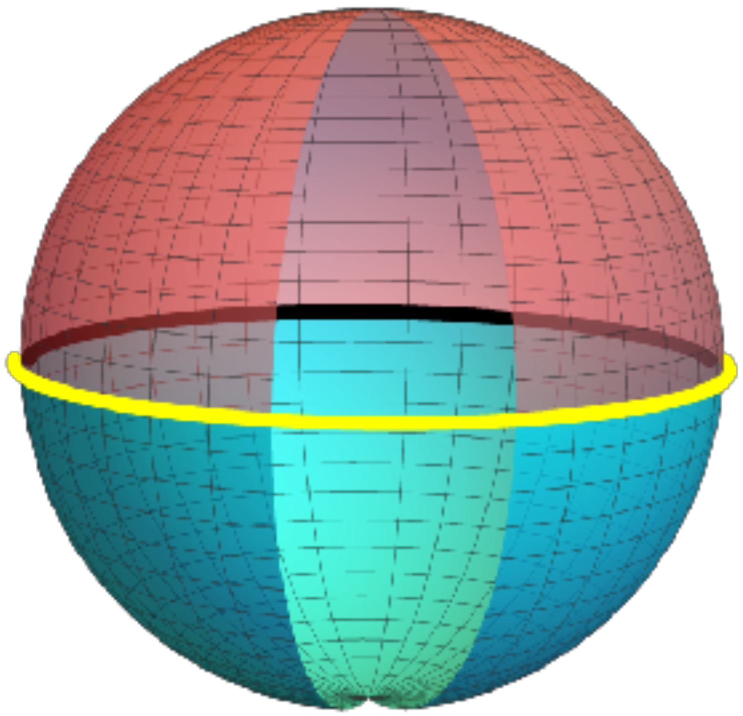
“unoriented” surface

AB, T. Bzdusek, RJ Slager, Phys. Rev. B **102**, 115135 (2020)

Oriented double covering

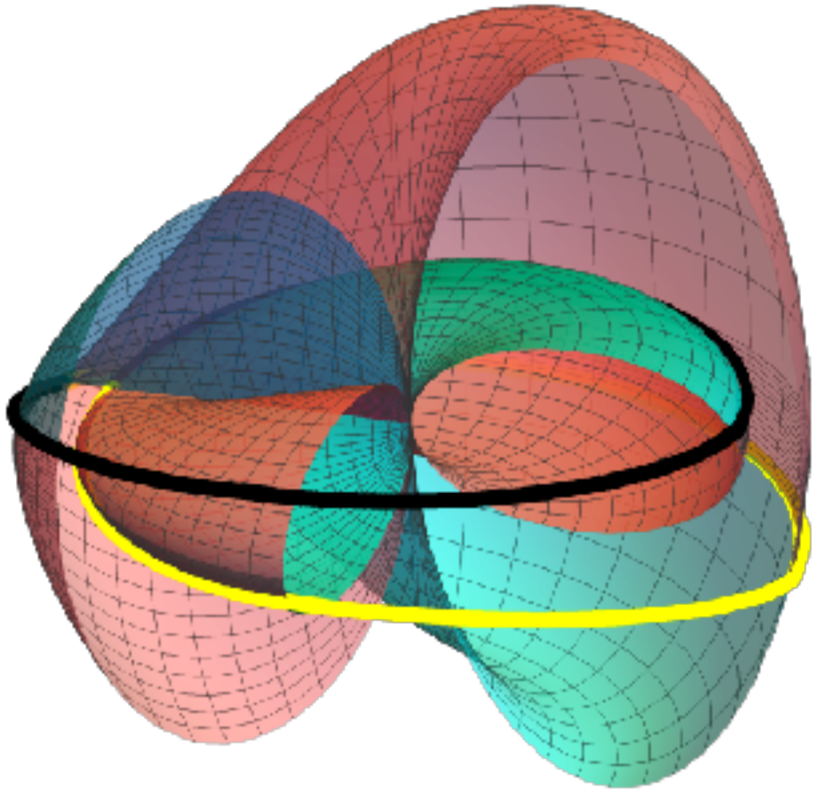
$$\mathbb{R}\mathrm{P}^2 = \mathbb{S}^2/\{x \sim -x\}$$

orientable



$\mathbb{S}^2$

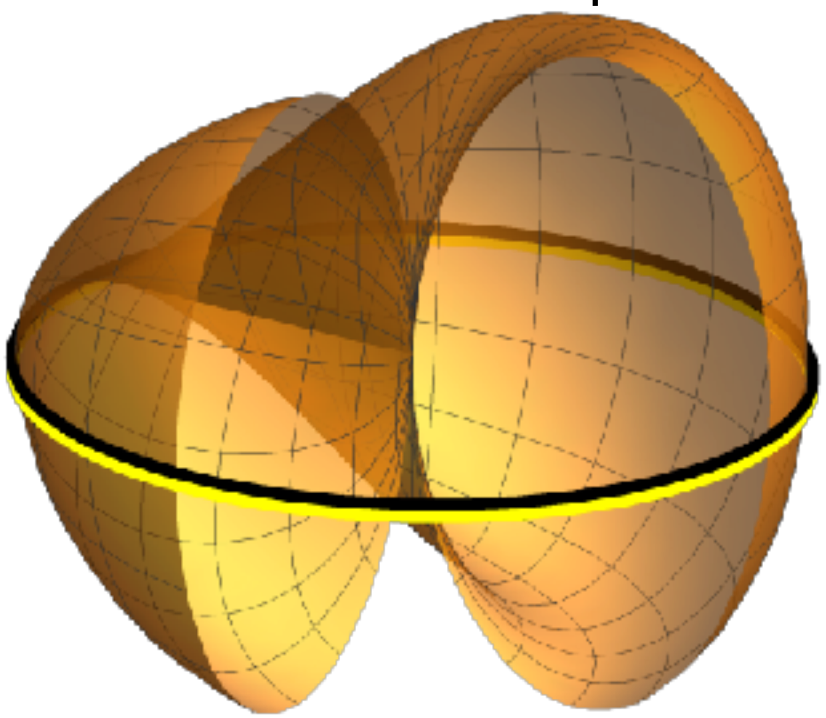
path-connected
simply connected



$\mathbb{S}^2 \to \mathbb{R}\mathrm{P}^2$

non-orientable

"cross-cap"



$\mathbb{R}\mathrm{P}^2$

path-connected

$\pi_1[\mathbb{R}\mathrm{P}^2] = \mathbb{Z}_2$

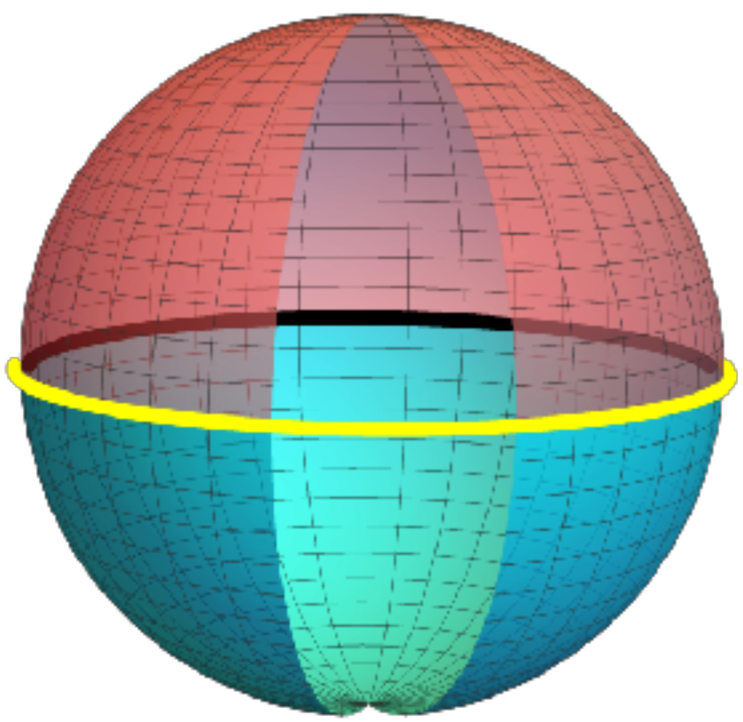
$$\pi_2[\mathbb{S}^2] = \mathbb{Z} \cong \pi_2[\mathbb{R}\mathrm{P}^2] = 2\mathbb{Z}$$

AB, T. Bzdusek, RJ Slager, Phys. Rev. B **102**, 115135 (2020)

Oriented double covering

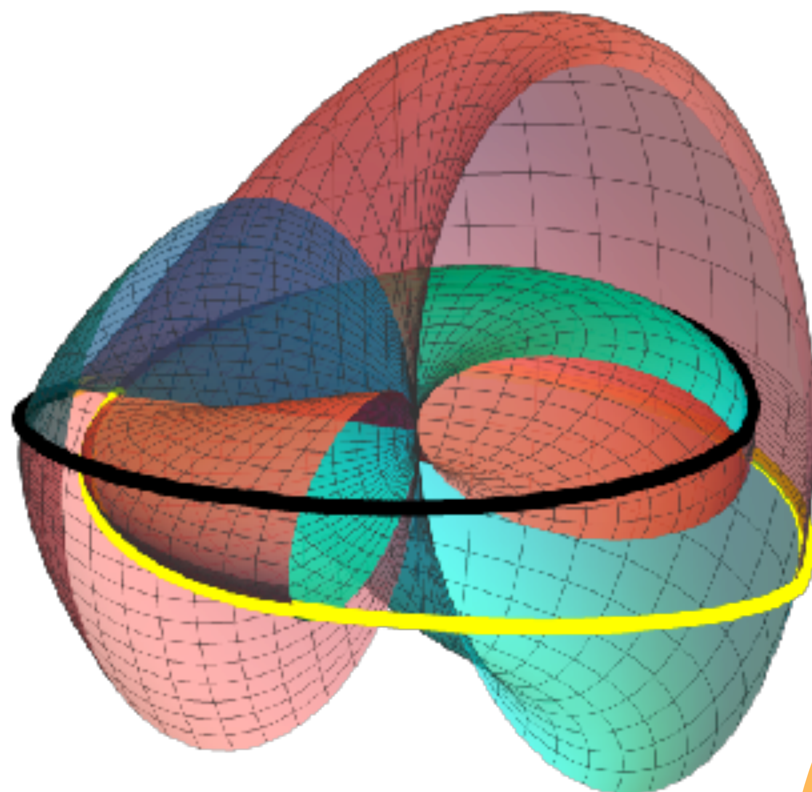
$$\mathbb{RP}^2 = \mathbb{S}^2/\{x \sim -x\}$$

orientable



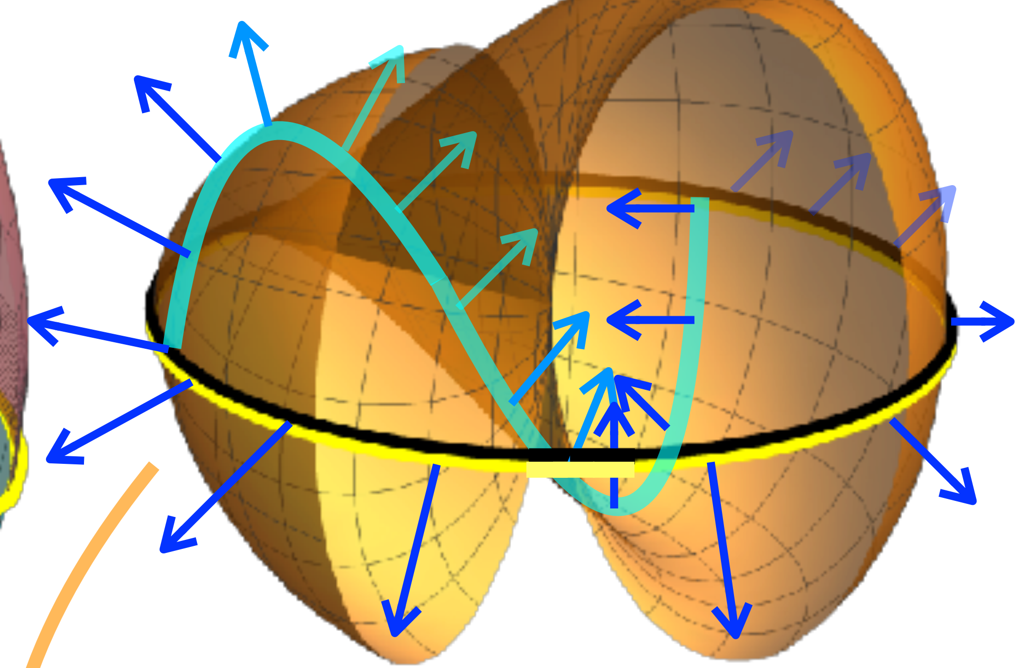
$\mathbb{S}^2$

path-connected
simply connected



$\mathbb{S}^2 \to \mathbb{RP}^2$

“cross-cap”



$\mathbb{RP}^2$

non-contractible loop

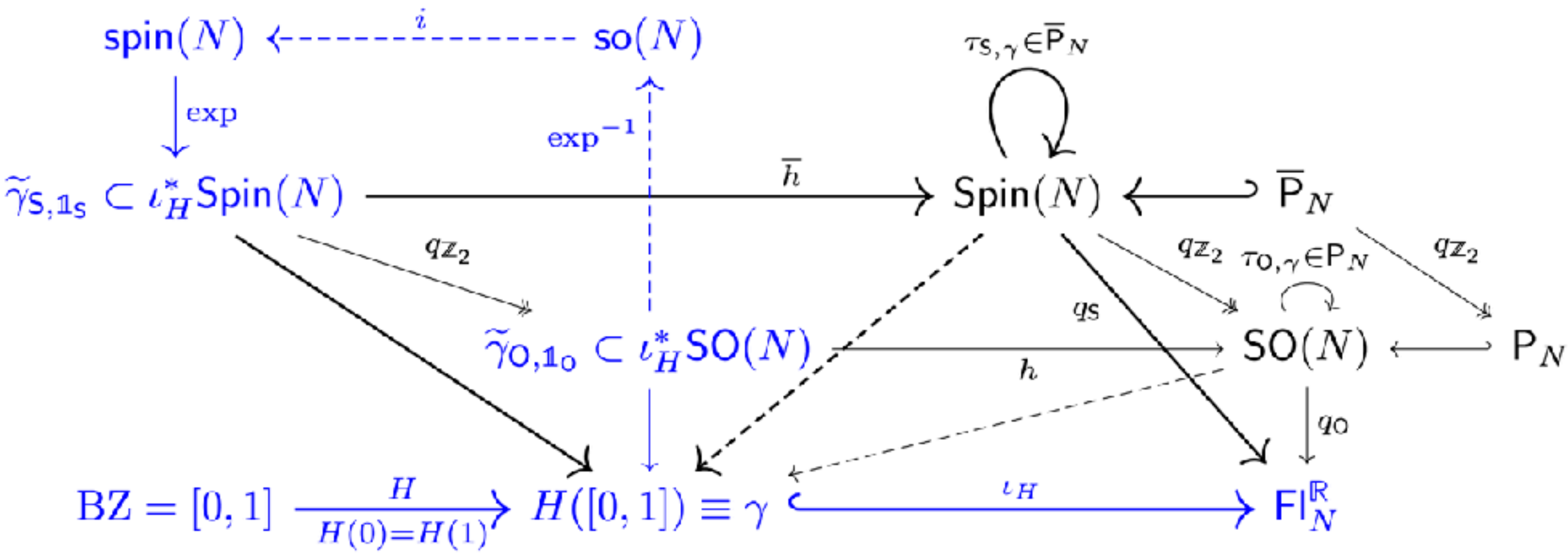
path-connected

$\pi_1[\mathbb{RP}^2] = \mathbb{Z}_2$

$$\pi_2[\mathbb{S}^2] = \mathbb{Z} \cong \pi_2[\mathbb{RP}^2] = 2\mathbb{Z}$$

AB, T. Bzdusek, RJ Slager, Phys. Rev. B **102**, 115135 (2020)

Computation of non-Abelian charges: lift diagram



monodromy representation = holonomy computation

Contents

Patch Euler number (gauge invariance of nodal points)

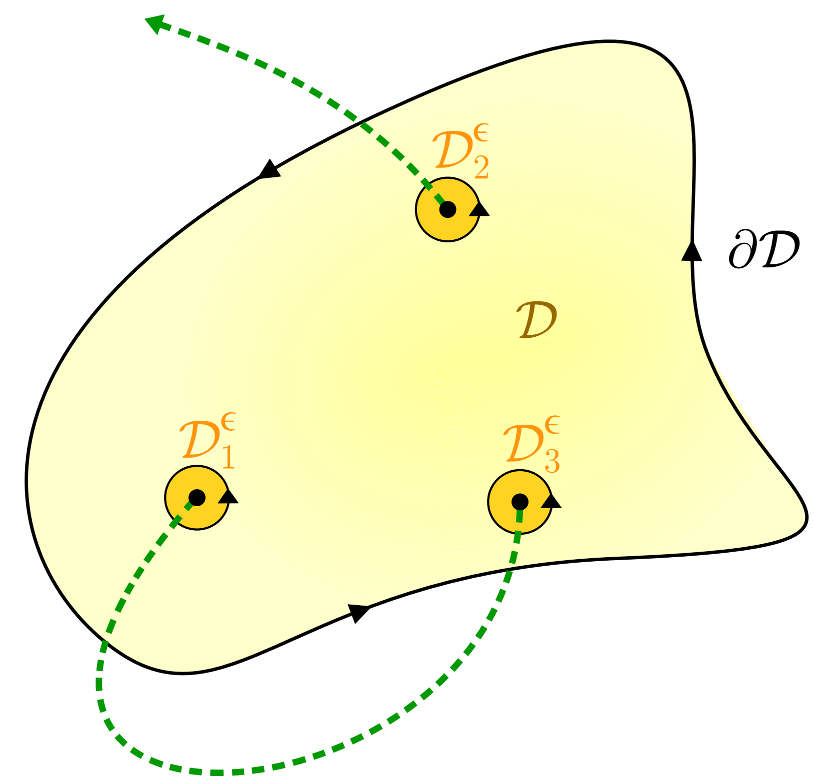
Euler class:

$$2\chi(\mathcal{D}) = \frac{1}{\pi}\left[\int_{\mathcal{D}} \mathrm{Eu} - \oint_{\partial\mathcal{D}} \mathrm{a}\right]$$

$$= \frac{1}{\pi}\sum_n \left[\int_{\mathcal{D}_n^\epsilon} \mathrm{Eu} - \oint_{\partial\mathcal{D}_n^\epsilon} \mathrm{a}\right]$$

$$= \sum_n W_n \in \mathbb{Z}$$

The patch *D* contains principal nodes and avoids adjacent ones



The Euler connection and Euler form are continuous except at the principal nodes,
while the Euler form is not exact (Eu ≠ da),
it is nevertheless integrable !