NORDITA

UNIVERSITY OF CAMBRIDGE

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

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# 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

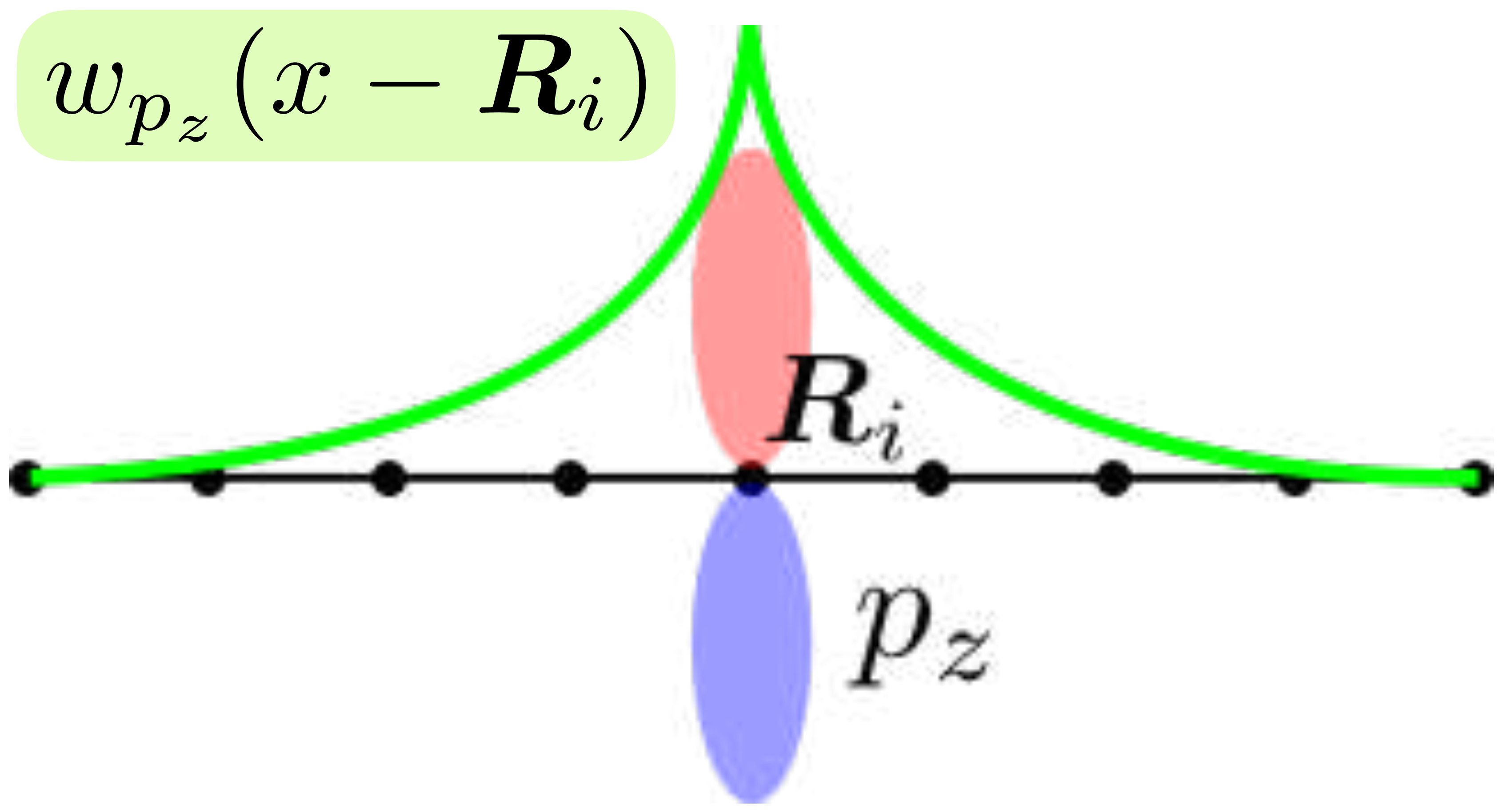
$$H_{\alpha\beta}(\boldsymbol{k}) = \sum_{\boldsymbol{R}_j} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_j}\ t_{\alpha\beta}(\boldsymbol{R}_j - \boldsymbol{0})$$

Bloch picture:

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

**Wannier functions**

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




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

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

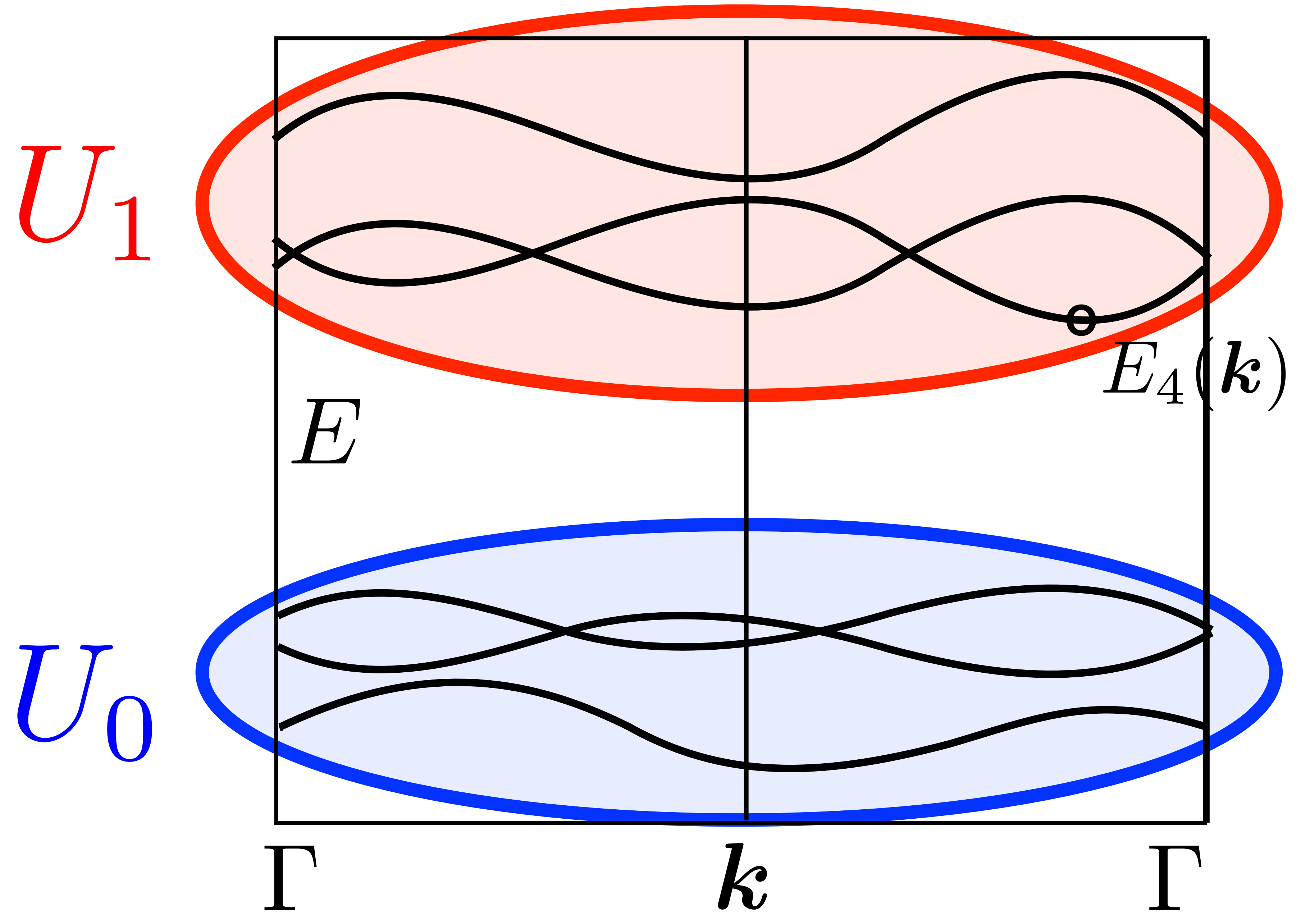
## Grassmannian modeling of gapped band structures

Bloch Hamiltonian:

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

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

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




flattened Hamiltonian:

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

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*₂*T*** symmetry (spinful or spinless), spinless ***PT*** symmetry

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

$$\mathcal{A}^2 = +\mathbf{1} \quad \longrightarrow \quad \text{no Kramers degeneracies:} \quad \left| \begin{array}{l} \mathcal{A} = D\mathcal{K} \\ D = \mathrm{diag}\{\mathrm{e}^{\mathrm{i}\varphi_j}\}_{j=1}^{N} \end{array} \right.$$

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

**within the $C_2T$ plane:**

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

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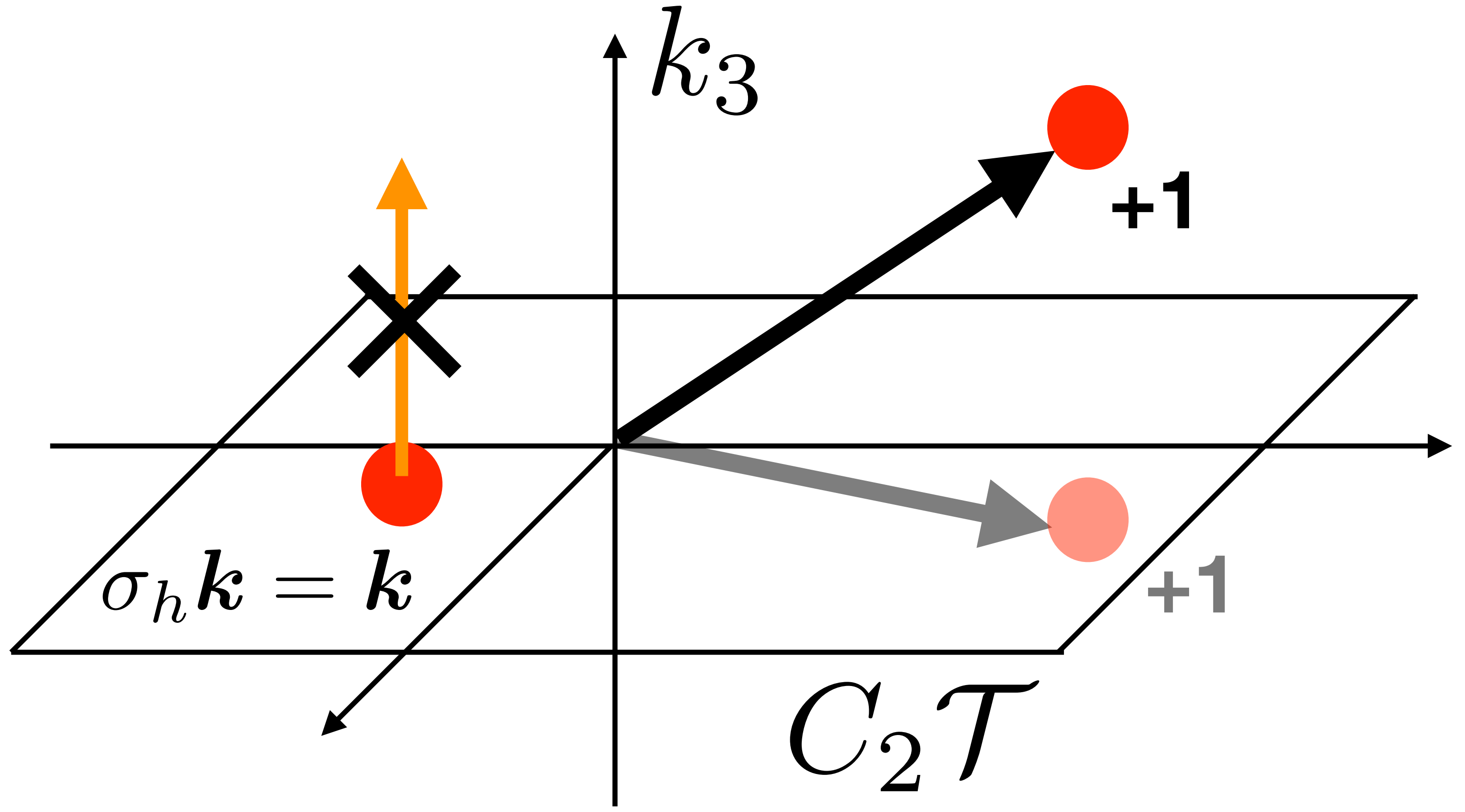


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# “Real” topologies

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

# “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, ***$C_2$T, PT*** | Graphene, SSH insulators |
| 2D | spinful or spinless ***$C_2$T*** 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

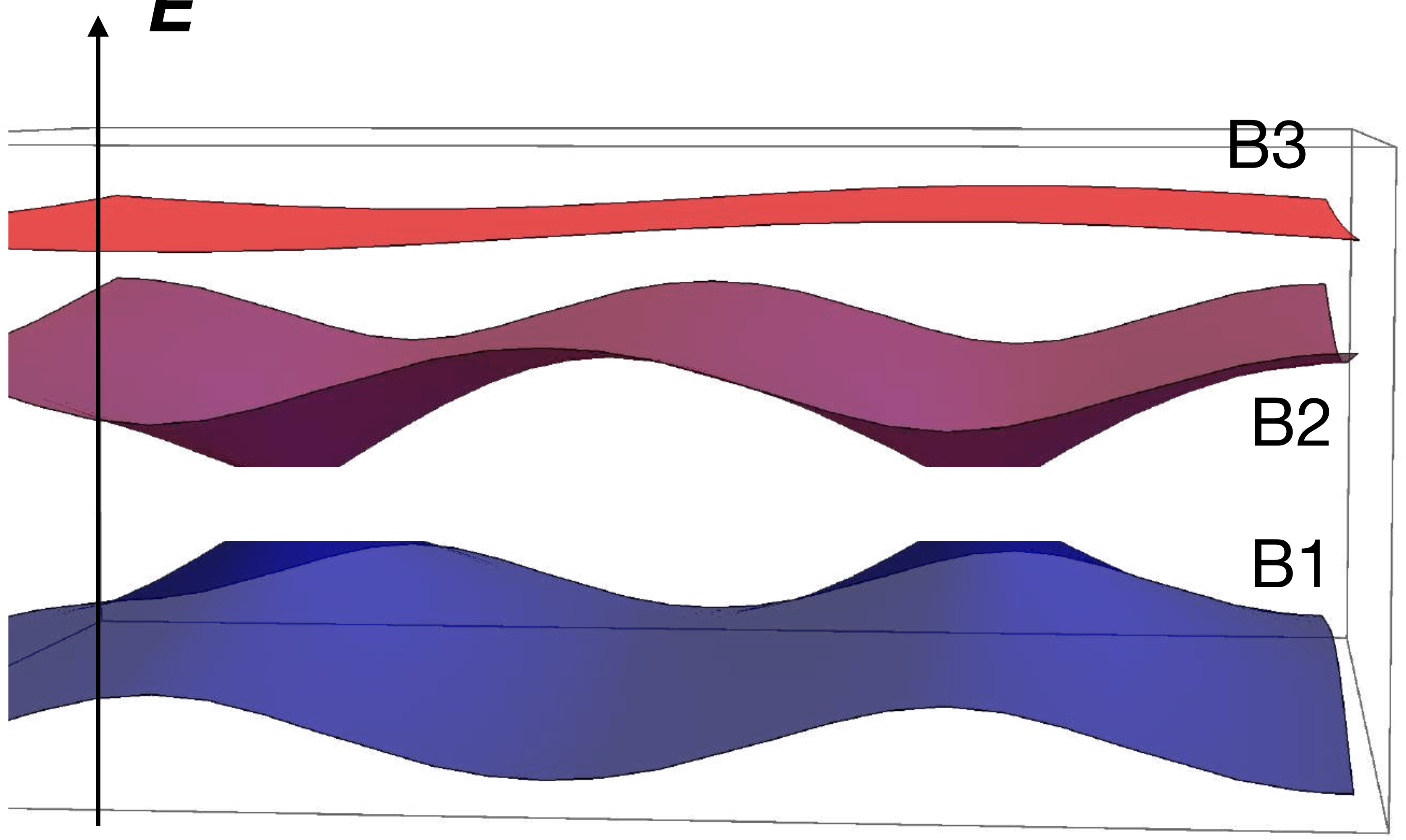
# 1.5D topology of three-level system

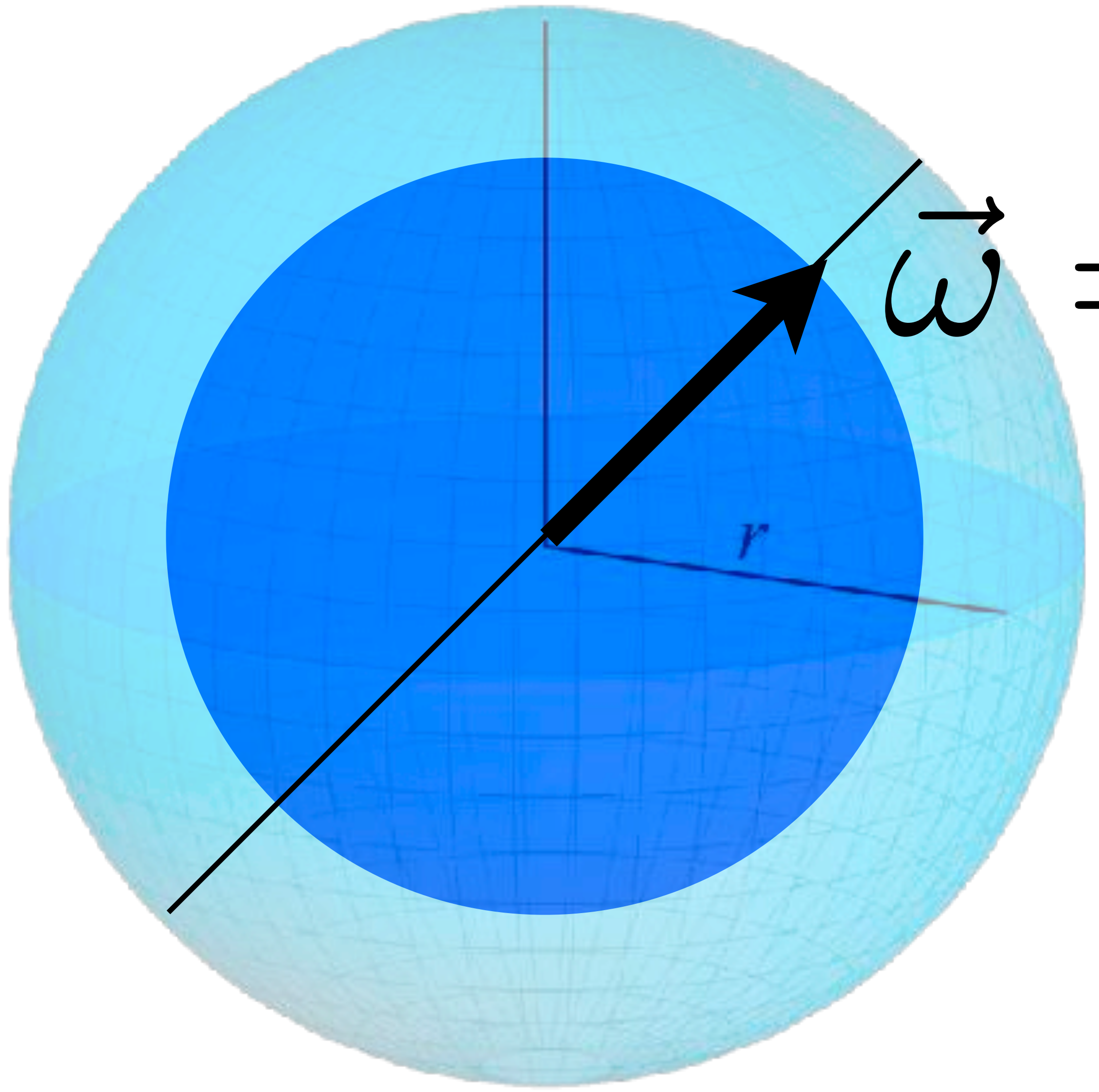
$$\widetilde{H}(\boldsymbol{k}) = R(\boldsymbol{k})\mathcal{E}(\boldsymbol{k})R^T(\boldsymbol{k}) \qquad R(\boldsymbol{k}) = (\boldsymbol{e}_1\ \boldsymbol{e}_2\ \boldsymbol{e}_3)$$

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

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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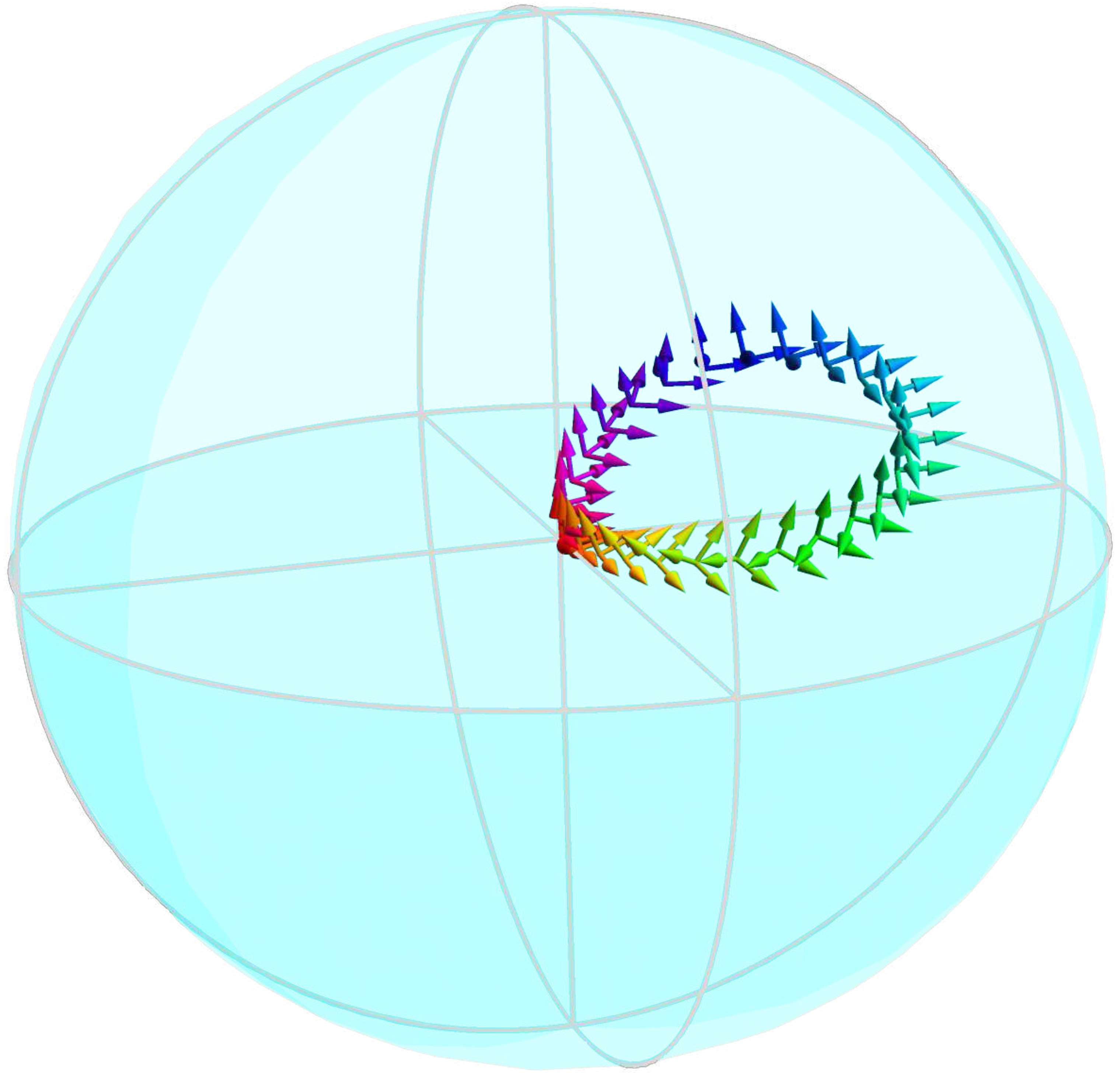
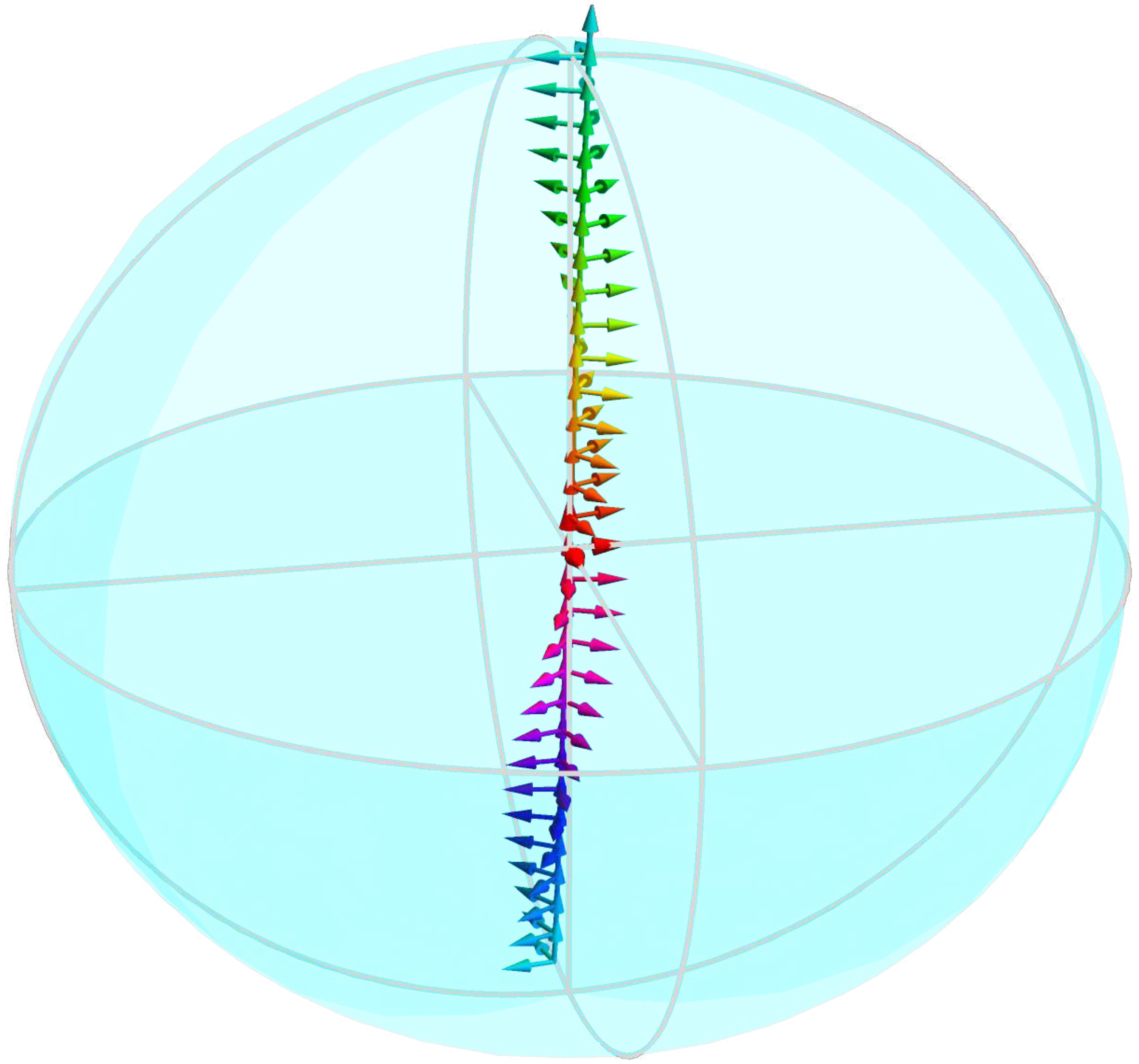
**Topology over a loop in the BZ:**

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

accumulated {0, 2$\pi$}-frame rotation,





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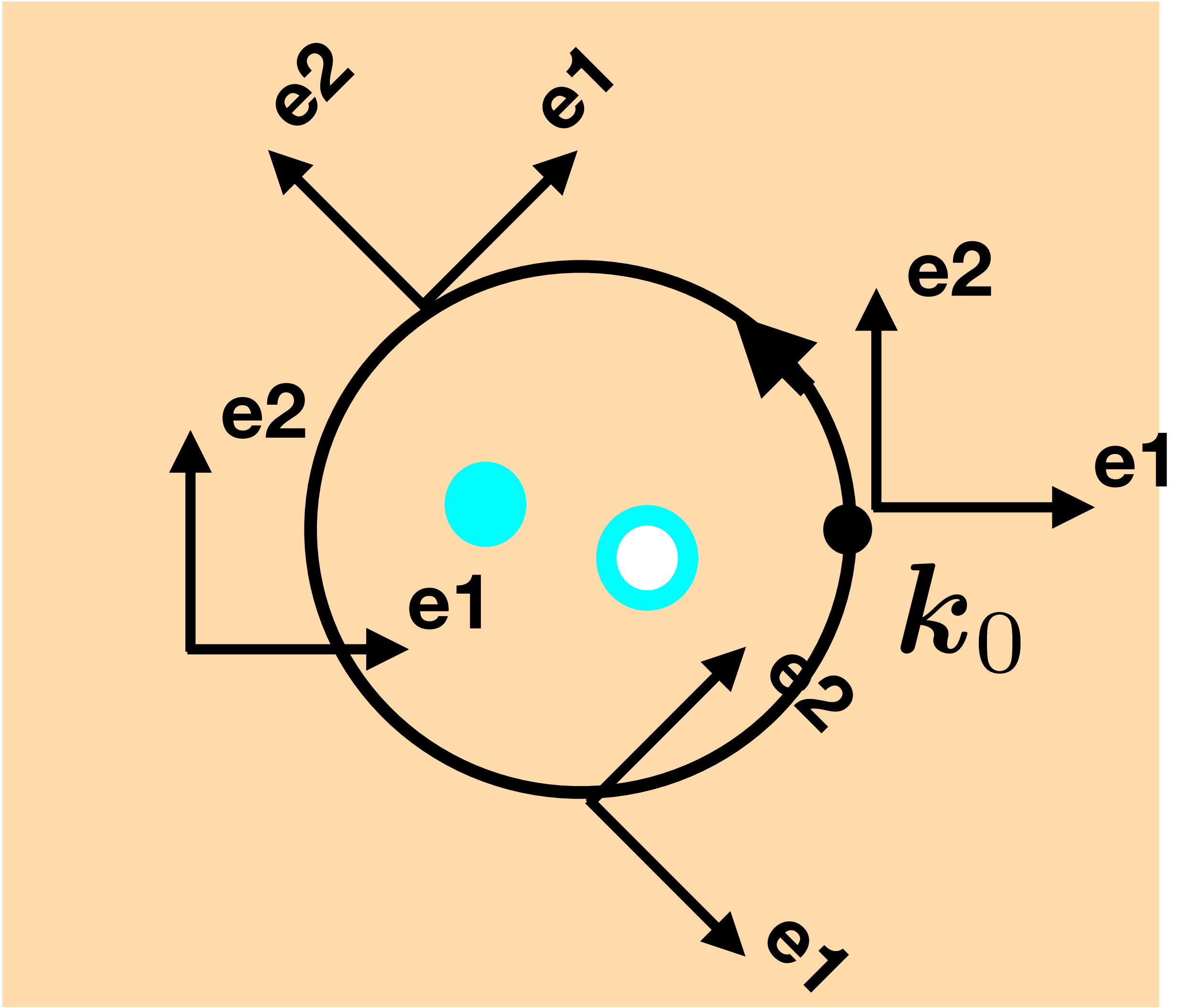
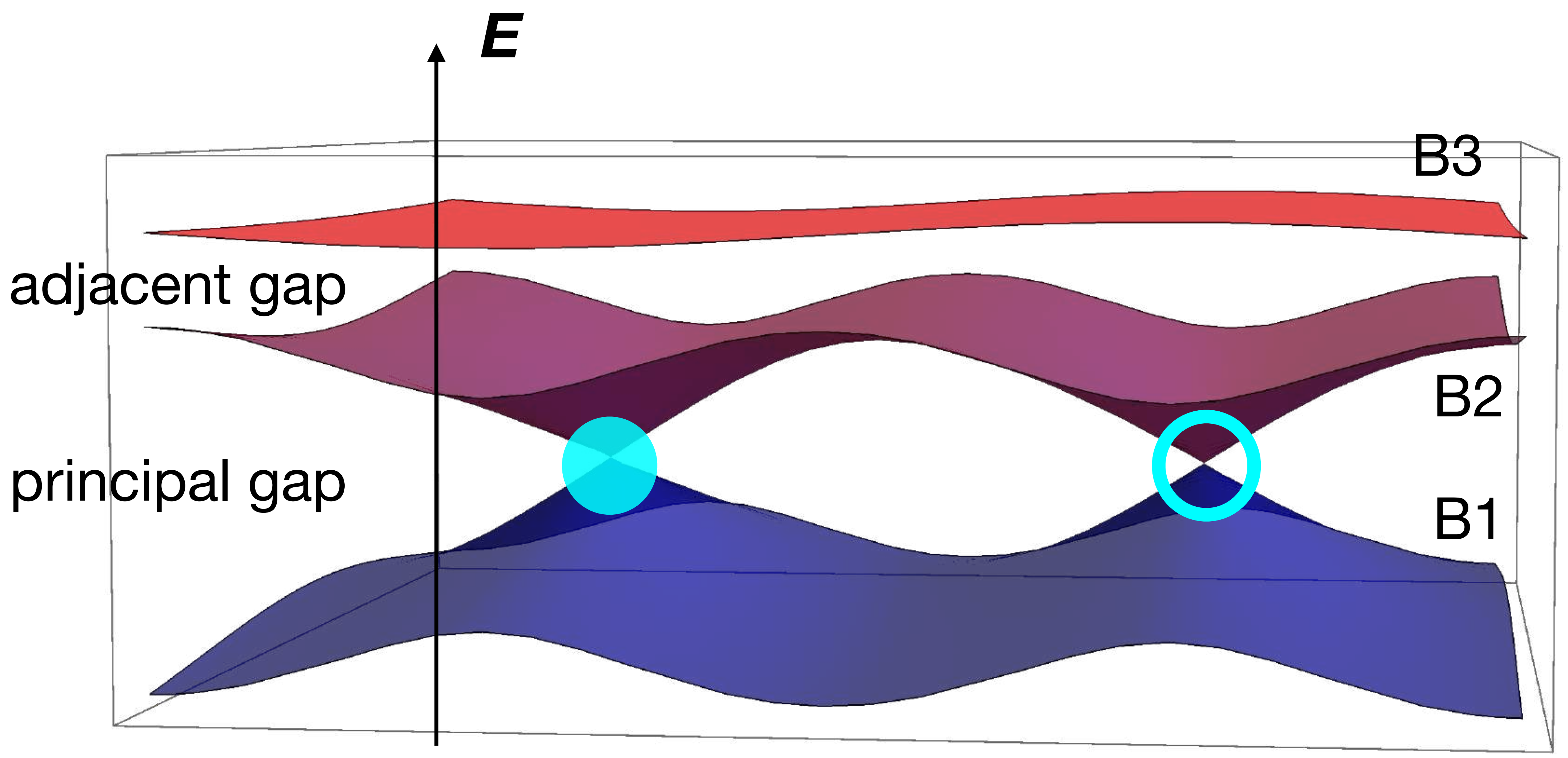
stability of Nodal-Points pair

Nodal-Point charge has two signs!

0−frame rotation around $e_3$



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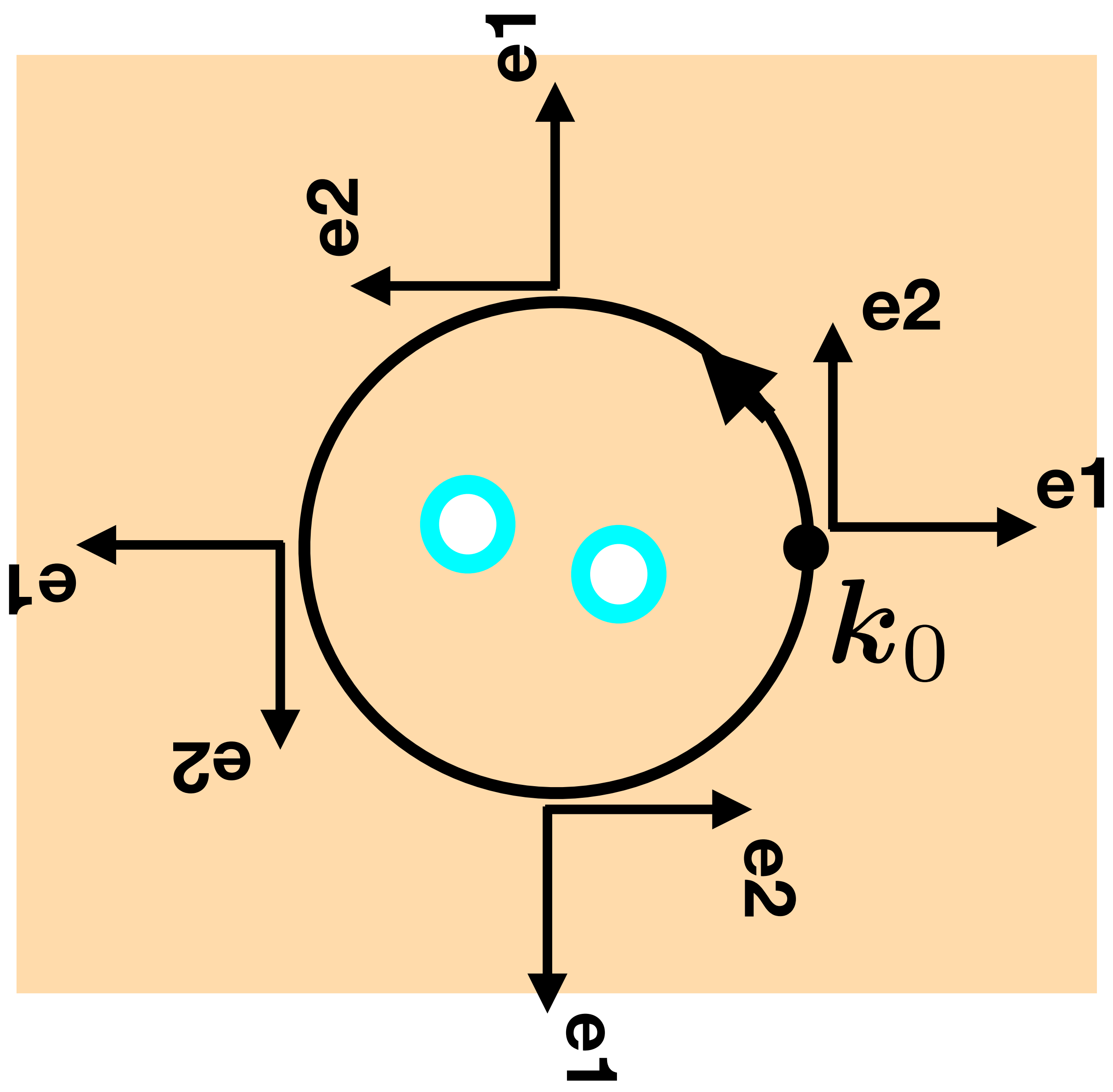
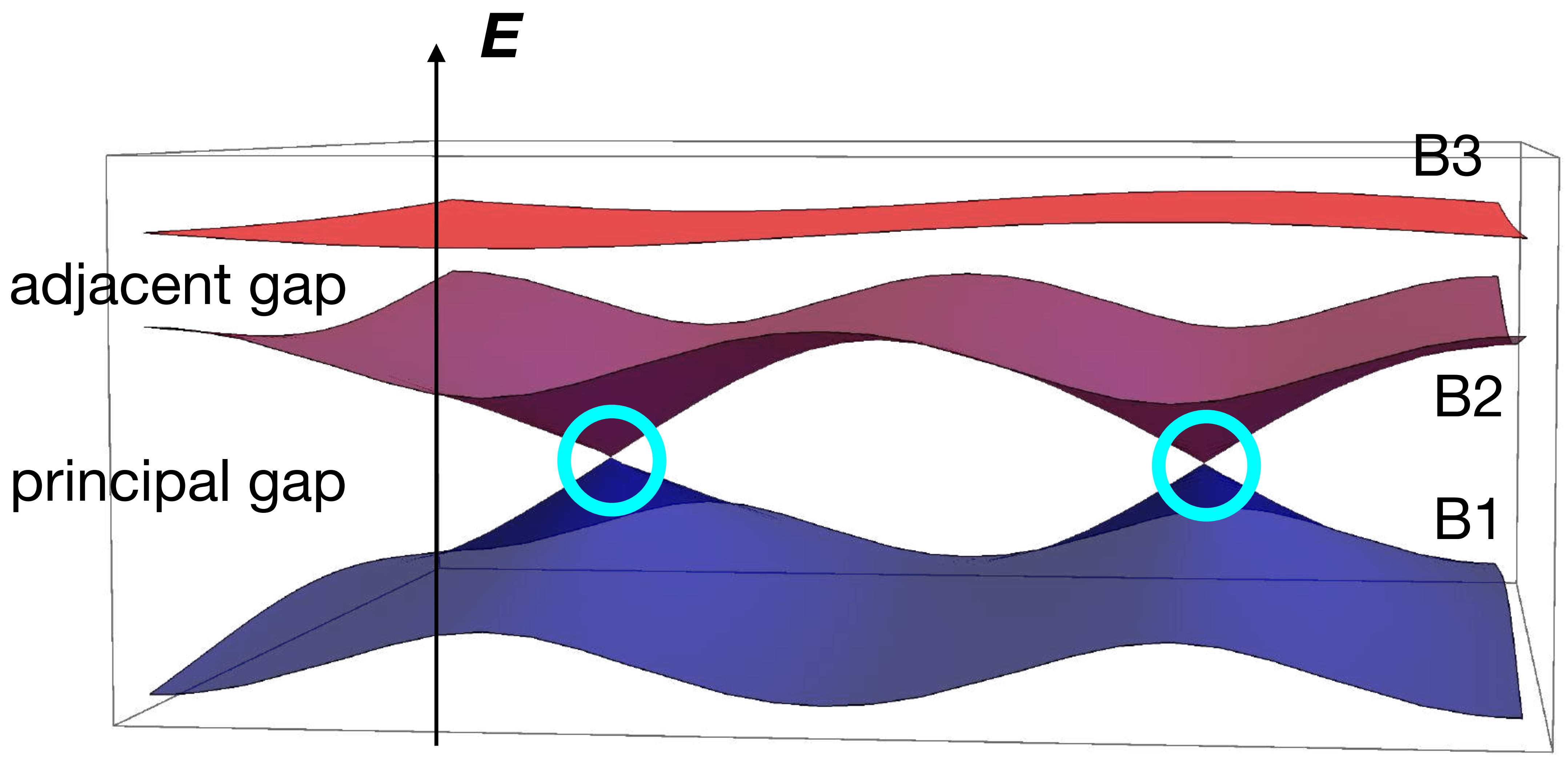
**$2\pi$−frame rotation around $e_3$**



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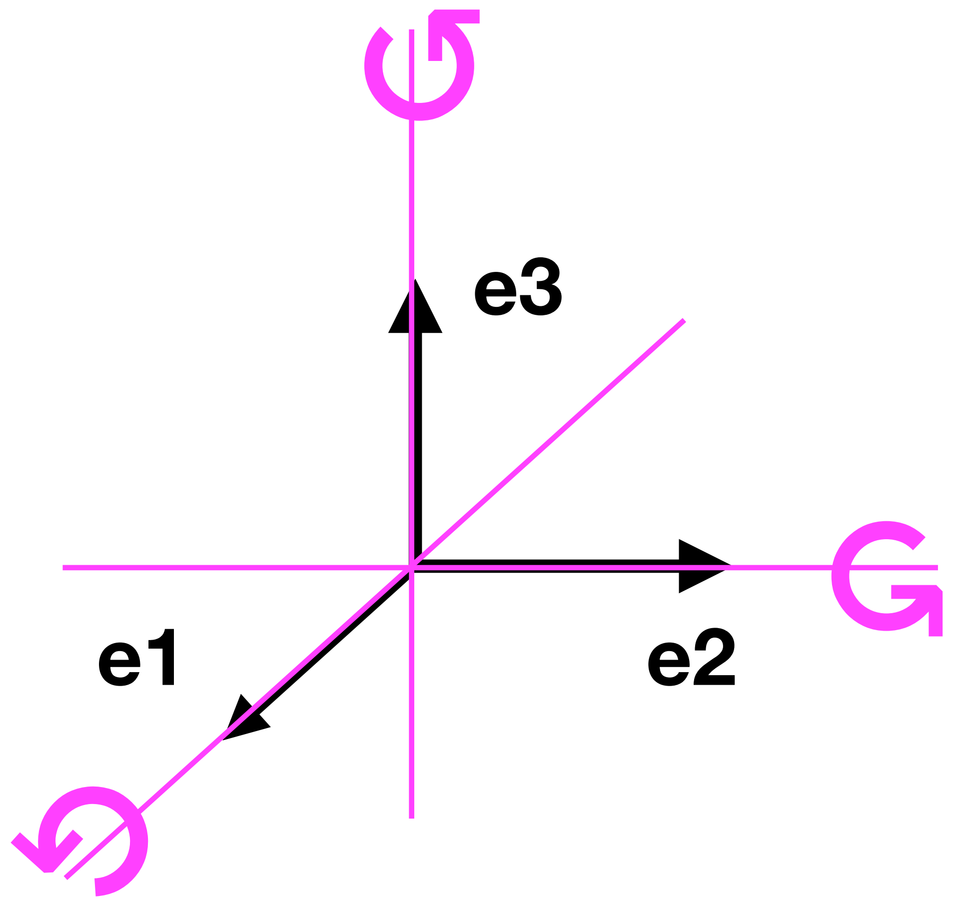
$$\widetilde{H}(\boldsymbol{k}) = R(\boldsymbol{k})\mathcal{E}(\boldsymbol{k})R^T(\boldsymbol{k}) \qquad R(\boldsymbol{k}) = (\boldsymbol{e}_1\ \boldsymbol{e}_2\ \boldsymbol{e}_3) \sim (\pm\boldsymbol{e}_1\ \pm\boldsymbol{e}_2\ \pm\boldsymbol{e}_3)$$

Group of gauge freedom: $\mathsf{O}(1)^3 = \mathsf{C}_i \times \mathsf{D}_2 = \{E, I\} \times \{E, C_{2z}, C_{2y}, C_{2x}\}$

$\mathsf{D}_2$ : dihedral point group,

$\pi$-frame rotation around $e_1$, $e_2$, $e_3$




Bdzusek *et al*, Science (2019)

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Flag manifold

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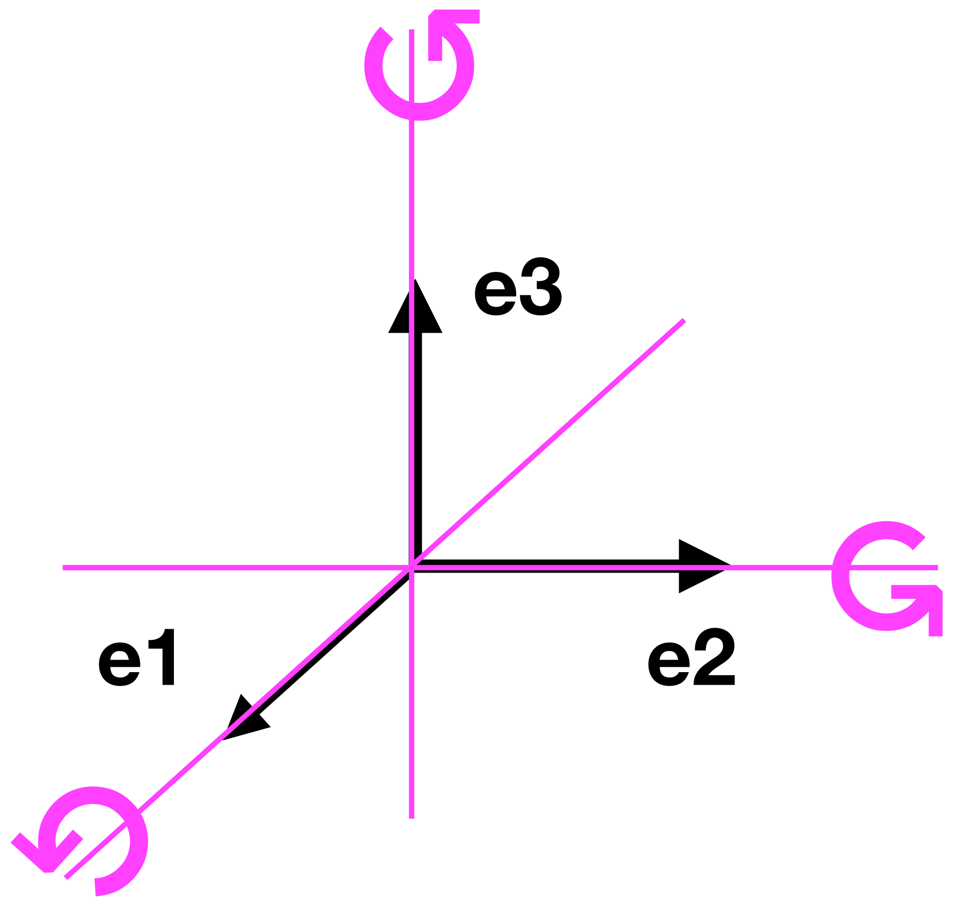


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Lie algebra representation

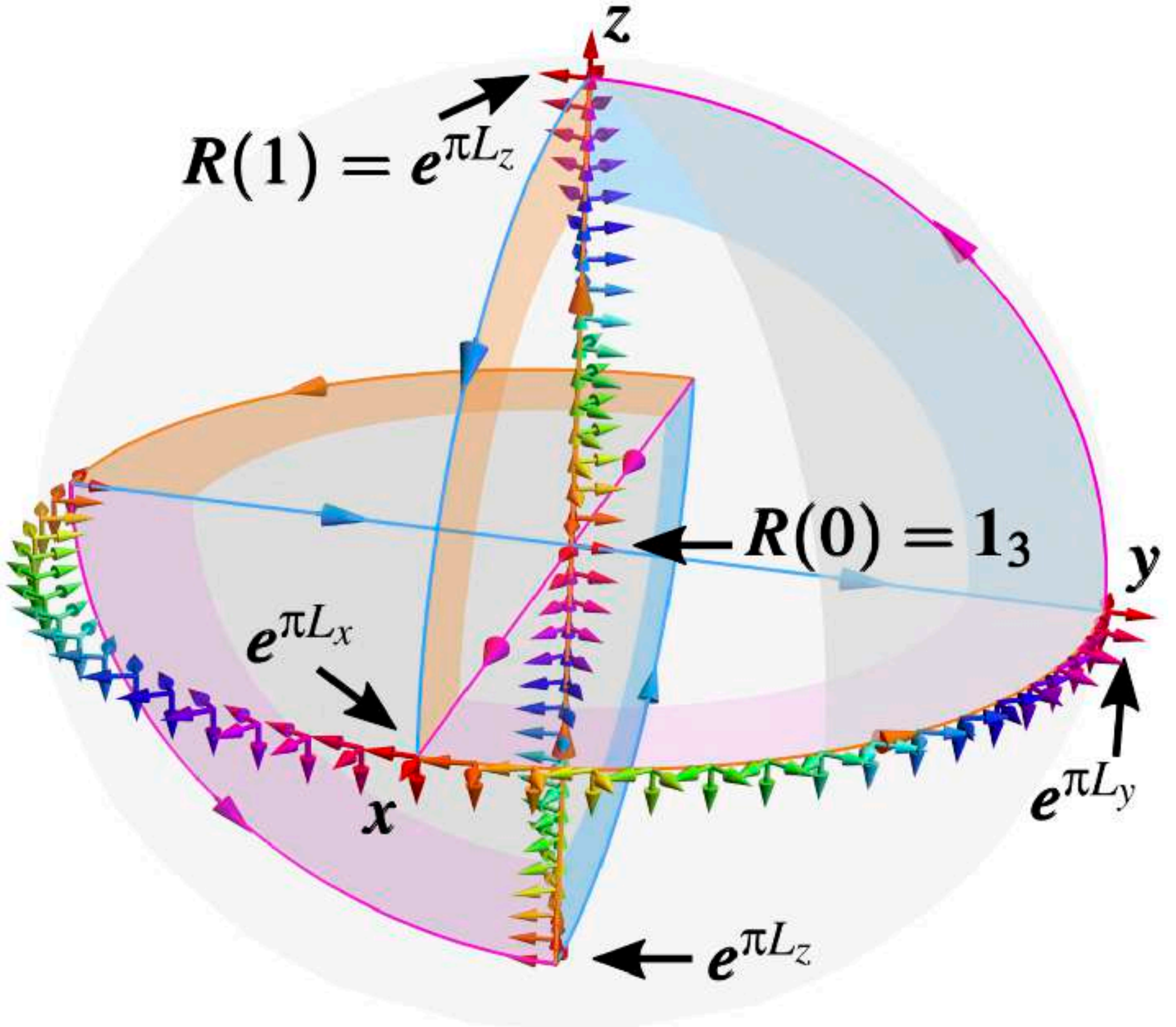
accumulated rotation of parallel transp. frame

Flag manifold

$$\mathsf{Fl}^{\mathbb{R}}_{1,1,1} = \frac{\mathsf{O}(3)}{\mathsf{O}(1)^3} = \frac{\mathsf{SO}(3)}{\mathsf{D}_2}$$

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

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

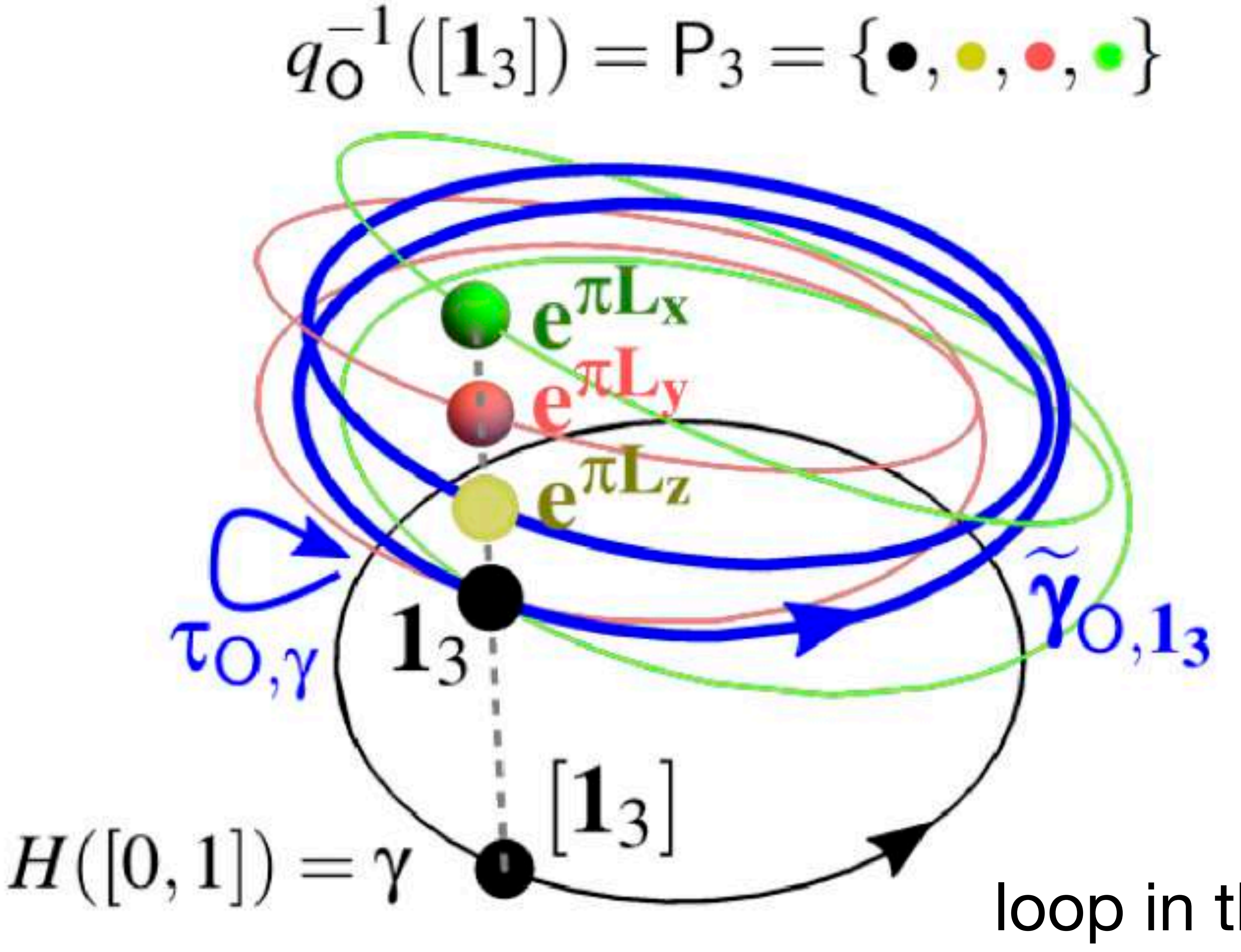


# Monodromy representation

principal fiver bundle
with discrete structure group

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

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




loop in the flag

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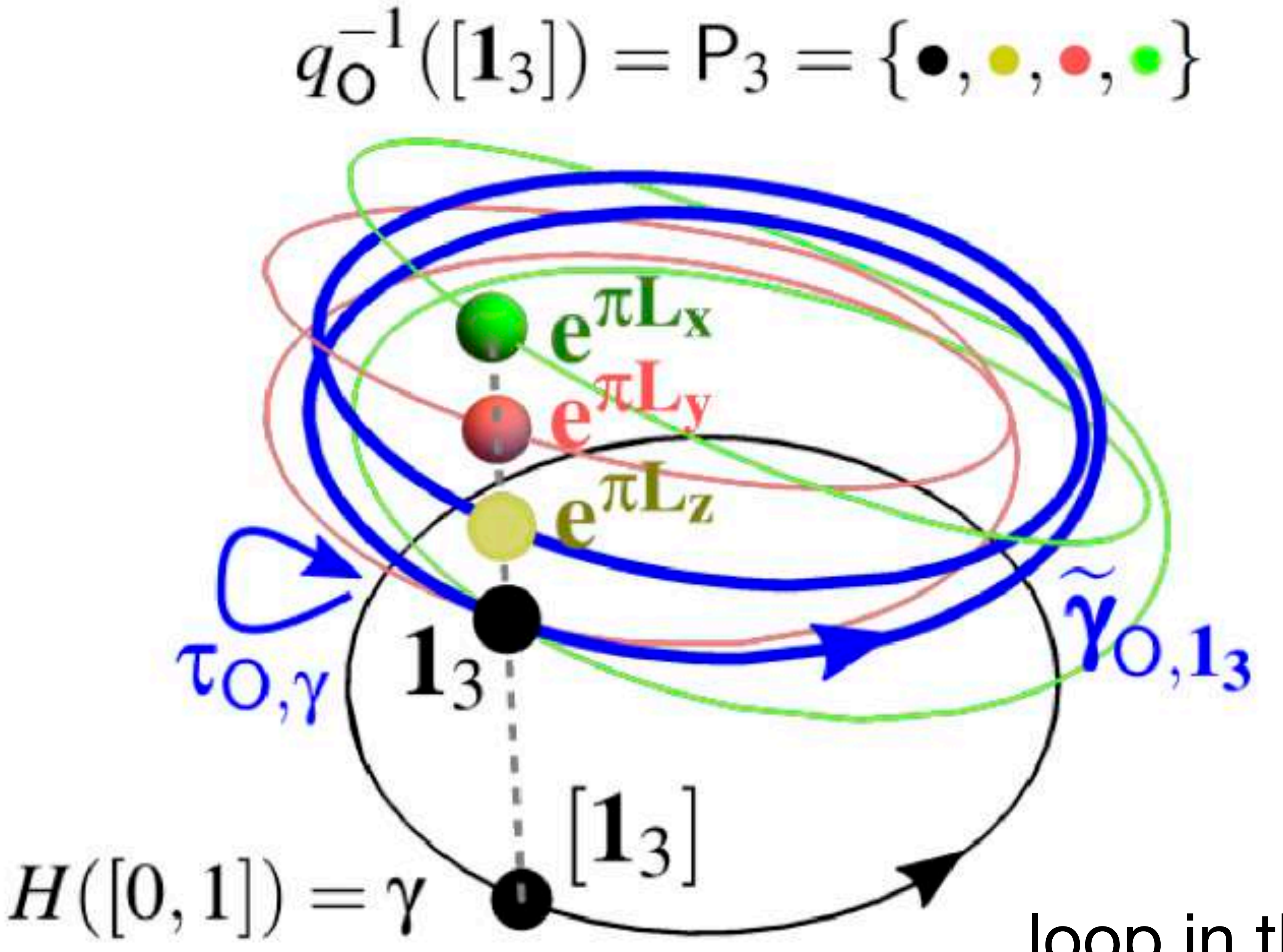



loop in the flag

It does not distinguishes a

$\pi$-rotation

from a

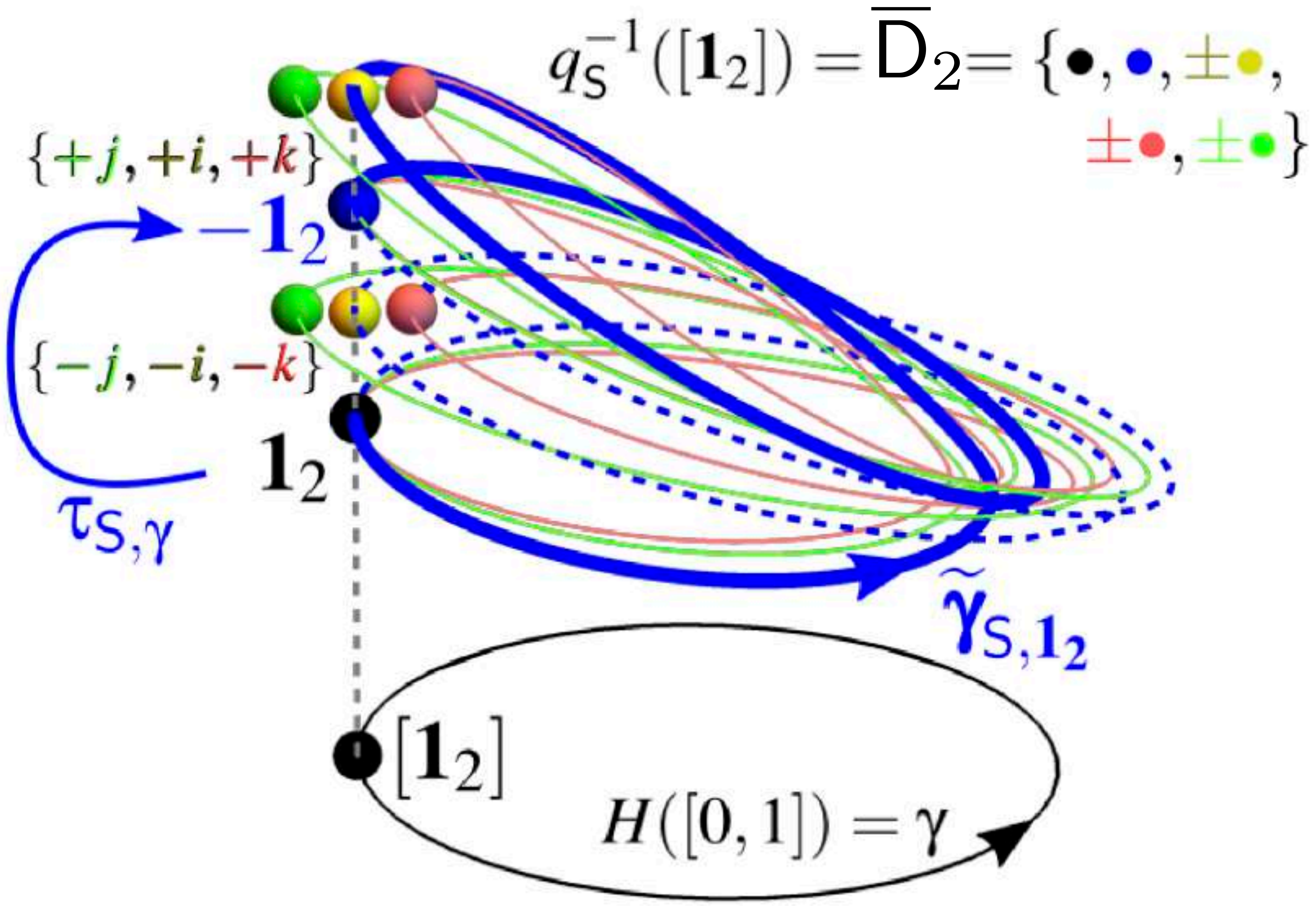
($-\pi$)-rotation around **$e_3$**

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

# Monodromy representation,
# 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 $\pi_1\left(\mathsf{SO}(3)/\mathsf{D}_2\right) = \overline{\mathsf{D}}_2$




$\pi$-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: holonomy rep.

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

# Non-Abelian topological invariant of nodal points

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

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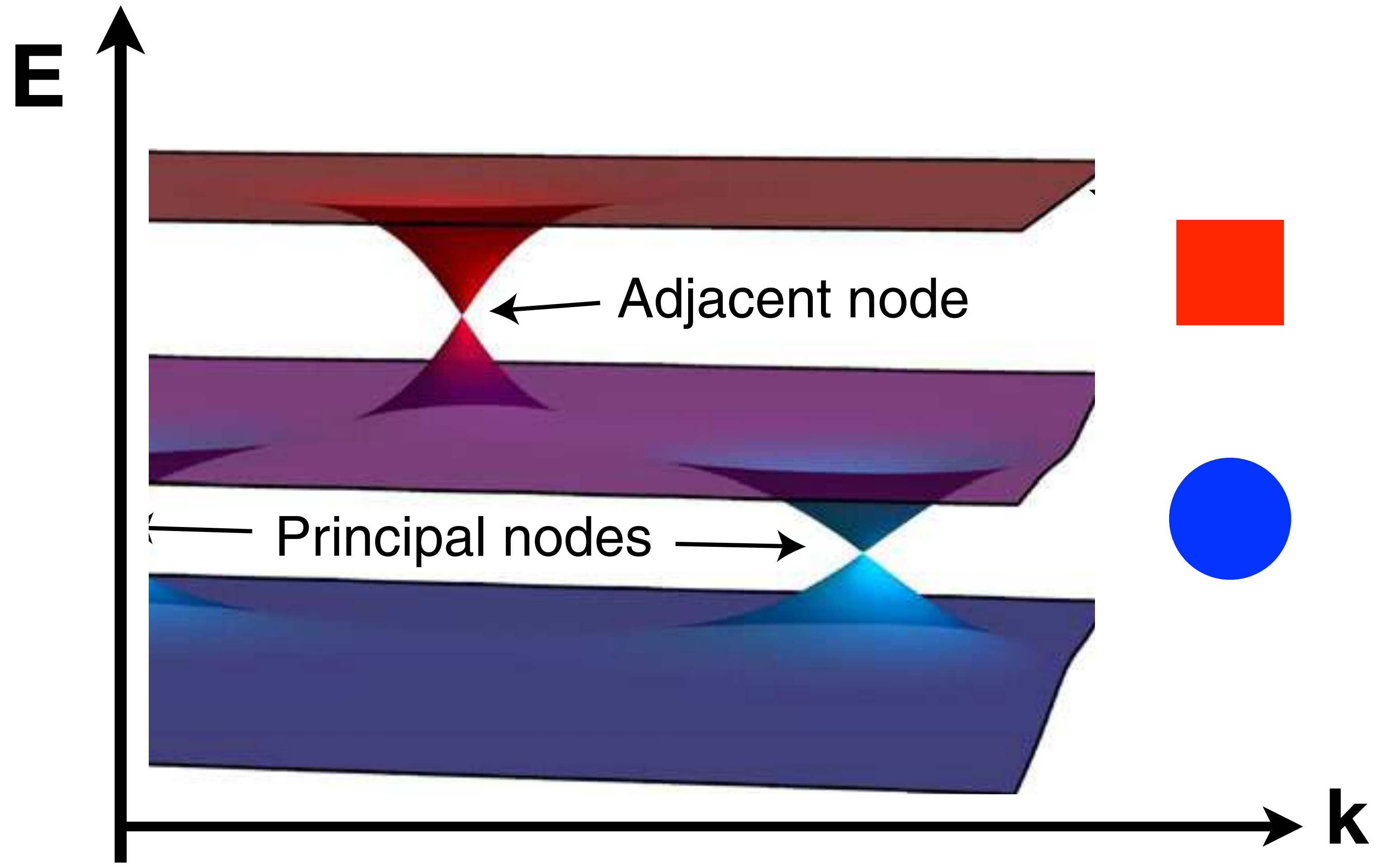
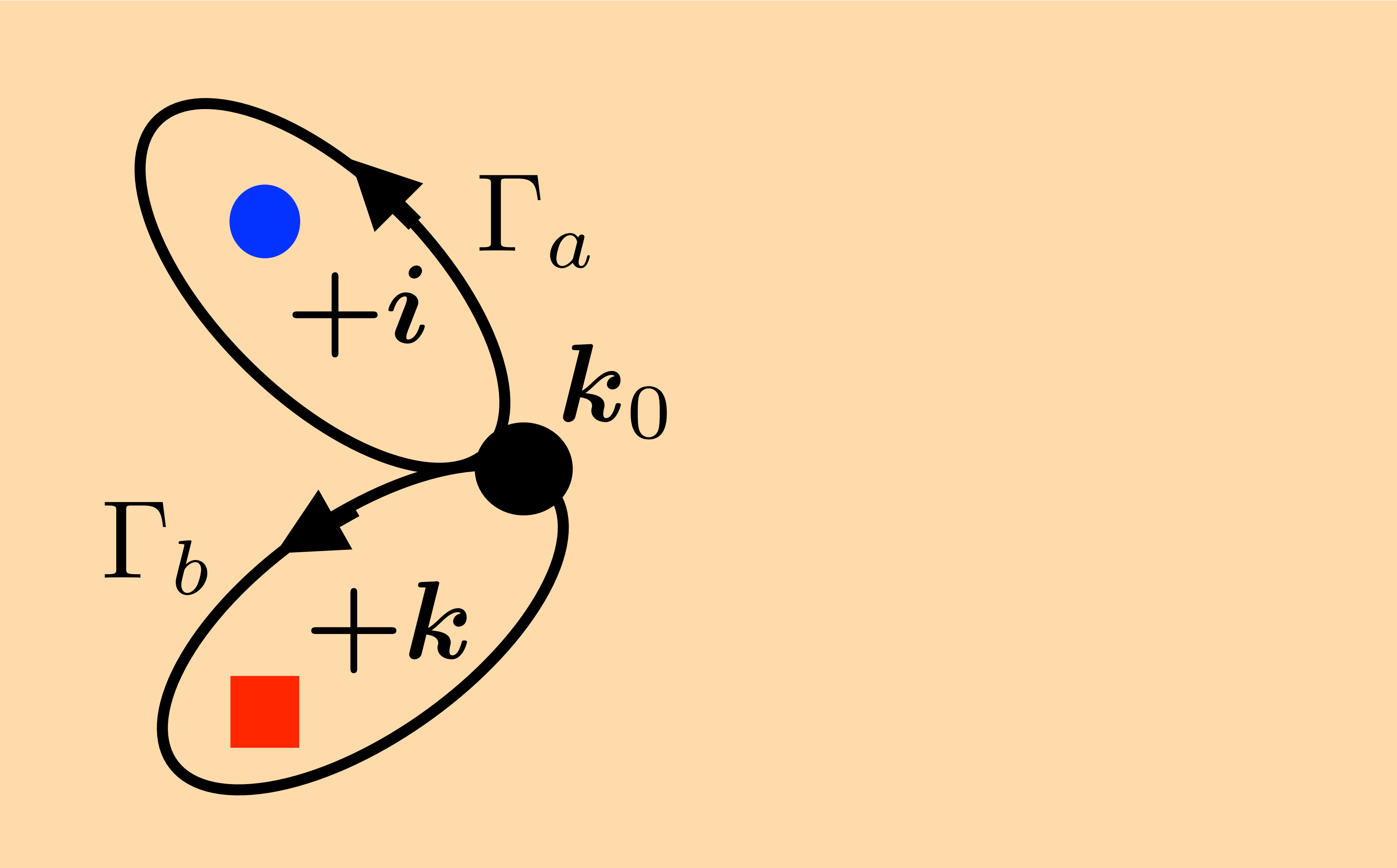
quaternion group:

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

accumulated frame rotations
around multi-gap nodes

Bdzusek *et al*, Science (2019)



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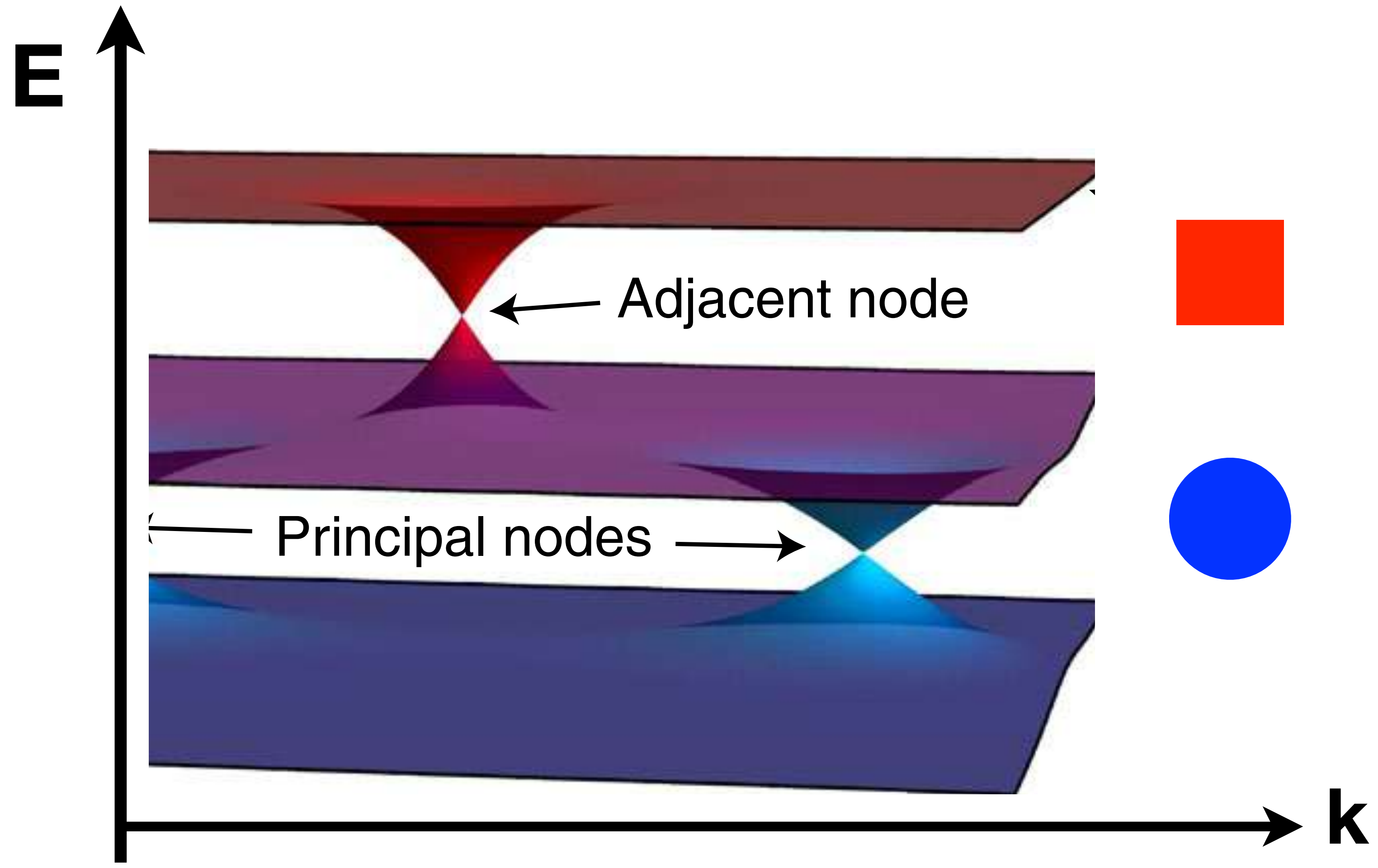
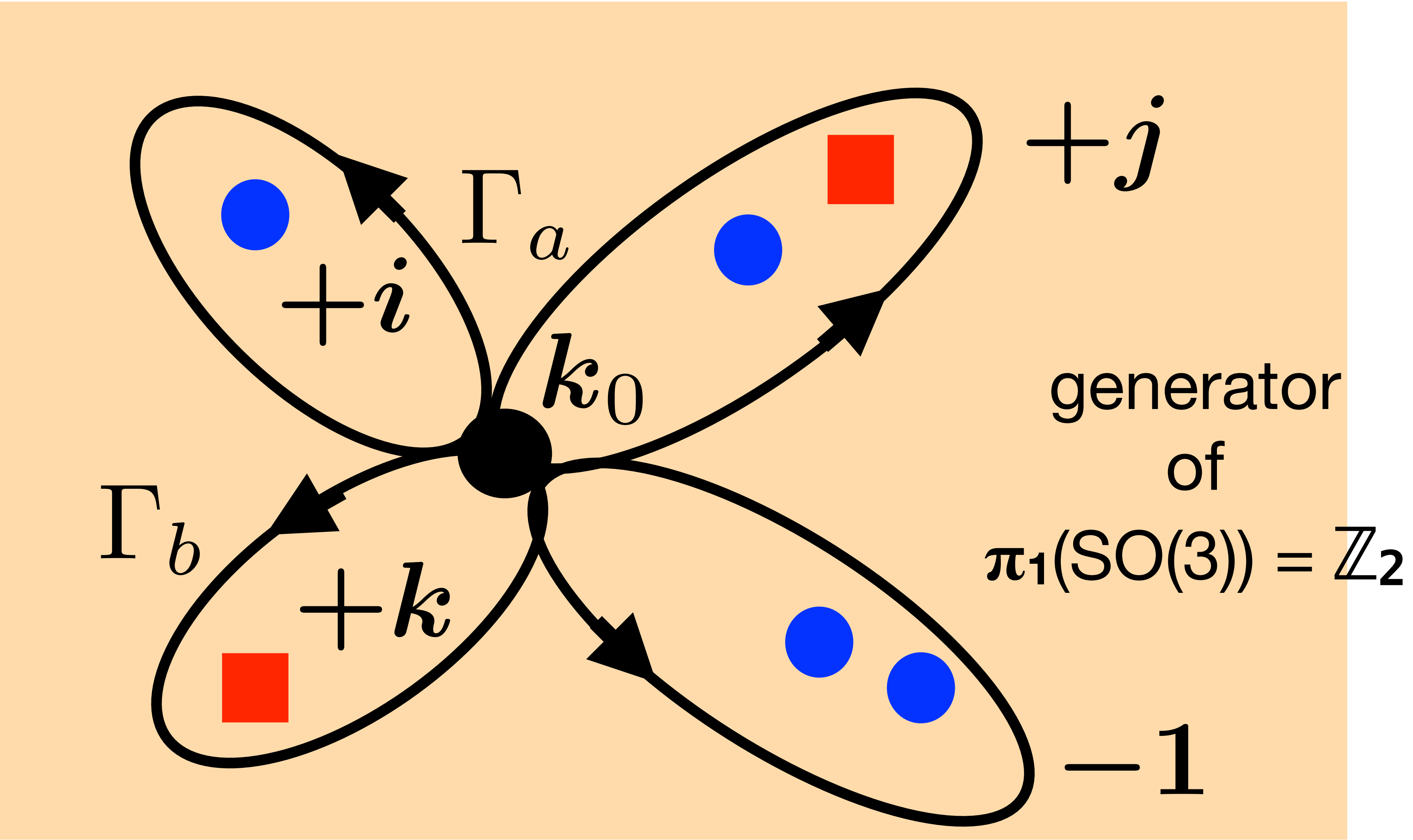
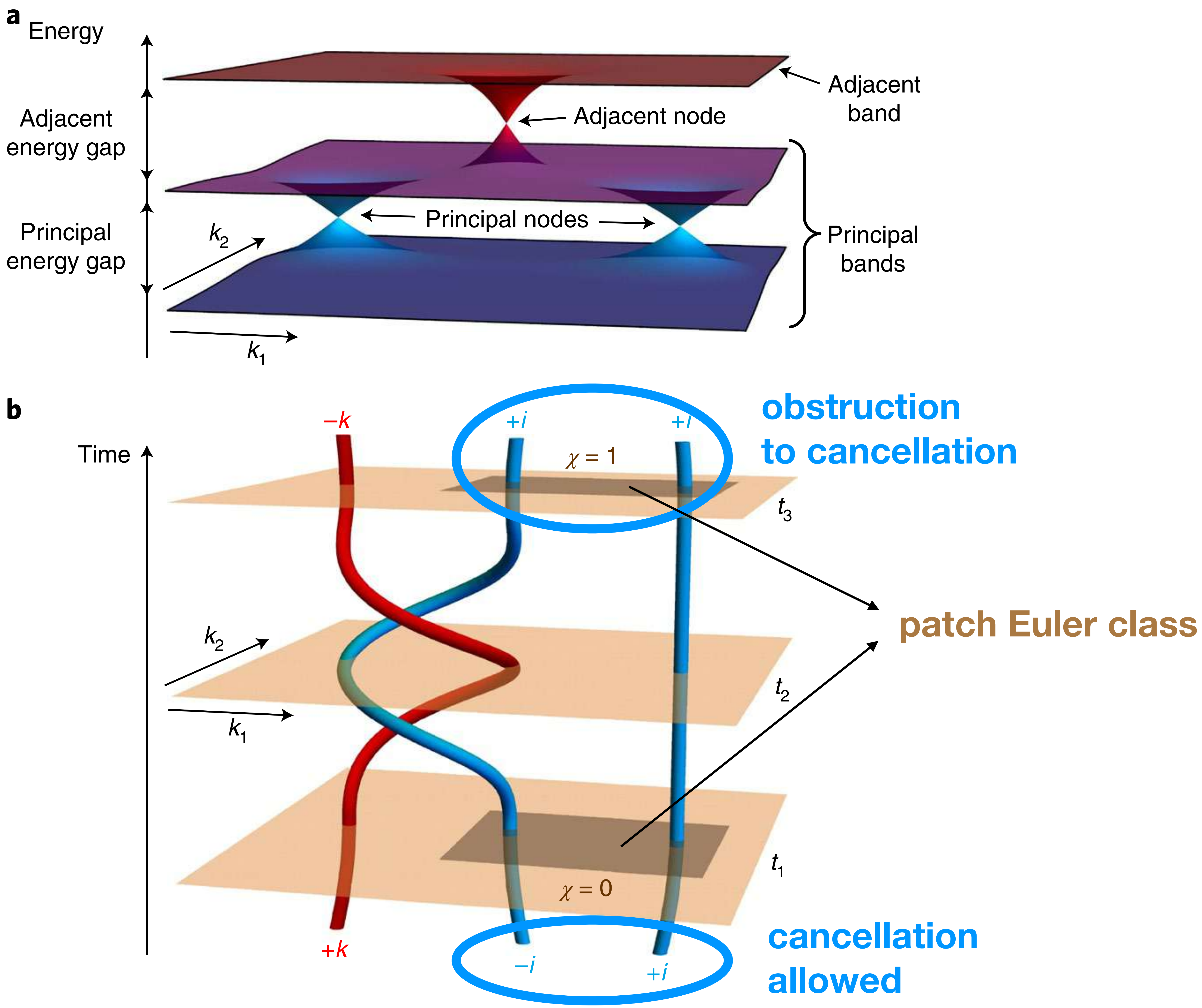


# Reciprocal braiding of Weyl points in a $C_2T$-plane




AB, et al Nature Physics 16, 1137 (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)

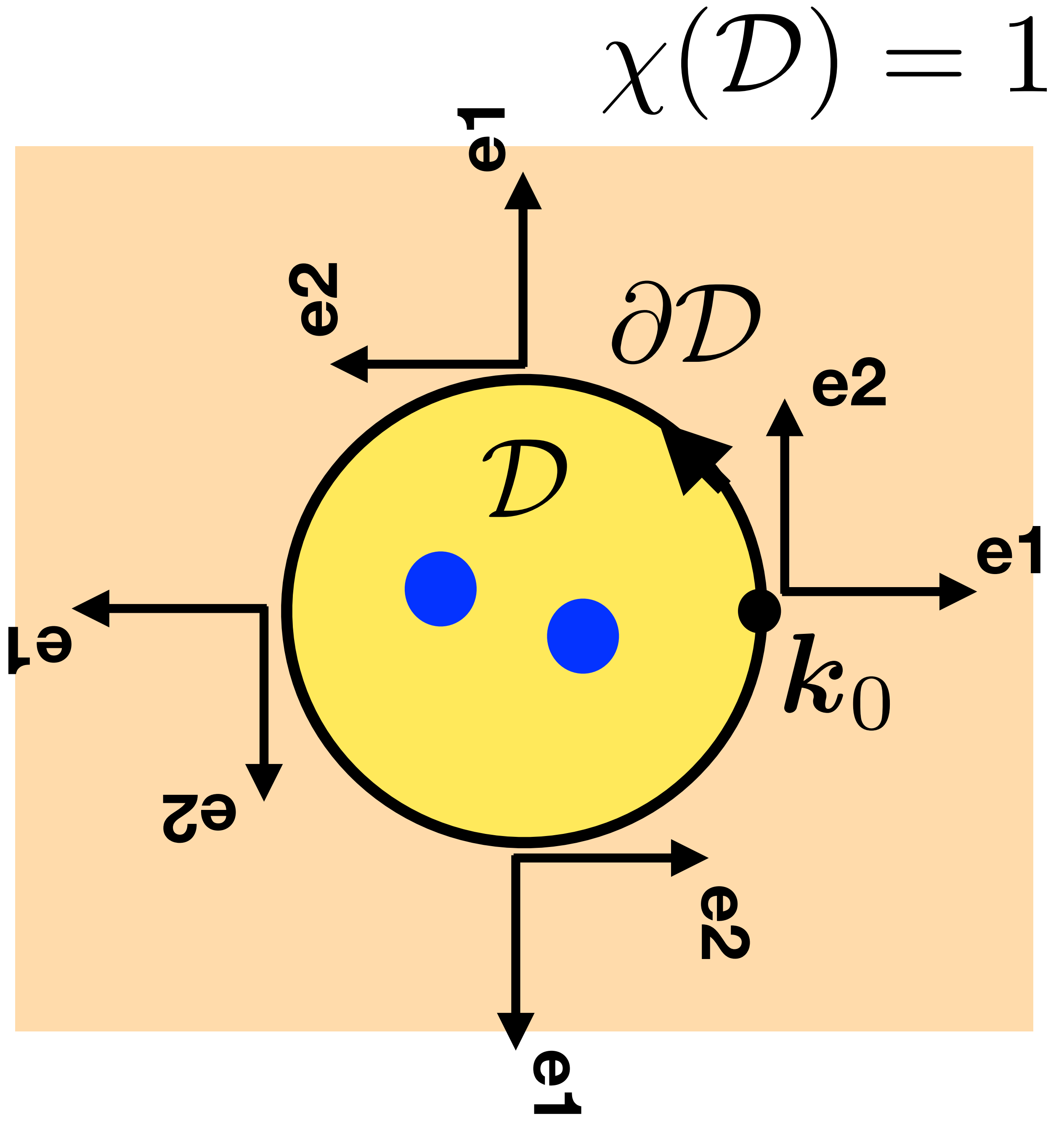
Euler form: $\mathrm{Eu} = d\mathrm{a}$

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

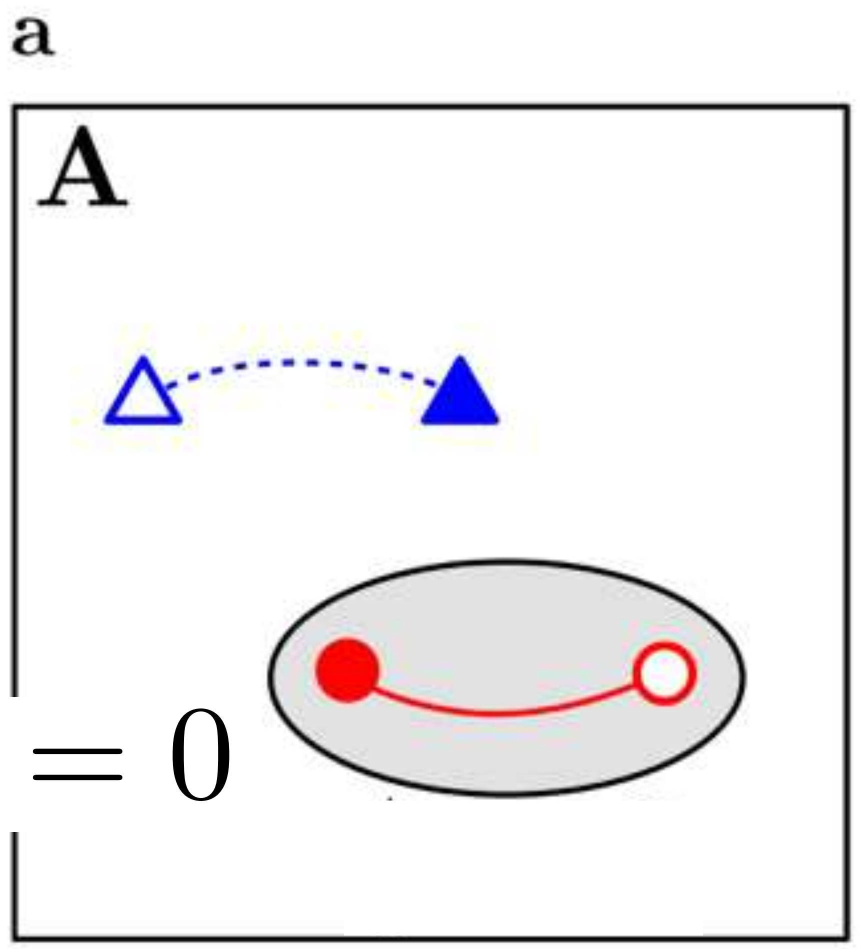
# Patch Euler number (gauge invariance of nodal points)

Euler number:

$$\chi(\mathcal{D}) = \frac{1}{\pi}\left[\int_{\mathcal{D}} \mathrm{Eu} - \oint_{\partial\mathcal{D}} \mathrm{a}\right]$$
$$= \frac{1}{\pi}\sum_n \left[\int_{\mathcal{D}_n^\epsilon} \mathrm{Eu} - \oint_{\partial\mathcal{D}_n^\epsilon} \mathrm{a}\right]$$
$$= \sum_n W_n \in \mathbb{Z}$$



# Braiding rules in terms of Dirac string and patch Euler class




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

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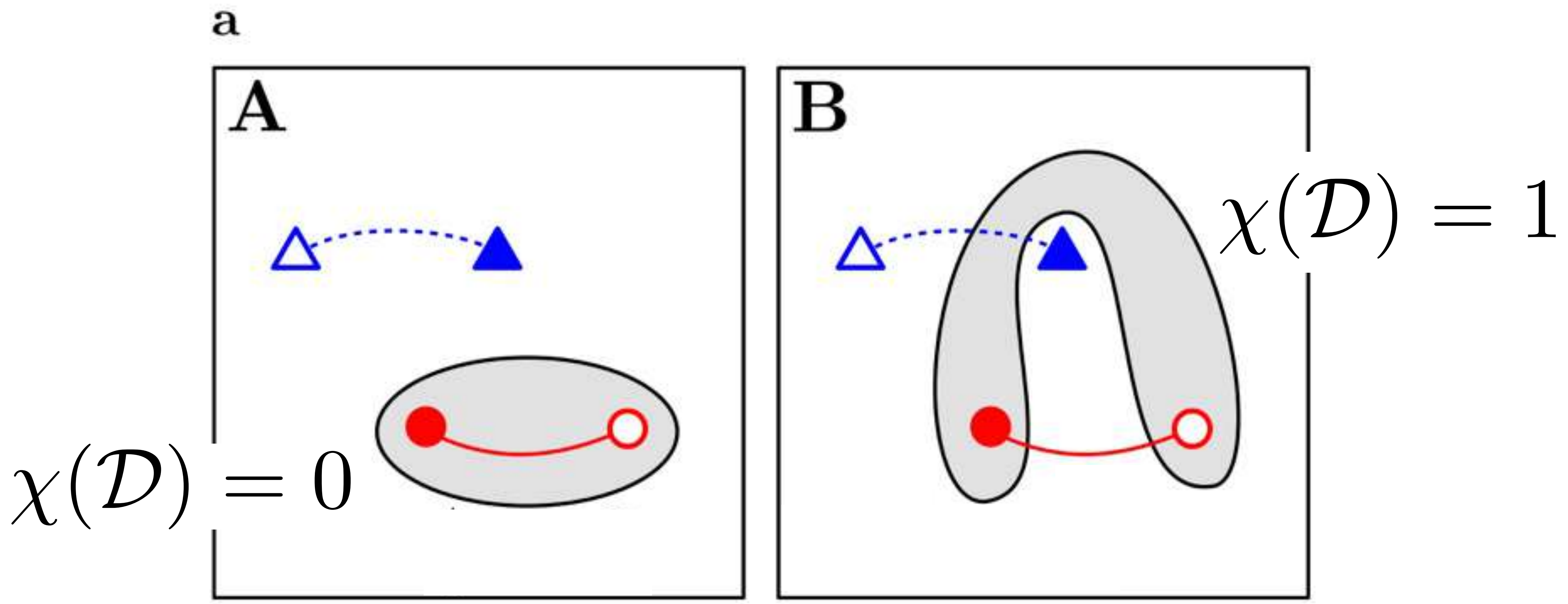

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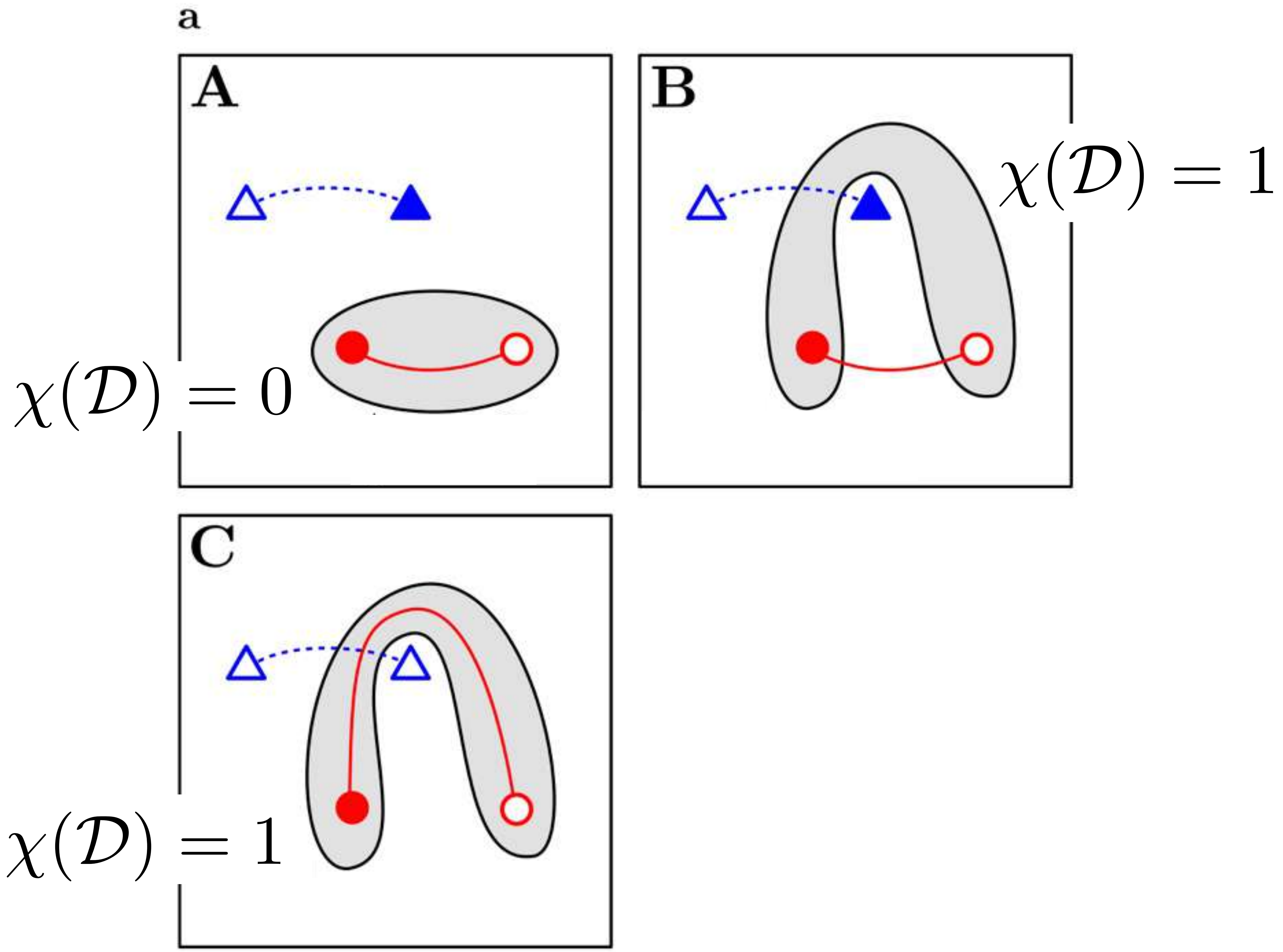

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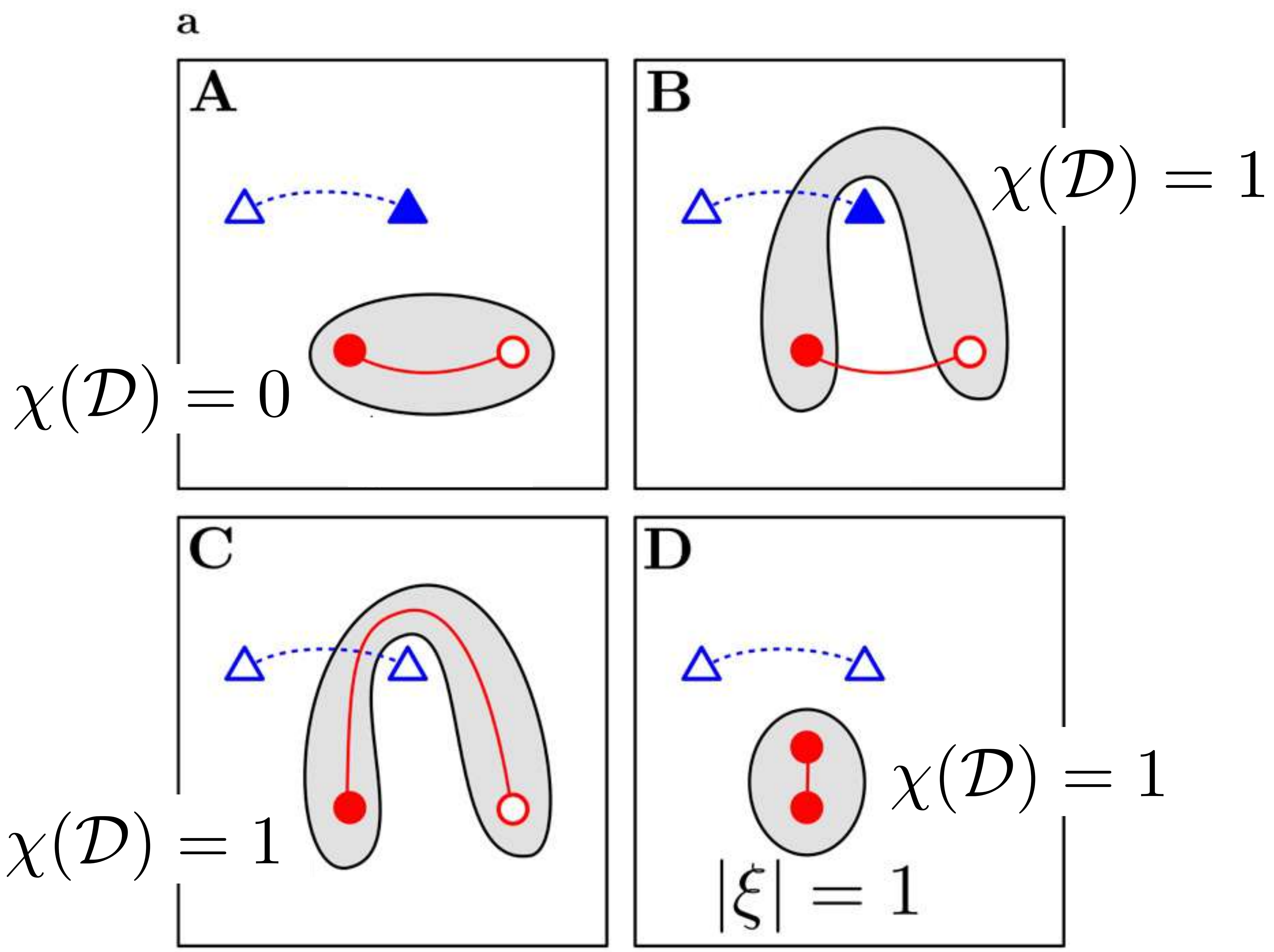
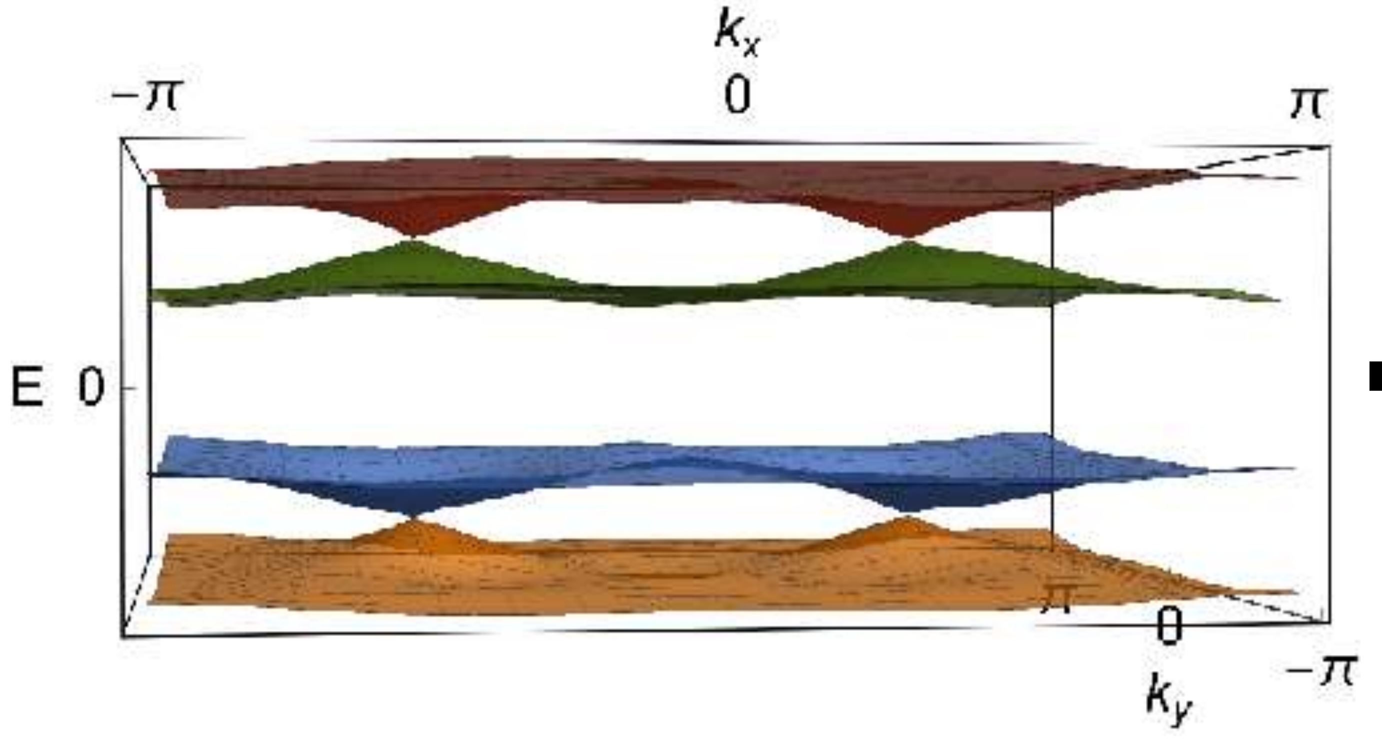
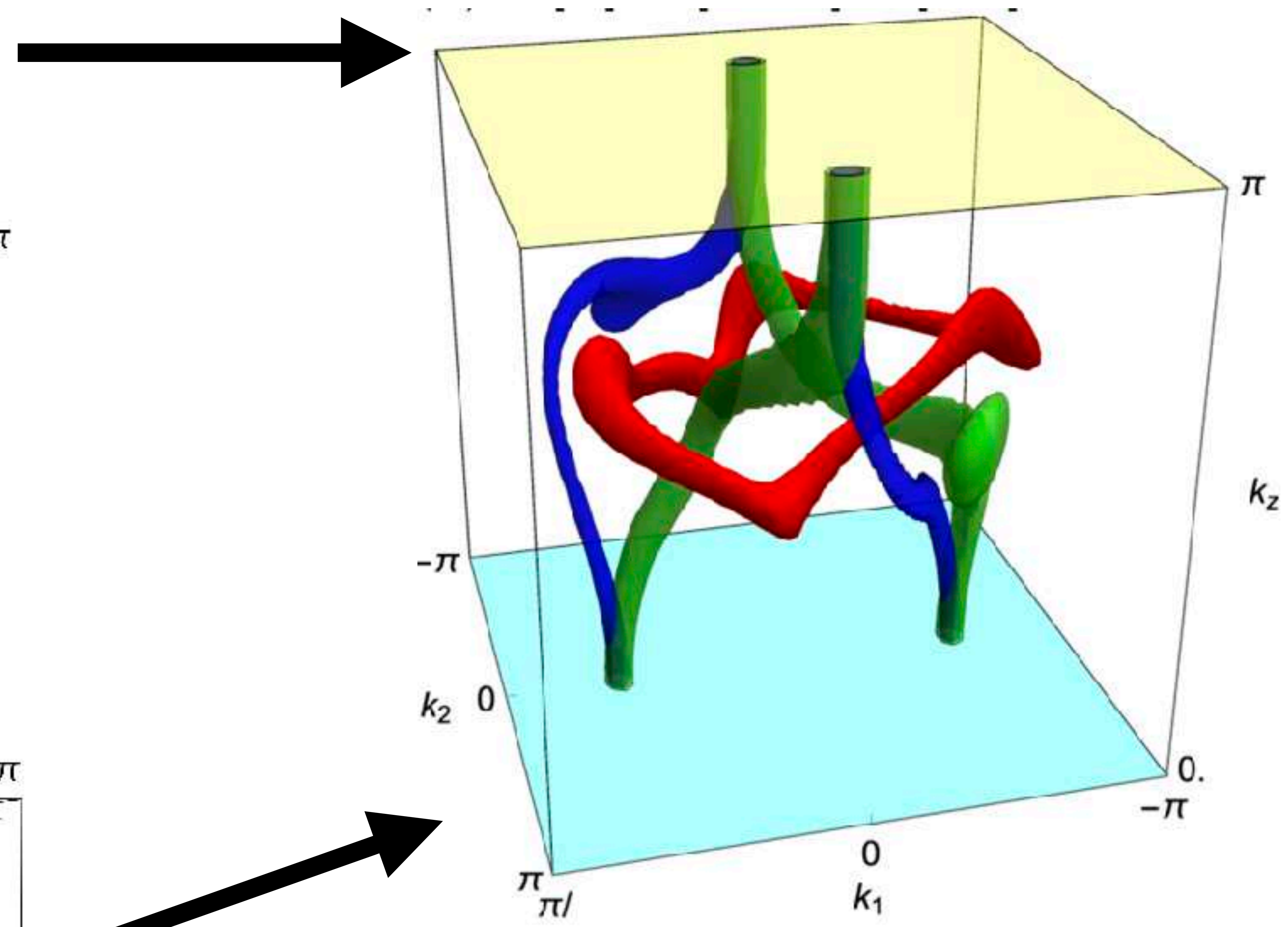


# Euler number conversion via braiding of Weyl points

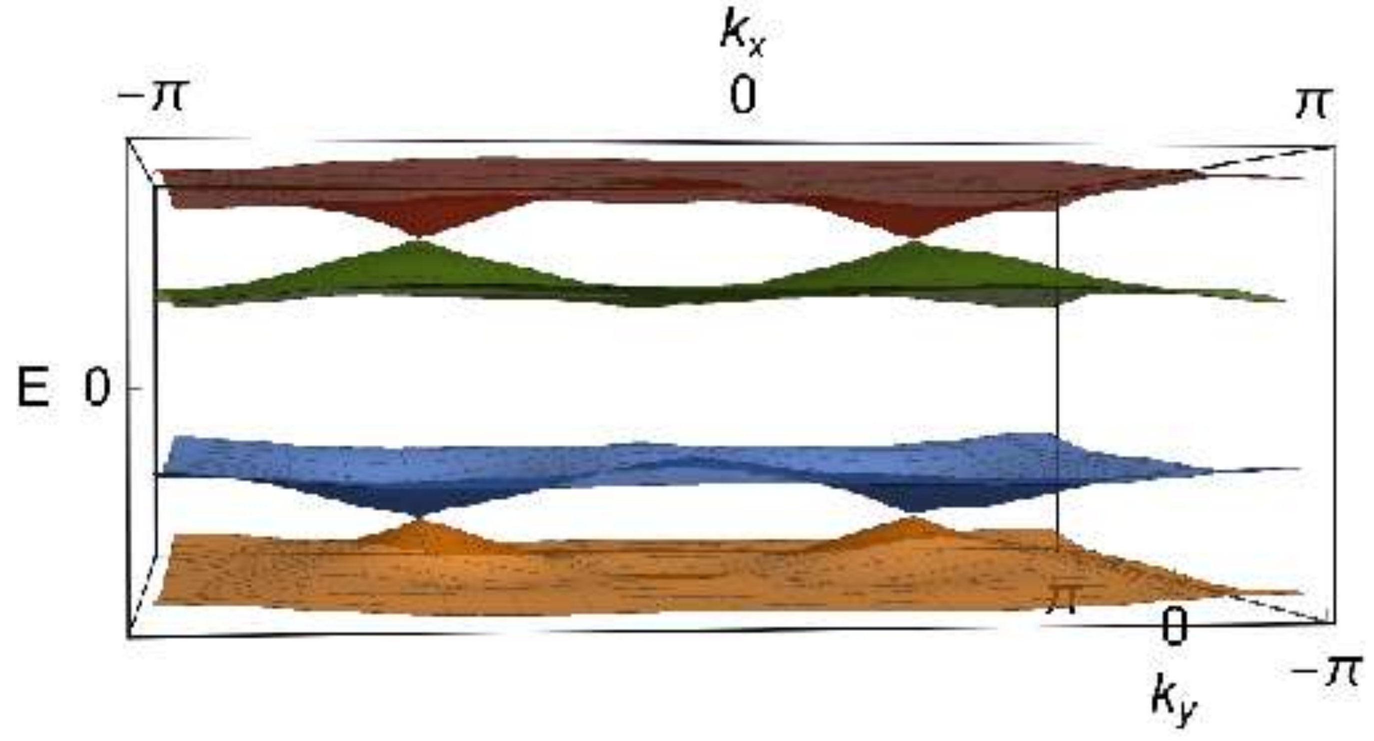
$$(\chi_I, \chi_{II}) = (1, 1)$$




Linked nodal rings = braiding trajectories of NP

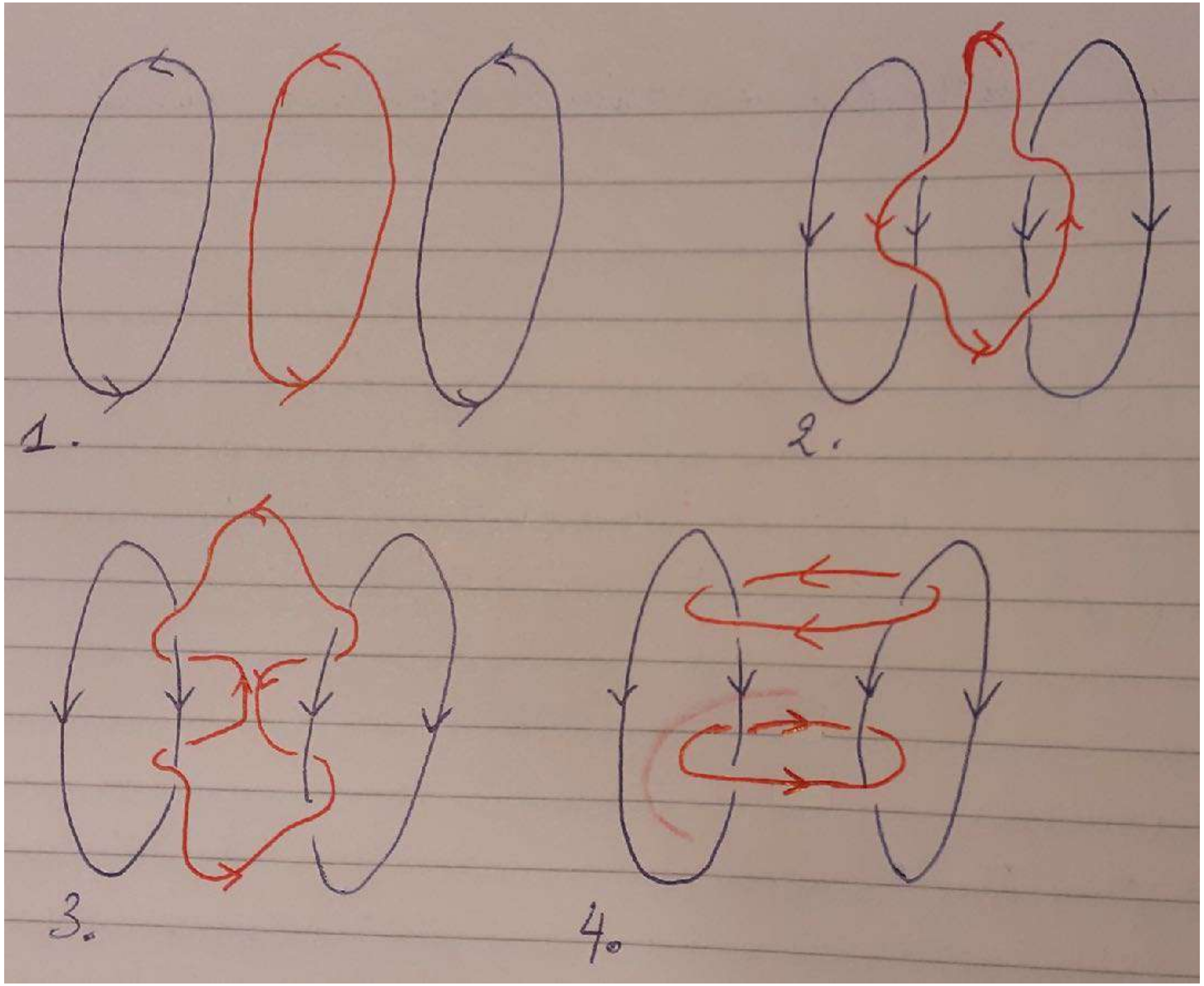



$$(\chi_I, \chi_{II}) = (1, -1)$$

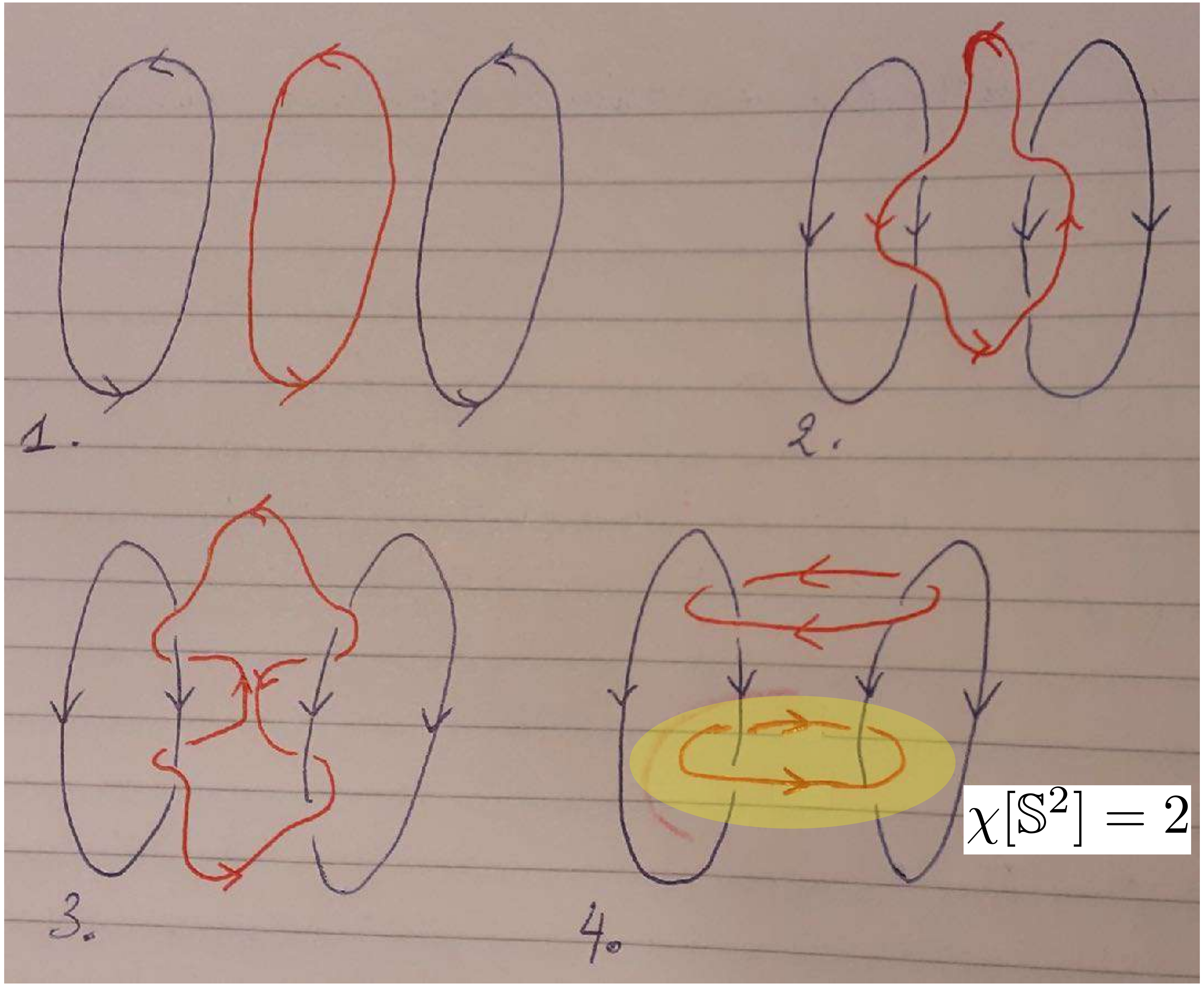



AB, RJ Slager, arxiv:2203.16741

# Braiding of nodal rings in 3D PT phases



# Braiding of nodal rings in 3D PT phases



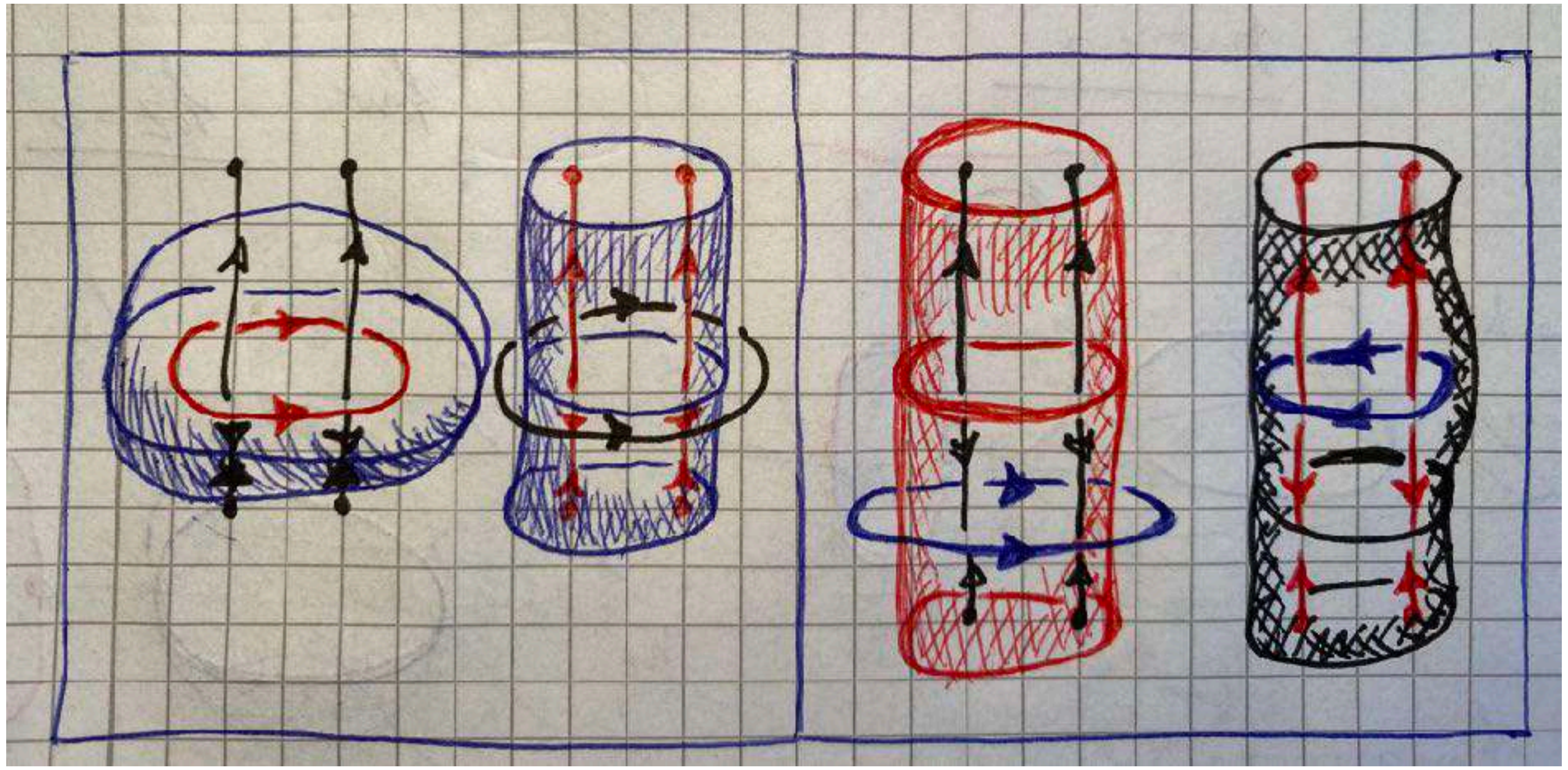
# Higher dimensional Euler insulators

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:

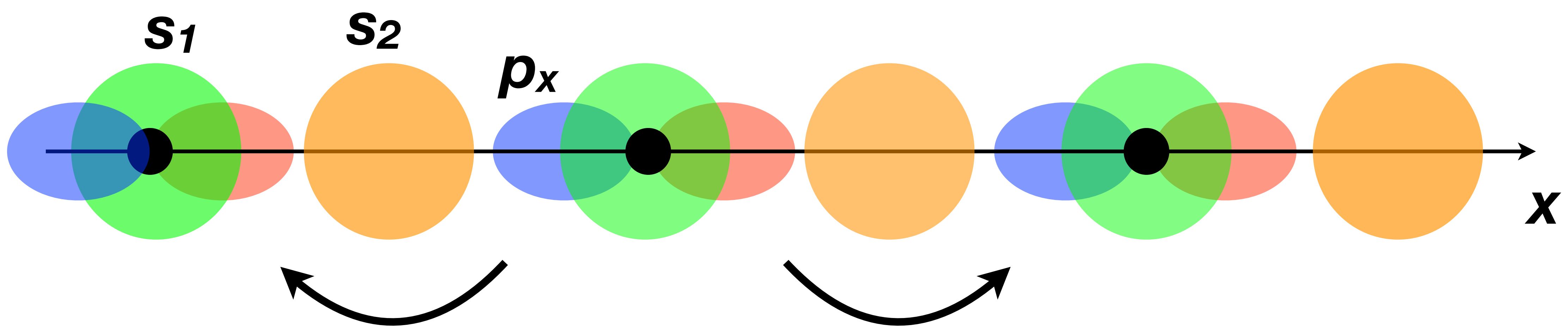


arxiv:2301.08827

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

# Intrinsic or projected 1D topology

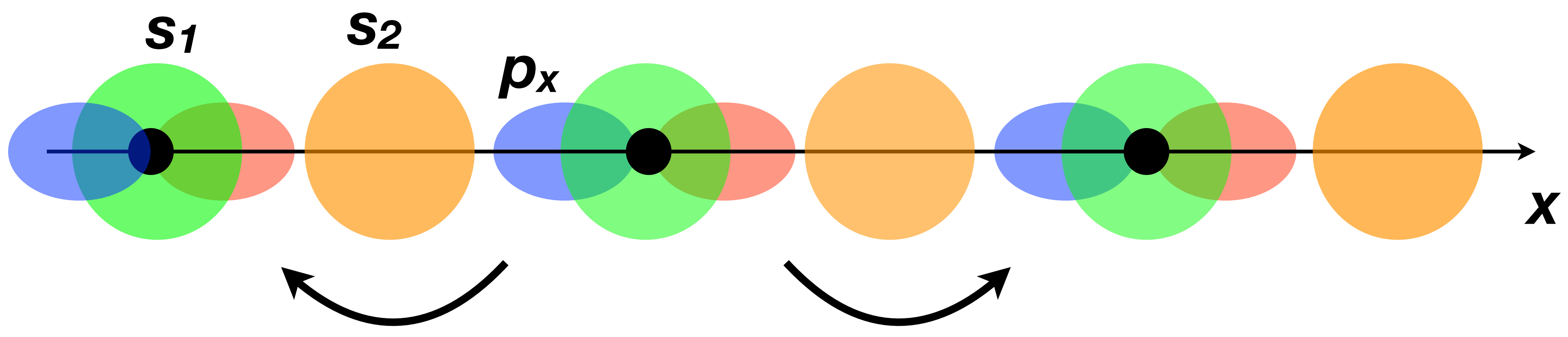
intrinsic: atomic-like orbitals
projected: hybrid Wannier functions



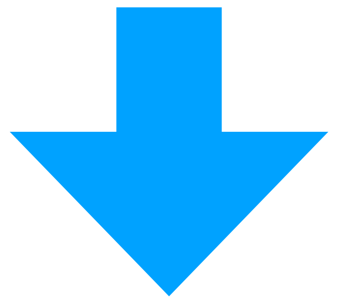

In $C_2T$ (mT, PT) only the unitary part acts on the position operator!

# 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

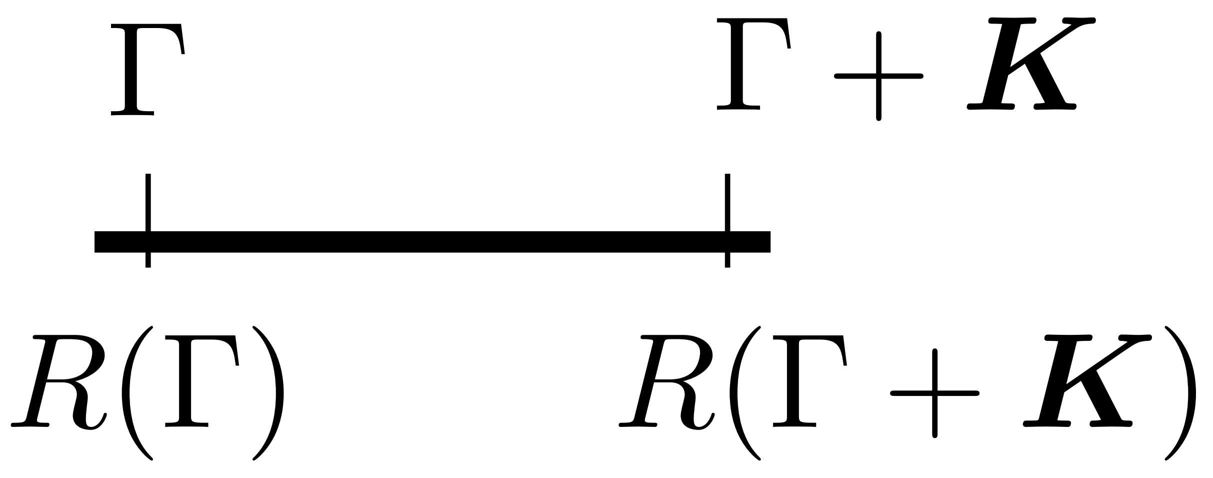
even though $C_2$ (m,P) is not a symmetry of the Bloch Hamiltonian

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




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

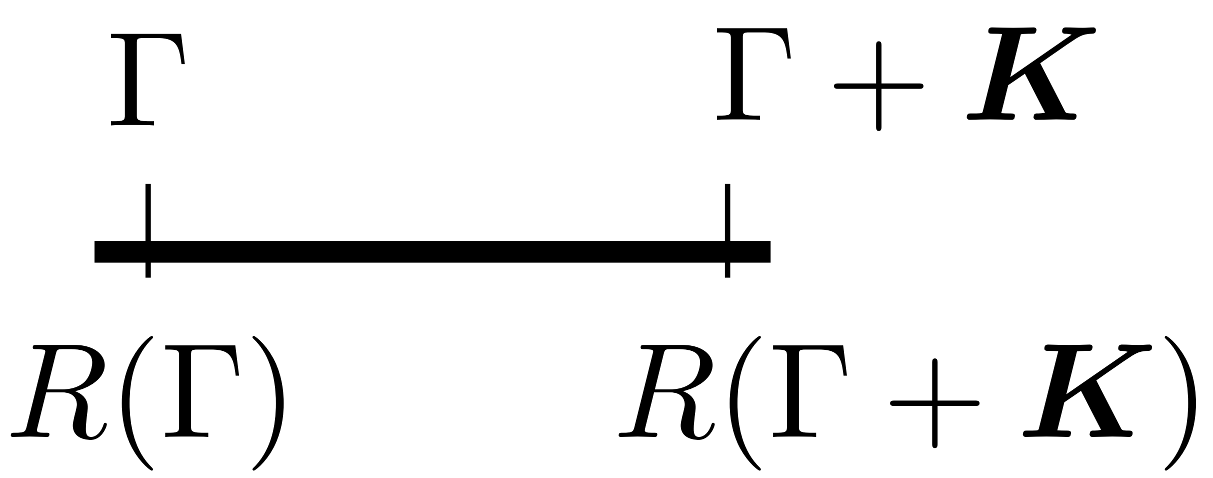
translation sym:

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

$$|\phi_\alpha, \boldsymbol{k}\rangle = \frac{1}{\sqrt{N}}\sum_n e^{i\boldsymbol{k}\cdot(\boldsymbol{R}_n+\boldsymbol{r}_\alpha)}|w_\alpha, \boldsymbol{R}_n + \boldsymbol{r}_\alpha\rangle$$

# 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:

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

# Intrinsic or projected 1D topology

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

$$g_{\boldsymbol{K}} = \begin{pmatrix} g_{\boldsymbol{K},11}^{\in \pm 1} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & g_{\boldsymbol{K},NN}^{\in \pm 1} \end{pmatrix} \in \mathsf{P}_N \quad \subset \mathsf{SO}(N)$$

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

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

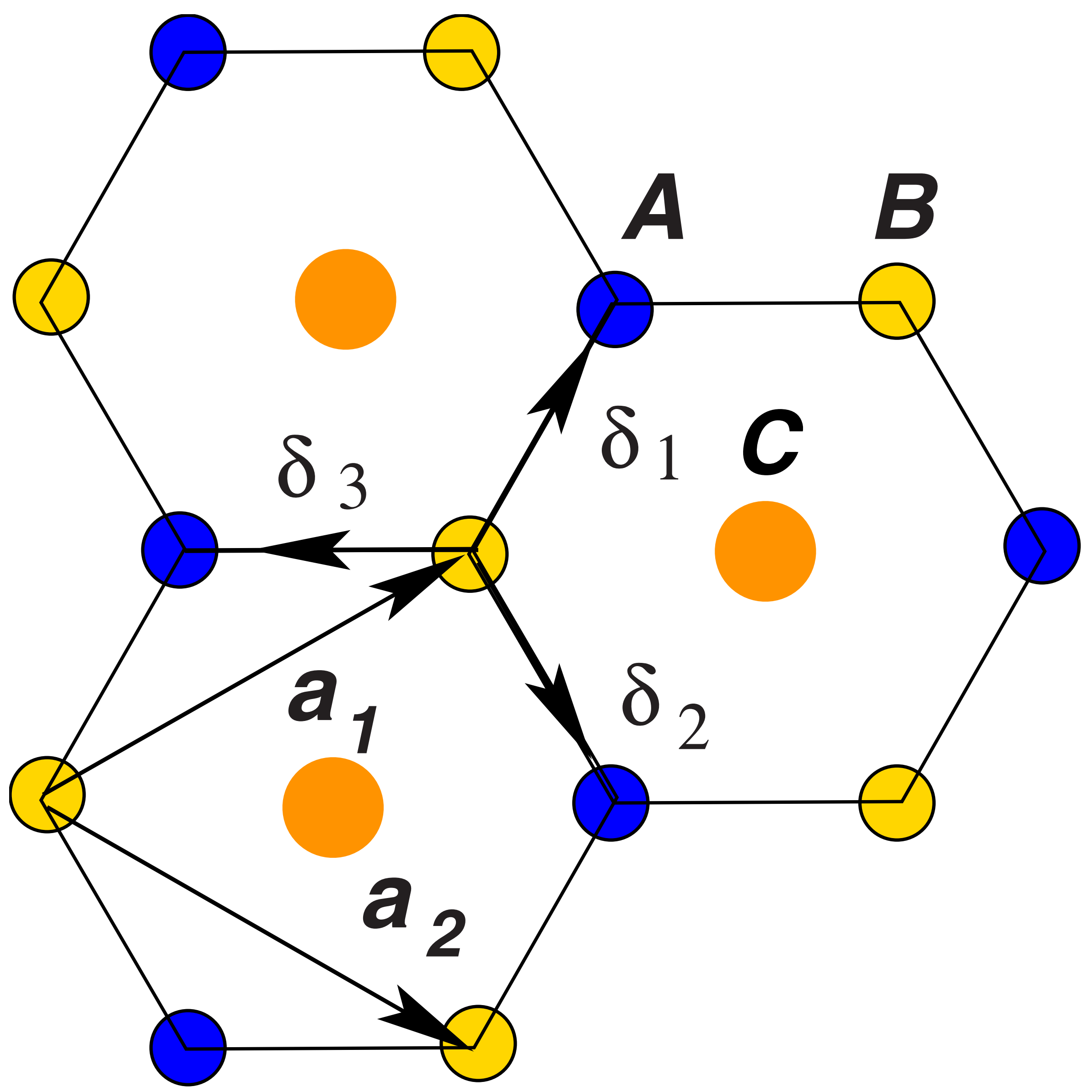
For any pair of orbitals located away from the Brillouin zone center and that are mapped onto-each other under $C_2$, we do change of gauge:

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

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

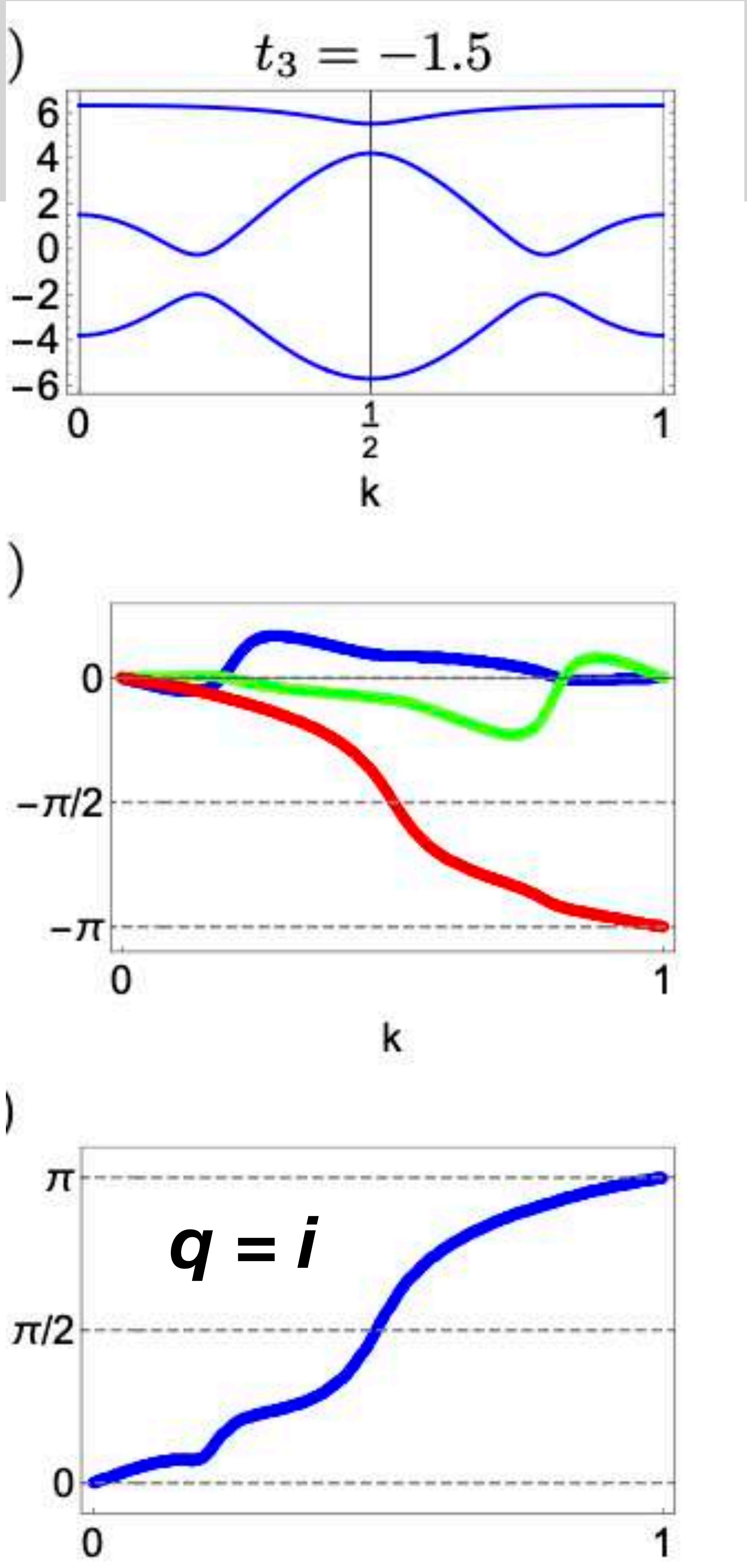
# Embedded 1D non-Abelian topology

Honeycom + triangular lattice

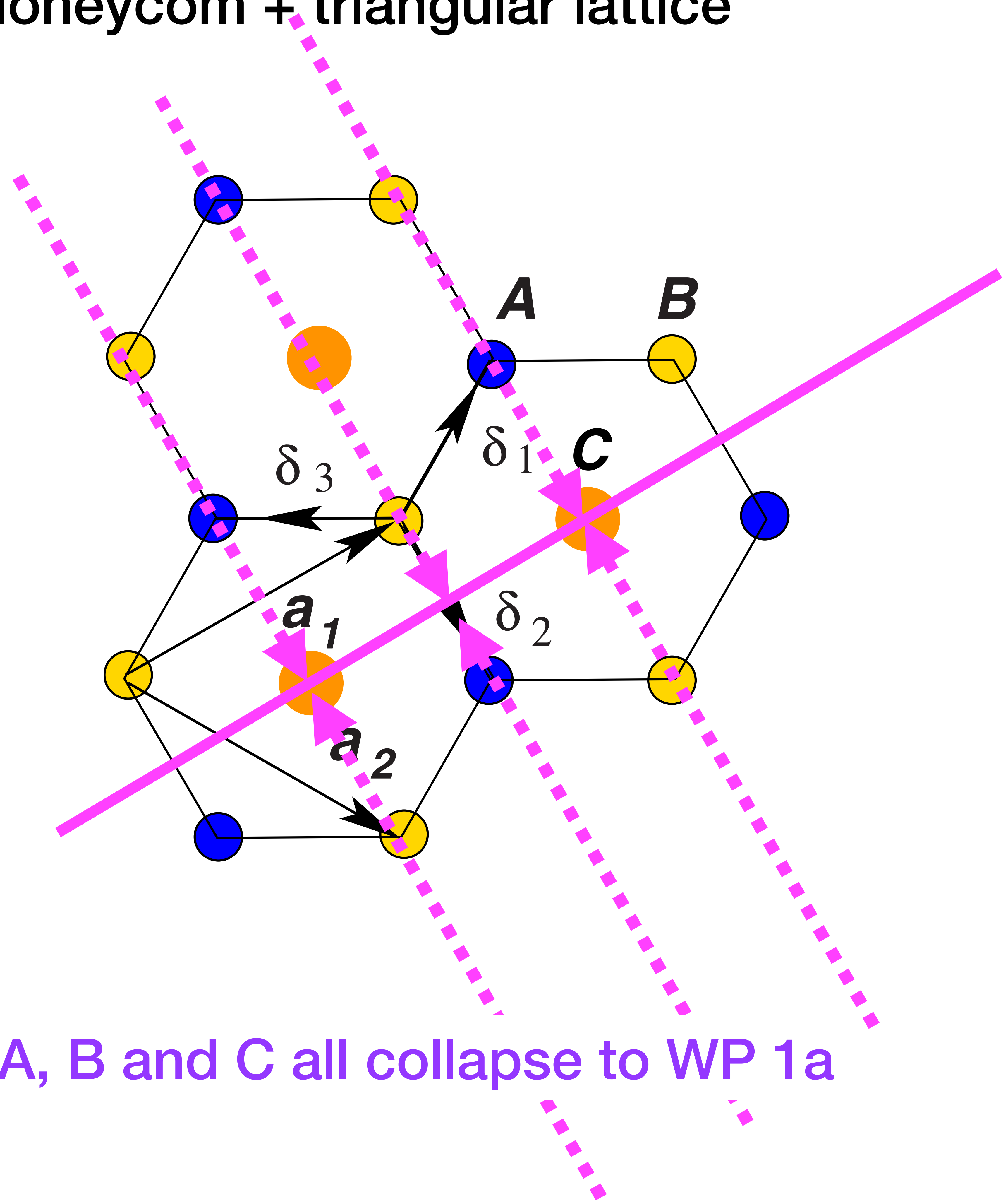



honeycomb sites (***A***,***B***): Wyckoff's position *2b*
triangular sites (***C***): Wyckoff's position *1a*

# Embedded 1D non-Abelian topology



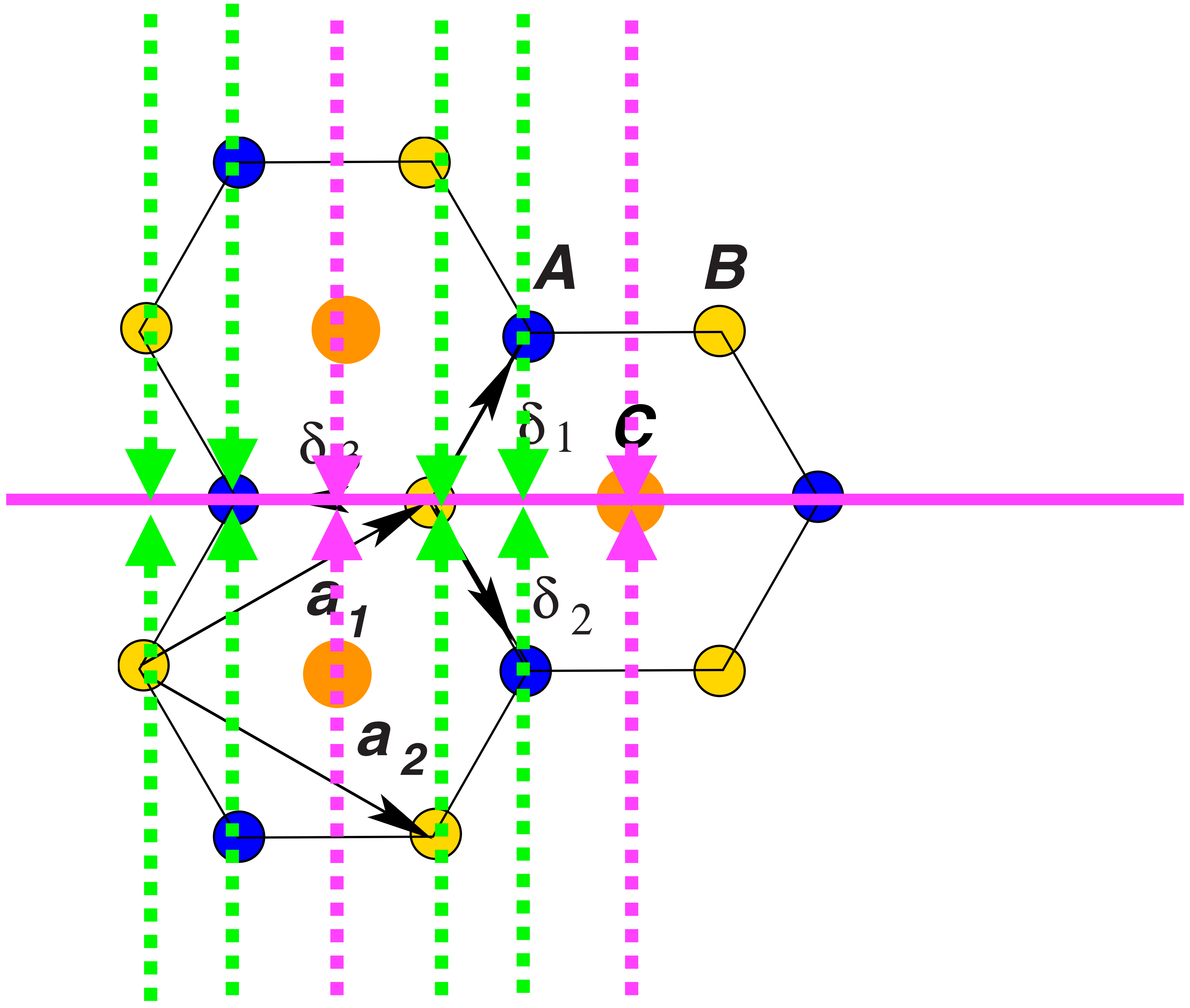

Honeycom + triangular lattice



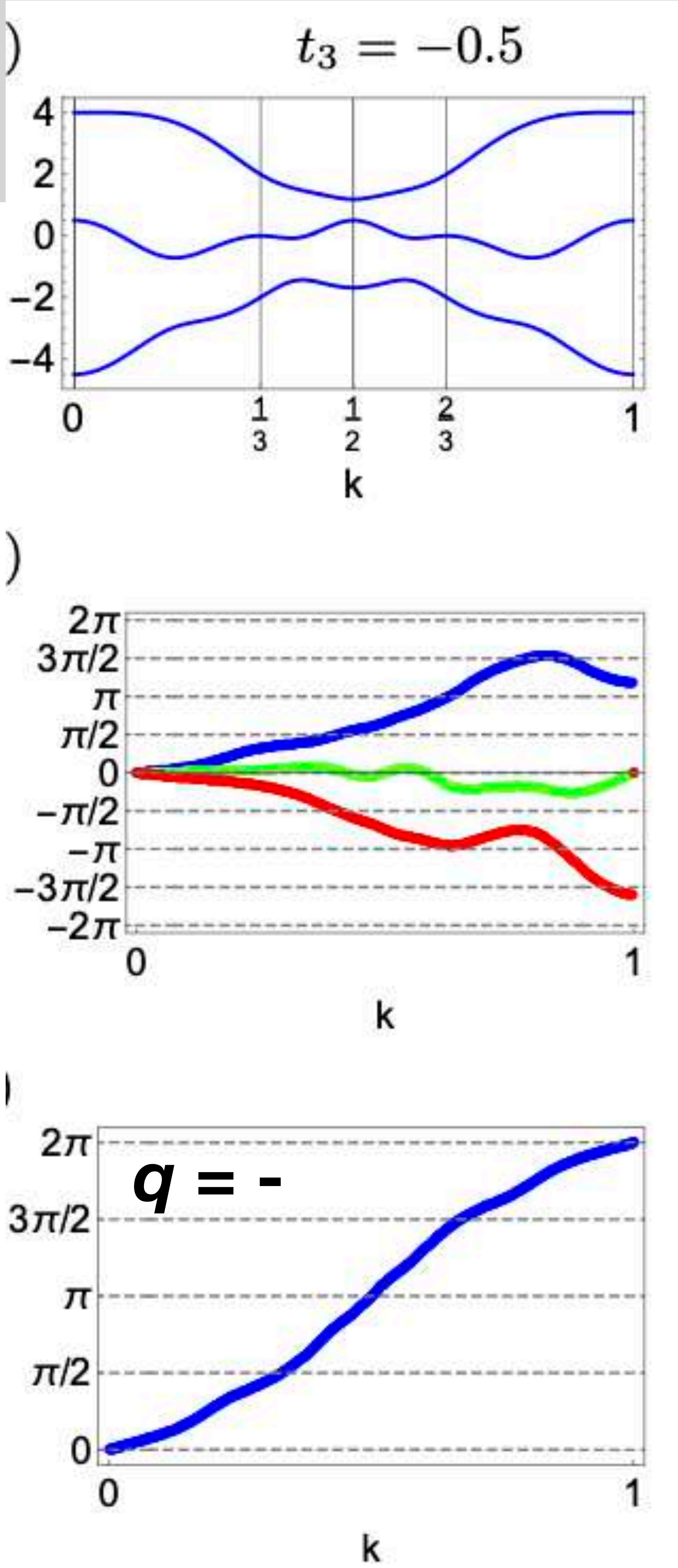

A, B and C all collapse to WP 1a

# Embedded 1D non-Abelian topology

Honeycom + triangular lattice

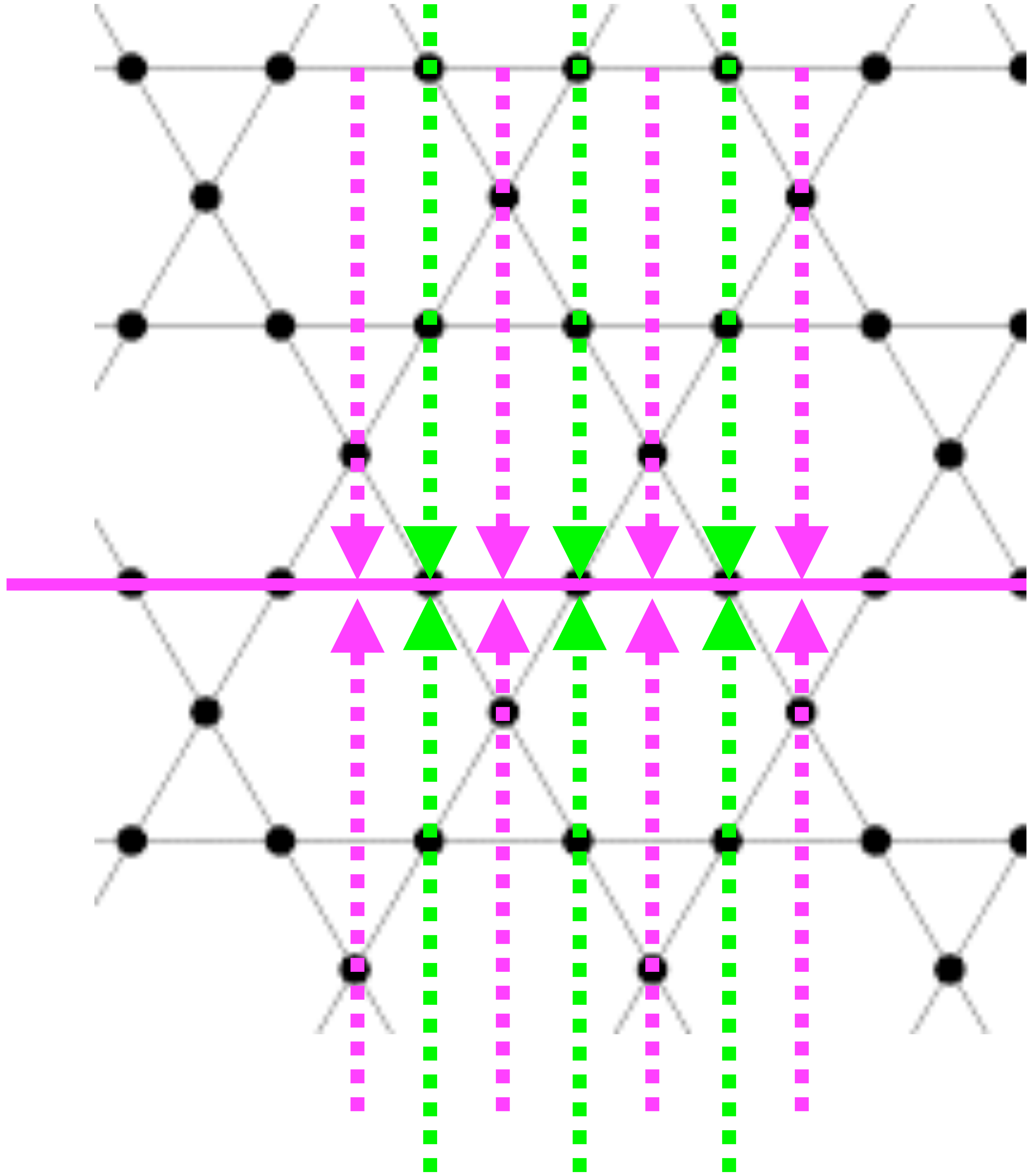



A image of B under $C_2$

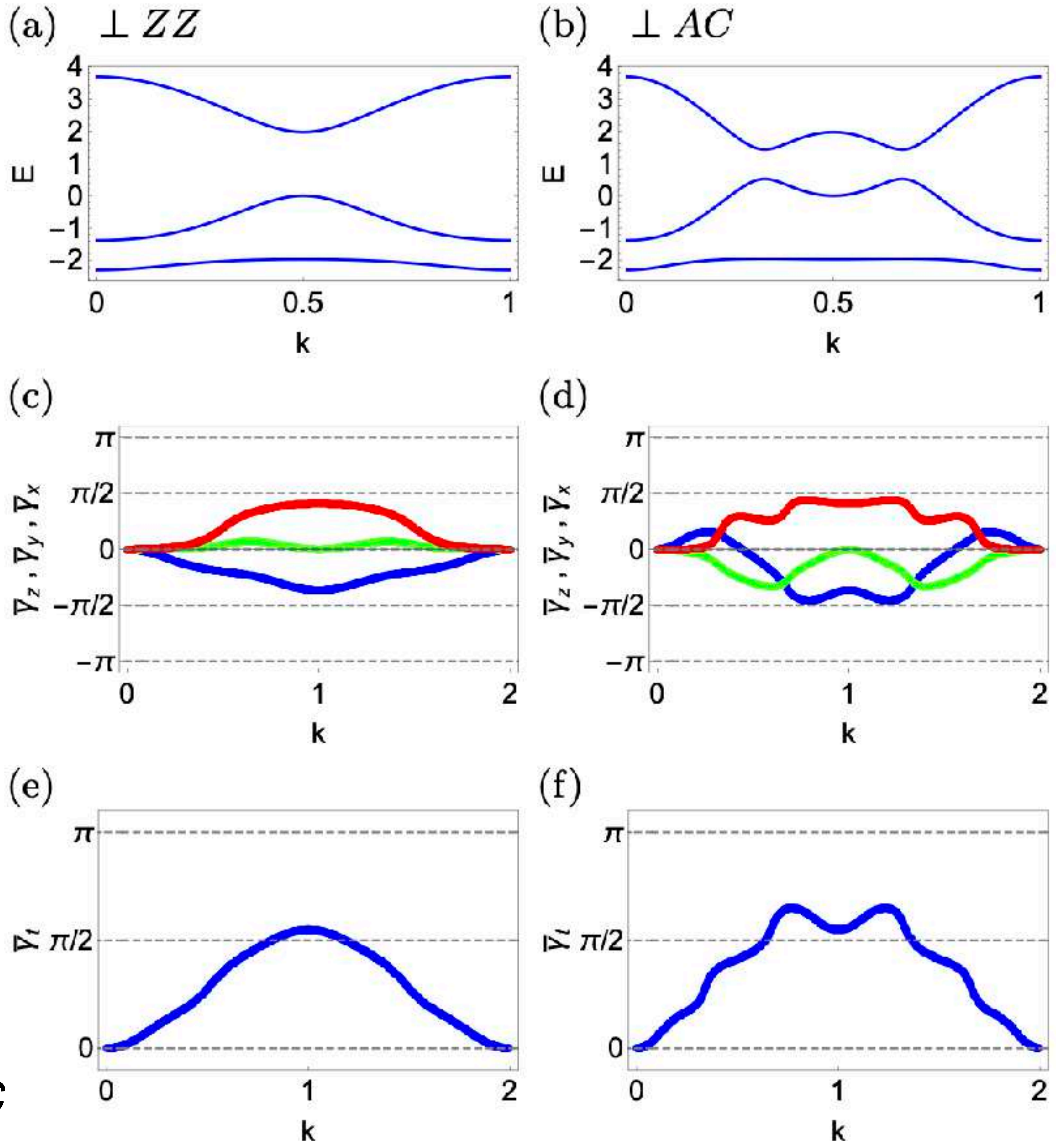


# Embedded 1D non-Abelian topology

Kagome lattice

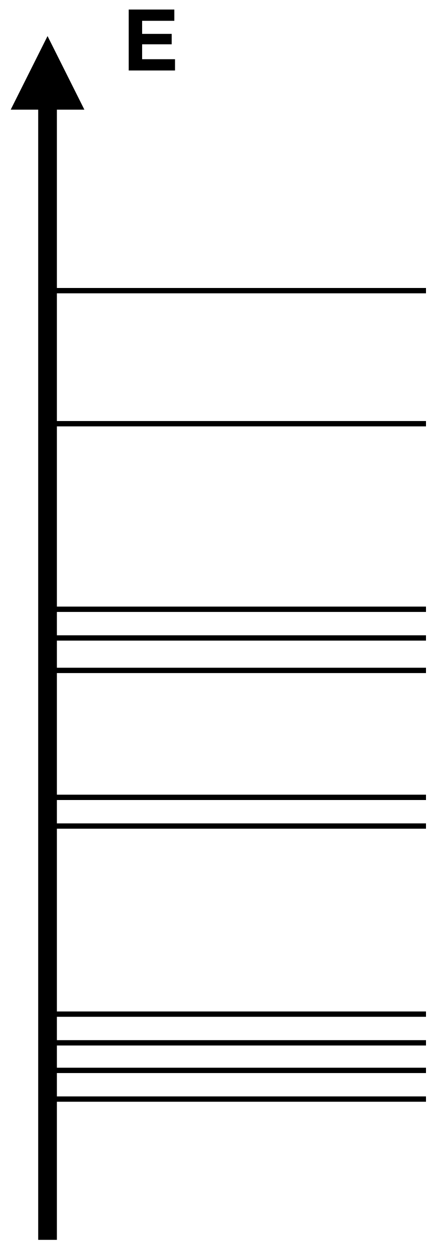


kagome sites: Wyckoff's position 3*c*



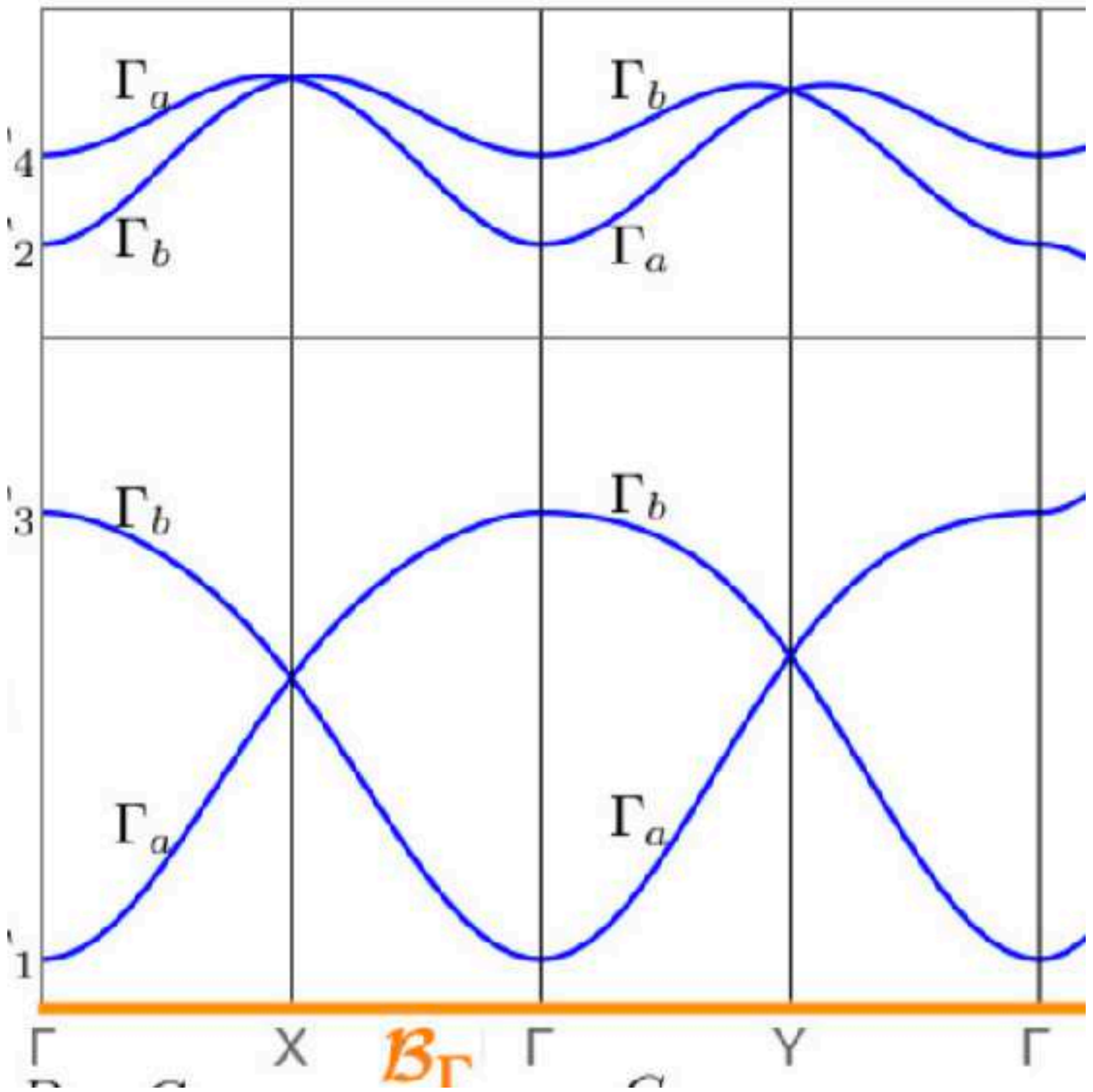
# To come

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