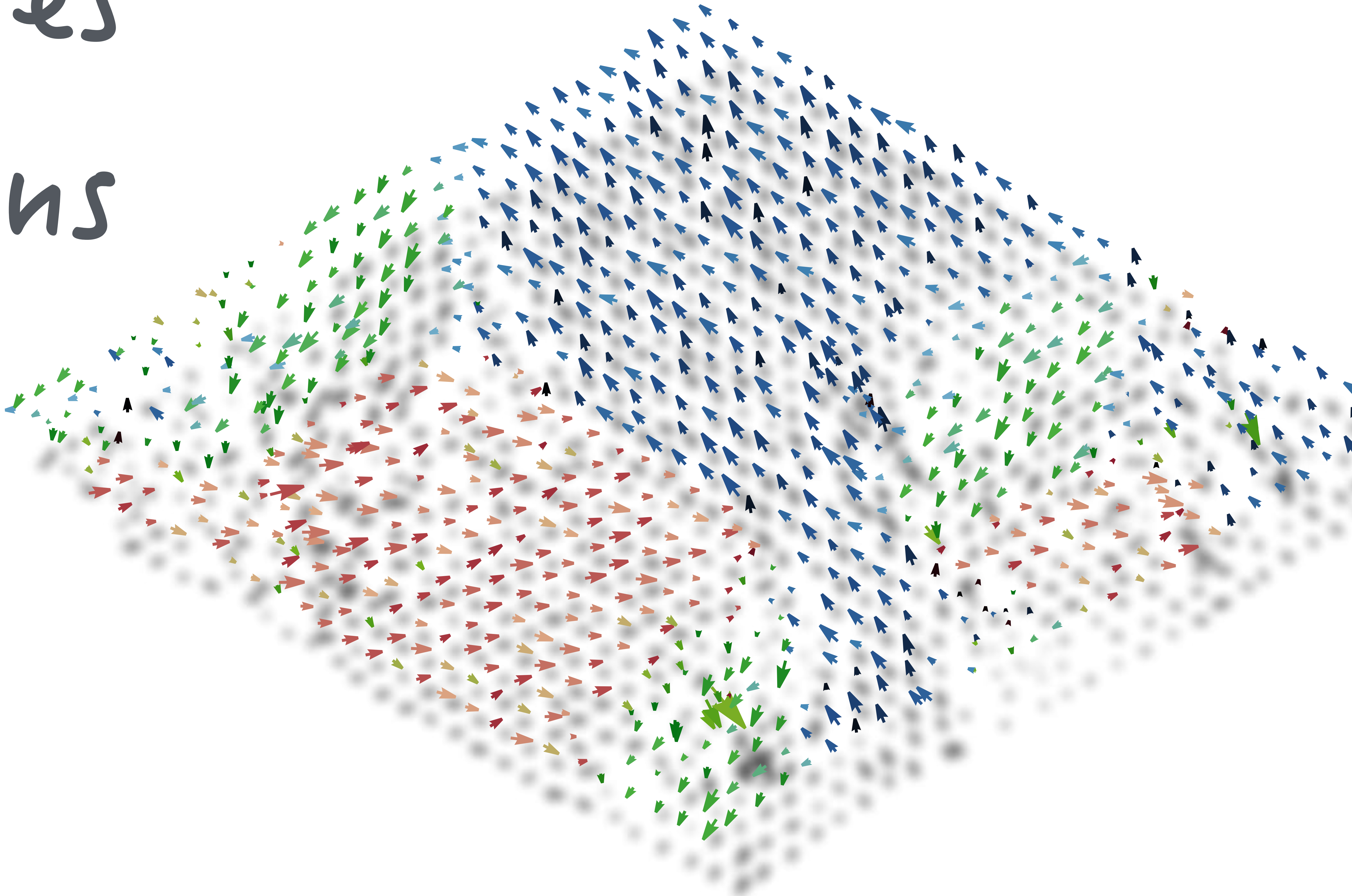
A glimpse into the world of

Topological phases in two dimensions

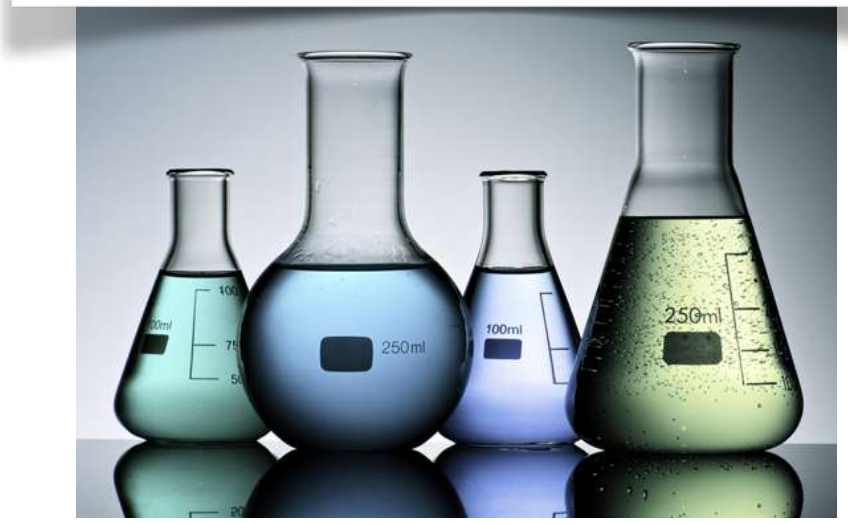
David Carpentier

CNRS and **E**cole **N**ormale **S**upérieure de **L**yon



Properties of Matter

mechanical properties



Liquid

Solid

Properties of Matter

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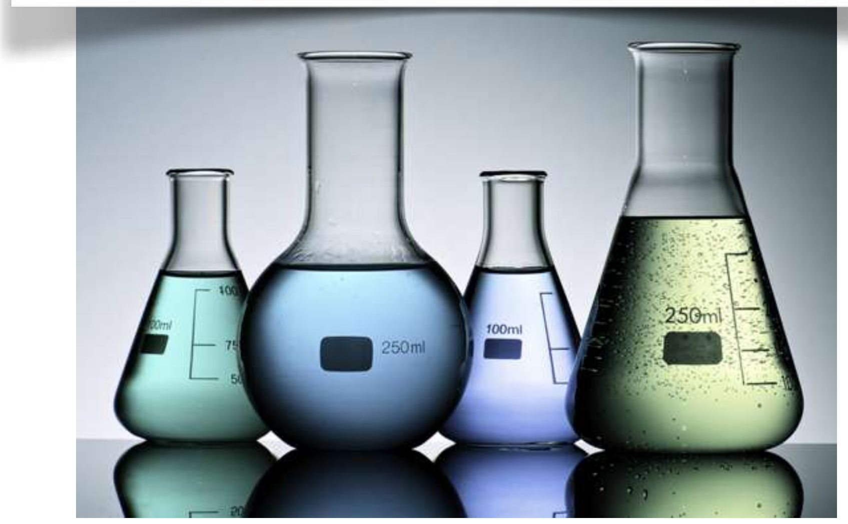

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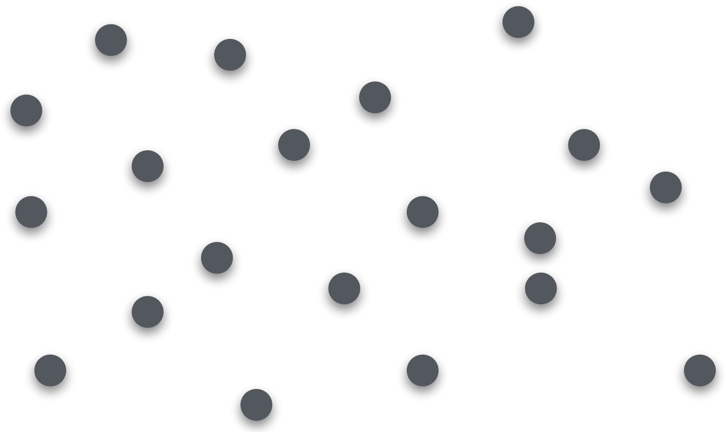
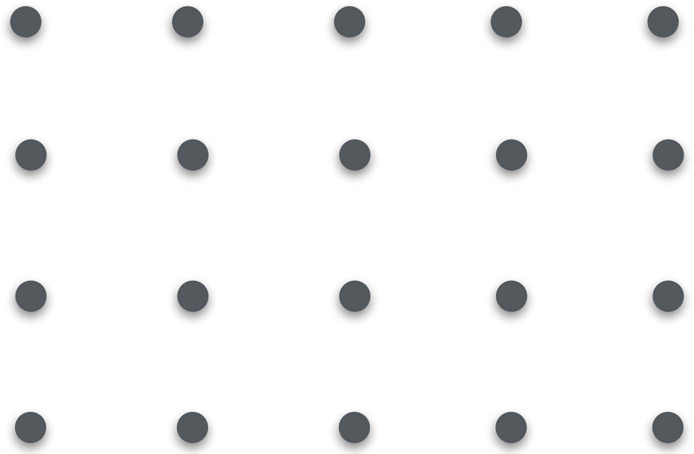
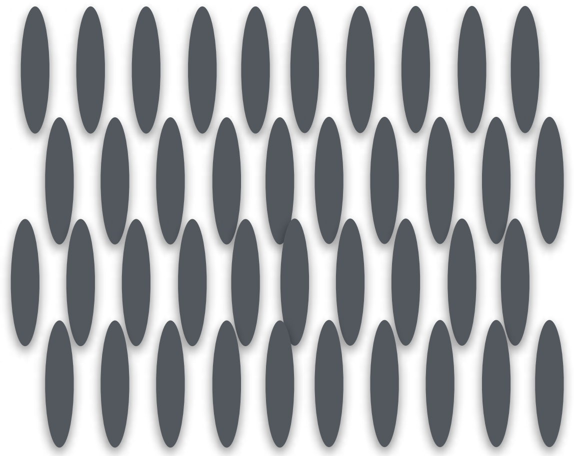


Solid



nematic



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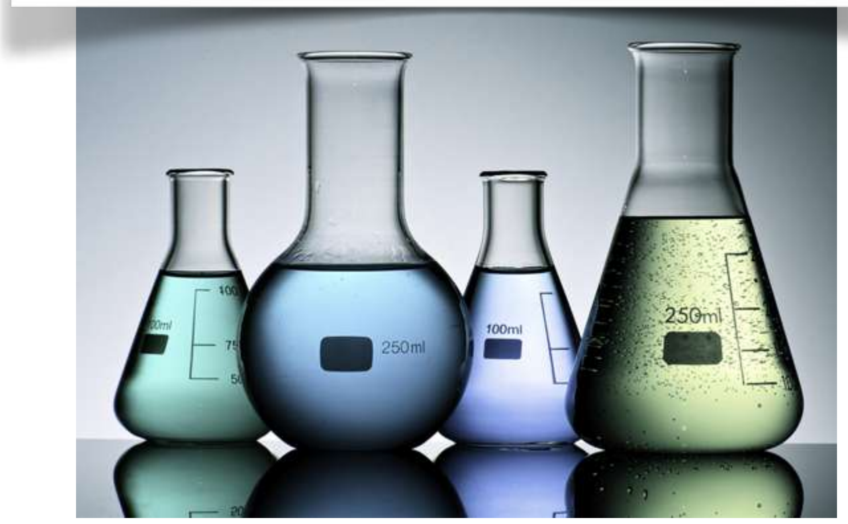

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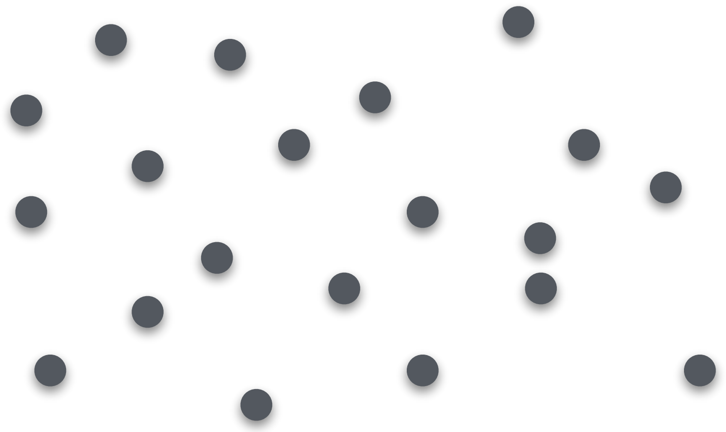

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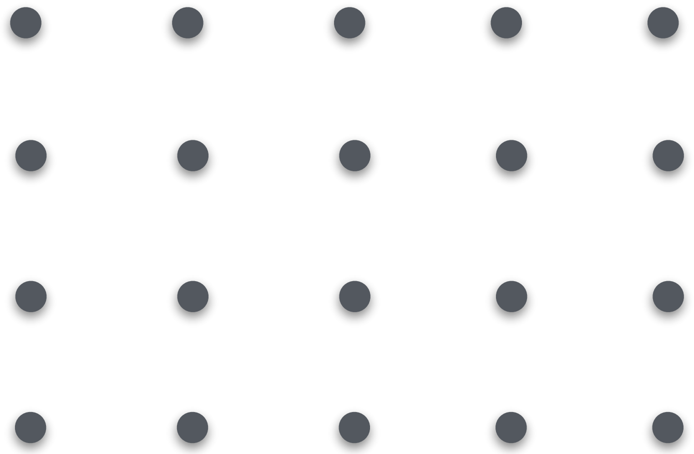

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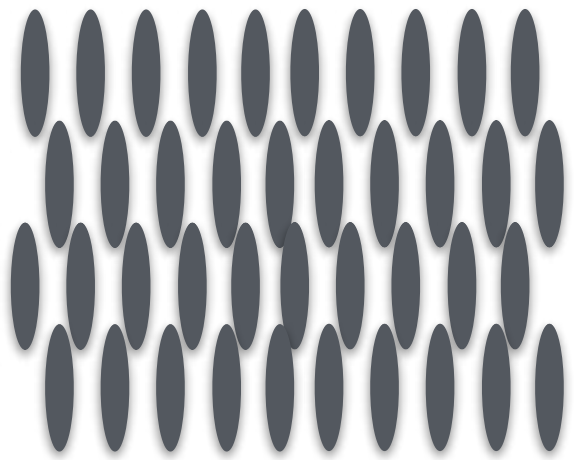
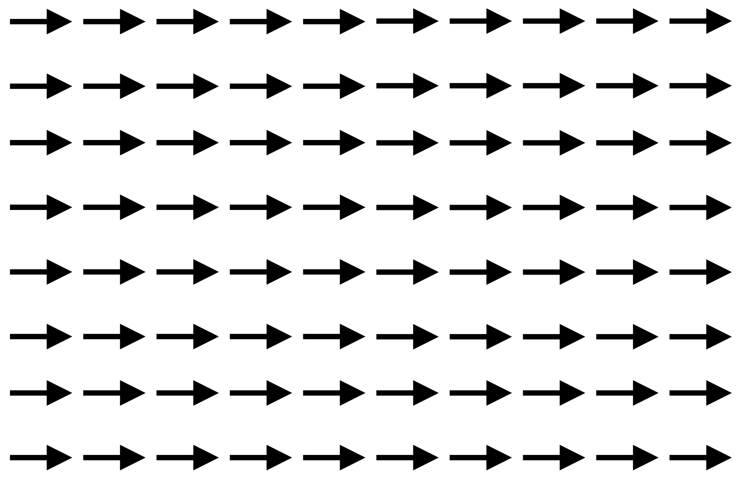


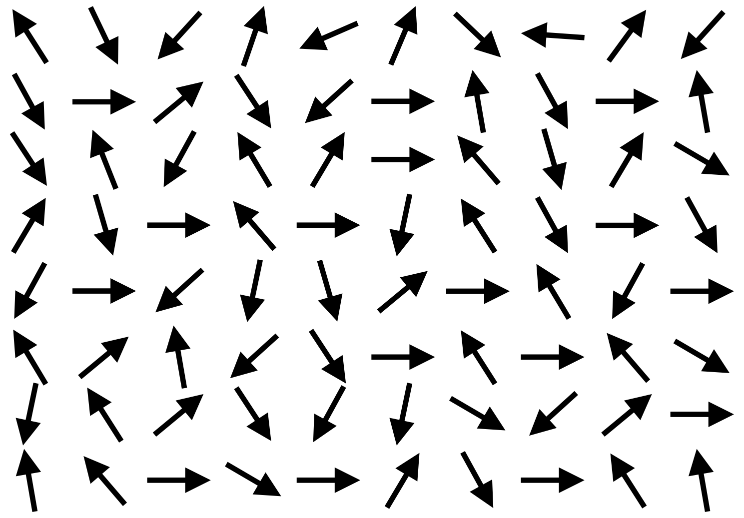
magnetic properties

electronic properties

Ferromagnet



Paramagnet

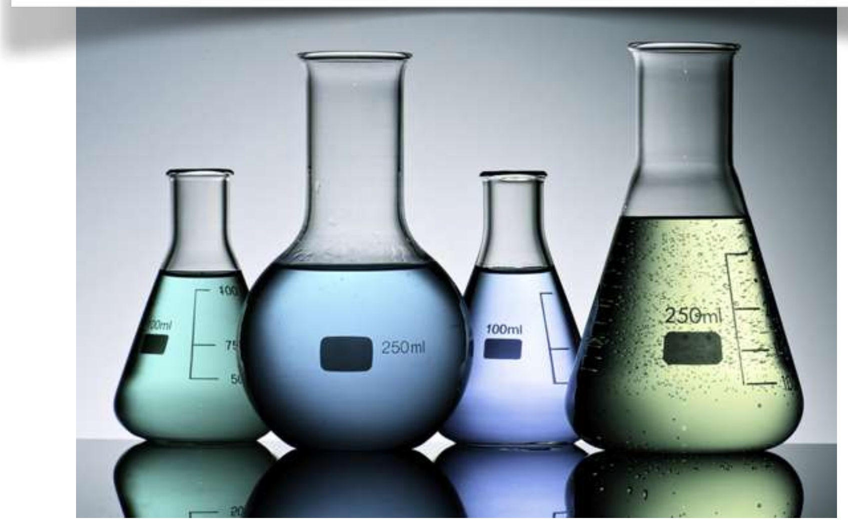


Metals

Insulators

Properties of Matter

mechanical properties



Symmetry : leaves the phase invariant

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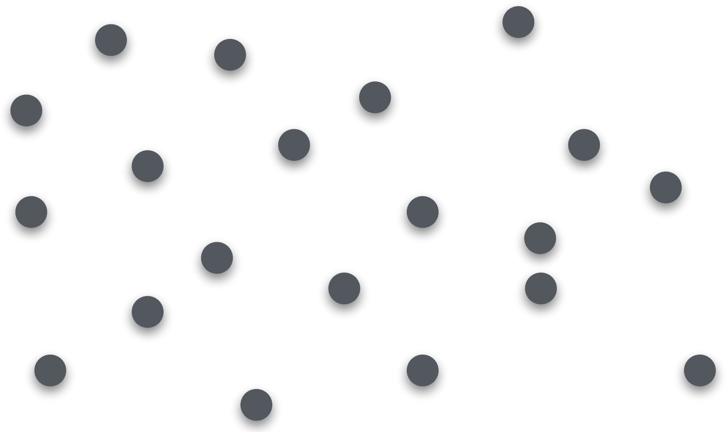

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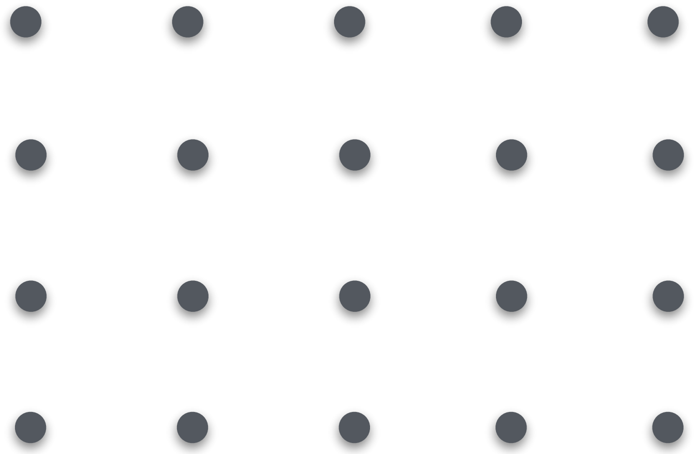

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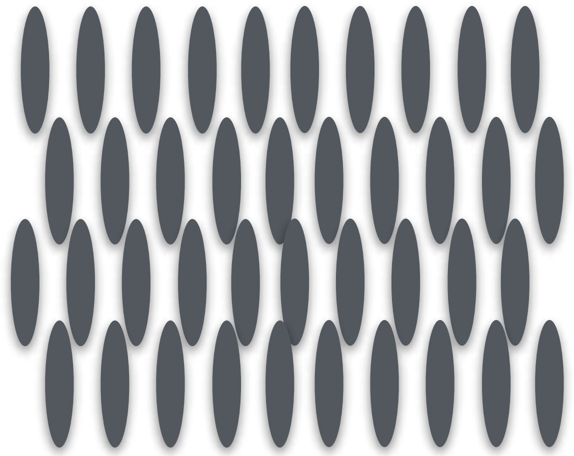

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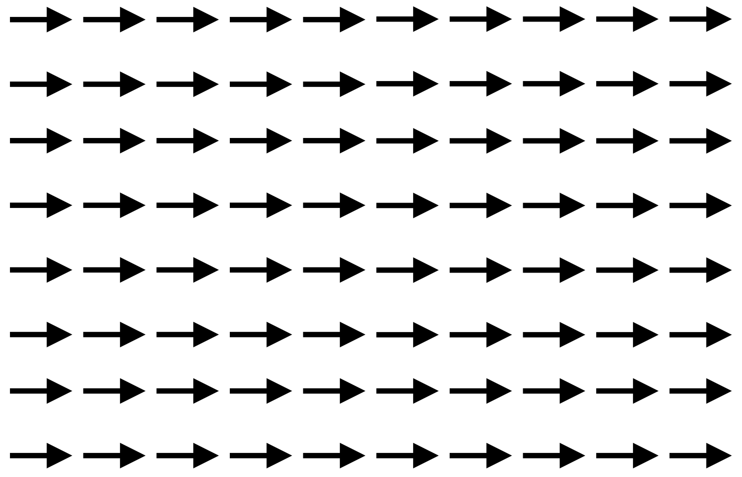

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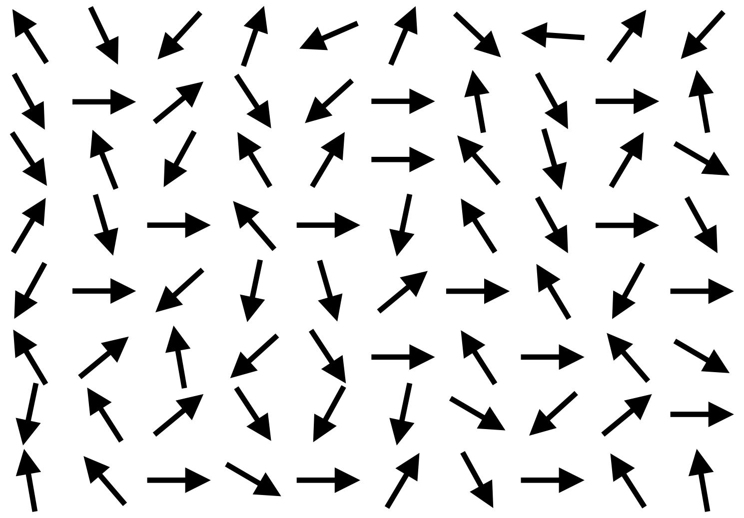

electronic properties

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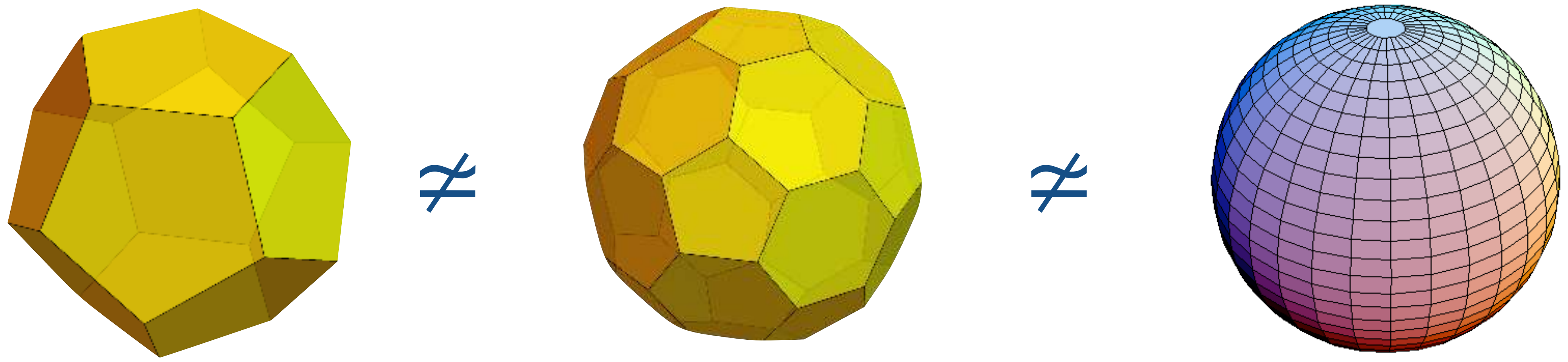
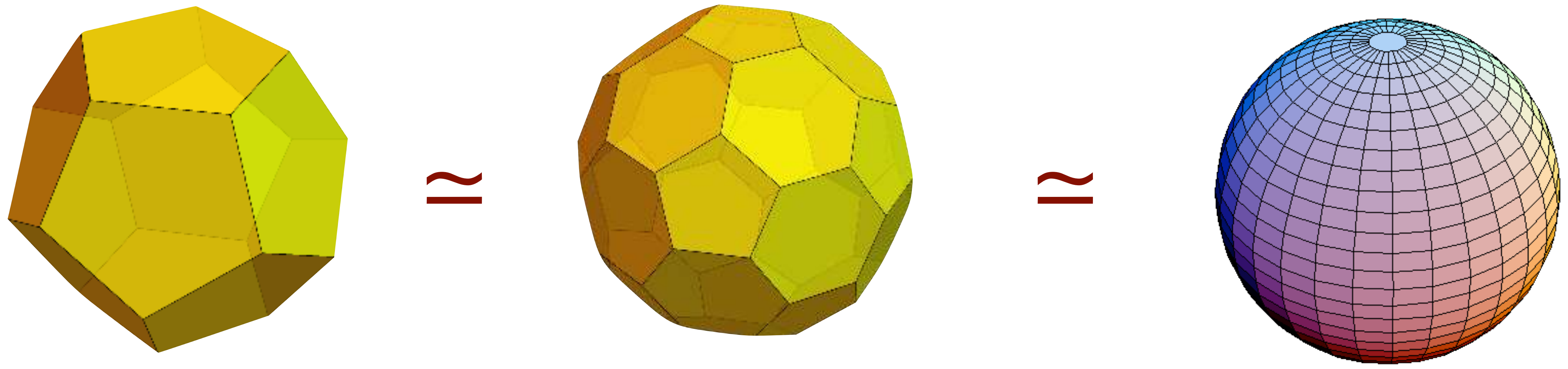
Topology versus Geometry

Symmetry : leaves the object invariant



Topology : global shape

the study of properties **unaffected by the continuous change** of shape or size



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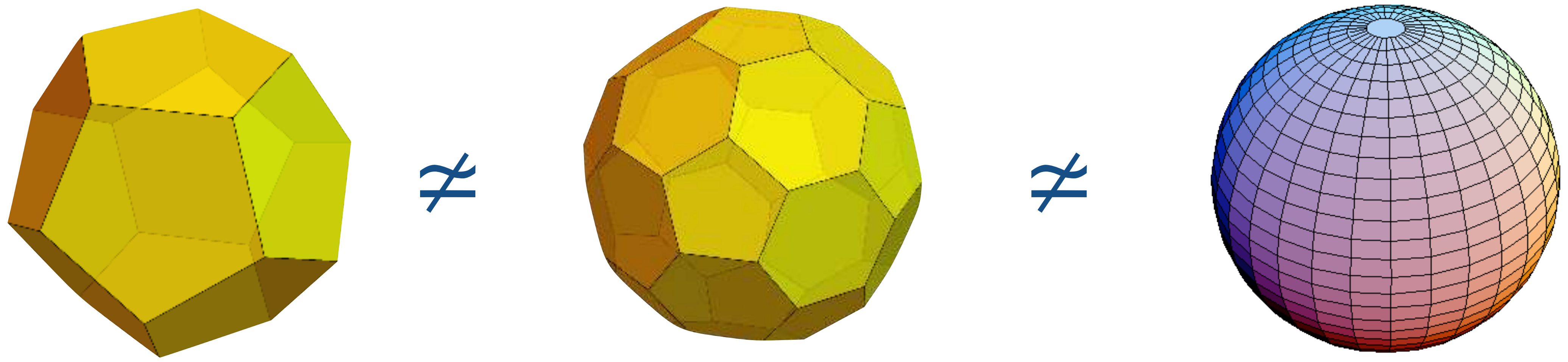

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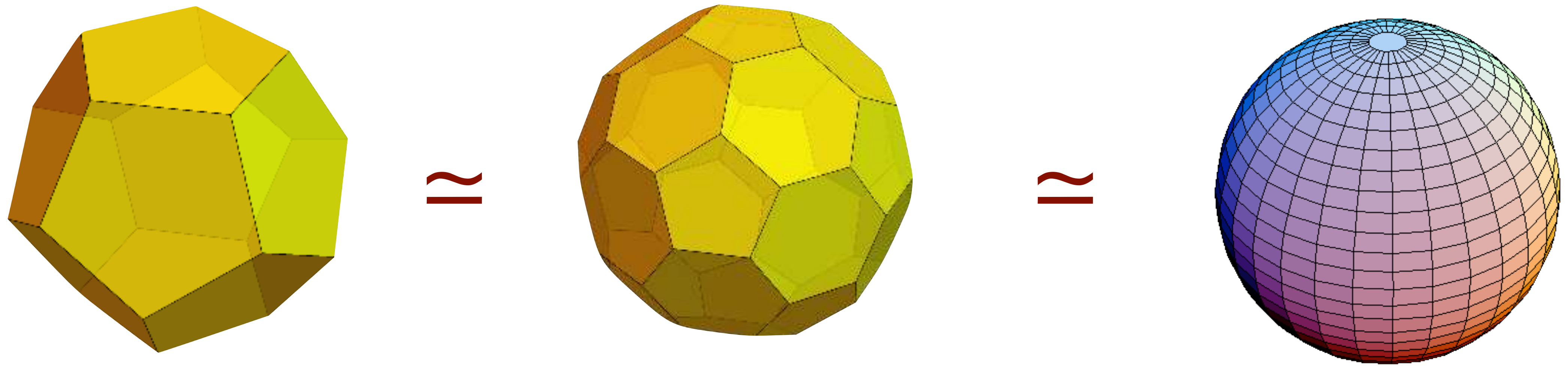

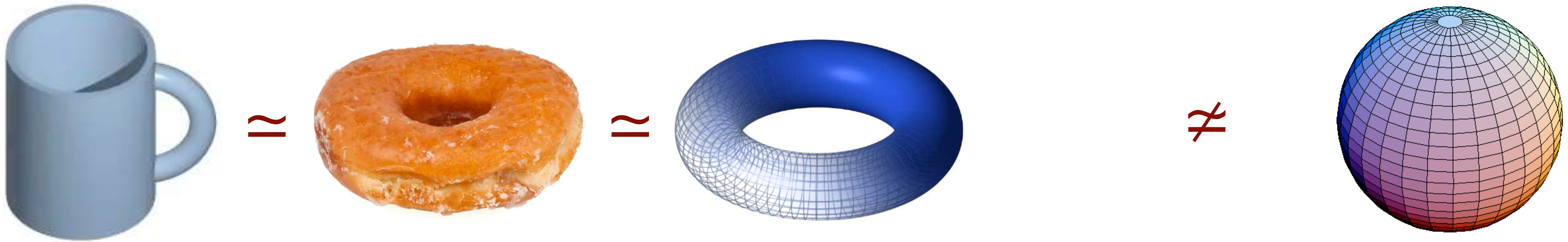

the famous «donut »

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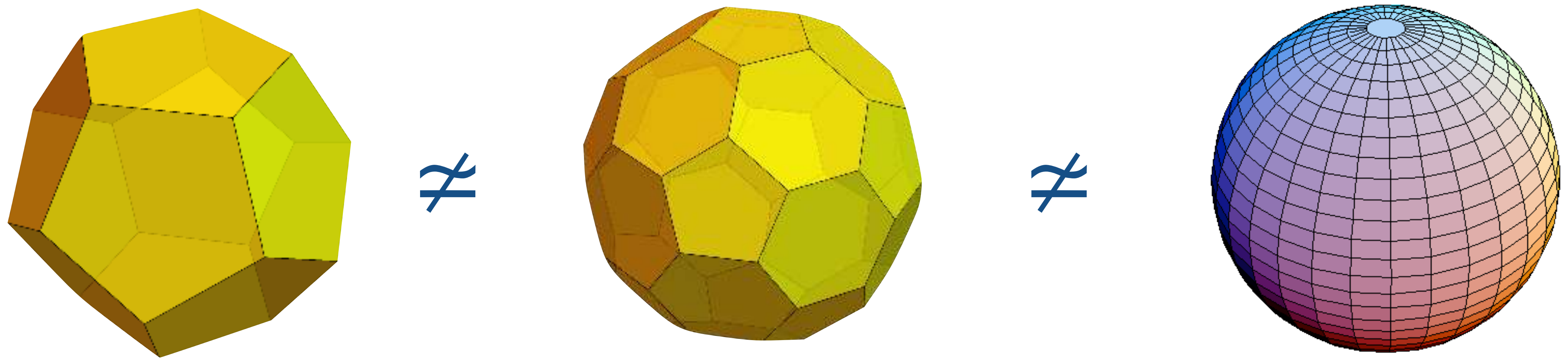

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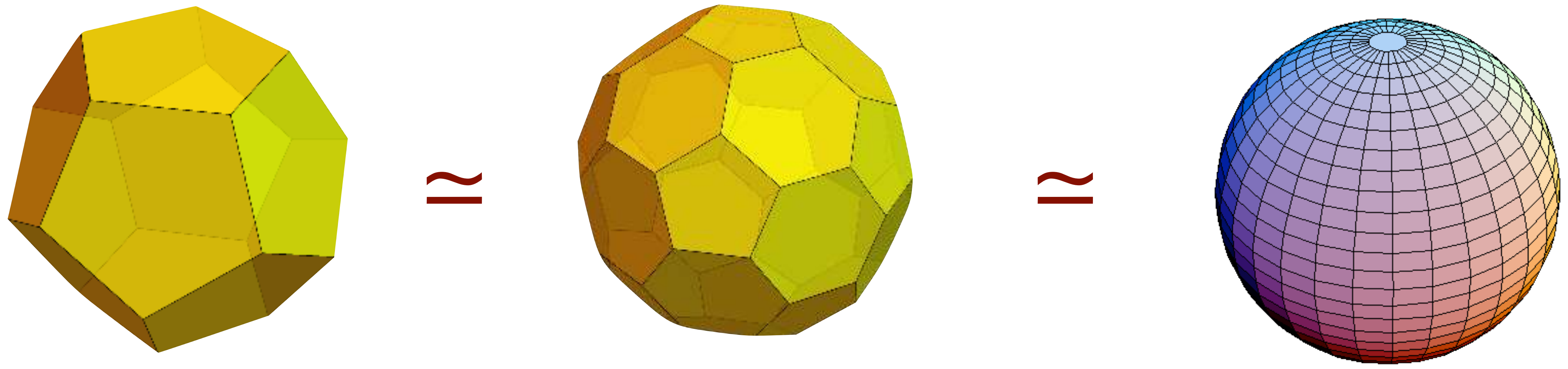

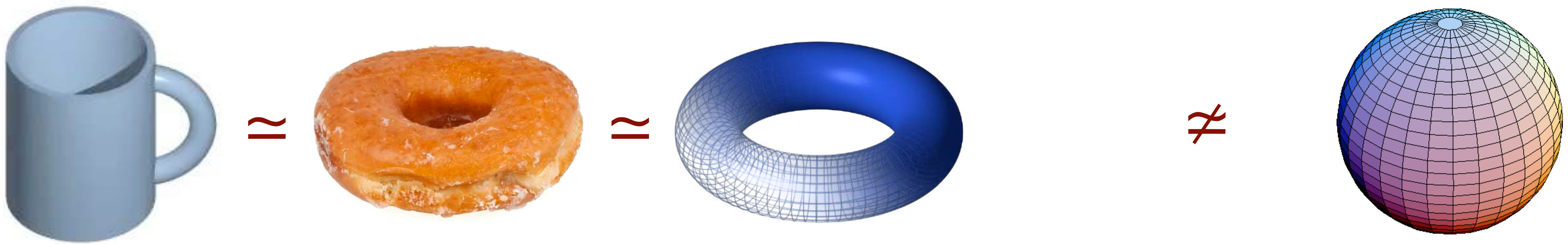

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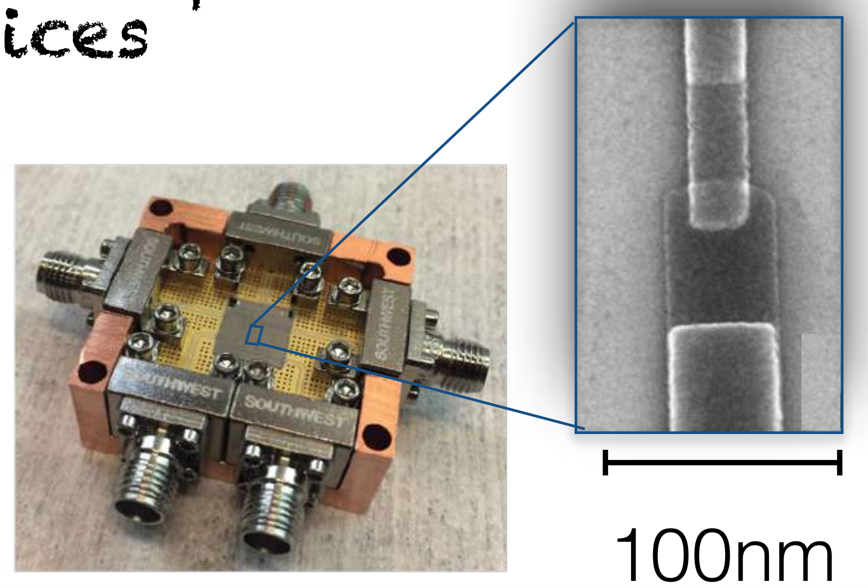
Topological Matter

Quantum Technologies

Robust quantum devices



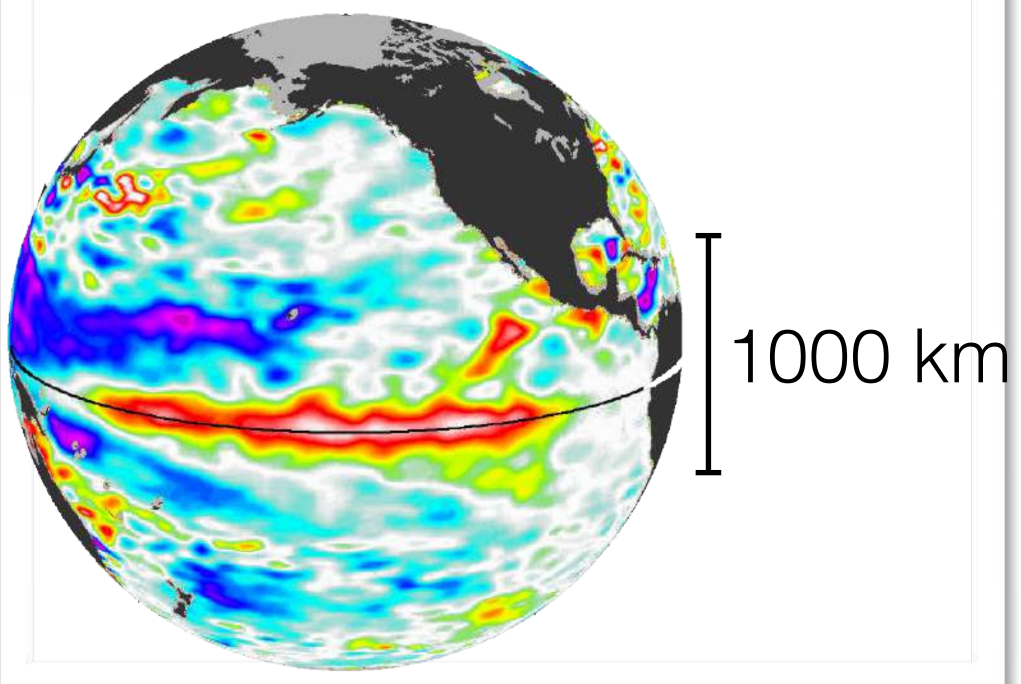
Electronic Properties of Quantum Matter

Topological Insulators

Topology
global shape

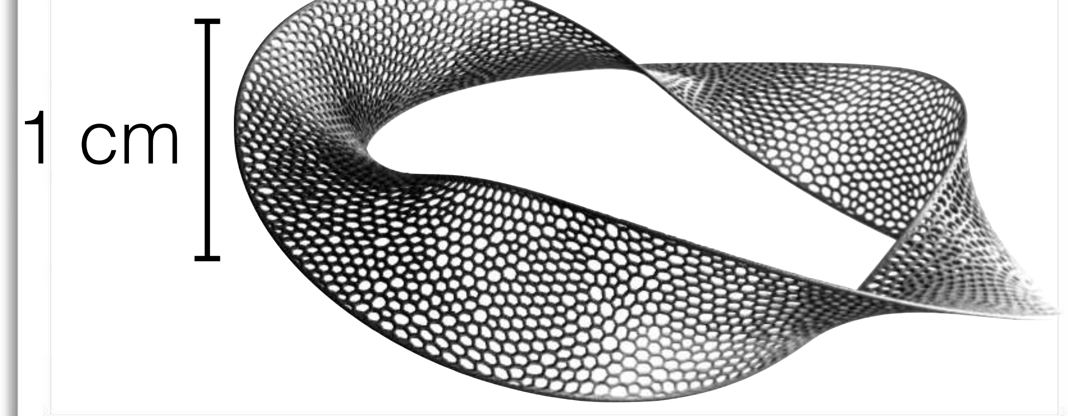
Geofluids

equatorial waves of topological origin



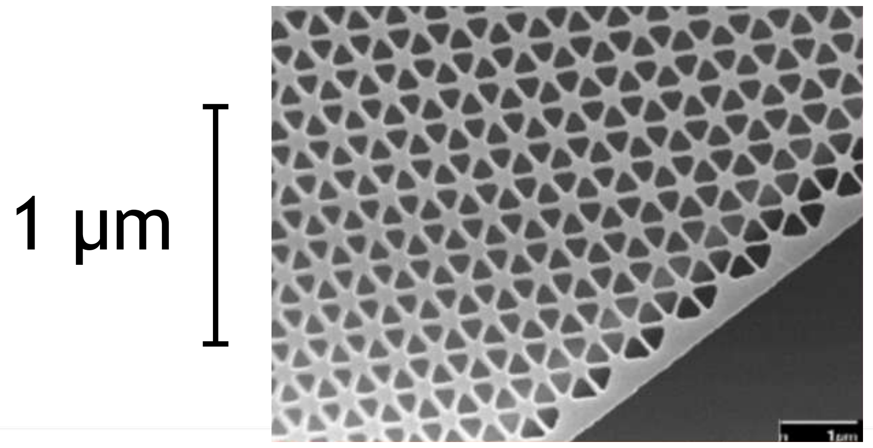
Mechanics / Metamaterials

deformations constrained by topology



Optics / Metamaterials

optical modes constrained by topology



Topological Matter

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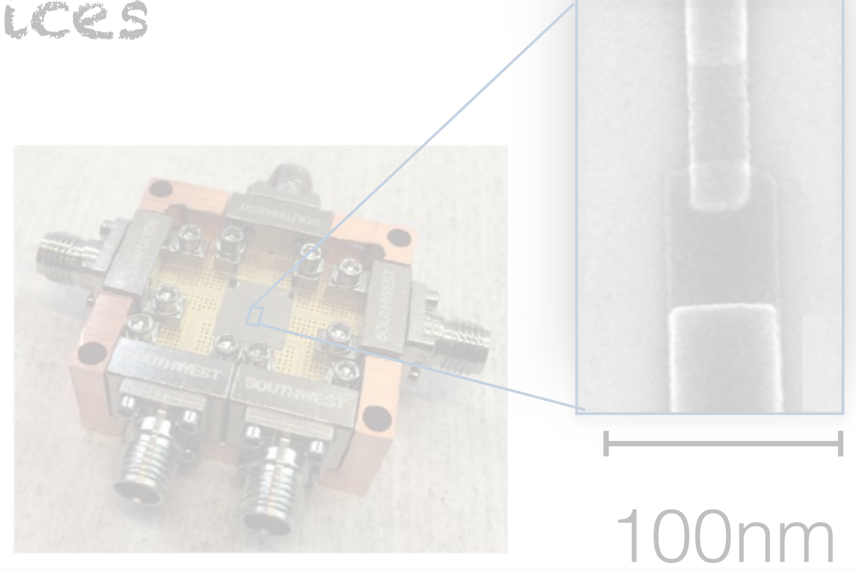

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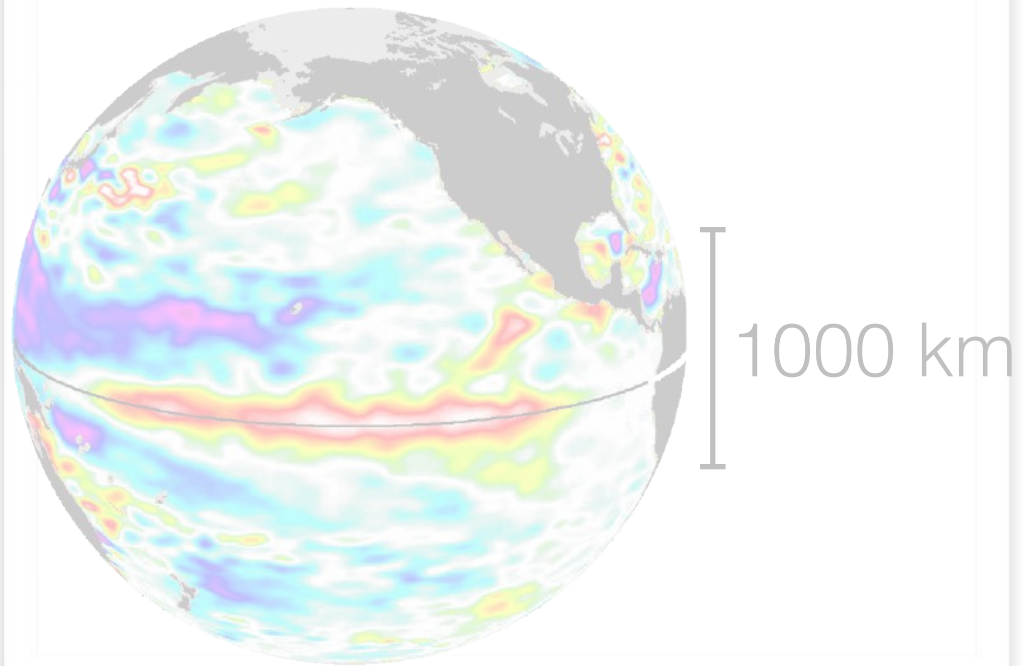

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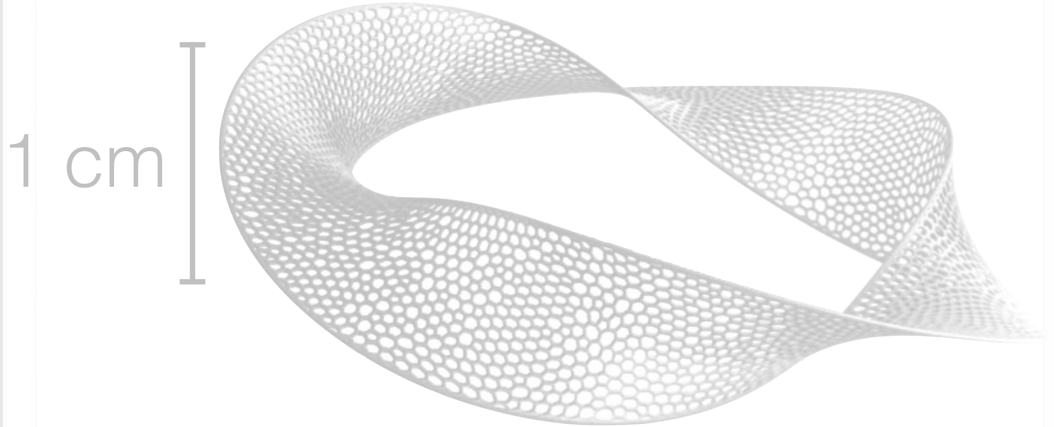


Optics / Metamaterials

optical modes constrained by topology

Topological Matter

Chern Topological Index
Quantum Hall Effect
Thouless, Kohmoto, Nightingale and den Nijs (1982)
Niu, Thouless, and Wu (1985)
Haldane (1985)

Topological Superconductor
formal 1D model
Kitaev (2001)

Topological Insulators
new Z_2 topological index constrained by T symmetry
Kane and Mele (2005)
Bernevig, Hughes, and Zhang (2006)
Fu, Kane et Mele (2007)
Moore and Balents (2007)
Roy (2009)

Topological Crystalline Insulators
constrained by crystal symmetries
Fu (2011)

Topological Dirac & Weyl metals
no gap

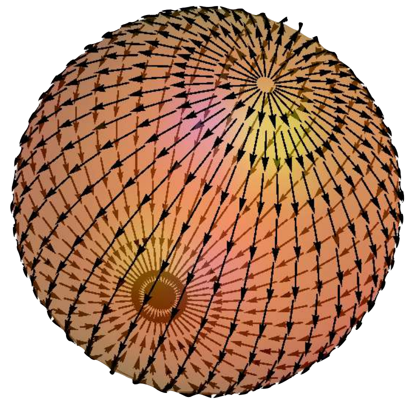
Nobel Prize in Physics (2016)
D.J. Thouless,
F.D. Haldane and J.M. Kosterlitz
« for theoretical discoveries of topological phase transitions and topological phases of matter »

Topological Quantum Chemistry
New band theory of materials (crystal symmetres & topology)

Outline

1. Notion of topological number

   Chern number for fields on a manifold



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3. How to calculate a topological number ?

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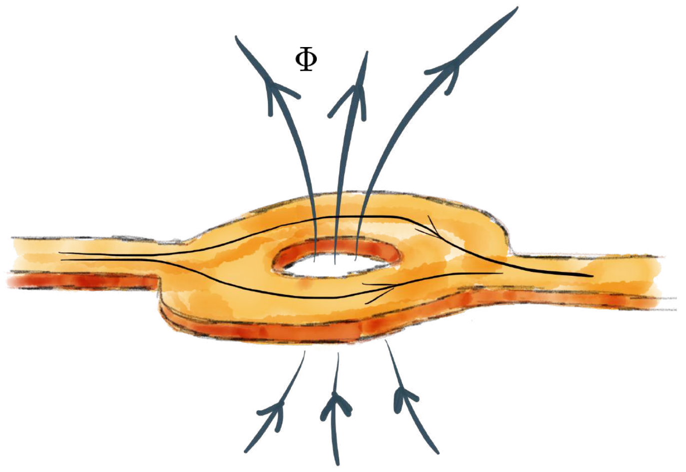
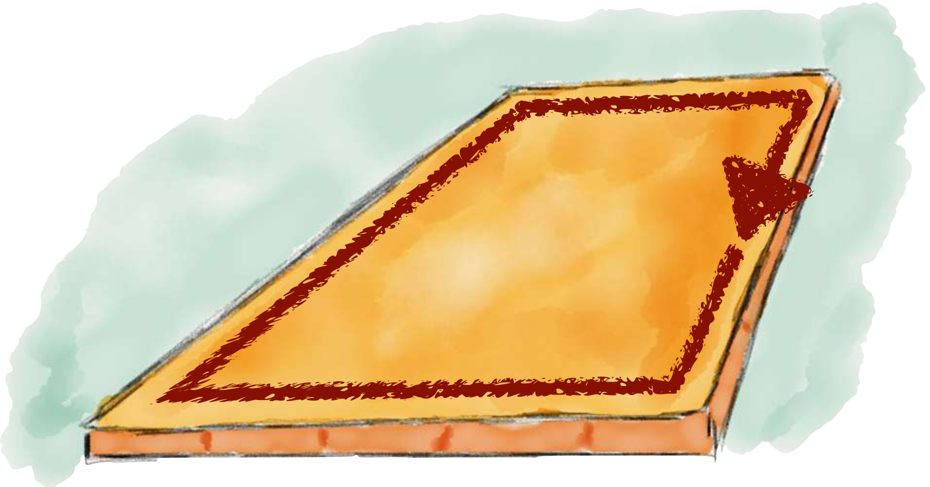


4. Surface/Interface states

   Between two inequivalent topological band structures :
   interface states



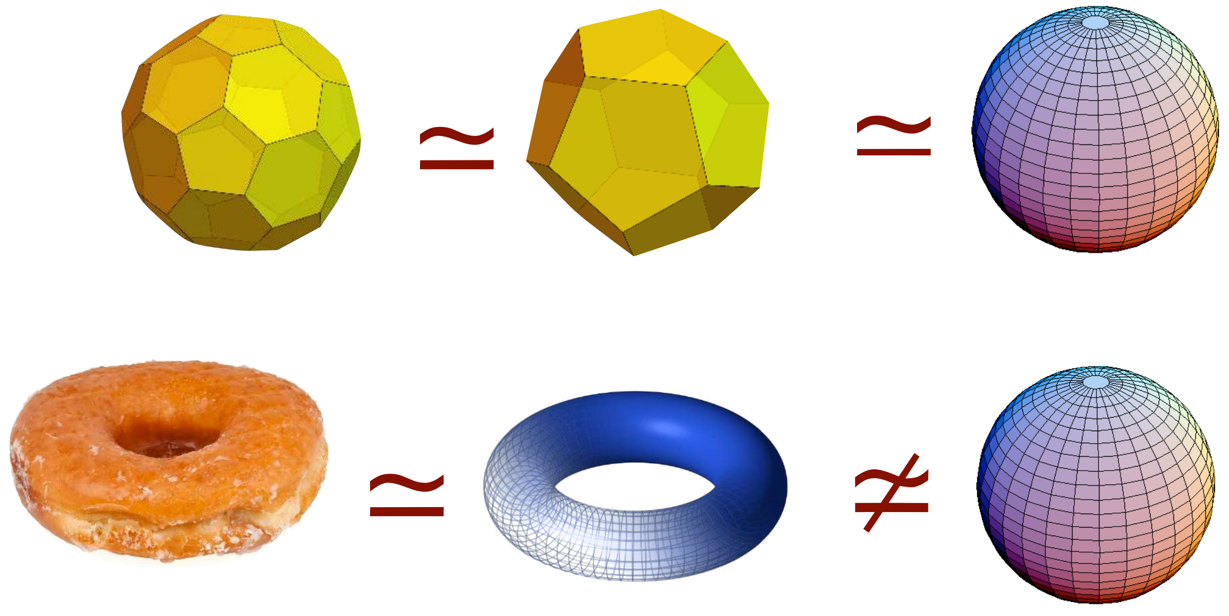
5. Topology and symmetries

   Time-reversal, chiral symmetry: topological insulators
   Crystalline symmetries: topological quantum chemistry

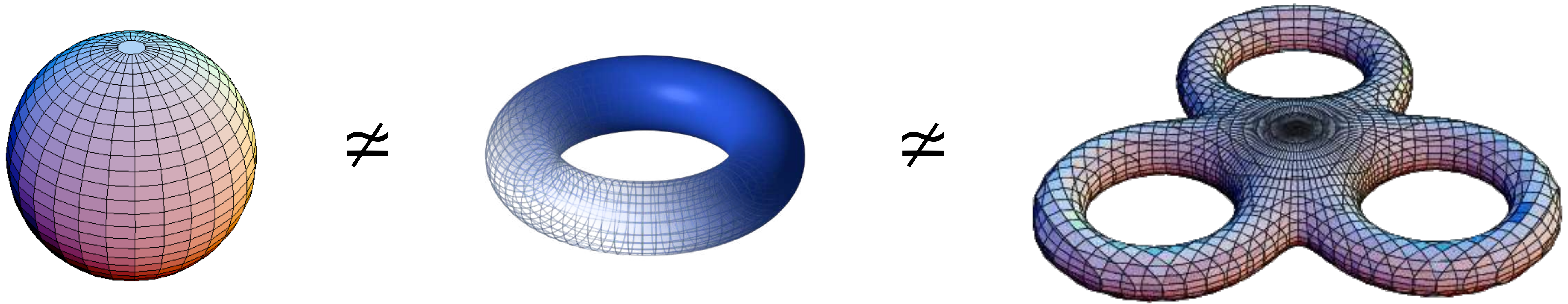
Topology

Topology: aims at classifying objects

- identifies properties of objects that are preserved under continuous deformations
- uses **integer number** to distinguish classes of objects



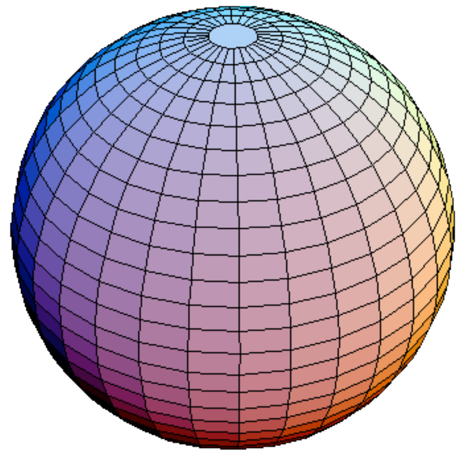
Example of 2d surfaces :



$\chi = 2$ $\quad$ $\chi = 0$ $\quad$ $\chi = -4$

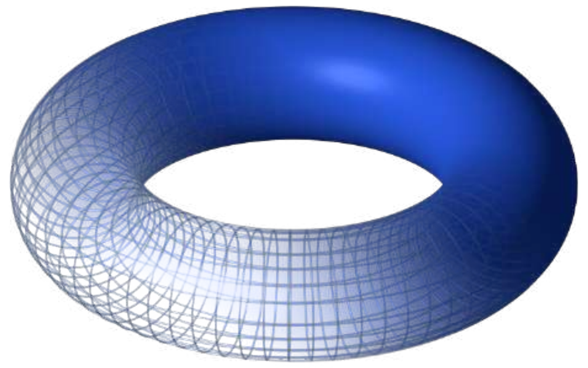
(Euler characteristic)

Topology



$\chi = 2$

$\neq$



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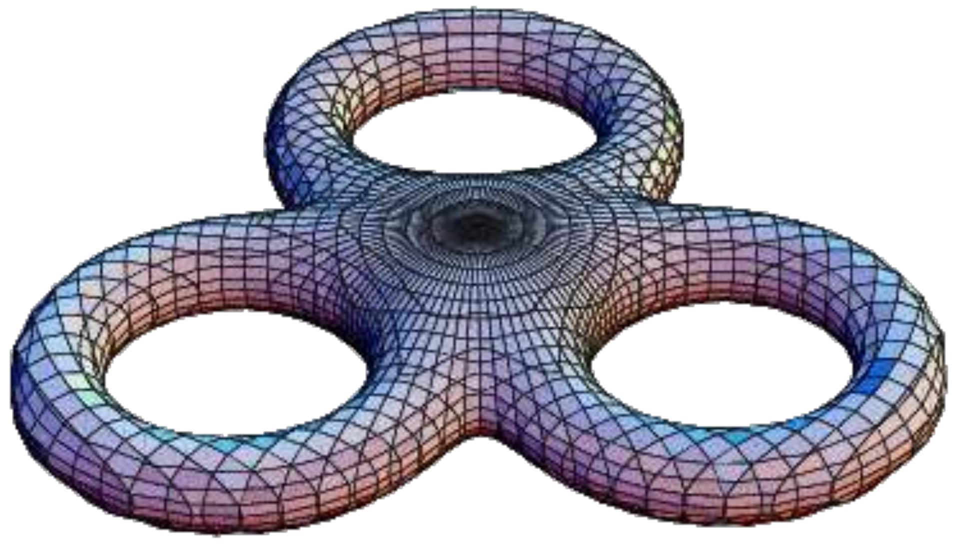
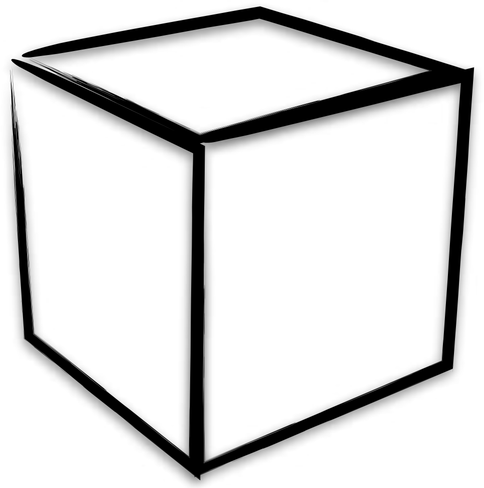
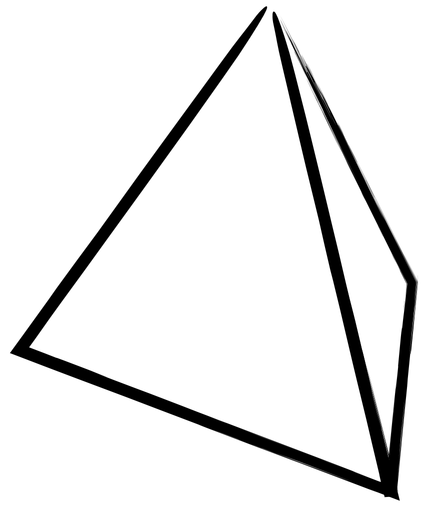


$\chi = -4$

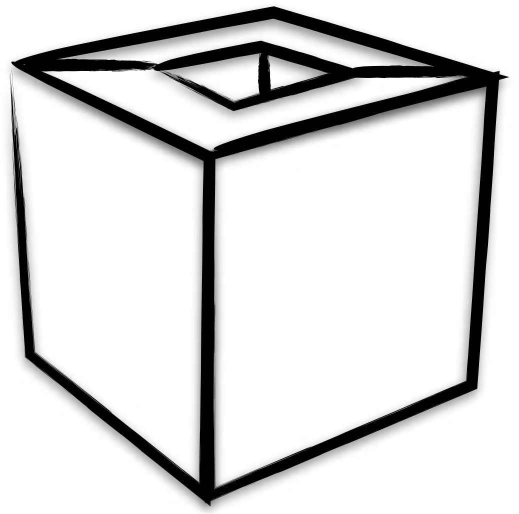
- For polygons: **Euler characteristic** χ = #vertices - # edges + # faces



$\chi = 8 - 12 + 6 = +2$

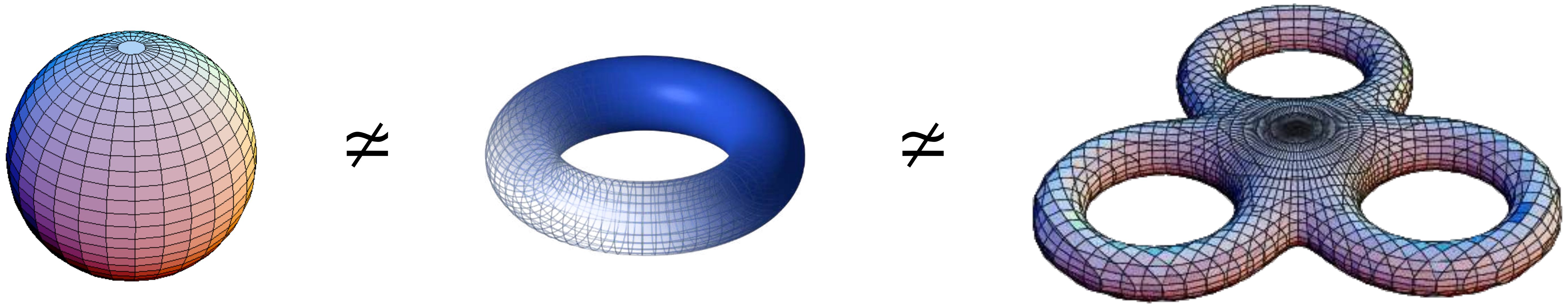


$\chi = 4 - 6 + 4 = +2$



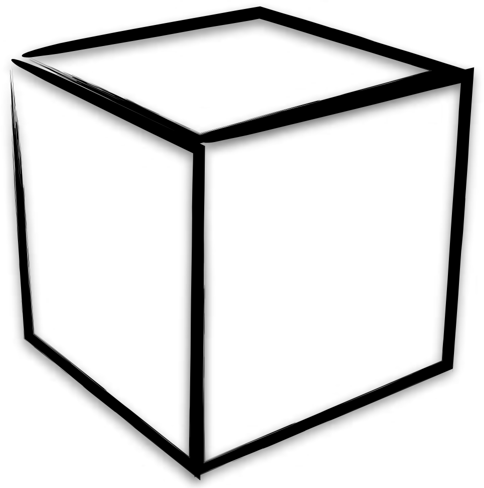
$\chi = 16 - 28 + 12 = 0$

Topology



$\chi = 2, g = 0$ $\neq$ $\chi = 0, g = 1$ $\neq$ $\chi = -4, g = 3$

- For polygons: **Euler characteristic** χ = #vertices - # edges + # faces



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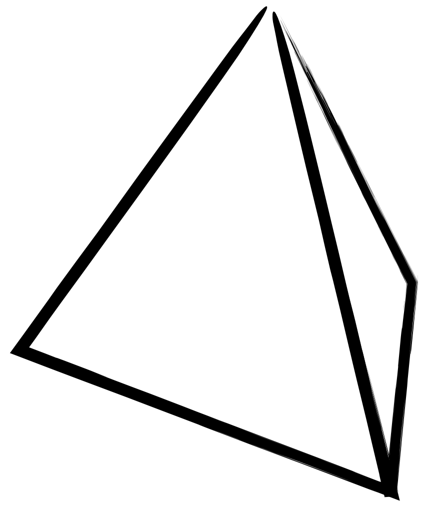

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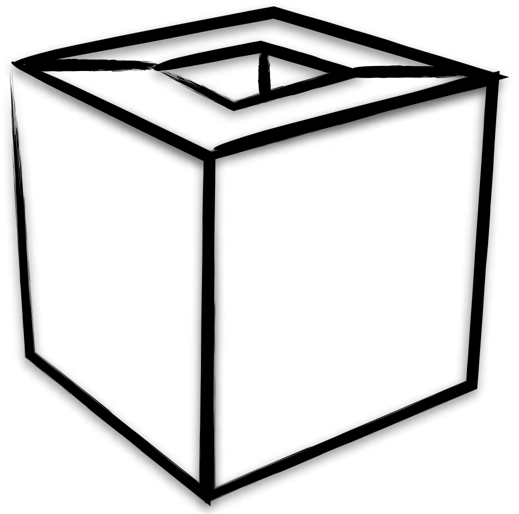


$\chi = 16 - 28 + 12 = 0$

- **Euler characteristic** ↔ genus g : $\chi = 2 - 2g$

- Gauss-Bonnet theorem $\chi = \int dS \; \kappa$

Gaussian curvature : $\kappa = 1/(R_1 R_2)$

– curvature : depends on «local properties»
– Integral of curvature : «global property» (topology)

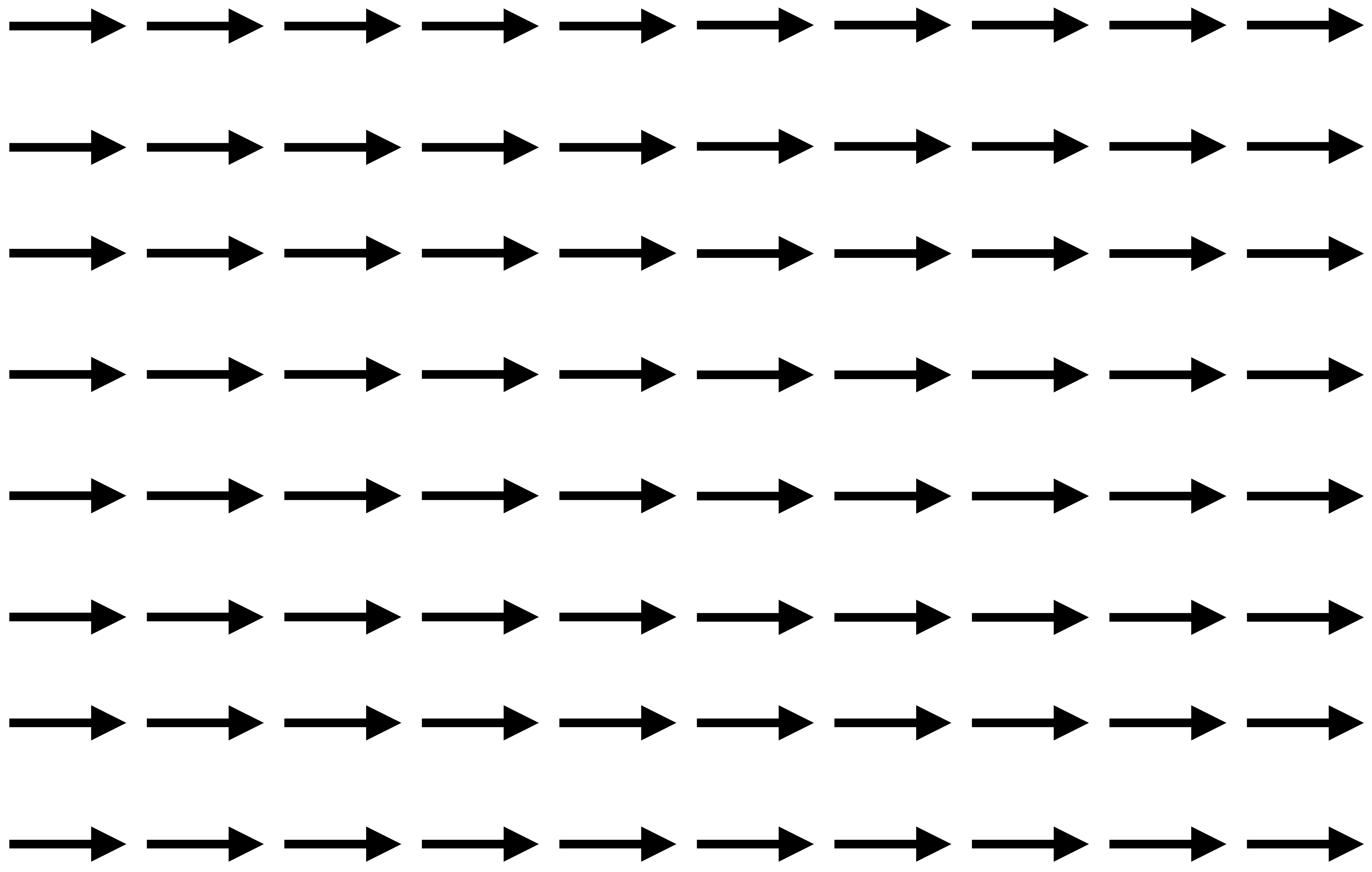
Topology

In condensed matter : **topological defects** of ordered phase / topological **textures**

- vortices (superfluid, superconductor, XY spins),
- dislocations and disclinations (solids, liquid crystals),
- hedgehog / skyrmions (SU(2) spins), etc.

Ordered phase :

- order parameter $\psi(x) \in \mathbb{C}$
- spatial order



d=2, complex order parameter

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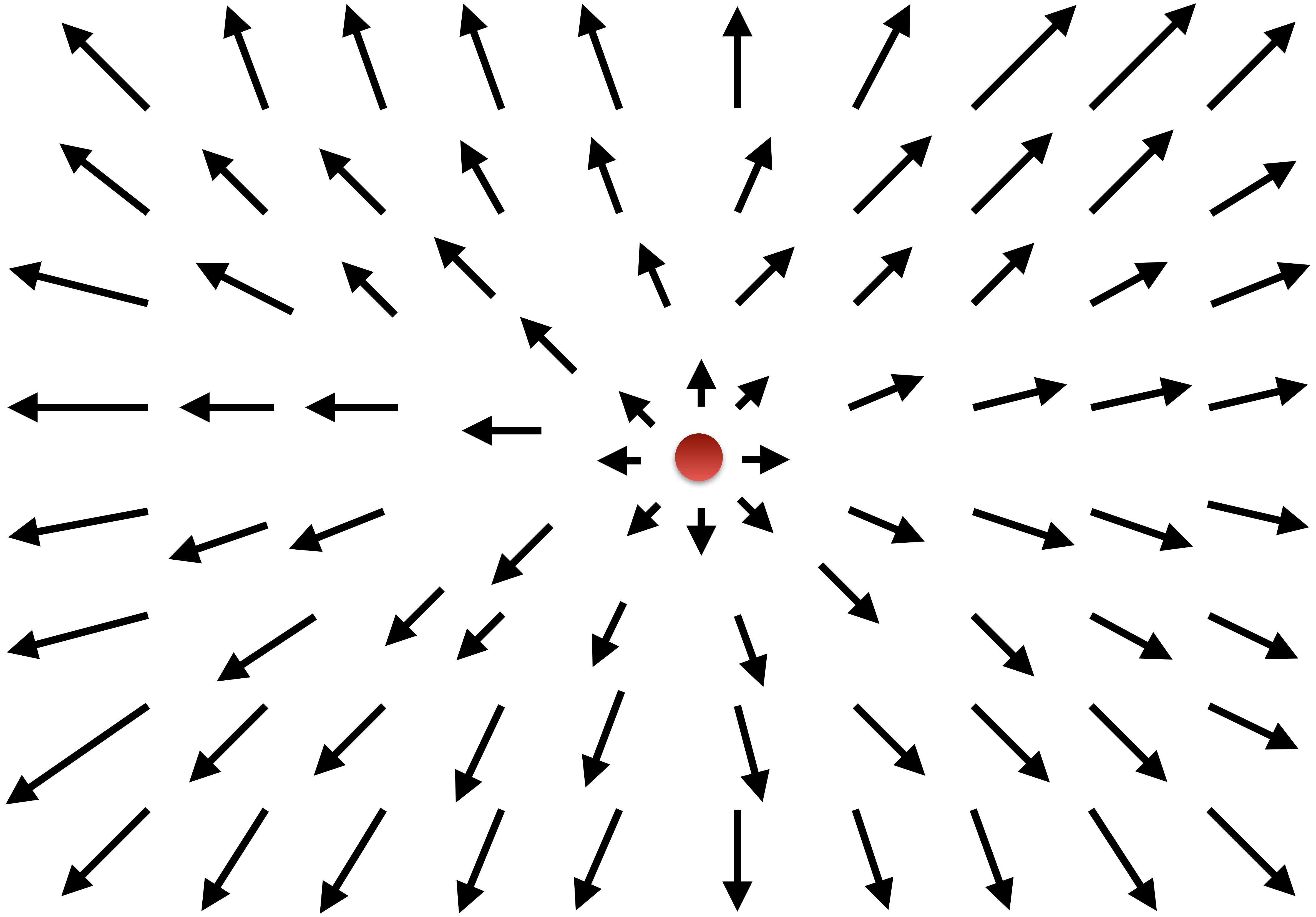

Ordered phase :

- order parameter
- spatial order

Associated Defect

- singularity of order field

d=2, complex order parameter

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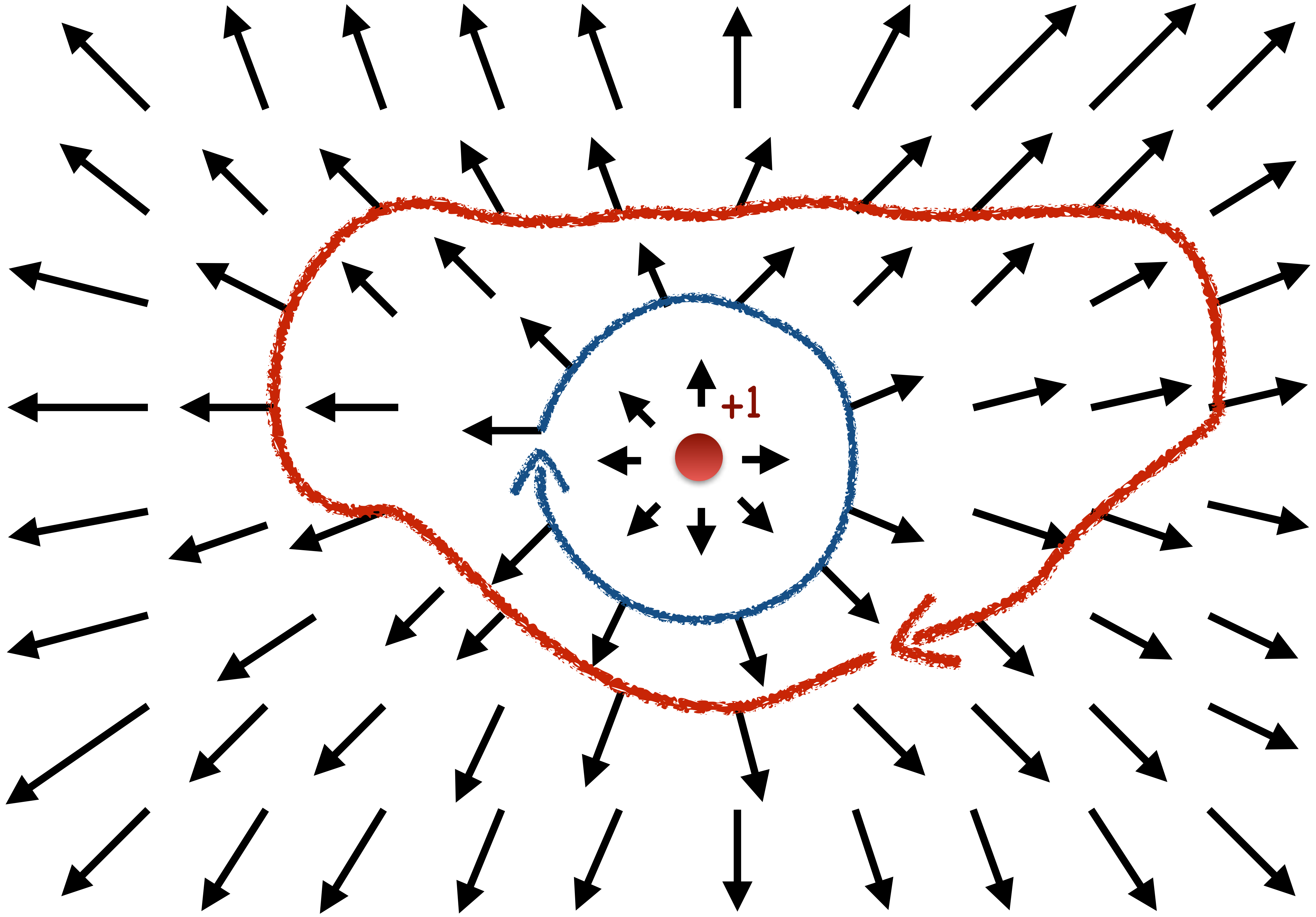
Ordered phase :

- order parameter
- spatial order

Associated Defect

- singularity of order field
- winding of order parameter : topological number

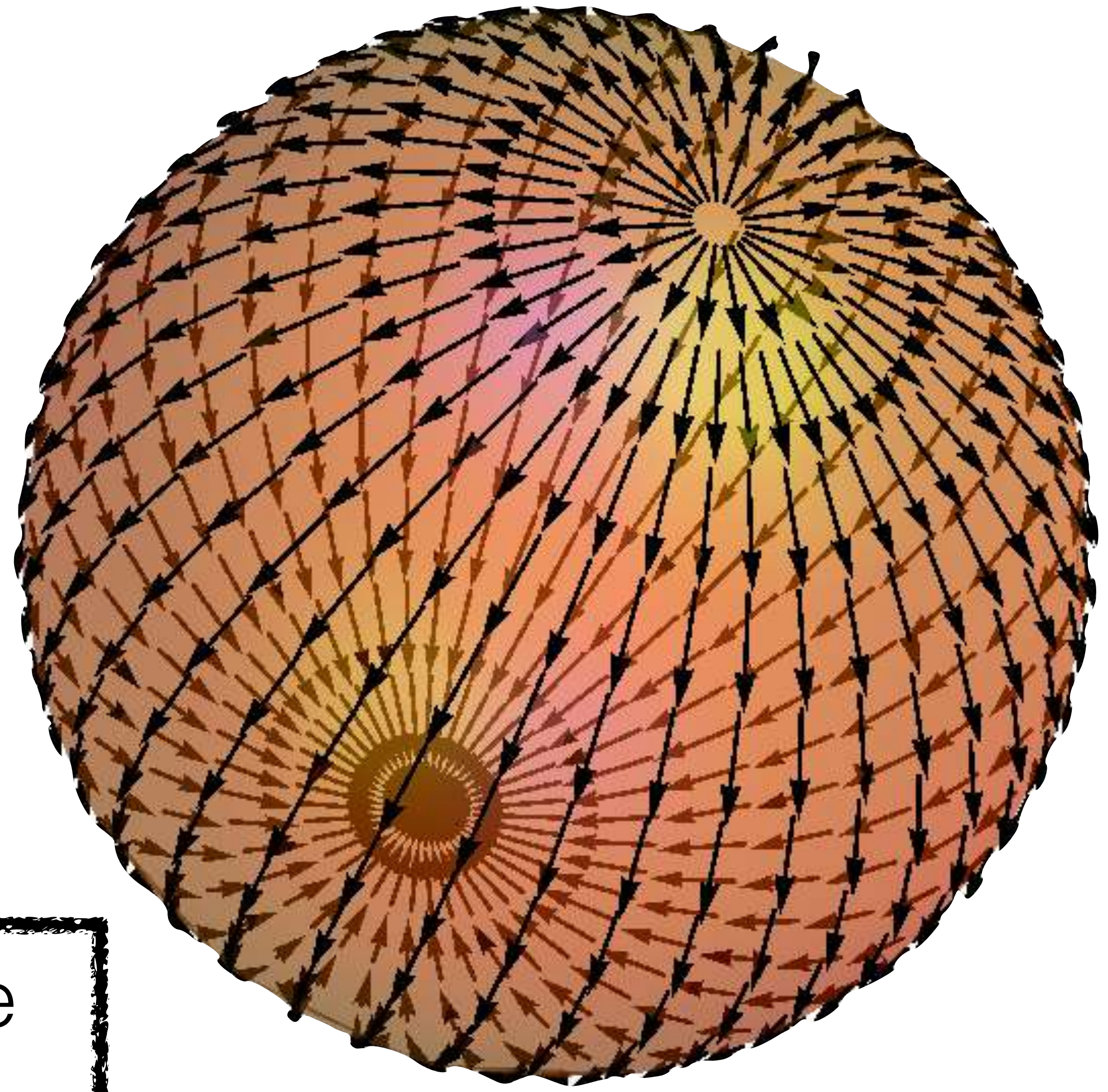


d=2, complex order parameter

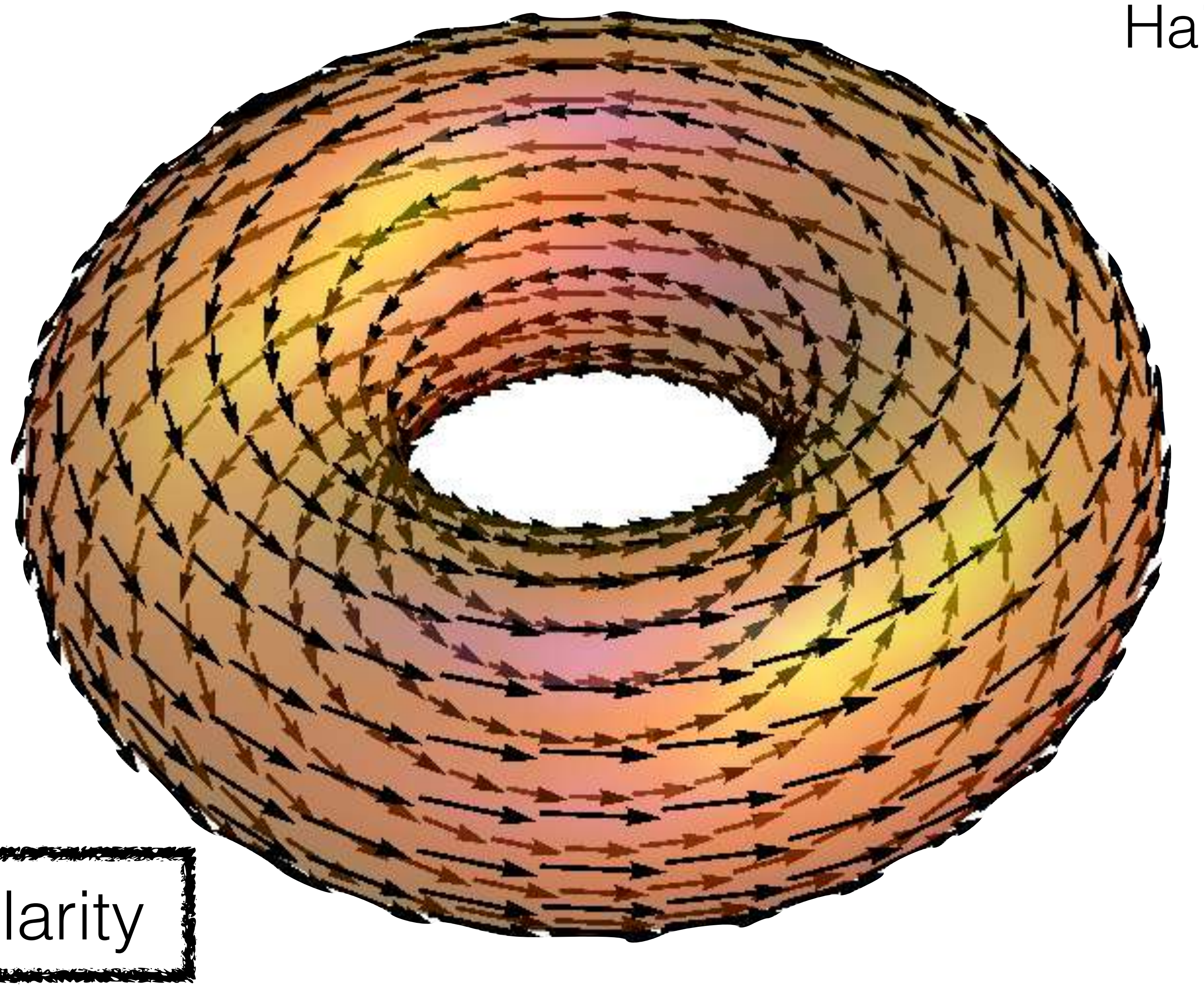
Topology

If vector field defined on a manifold : **non singular vector fields** do not necessarily exist

Hairy ball theorem



at least one singularity



no singularity

- defines a **vector bundle** (manifold + vector space above each point)
- all vector fields singular ↔ **non trivial vector bundle**
- **topological property**, associated with a « topological Chern number »

Outline

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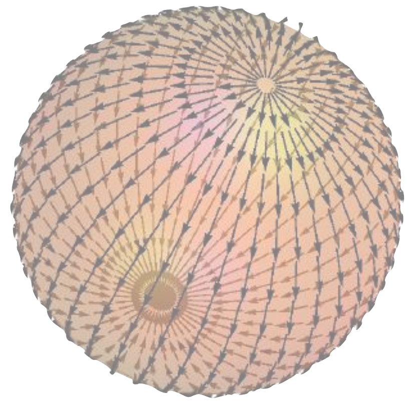
   Chern number for fields on a manifold



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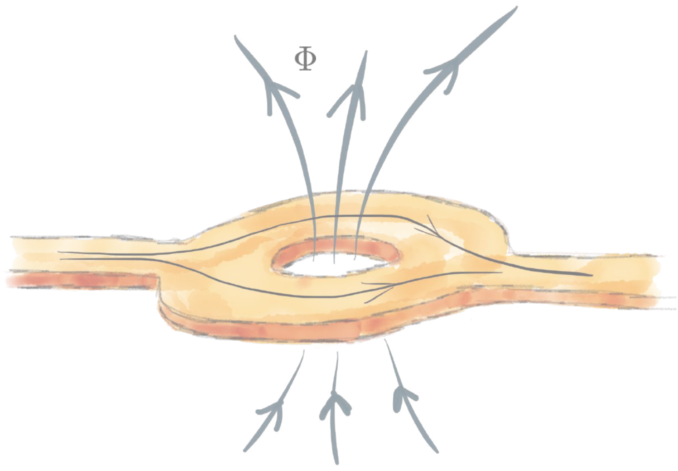

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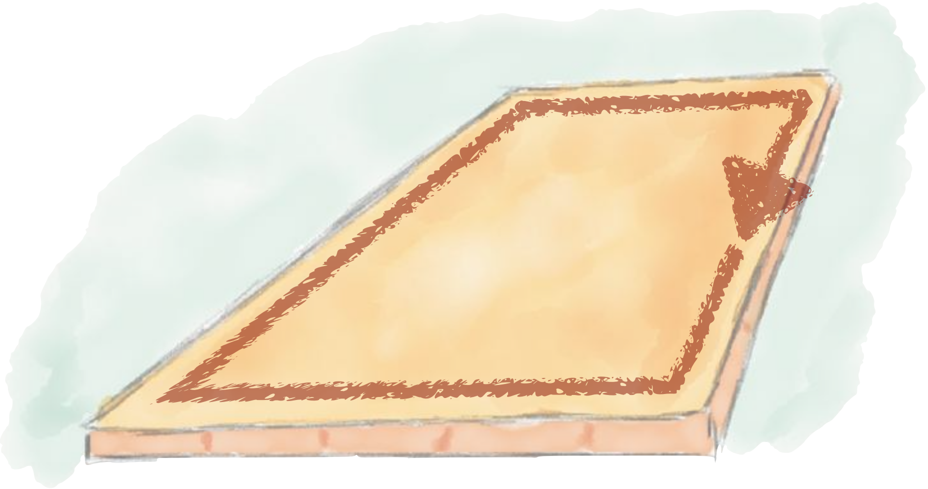

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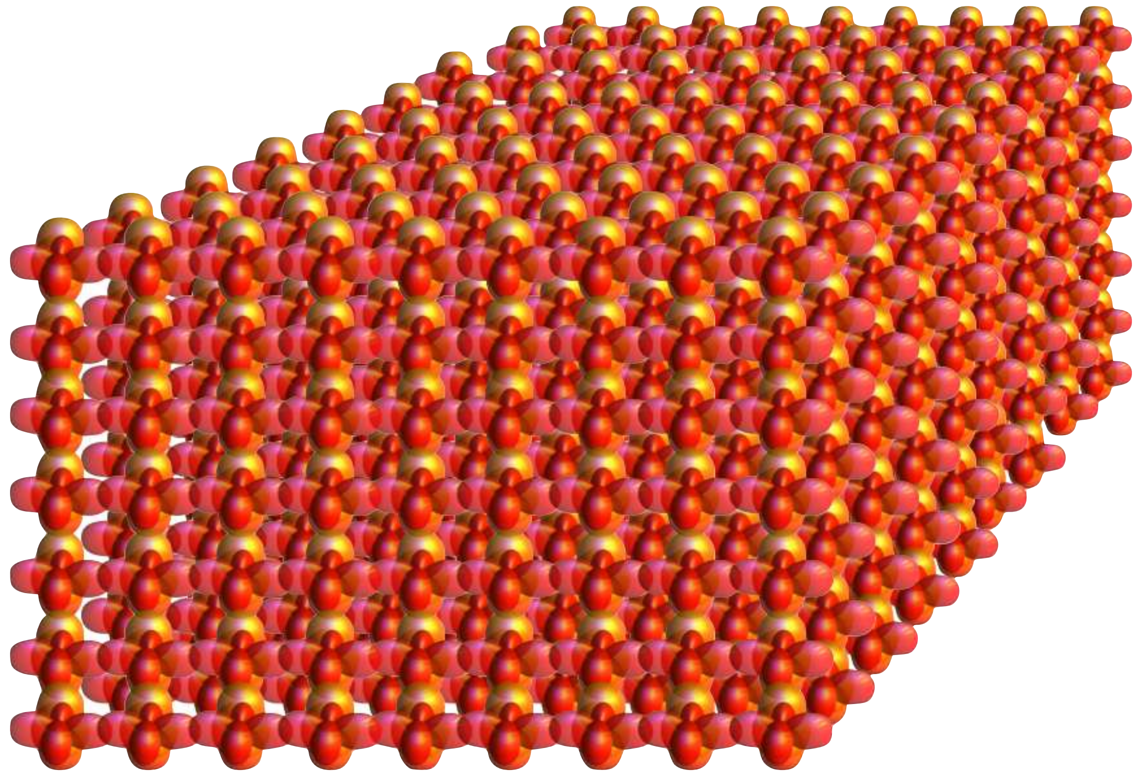
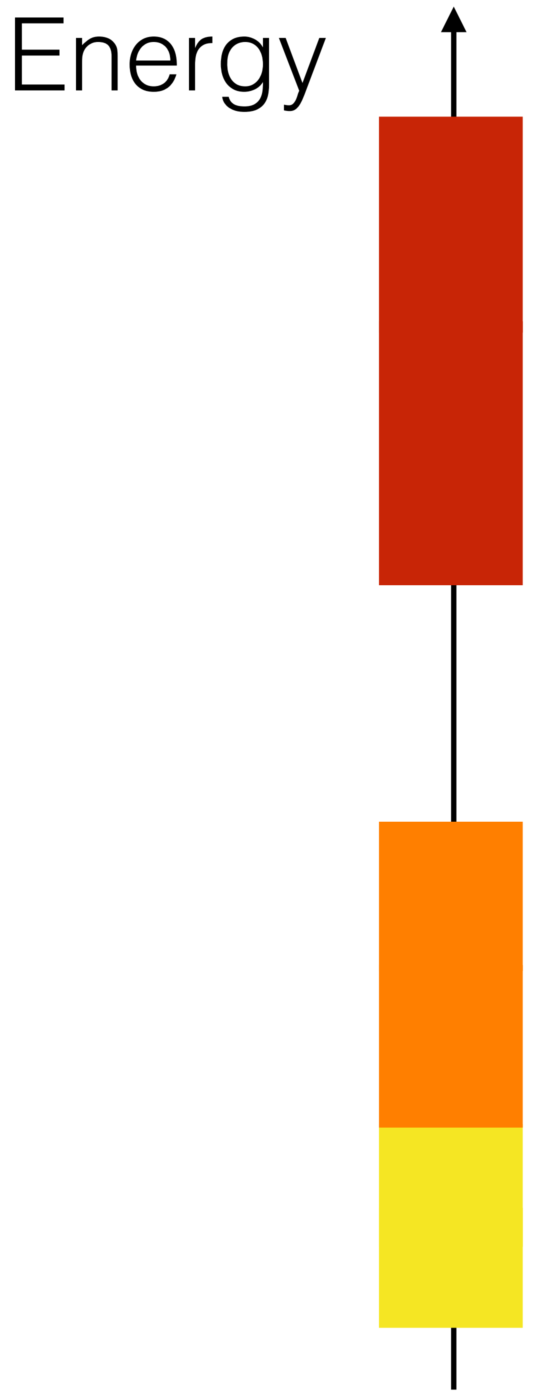
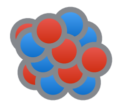
Band Theory of Electrons in Solids





Band Theory of Electrons in Solids

Electronic Orbitals



Single atom

Energy

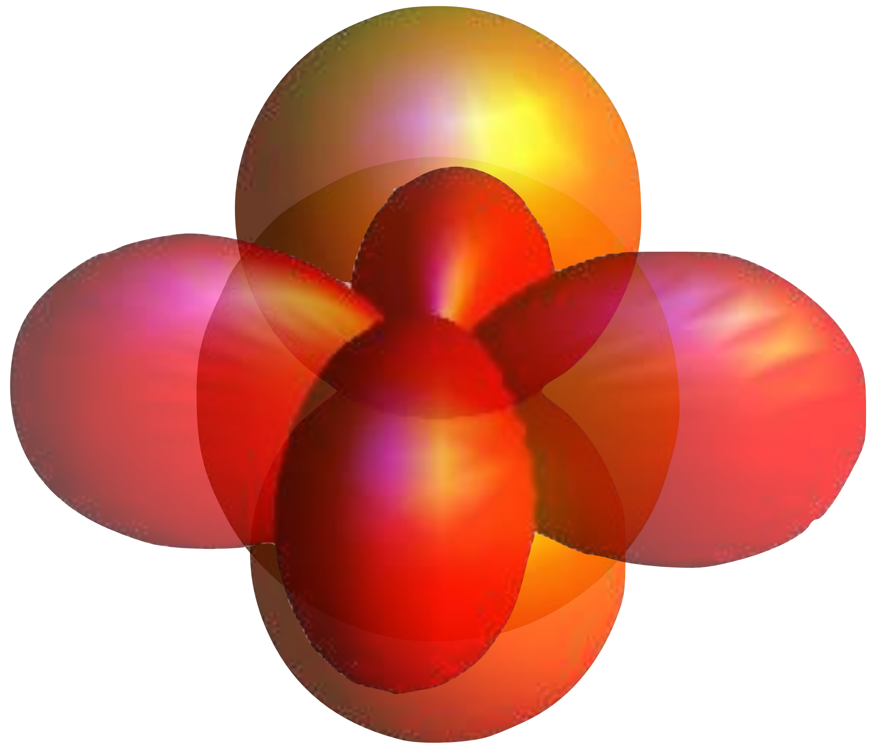
Discrete energy levels

Schrödinger equation :

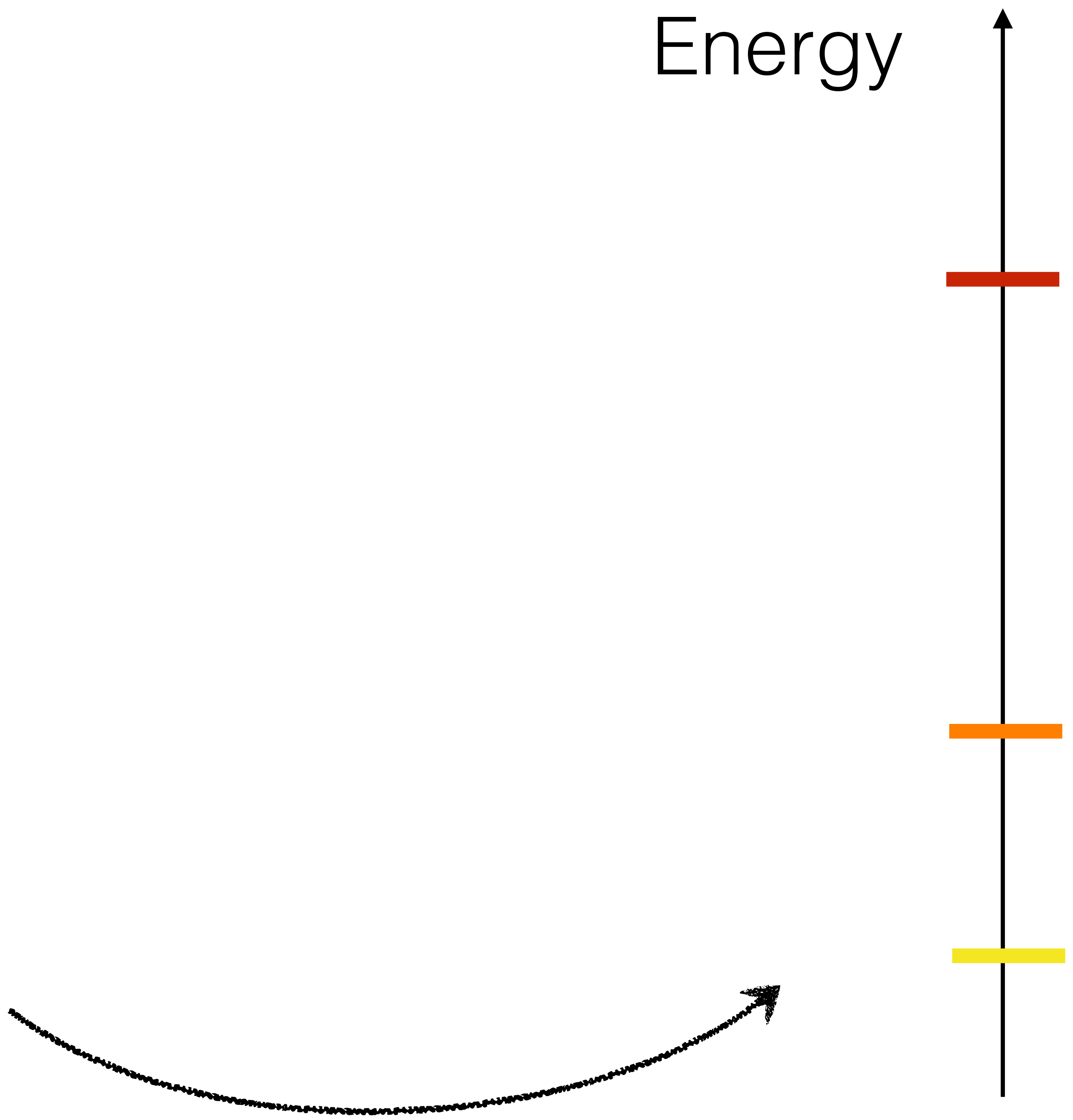
$$H|\psi\rangle = E\ |\psi\rangle$$

Band Theory of Electrons in Solids

Electronic Orbitals



Single atom



Discrete energy levels

Schrödinger equation :

$$H|\psi\rangle = E\ |\psi\rangle$$

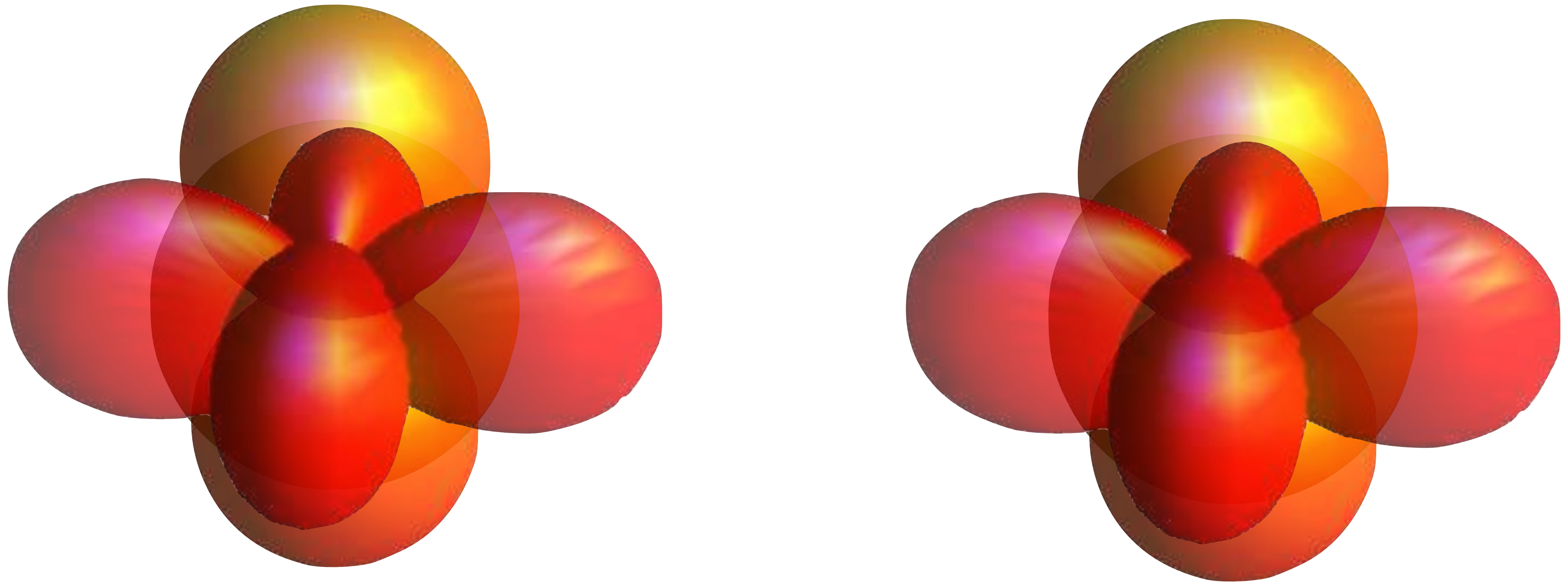
Band Theory of Electrons in Solids

Electronic Orbitals

1s

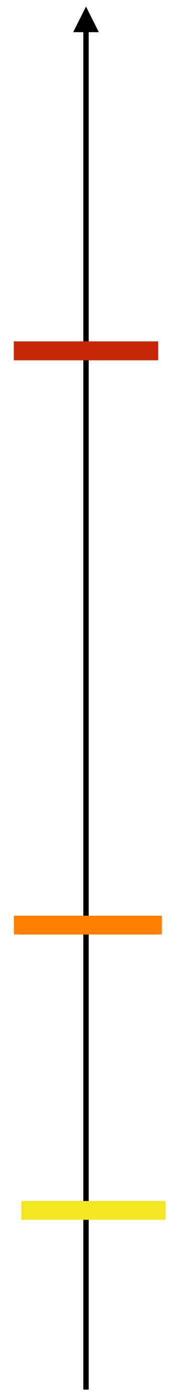
2p

3d



Two atoms

Energy



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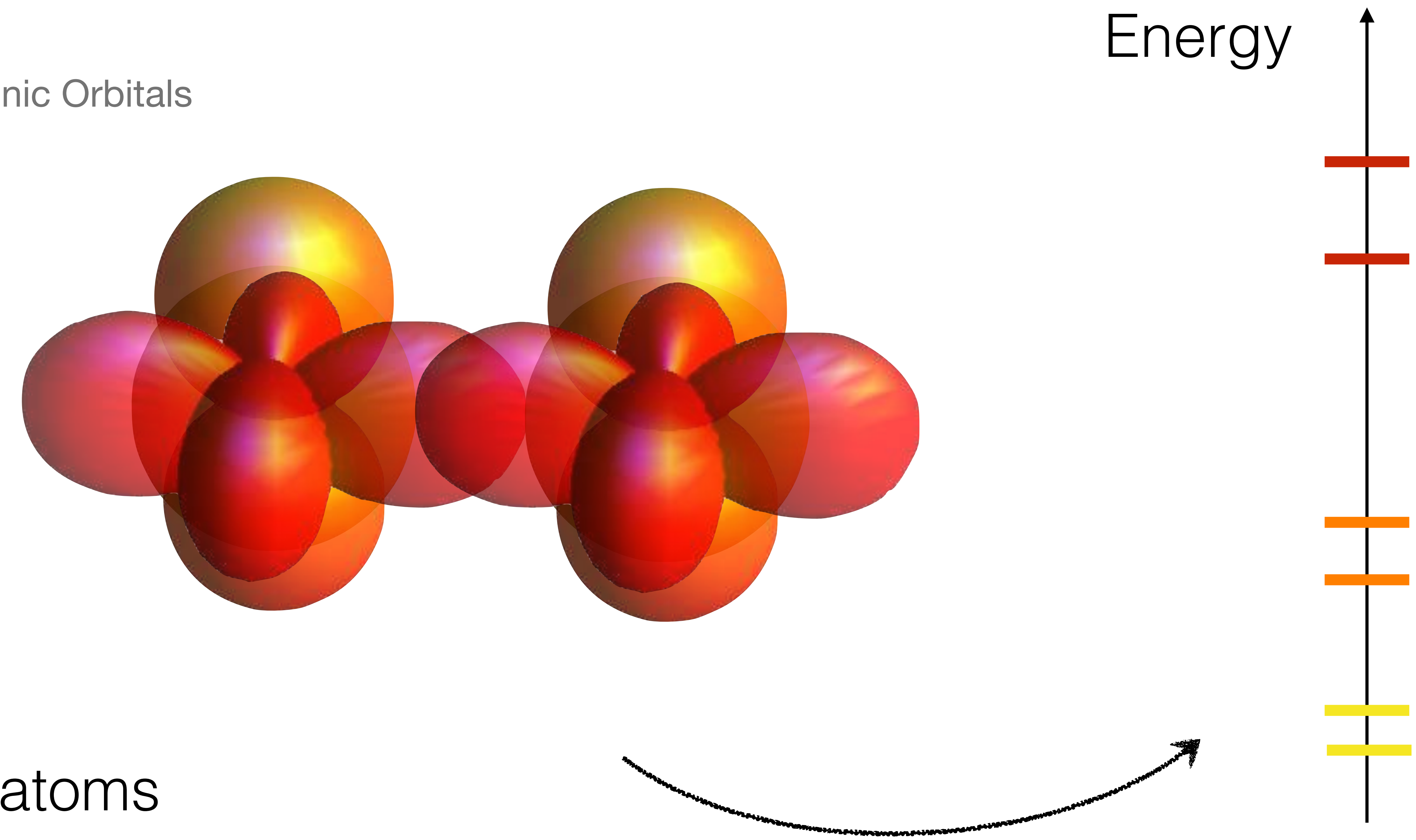

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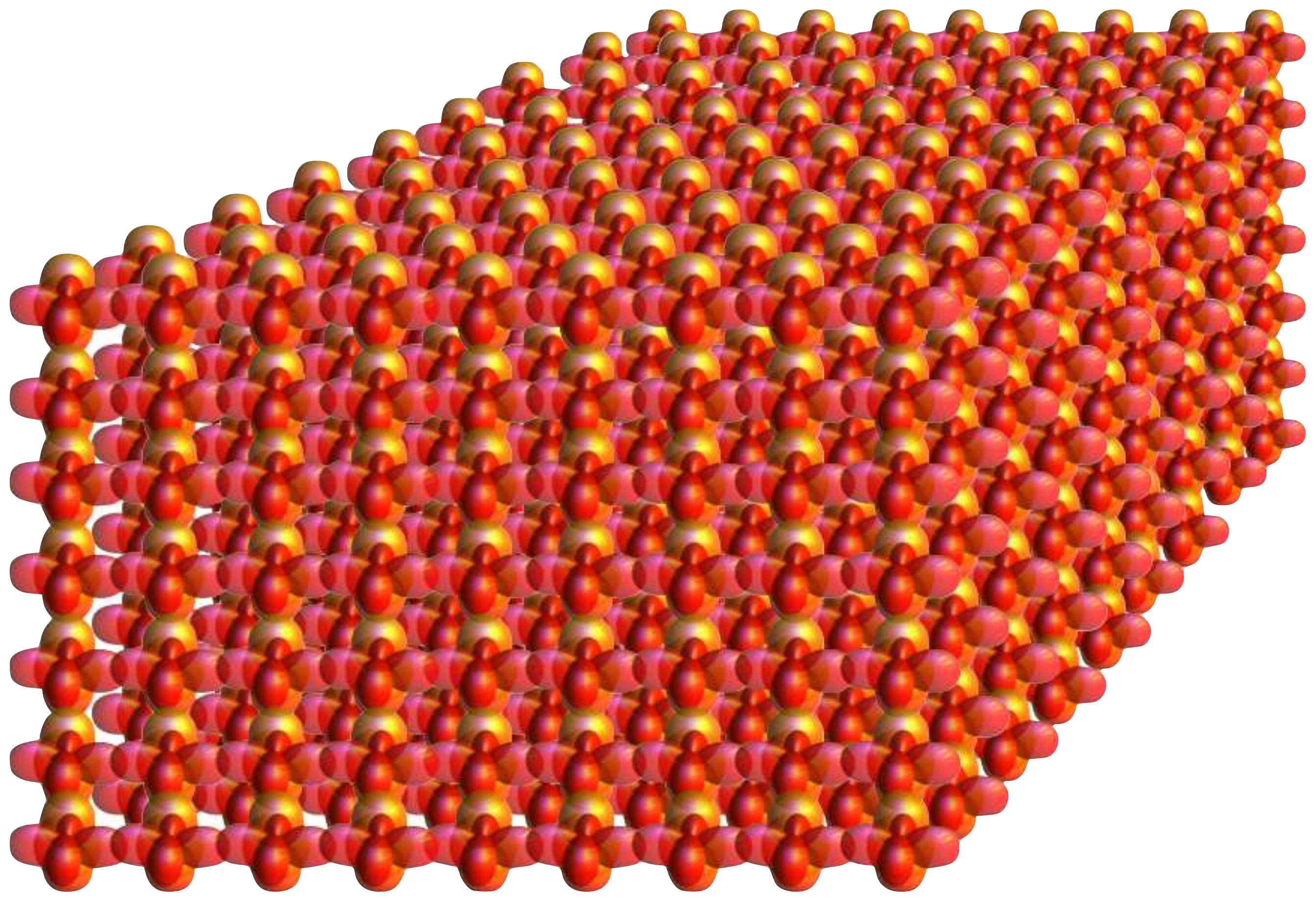
Electronic Orbitals



Solids : ~10^{23} atoms

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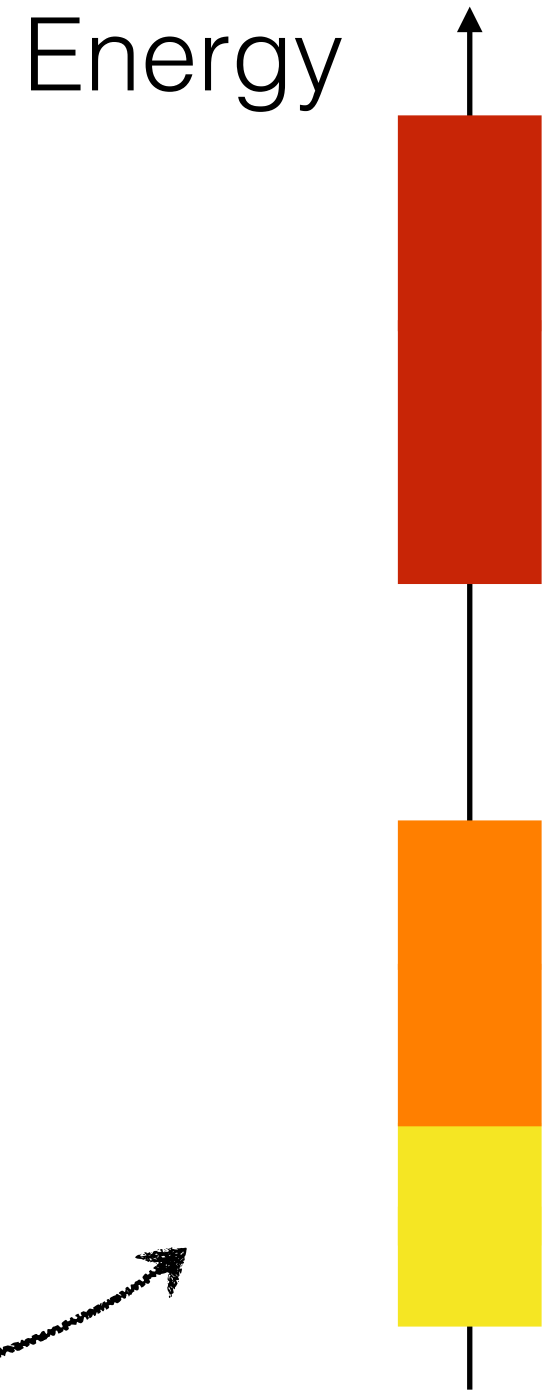

Discrete energy levels

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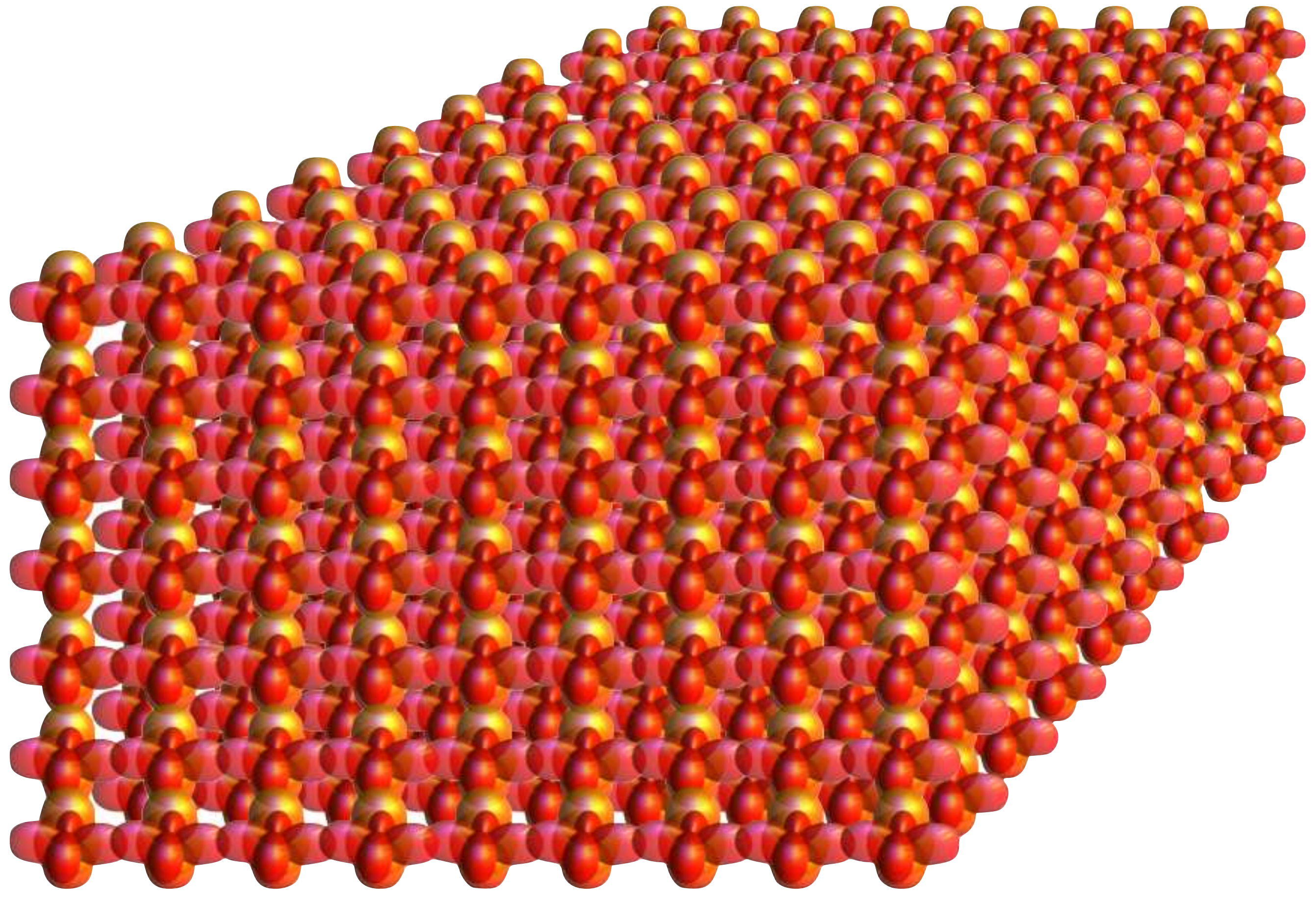
Continuous energy bands

Band Theory of Electrons in Solids

Electronic Orbitals



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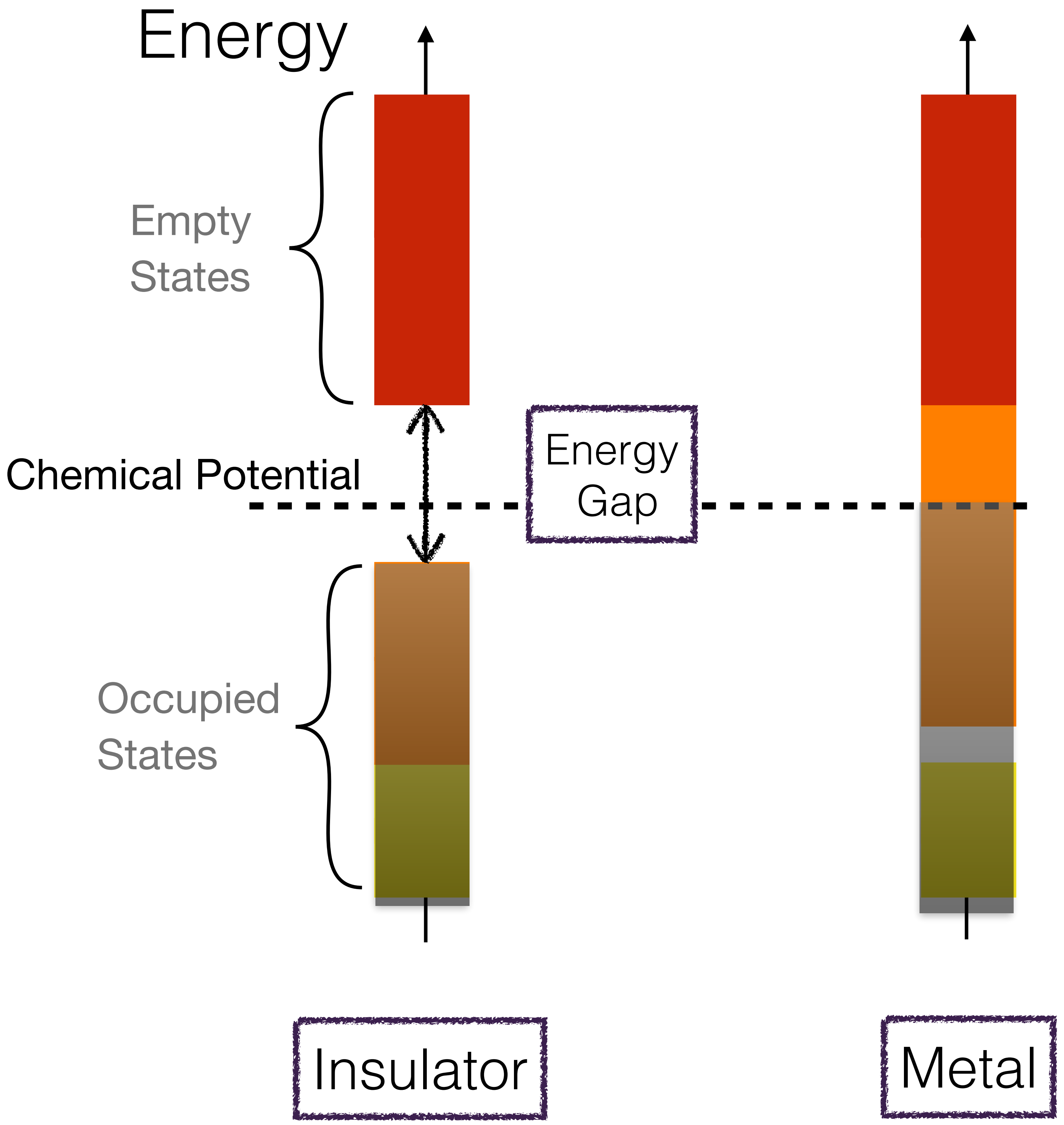
Continuous energy bands



Energy

Empty States

Chemical Potential

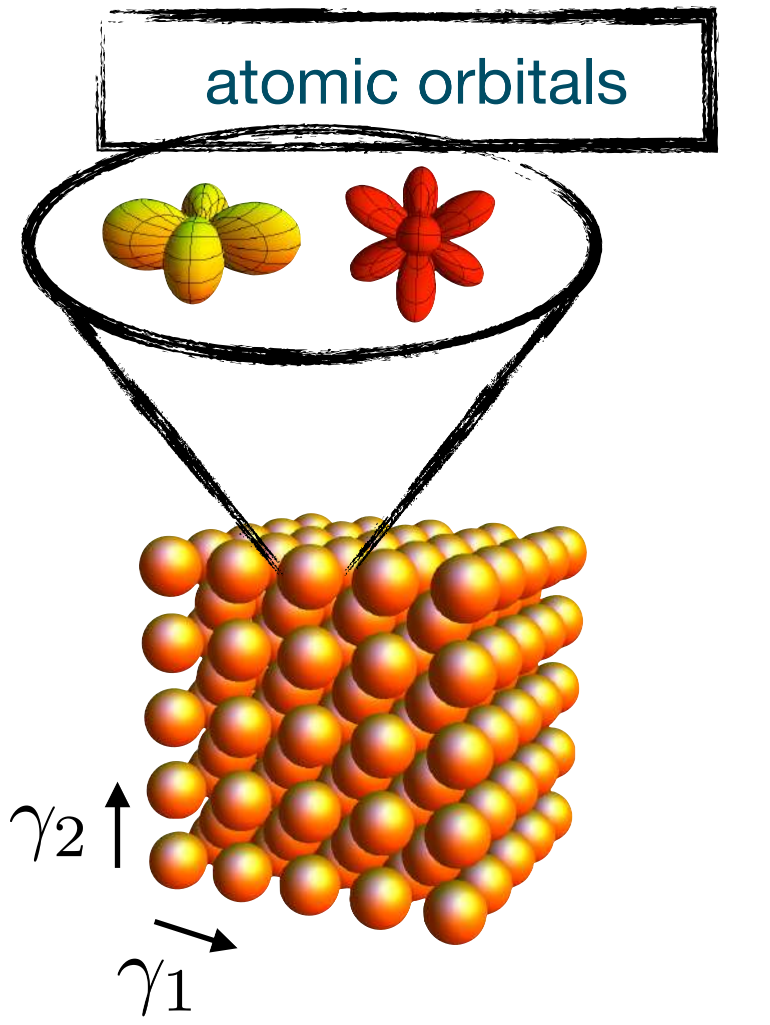
Energy Gap

Occupied States

Insulator

Metal

Band Theory of Solids

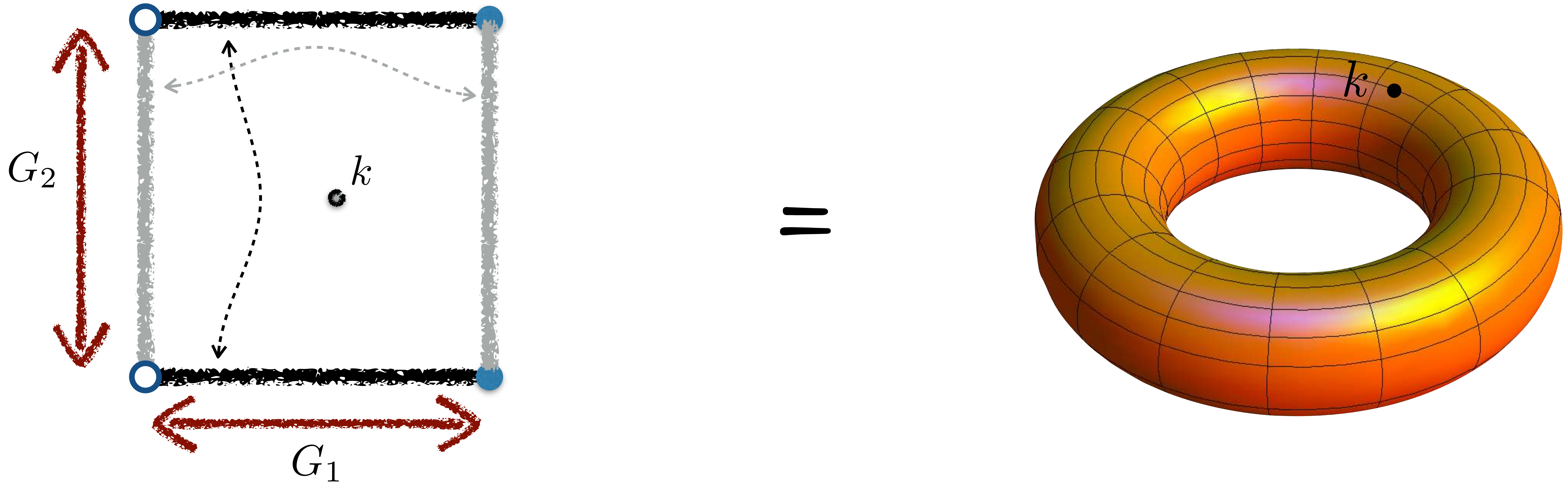


electrons on a lattice

- Band theory : single particle description of electronic states
  - Diagonalisation of a lattice Hamiltonian : $H_0|\psi\rangle = |\psi\rangle$
- Periodicity of lattice **(symmetry !)** :
  - Bravais lattice : translations T_γ that leave physical lattice invariant
  - if $|\psi\rangle$ eigenstate, then $T_\gamma|\psi\rangle$ also with same energy $T_\gamma\psi(x) = \psi(x-\gamma)$
  - diagonalize simultaneously H_0 and T_γ
- Bloch wavefunctions :
  - Eigenstates of translations : $T_\gamma\psi(x) = \psi(x-\gamma) = e^{ik.x}\psi(x)$
  - labelled by quasi-momentum k
  - k and $k+G$ label the same eigenvector $|\psi_k\rangle$ if

    $G.\gamma = n\ 2\pi,\ \ n \in \mathbb{Z}$ for all γ

Band Theory of Solids



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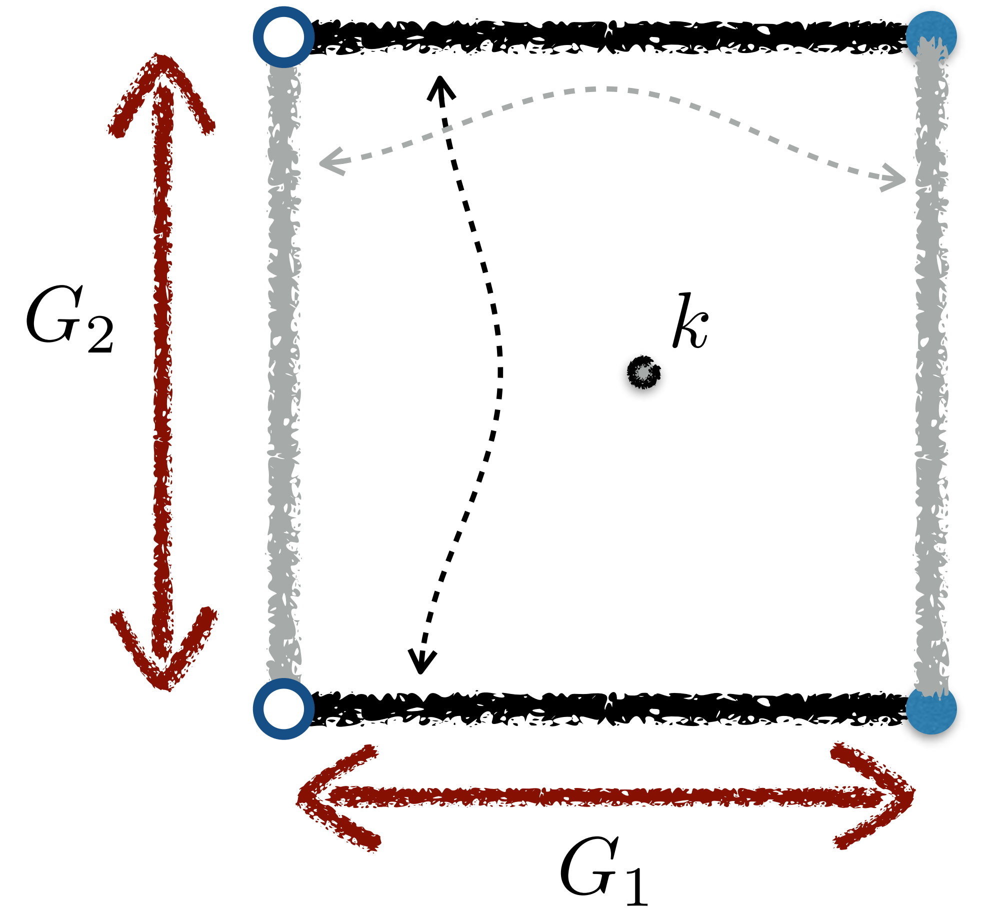
  - k lies in **Brillouin Zone**

Band Theory of Solids



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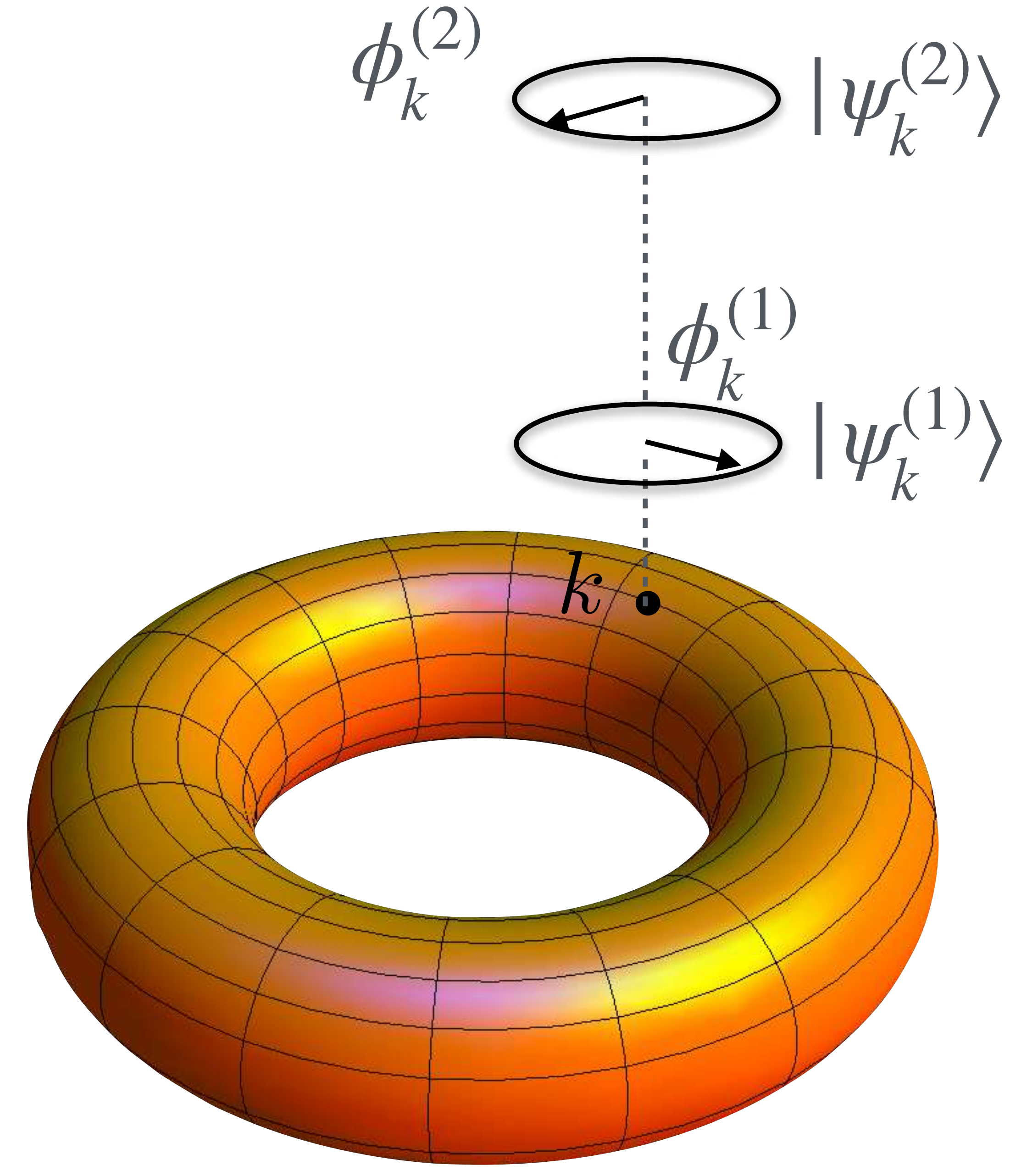
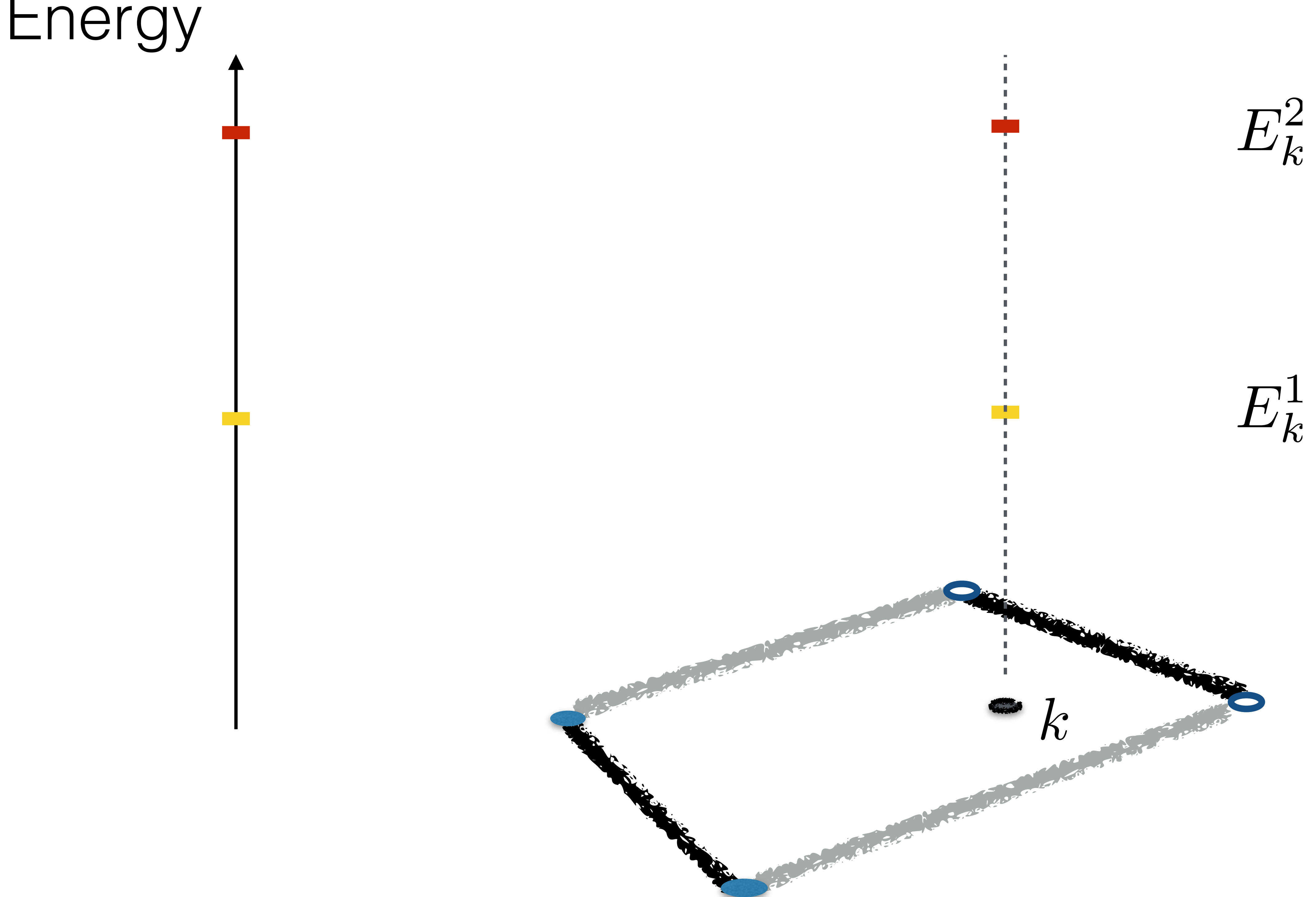
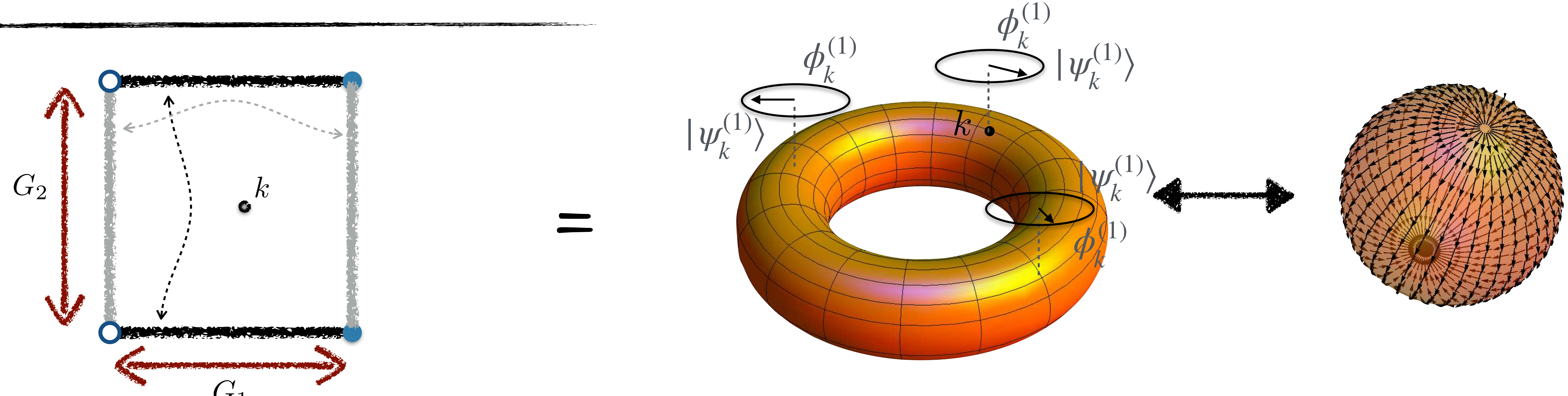
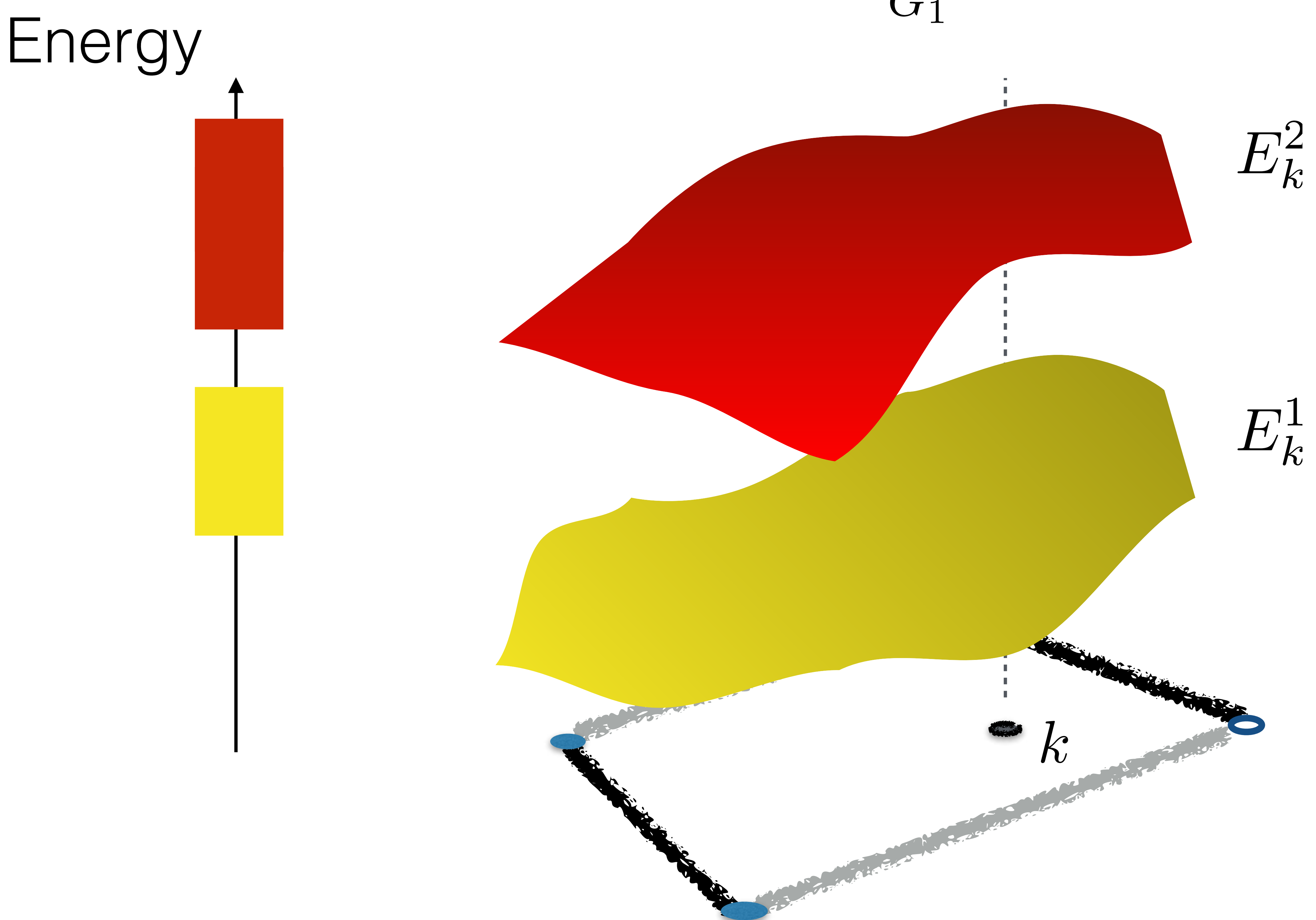




- Energy bands
  - Diagonalisation of Bloch Hamiltonian $H_k|\psi_k^{(\alpha)}\rangle = E_k^{(\alpha)}|\psi_k^{(\alpha)}\rangle$
  - Eigenvectors $|\psi_k^{(\alpha)}\rangle$ defined up to a phase $\phi_k^{(\alpha)}$

Band Theory of Solids





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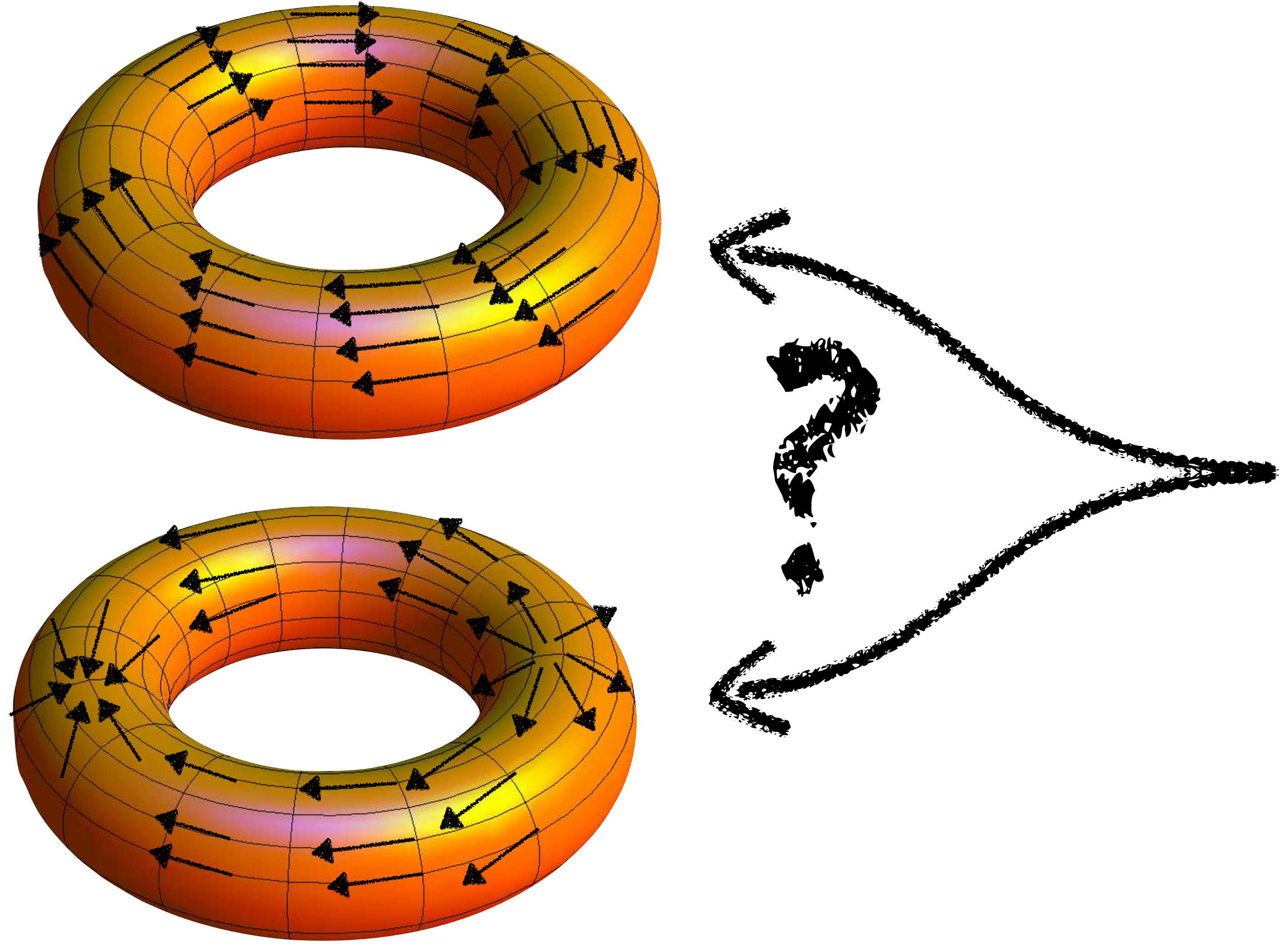
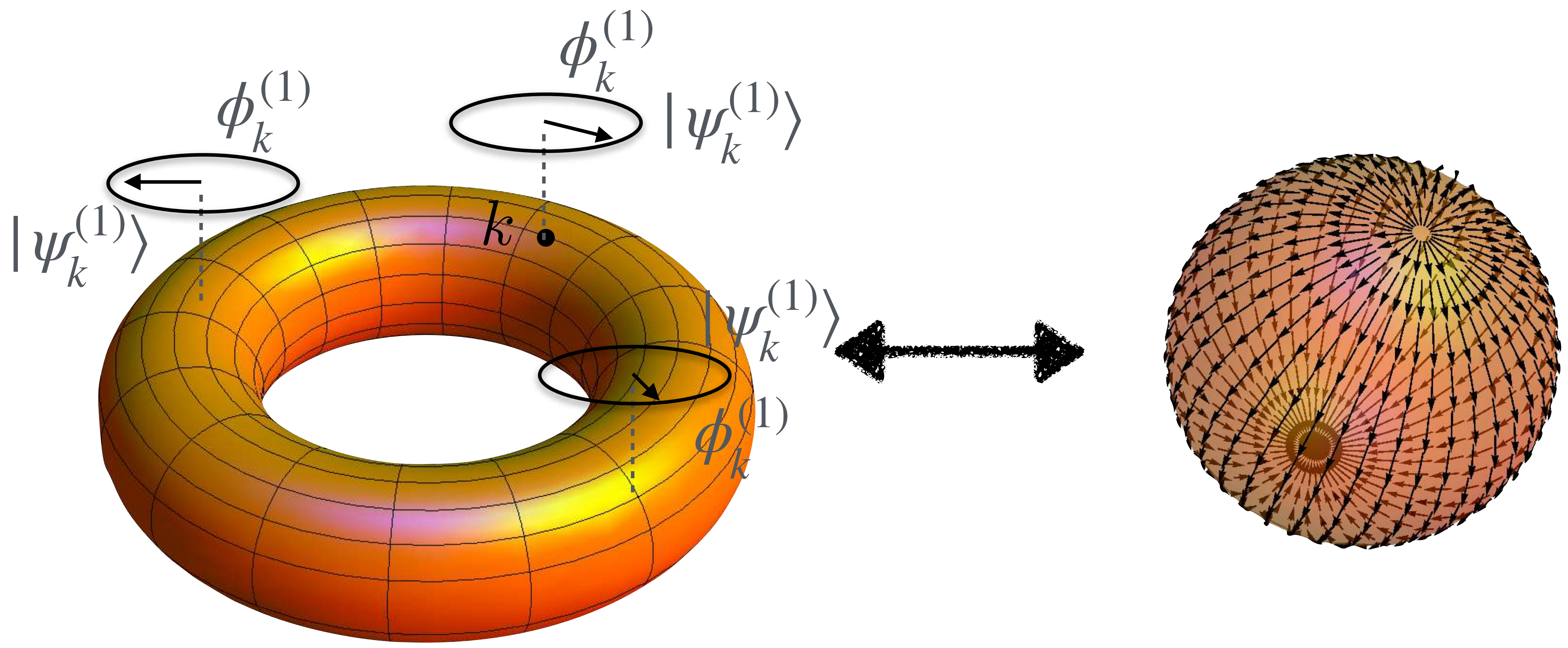
  - Each band: **Vector bundle** of $|\psi_k^{(\alpha)}\rangle$ over the Brillouin zone

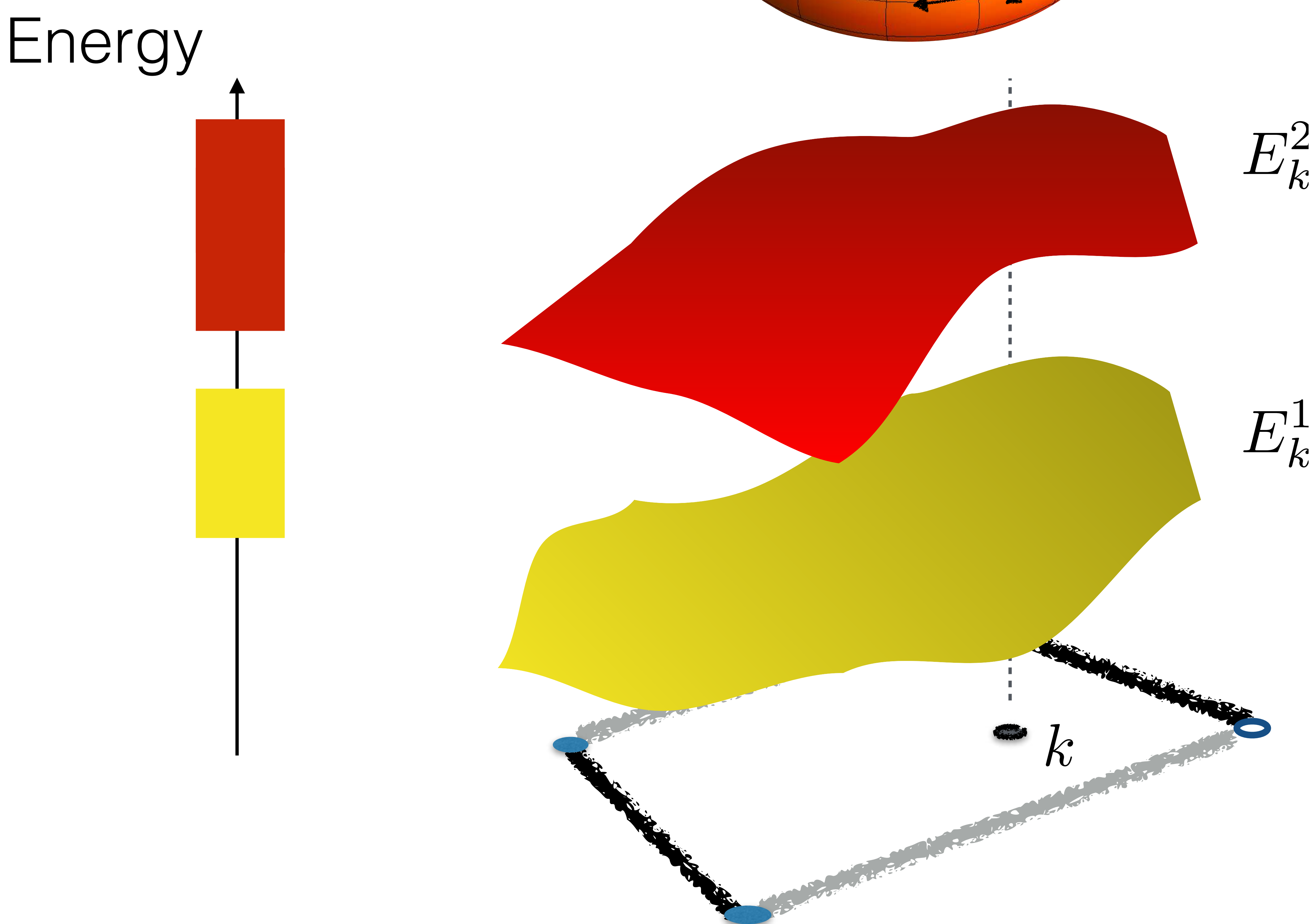
Band Theory of Solids

Is it always topologically trivial ?

(*i.e.* continuous vector field exists)







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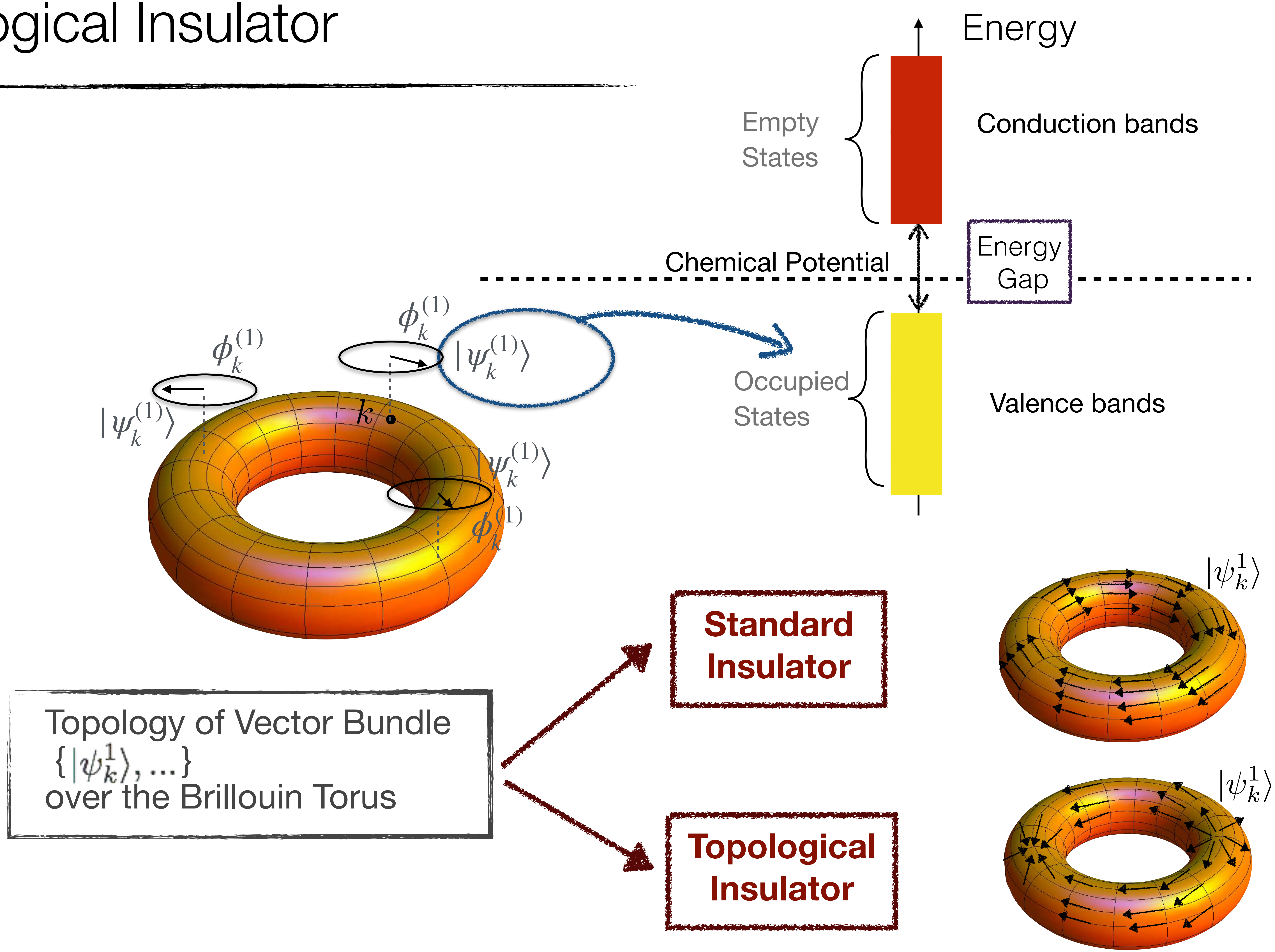
Topological Insulator



Energy

Empty States

Conduction bands

Chemical Potential

Energy Gap

Occupied States

Valence bands

Topology of Vector Bundle
$\{|\psi_k^1\rangle, \dots\}$
over the Brillouin Torus

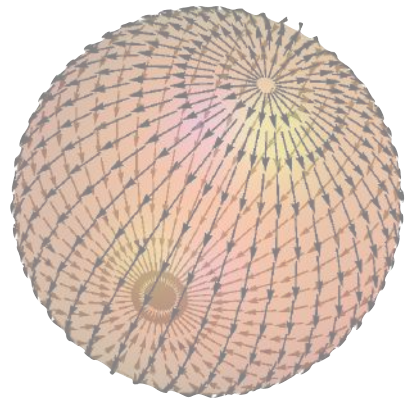
Standard Insulator

Topological Insulator

Outline

1. Notion of topological number

   Chern number for fields on a manifold



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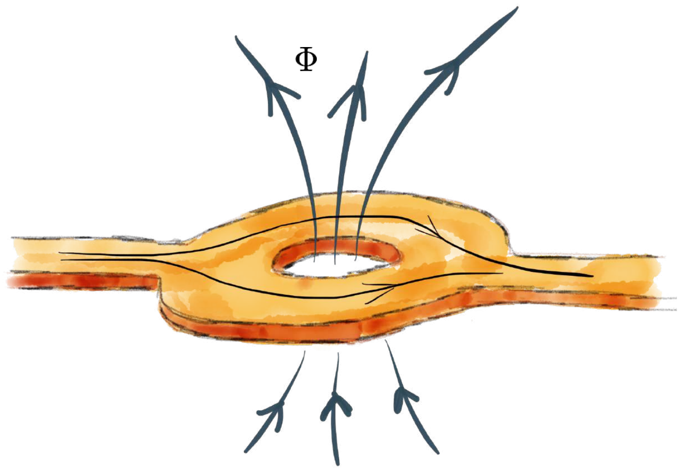
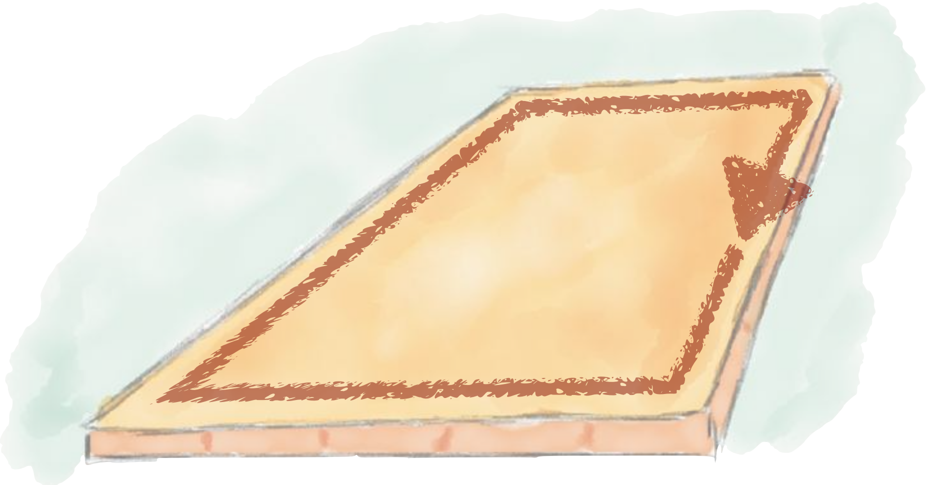
   Berry curvature, parallel transport, analogy with Aharonov-Bohm



4. Surface/Interface states

   Between two inequivalent topological band structures : interface states

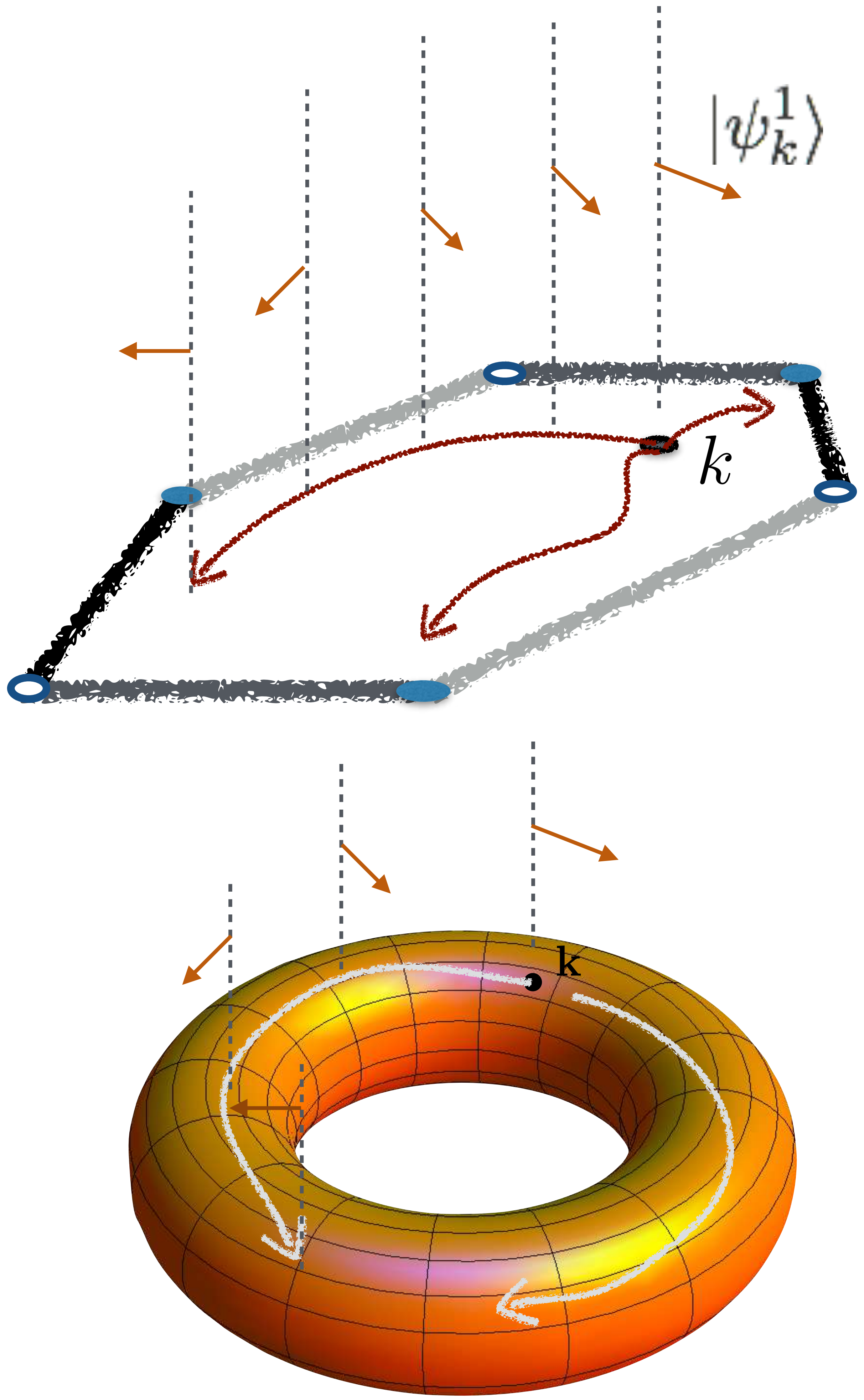


5. Topology and symmetries

   Time-reversal, chiral symmetry: topological insulators
   Crystalline symmetries: topological quantum chemistry

Continuous Vectors and Parallel Transport

ground state topology ↔ existence of non vanishing continuous eigenvector field

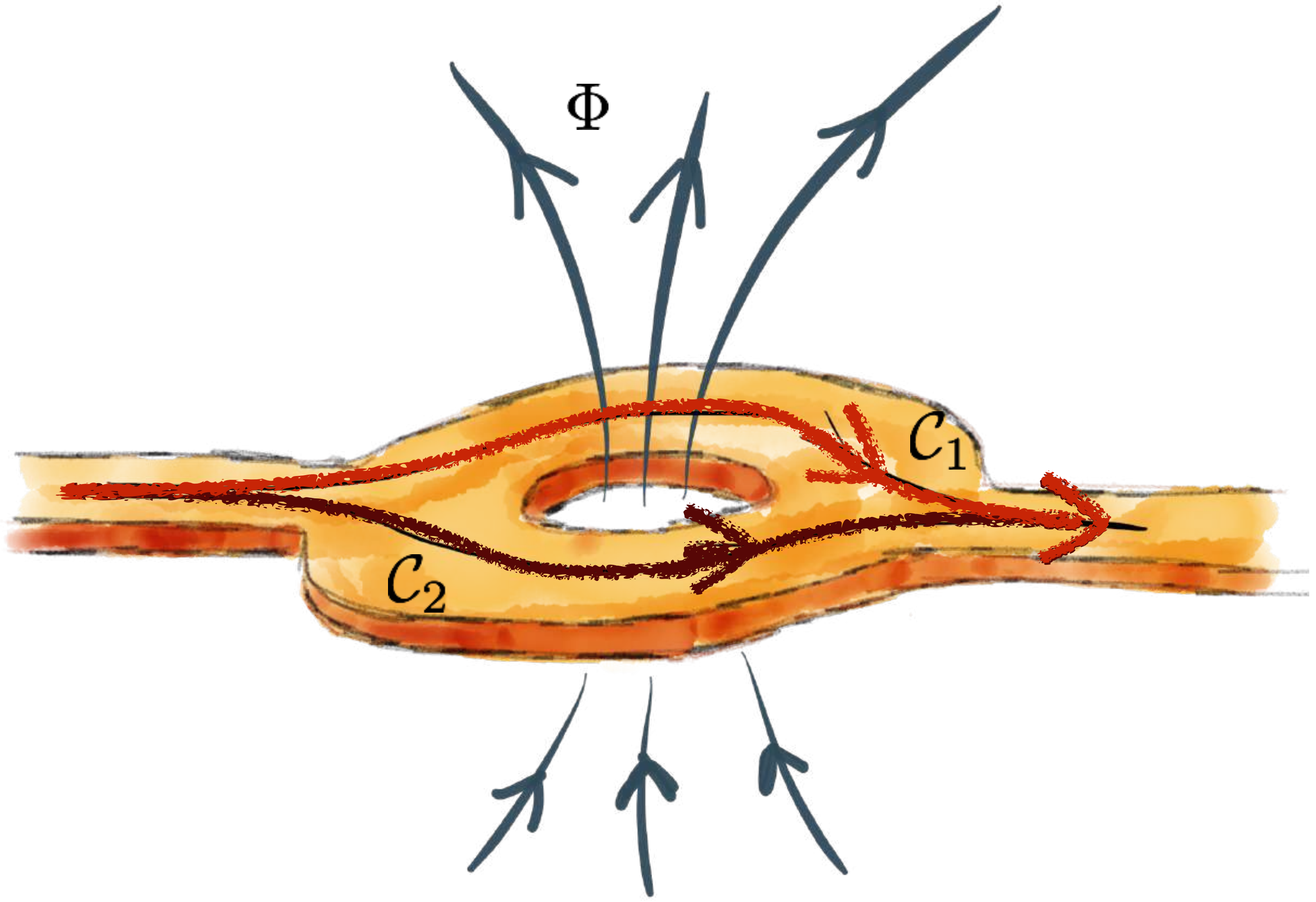


- Continuous eigenvectors not natural :
  - Phase of eigenvector often irrelevant
  - identify $|\psi_k^{(\alpha)}\rangle$ up to a (discontinuous) phase $\phi_k^{(\alpha)}$

➡ prescription to define continuous vectors

- Analogous situations (evolution of phase) :
  - Phase induced by a magnetic flux (Aharonov-Bohm)
  - Berry phase in adiabatic evolution of eigenstates

Aharonov-Bohm Phase



- Phase acquired due to the magnetic potential (gauge dependent) along a path

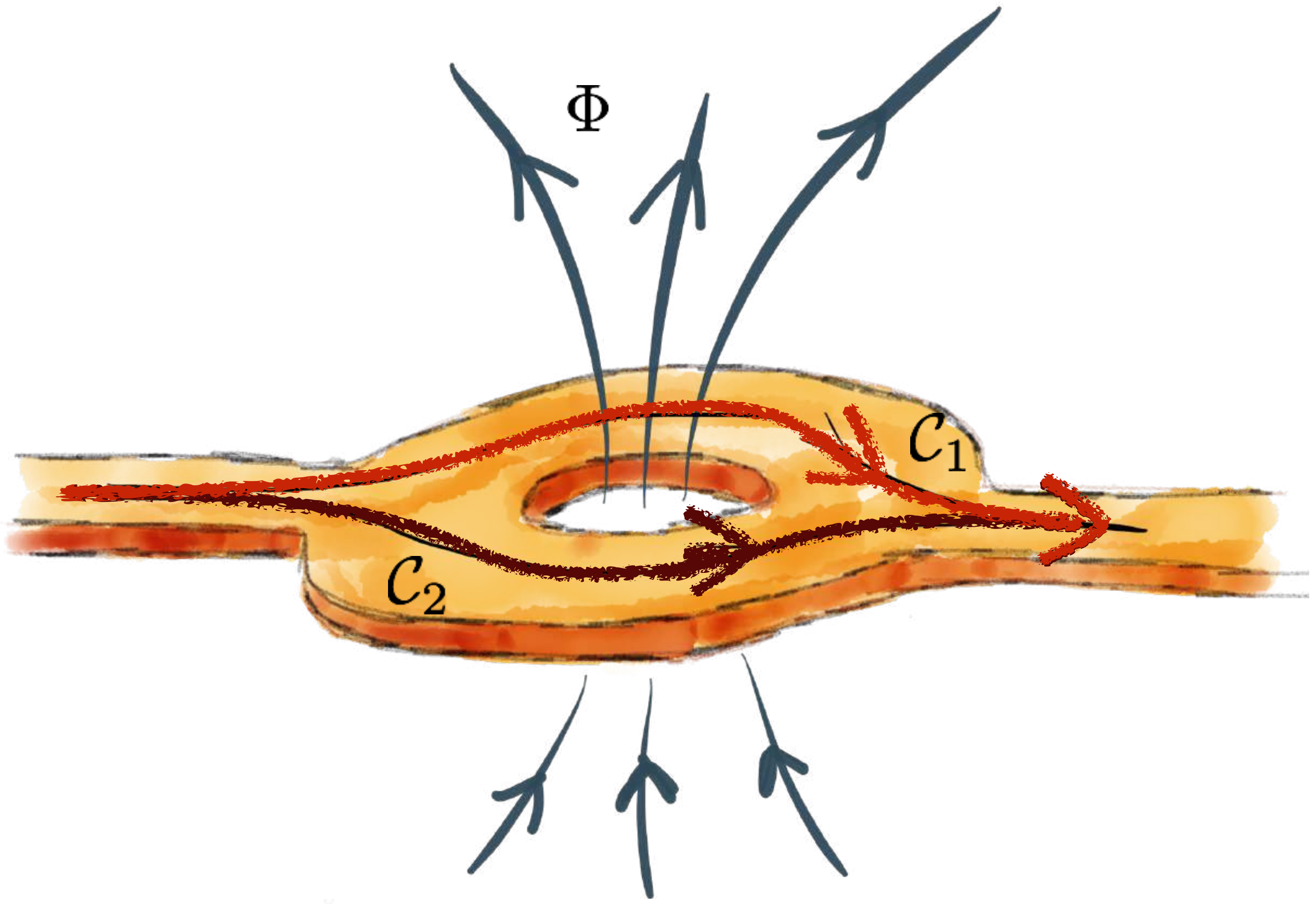
$$\theta_C = -\frac{e}{\hbar}\int_C A(x).dx$$

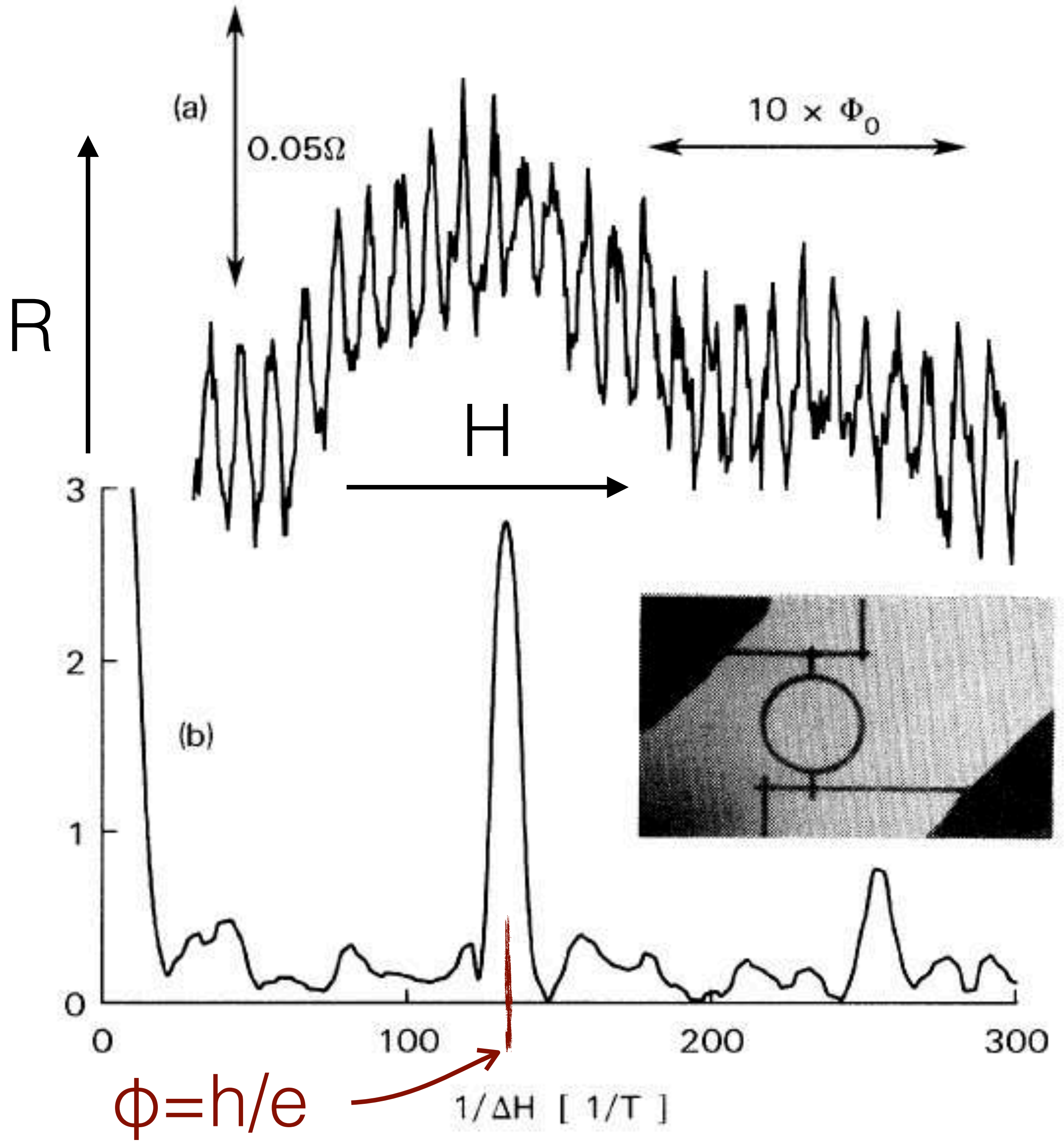
- Relative phase (gauge independent) between two paths

$$\theta_1 - \theta_2 = \frac{e}{\hbar}\oint_{\mathcal{C}_1 U \mathcal{C}_2} A(x).dl$$

$$= 2\pi\frac{\phi}{\phi_0} \qquad \phi_0 = h/e$$

Aharonov-Bohm Phase





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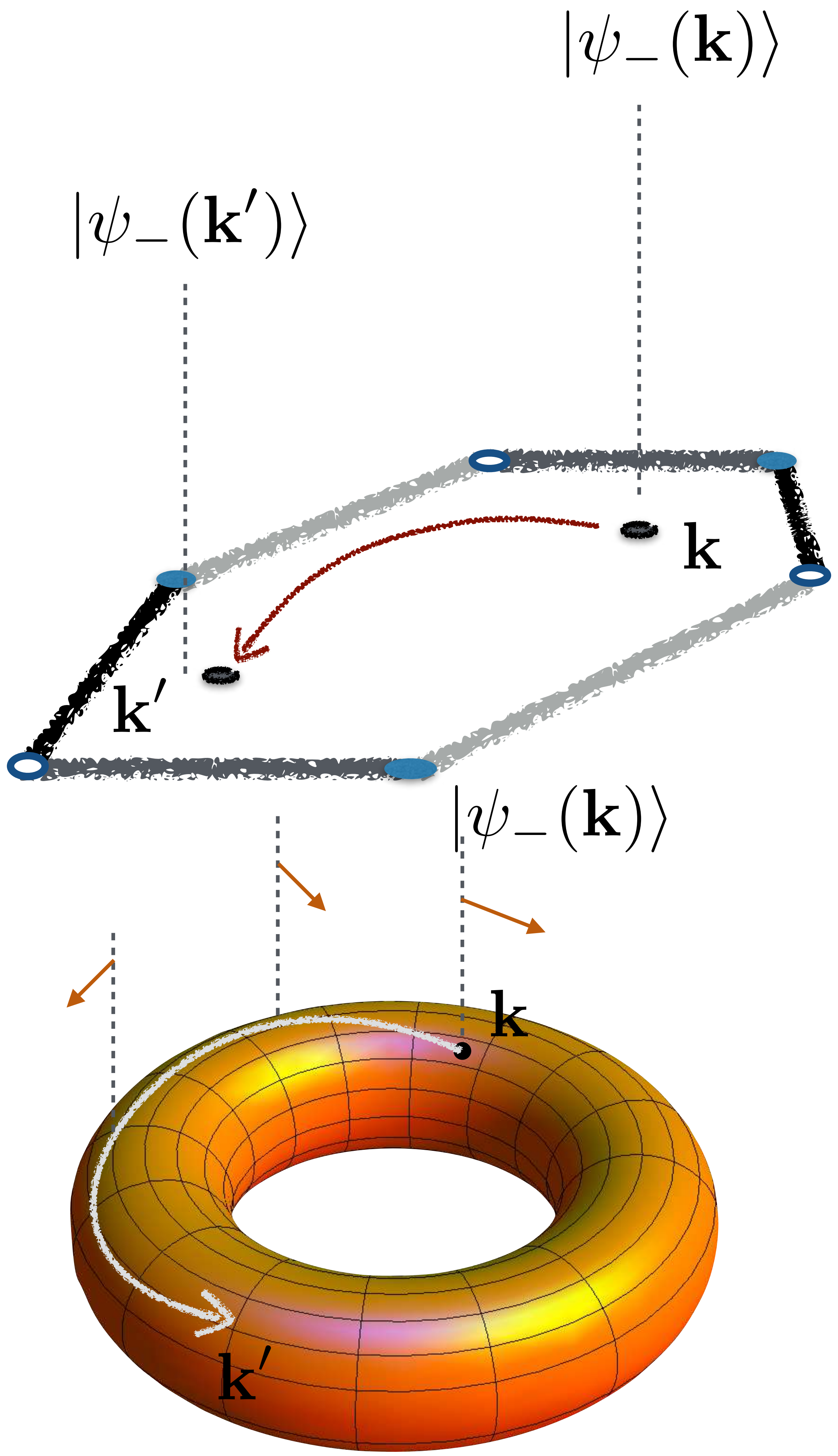
- Interference induce a modulation of the current $I(\phi)$ through a gold ring (diameter of the loop is 784nm) at low temperature T = 0.01K

R. A. Webb *et al.*, PRL (1985)

Parallel Transport of States and Berry Phase

Thouless *et al.*, (1982)
Berry (1984)
see also Fruchart *et al.*, (2014)



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  - Phase of eigenvector often irrelevant
  - identify $|\psi_-(\mathbf{k})\rangle$ up to a (discontinuous) phase
  - ➡ prescription to define continuous vectors
- **Berry Connexion** form (analogous to electr. potential)

$$|\psi_-(\mathbf{k})\rangle = e^{i\mathbf{k}.\hat{r}}|u_-(\mathbf{k})\rangle$$

$$\mathbf{A}_-(\mathbf{k}) = \frac{1}{i}\langle u_-(\mathbf{k})|\nabla_{\mathbf{k}}|u_-(\mathbf{k})\rangle$$

- **Berry phase** along a path $\mathcal{C}_1$in Brillouin zone :

$$\theta_{\text{Berry}} = \int_{\mathcal{C}_1} \mathbf{A}_-(\mathbf{k})$$

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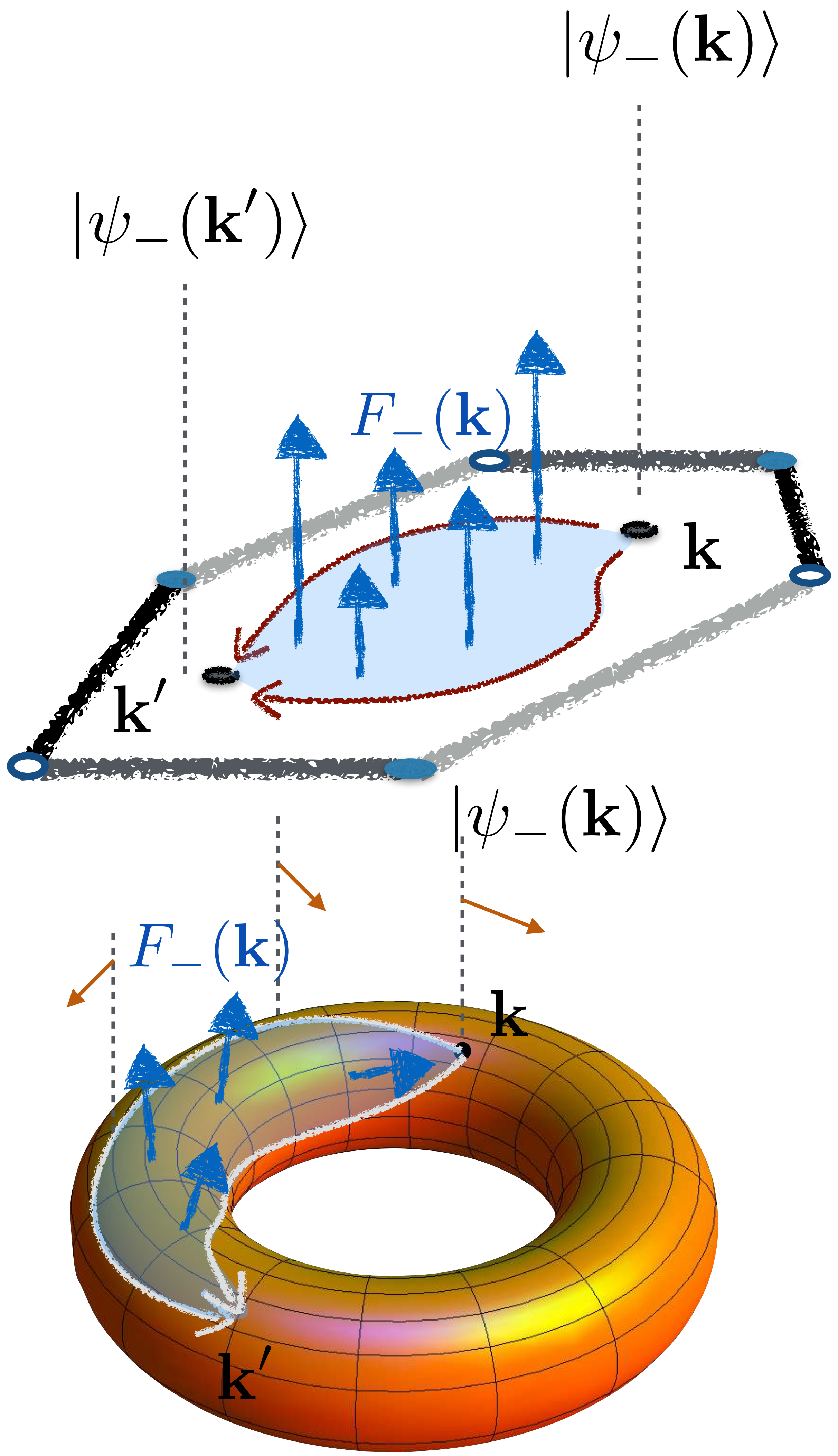

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- **Berry curvature** (analogous to Flux) :

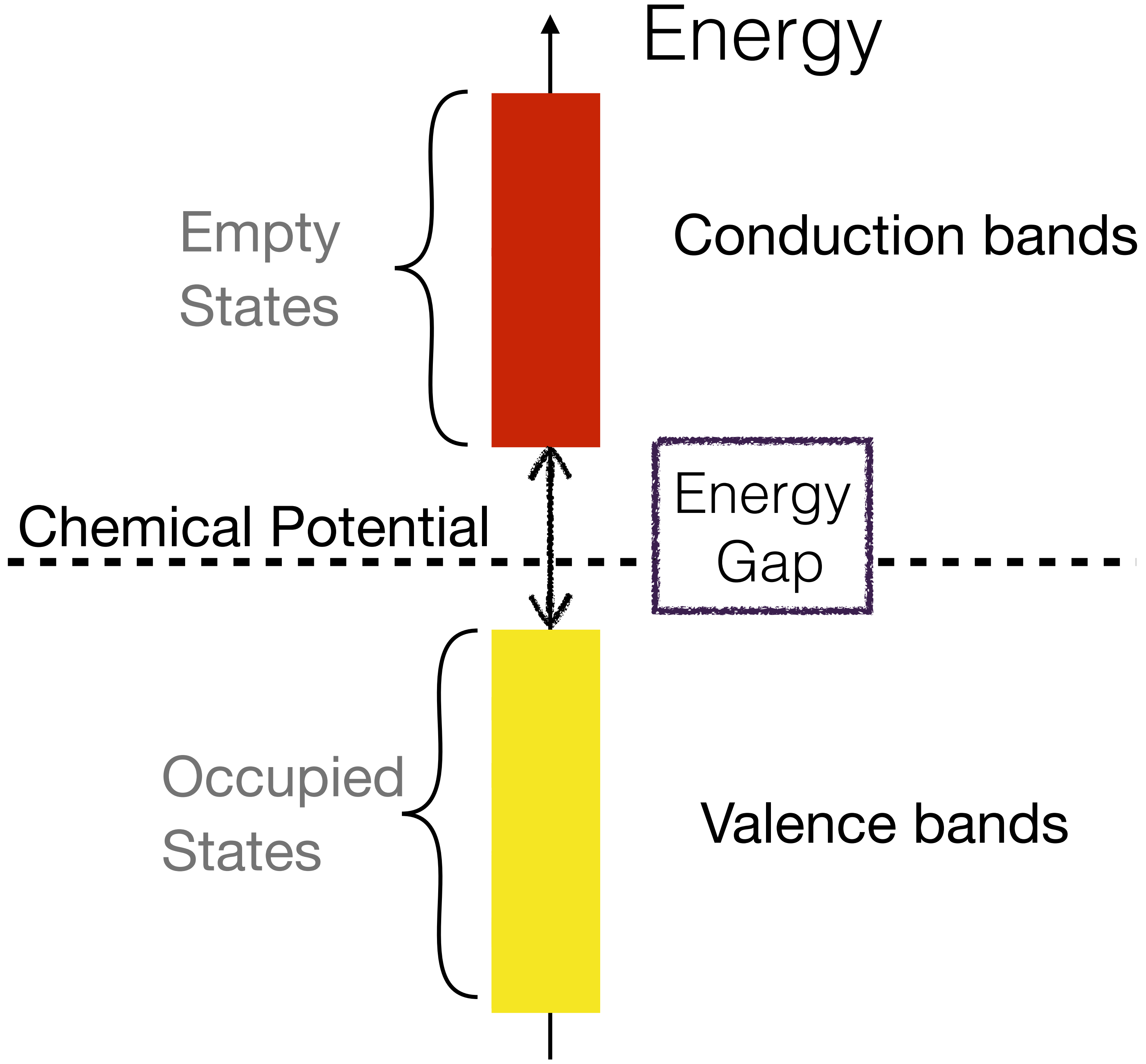
$$F_-(\mathbf{k}) = \boldsymbol{\nabla}_{\mathbf{k}} \times \mathbf{A}_-(\mathbf{k})$$

  - Relative phase between two paths :

$$\theta_{\mathcal{C}_1} - \theta_{\mathcal{C}_2} = \int_{\mathcal{C}_1} A_-(\mathbf{k}) - \int_{\mathcal{C}_2} A_-(\mathbf{k}) = \int_{\mathcal{S}} F_-(\mathbf{k})$$

Topological index for bands

Thouless *et al.*, (1982)
Berry (1984)
see also Fruchart *et al.*, (2014)



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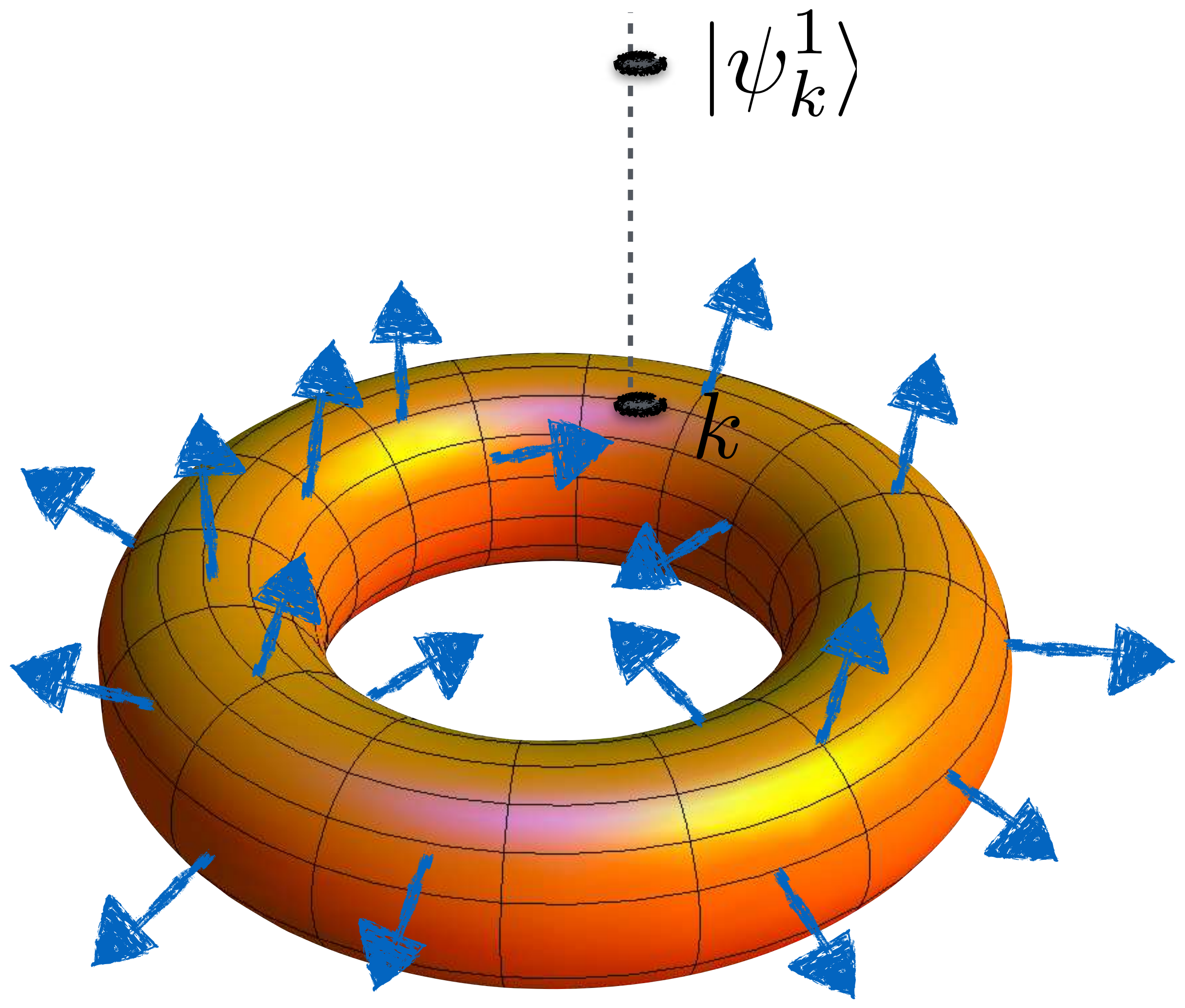
- **Berry curvature** (analogous to Flux) :

$$F_k = \nabla_k \times A_k$$

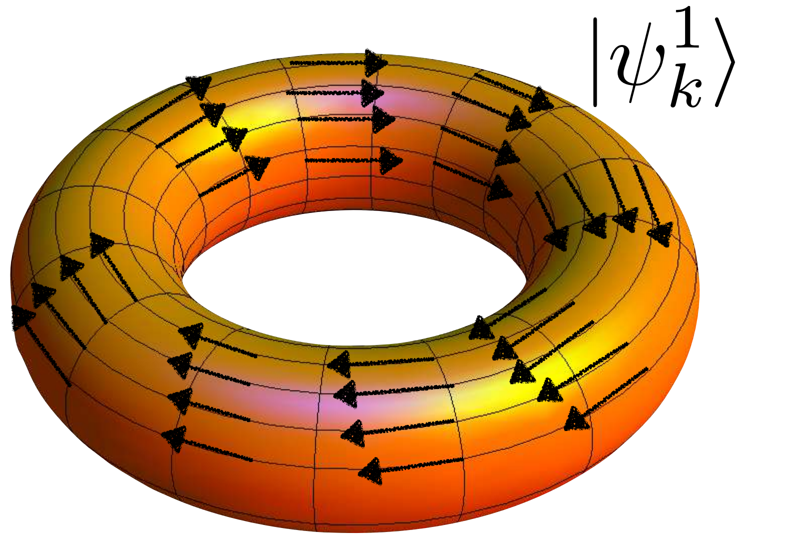
- **Topological number** : Chern number

$$C_1 = \frac{1}{2\pi}\int_{\mathrm{BZ}} F$$

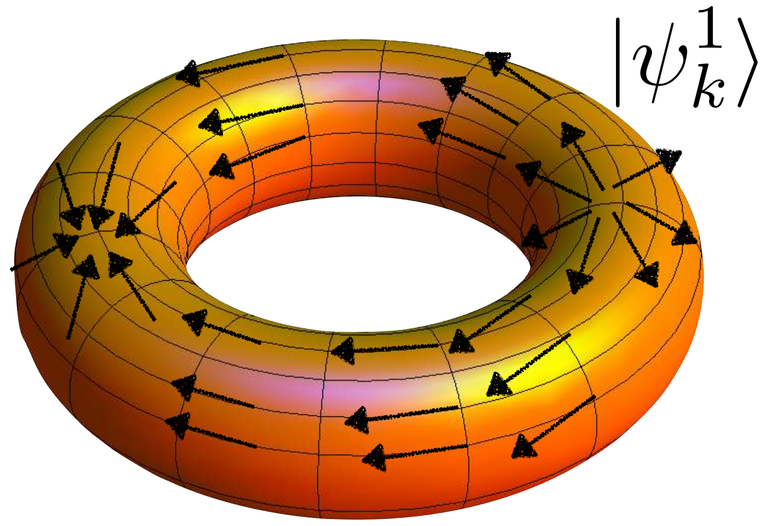
cf Gauss-Bonnet theorem



Trivial band (C = 0)



Topological band (C ≠ 0)

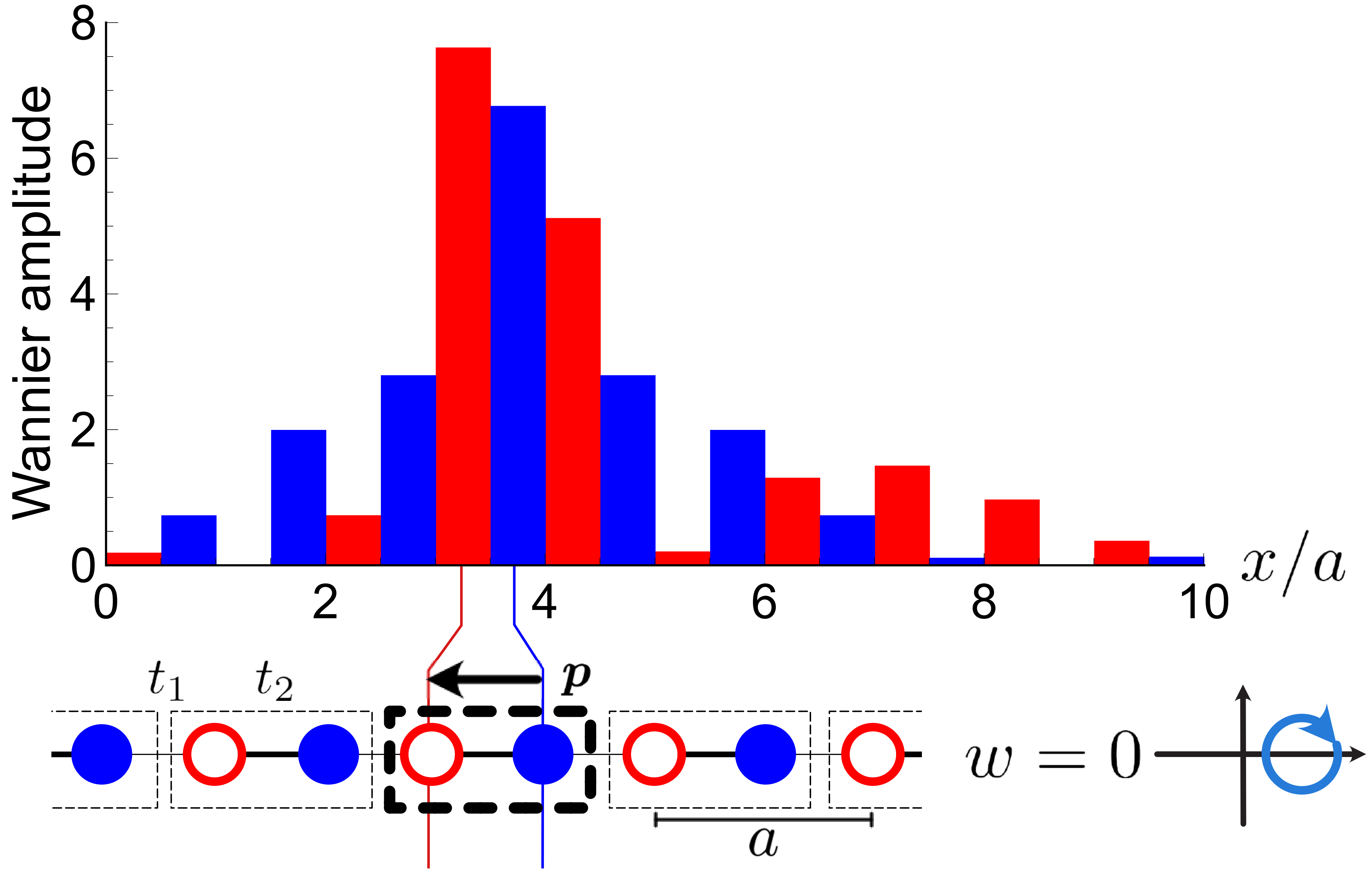


Topological band in real space

Bradlyn *et al.*, (2017)
Po *et al.*, (2017)

- Wannier function
  - Inverse FT $|w_{\mathbf{R}}^{(\alpha)}\rangle = \frac{V_{\text{cell}}}{(2\pi)^d}\int_{\text{BZ}} e^{-i\mathbf{k}.\mathbf{R}}|\psi_{\mathbf{k}}^{(\alpha)}\rangle d^d\mathbf{k}$
  - $w_{\mathbf{R}}^{(\alpha)}(\mathbf{r})$ decays as a function of $\mathbf{r}-\mathbf{R}$
  - center of charge of a Wannier function $\mathbf{r}^{(\alpha)} = \langle w_{\mathbf{R}}^{(\alpha)}|\hat{\mathbf{r}}|w_{\mathbf{R}}^{(\alpha)}\rangle$

- Topological band : obstruction to exponentially-localize Wannier function



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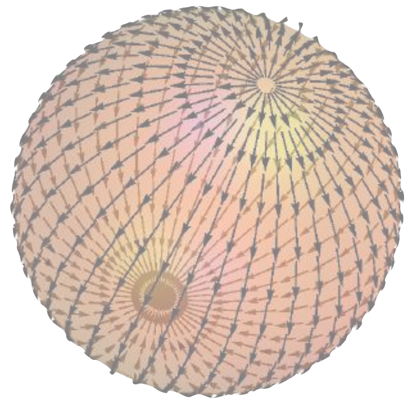

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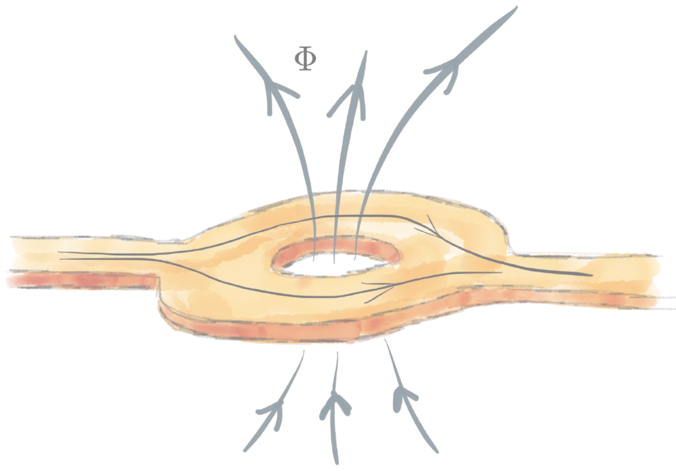
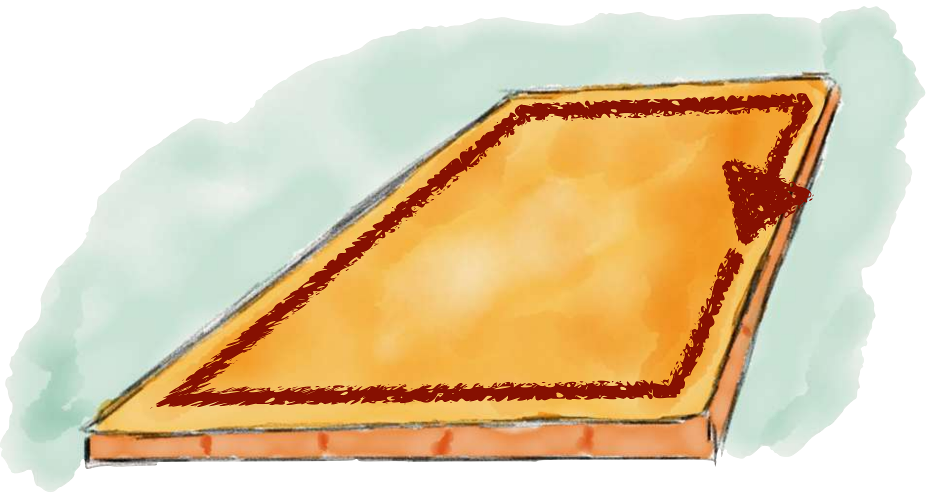


4. Surface/Interface states

   Between two inequivalent topological band structures :
   interface states



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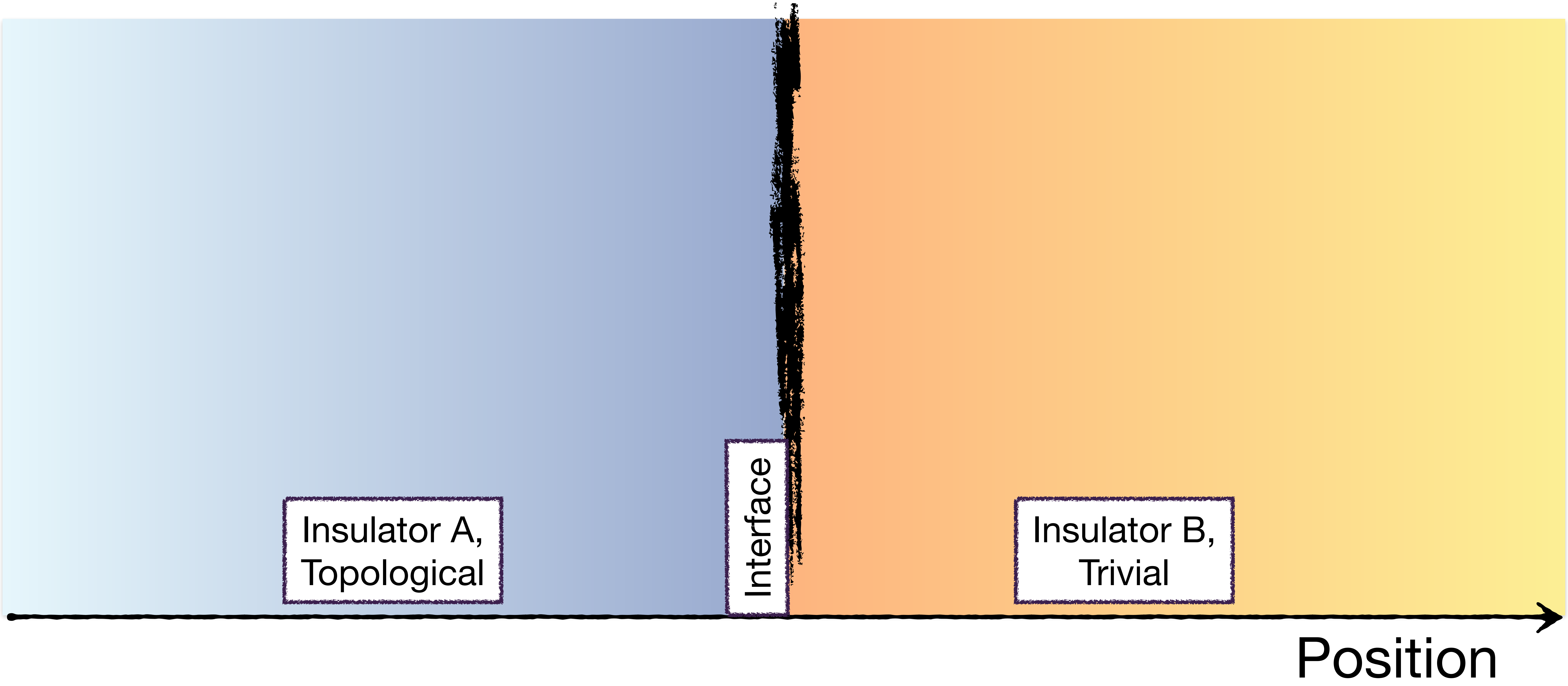
   Time-reversal, chiral symmetry: topological insulators
   Crystalline symmetries: topological quantum chemistry

Interface between Insulators



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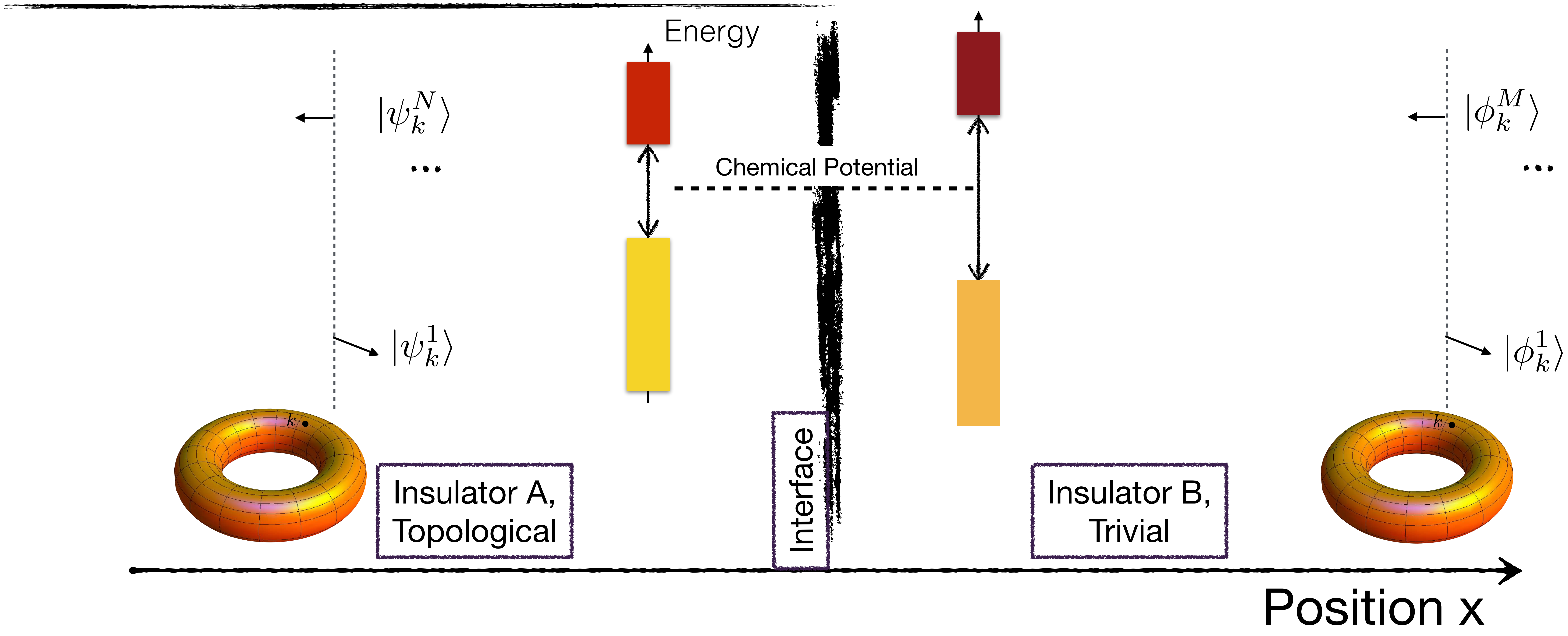
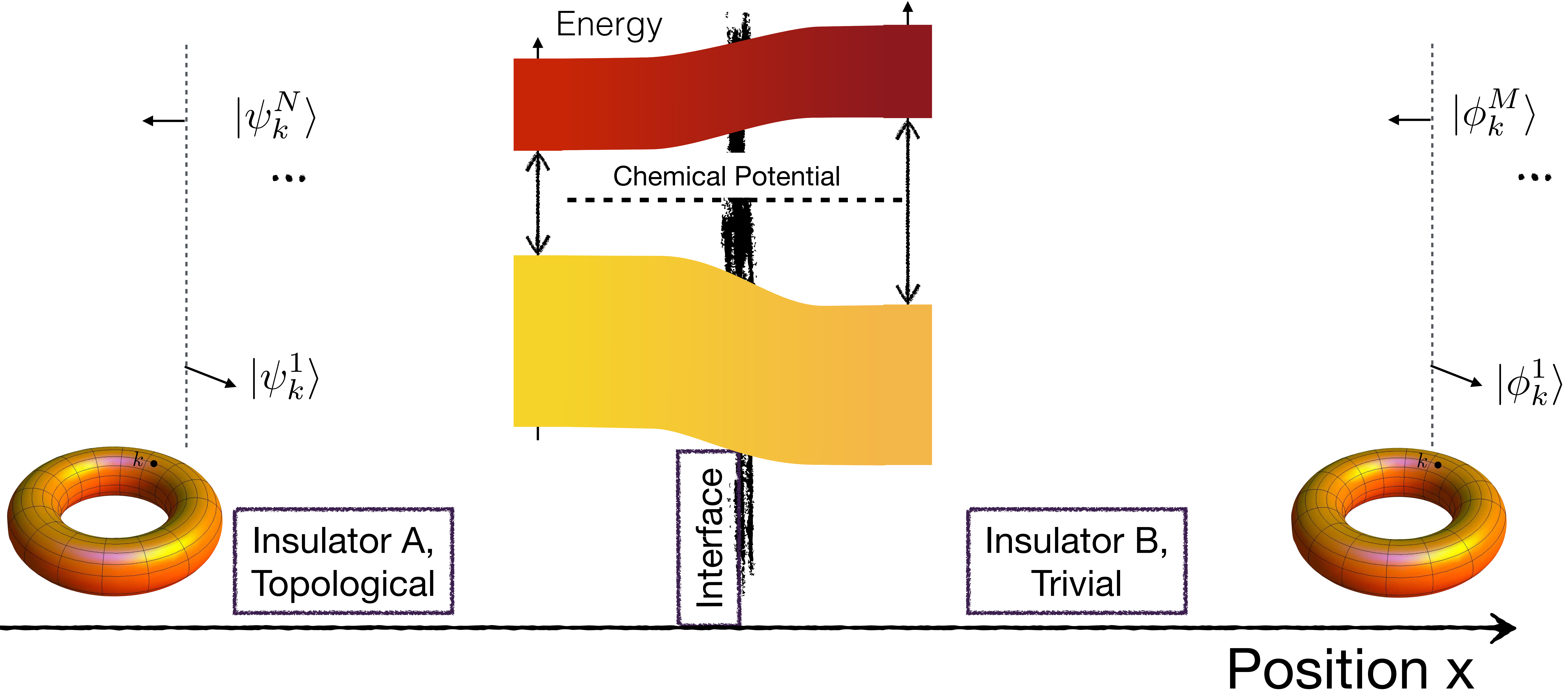


Description of the interface :

- consider eigenstates $\{|\psi_k^\alpha\rangle\}$ and $\{|\phi_k^\beta\rangle\}$of materials on both sides
- extrapolate (position dependent Hamiltonian H(x))

Interface between Insulators



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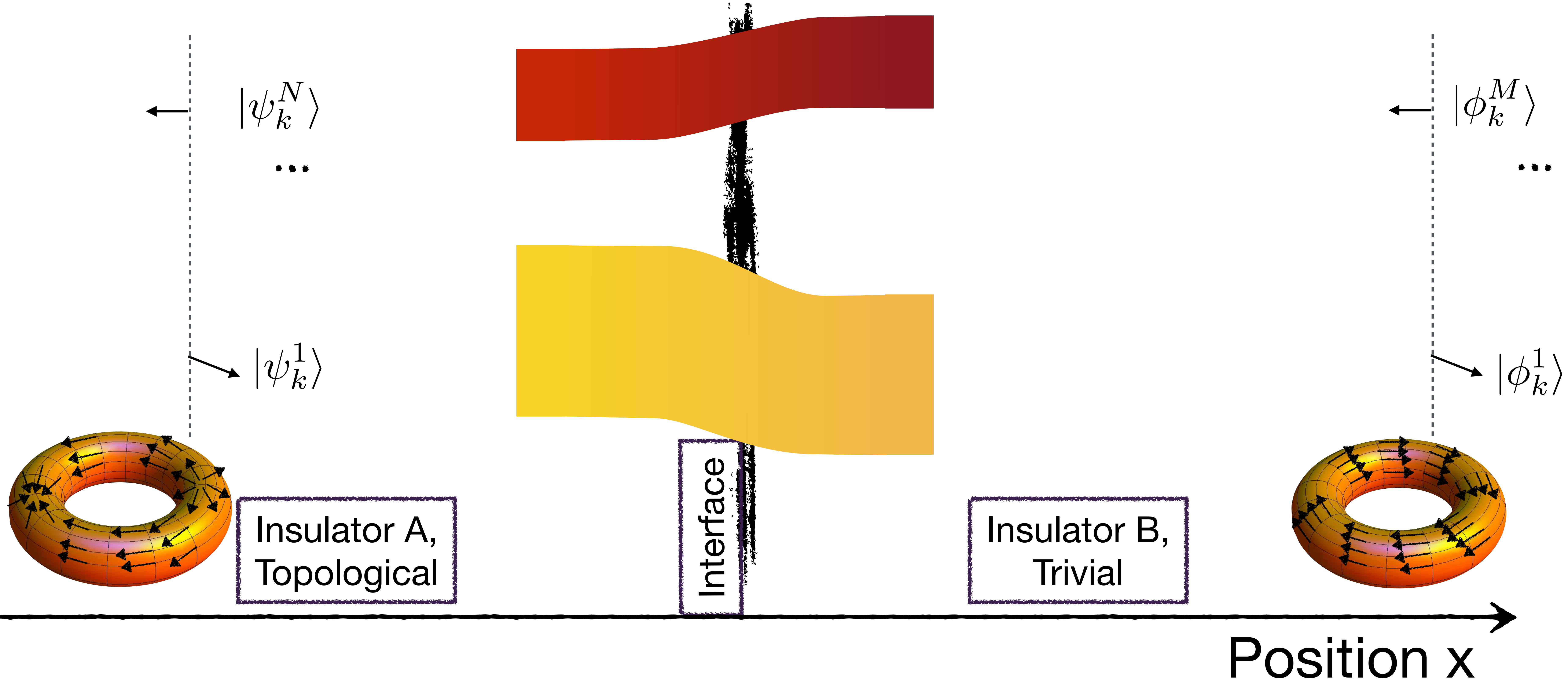

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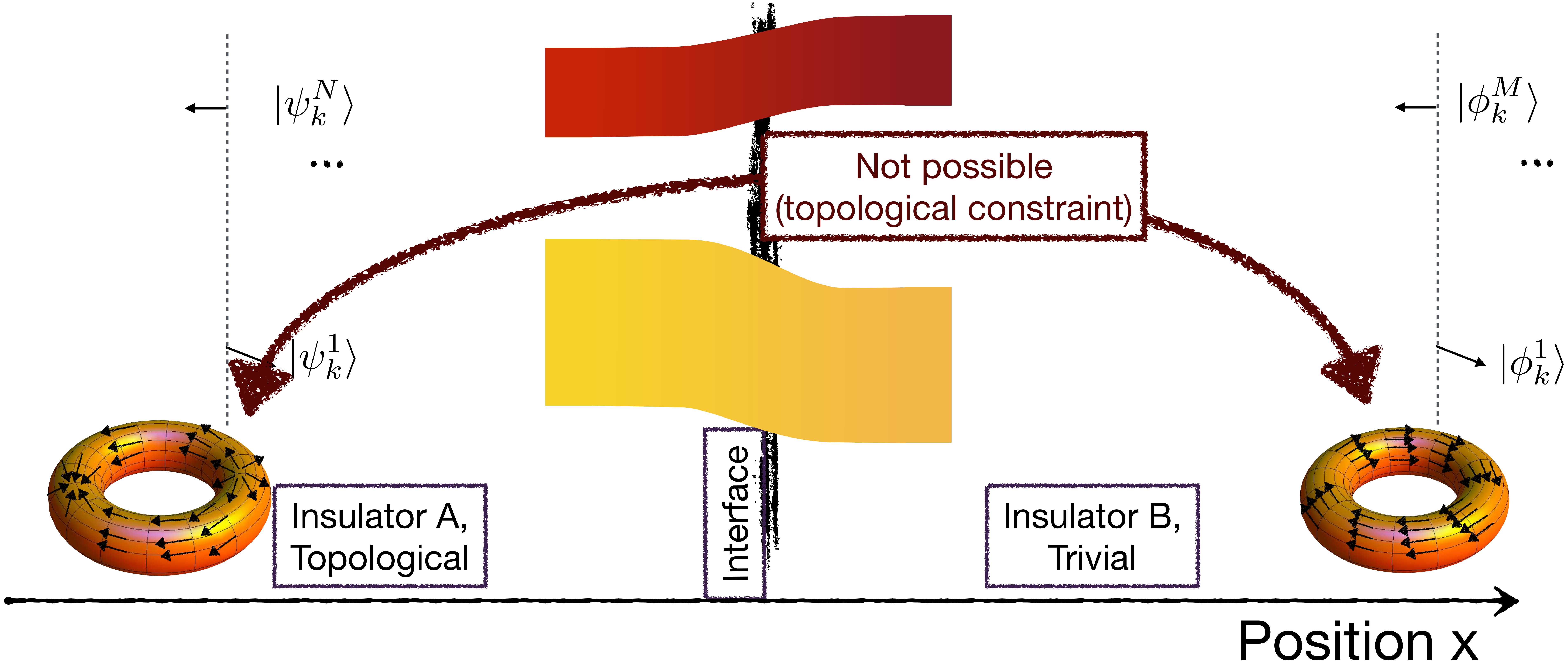

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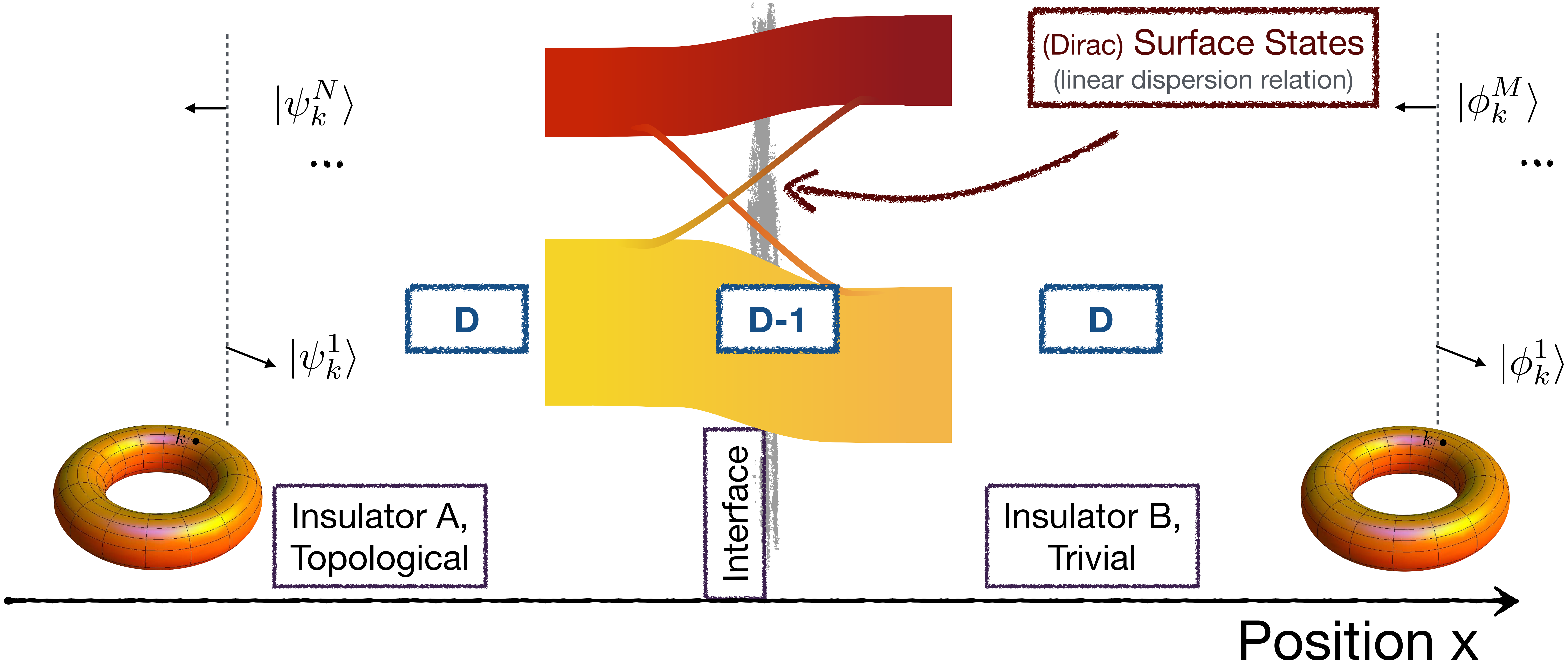

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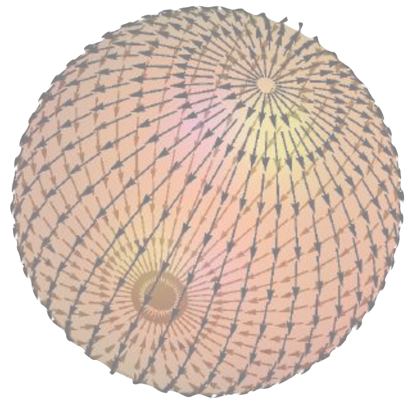

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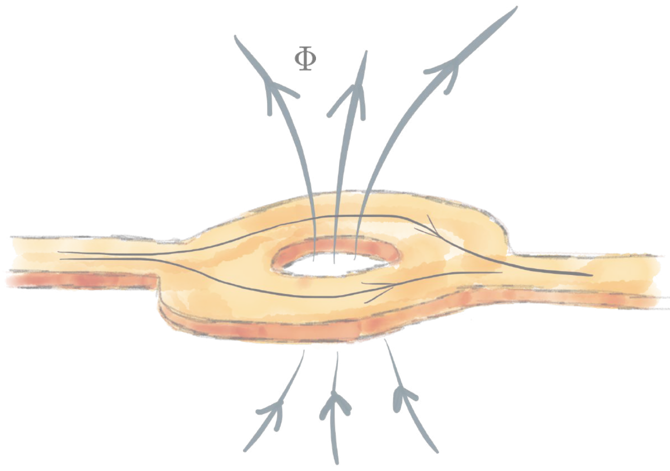

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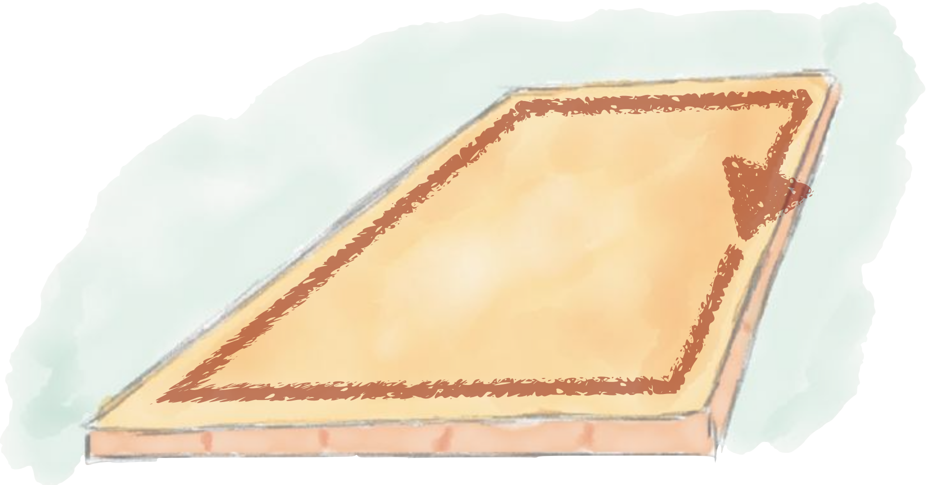

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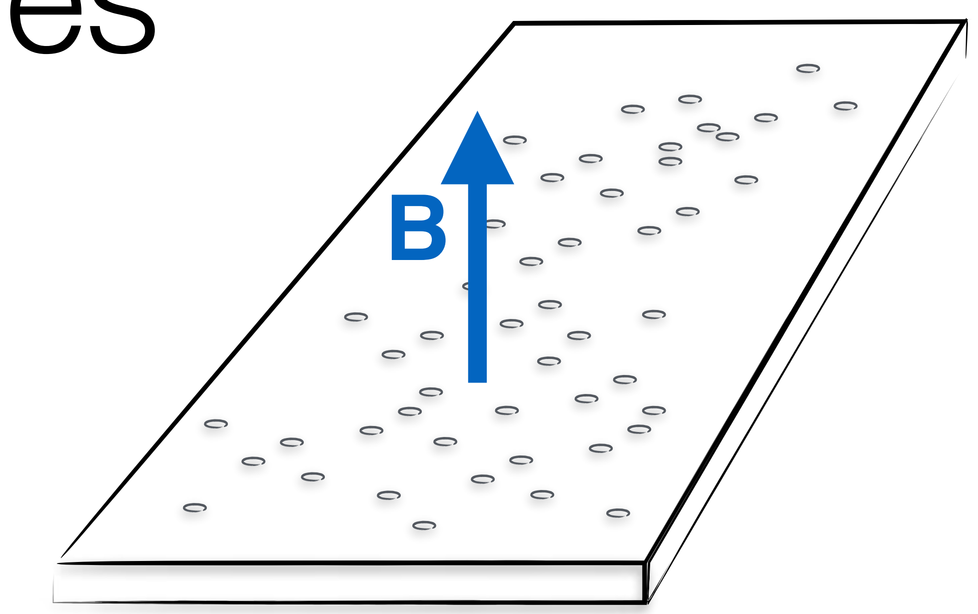
   Time-reversal, chiral symmetry: topological insulators
   Crystalline symmetries: topological quantum chemistry

Topological Property in Insulators and Symmetries

- Chern Topological Index (Quantum Hall Effect) :
  - breaking of time-reversal (e.g. **Magnetic Field**)
  - no Spin (a single Chern number per band)
  - **only d=2**



2DEG (Heterojunction GaAs/AlGaAs)

Thouless, Kohmoto, Nightingale and den Nijs (1982)
Niu, Thouless, and Wu (1985)
Haldane (1985)

- Z_2 Kane-Mele Topological Index :
  - spin dependent bands (S=½)
  - time reversal symmetry constraint, no Magnetic Field
  - induced by **strong spin-orbit coupling** (material property)
  - occurs in **d=2 and d=3**

➡New property of band structures !

- Topological superconductors

Kane and Mele (2005)
Bernevig, Hughes, and Zhang (2006)
Fu, Kane et Mele (2007)
Moore and Balents (2007)
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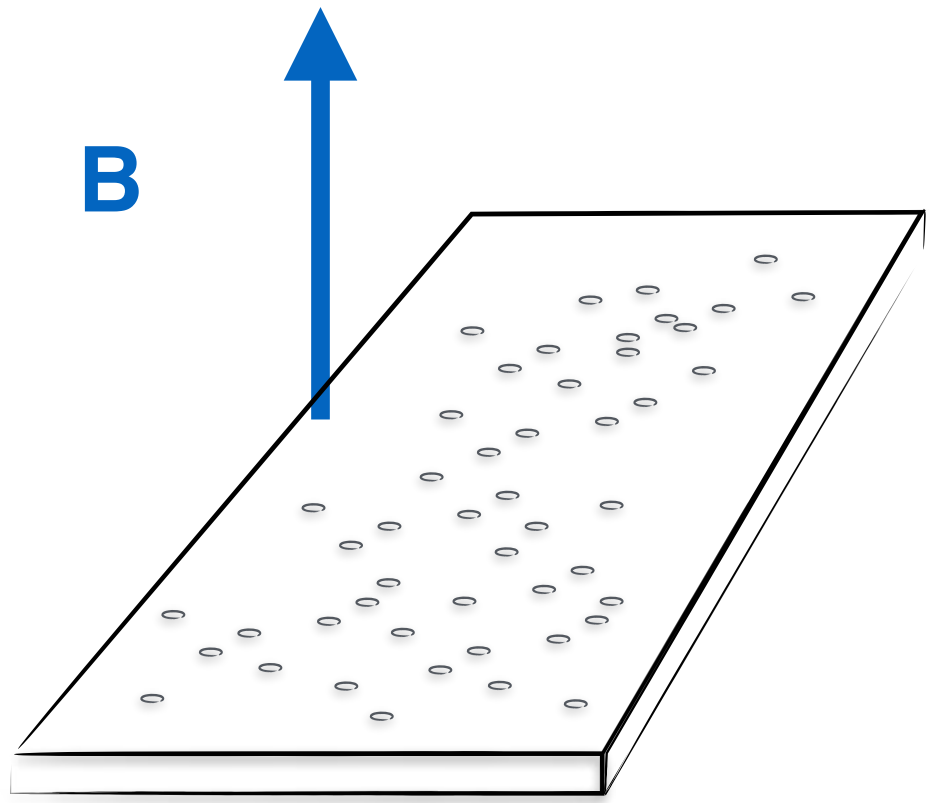
Fu and Kane (2007)

review : Fruchart *et al.* *CRAS* (2013)

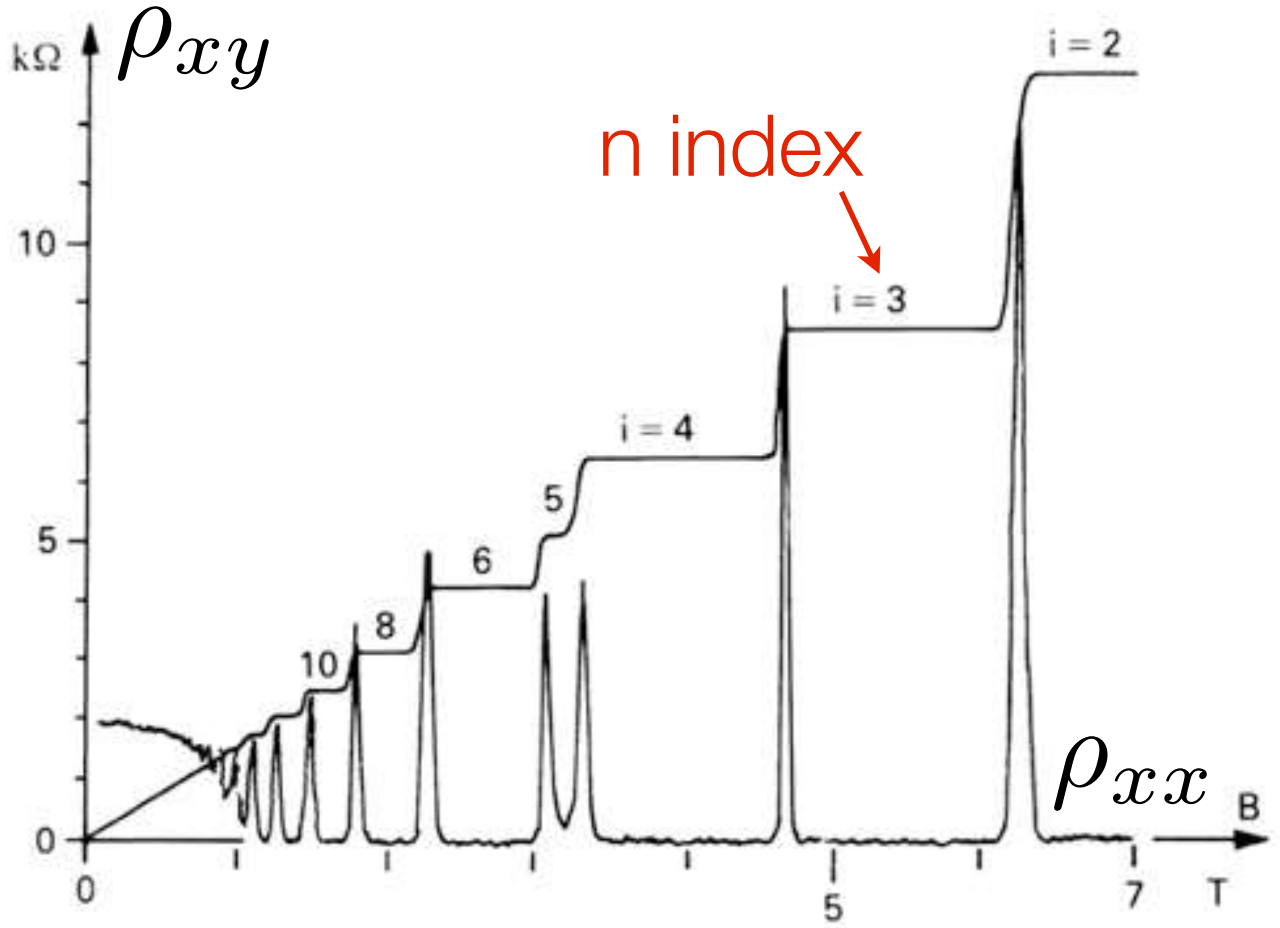
Quantum Hall Effect and Chern Topological Insulator



2DEG (Heterojunction GaAs/AlGaAs)

with high precision

$$\sigma_{xy} = n\frac{e^2}{h}$$

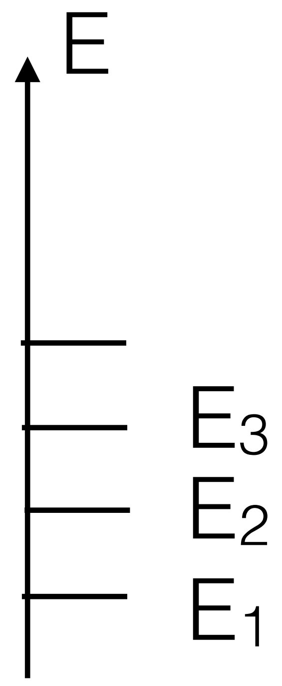


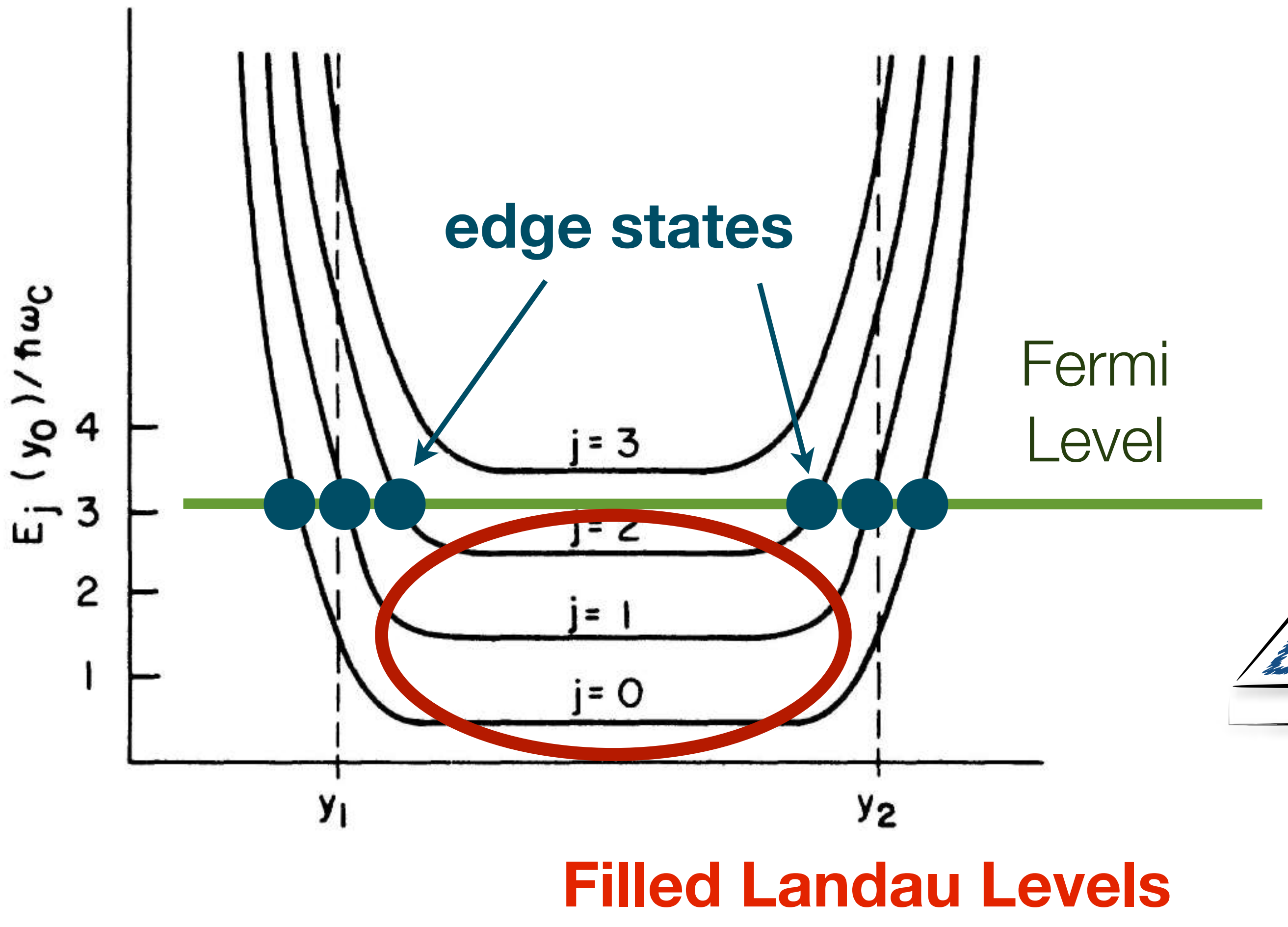
n is a topological invariant ⟷ number of (robust) edge modes

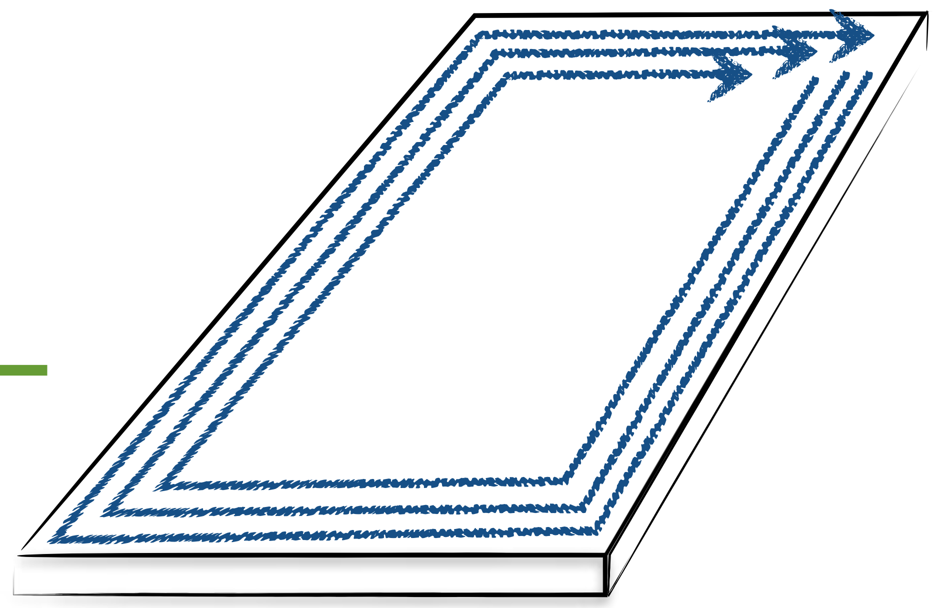
Thouless *et al.*. PRL **49** (1982)

M. Büttiker, PRB **38** (1988)

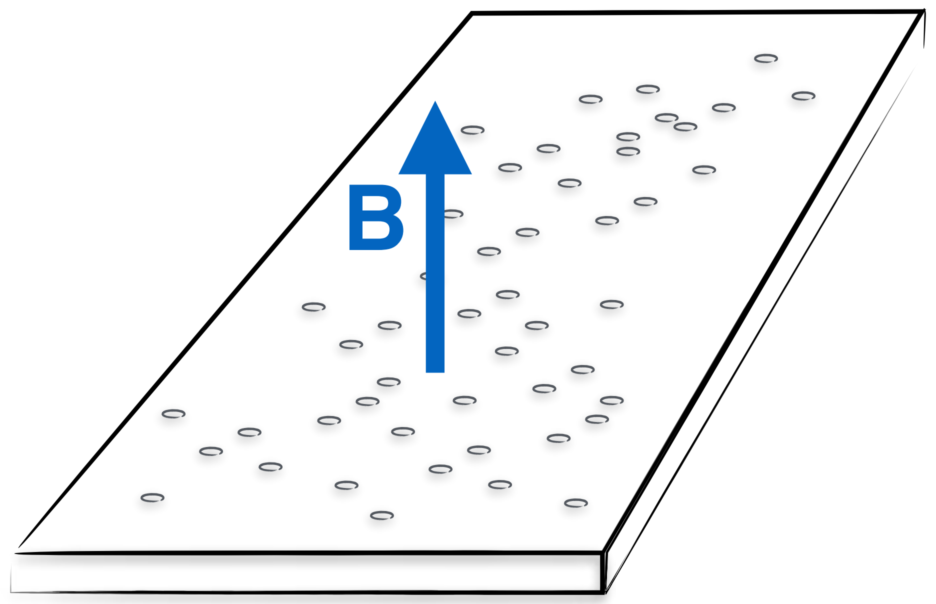
Landau Levels







Topological Property in Insulators



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Roy (2009)
Fu and Kane (2007)

review : Fruchart *et al.* *CRAS* (2013)

Symmetries and topology: (first) classification

Kitaev (2010)
Schnyder, Ryu, Furusaki, Ludwig (2008)

general (ubiquitous) symmetries

(superconductors)

Time Reversal Symmetry :

- anti unitary ($\Theta = UK$)
- states at same E, $[H, \Theta] = 0$
- $\Theta^2 = \pm\mathbb{I}$

Particle Hole Symmetry :

- anti unitary ($P = VK$)
- states at opposite E, $\{H, P\} = 0$
- $P^2 = \pm\mathbb{I}$

Chiral / Sublattice Symmetry :

- $C = \Theta.P$
- unitary
- states at opposite E, $\{H, C\} = 0$

Time Reversal Symmetry

Property of Time Reversal in Quantum Mechanics (for spin ½) :

- anti-unitary operator Θ : ***k*** →-***k*** ; σ →-σ ($\Theta = e^{\frac{i}{\hbar}\pi S_y} K$)
- $\Theta^2 = -\mathbb{I}$ (rotation by 2π of spin ½)
- Kramers degeneracy : if $|\psi\rangle$ is an eigenstate of H, then $\Theta|\psi\rangle$ is a distinct eigenstate with same energy

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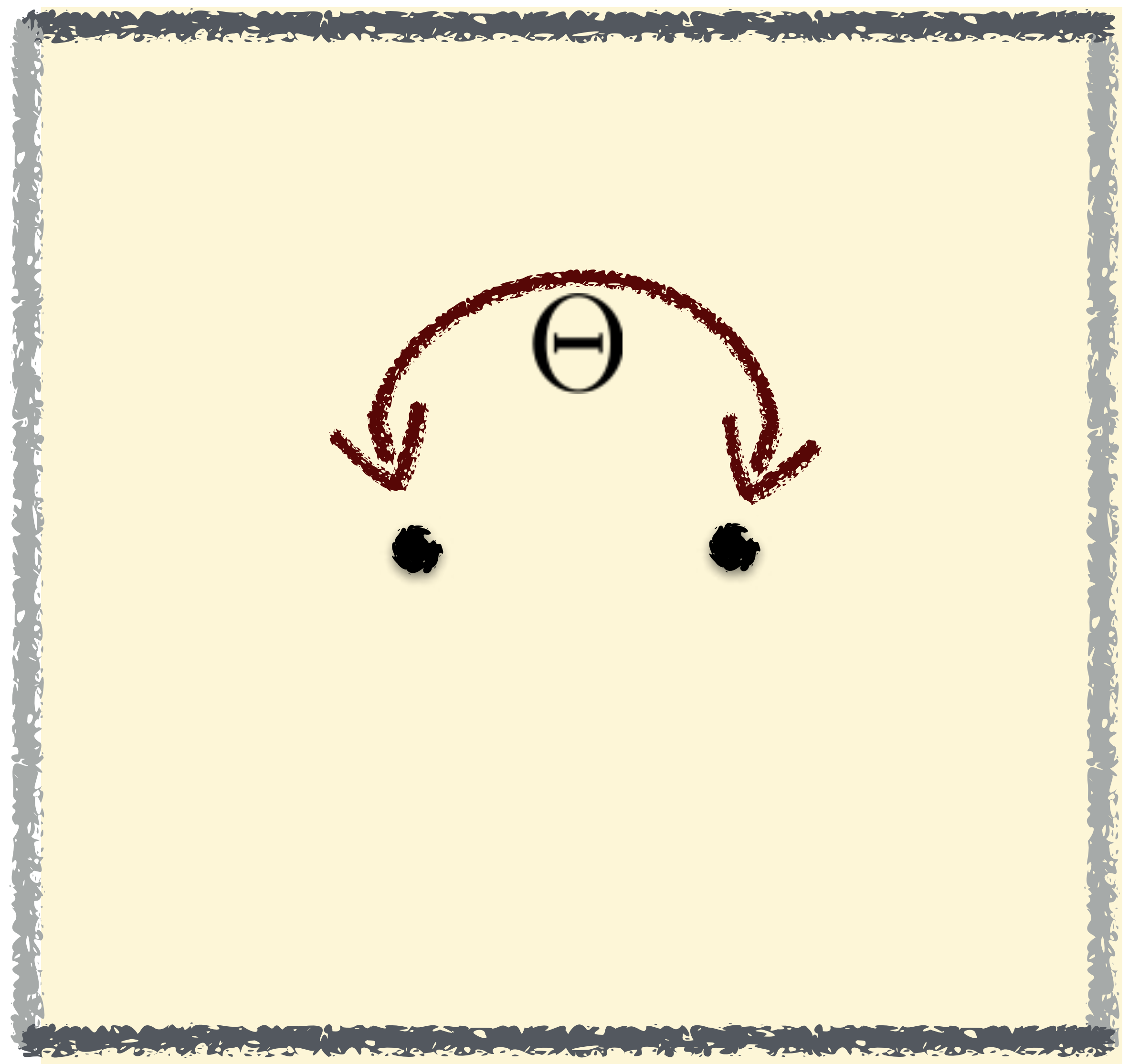
Application to **bands in a crystal** :

- Relates spectrum at k and $-k$

  $E_{k,\sigma} = E_{-k,-\sigma}$

  $\Theta|\psi_{k,\sigma}\rangle = |\psi_{-k,-\sigma}\rangle$



Brillouin Zone

Time Reversal Symmetry

Application to **bands in a crystal** :

- Relates spectrum at k and $-k$

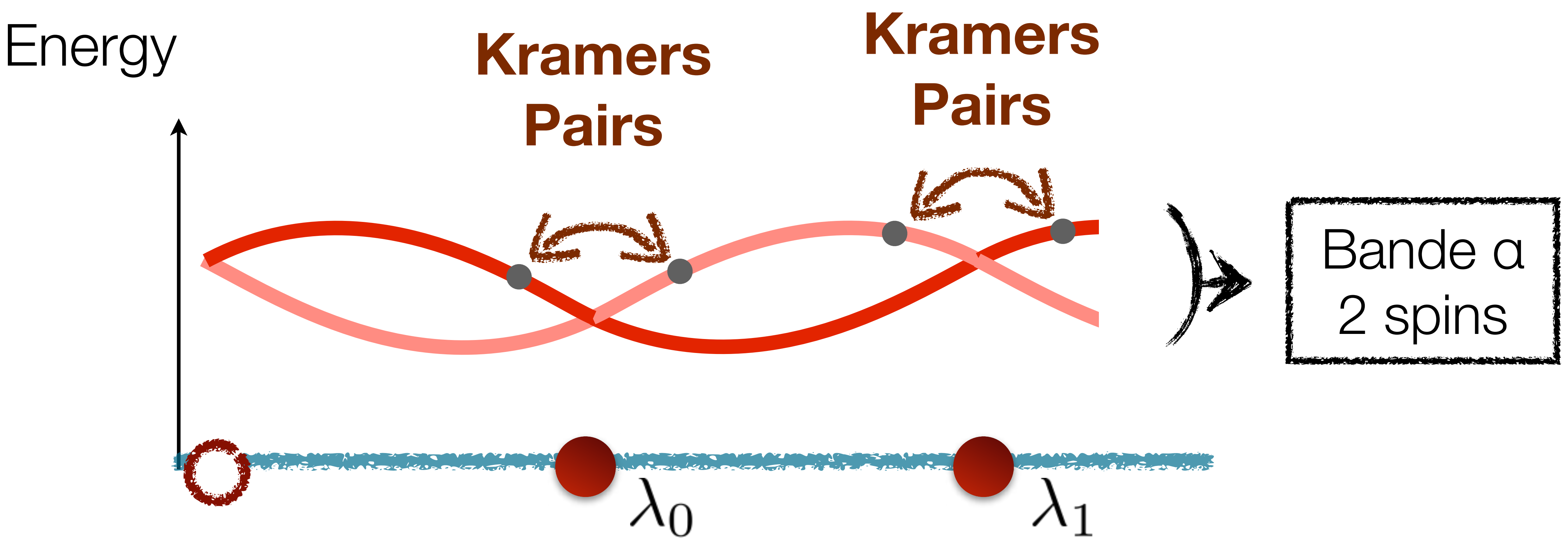
  $E_{k,\sigma} = E_{-k,-\sigma}$

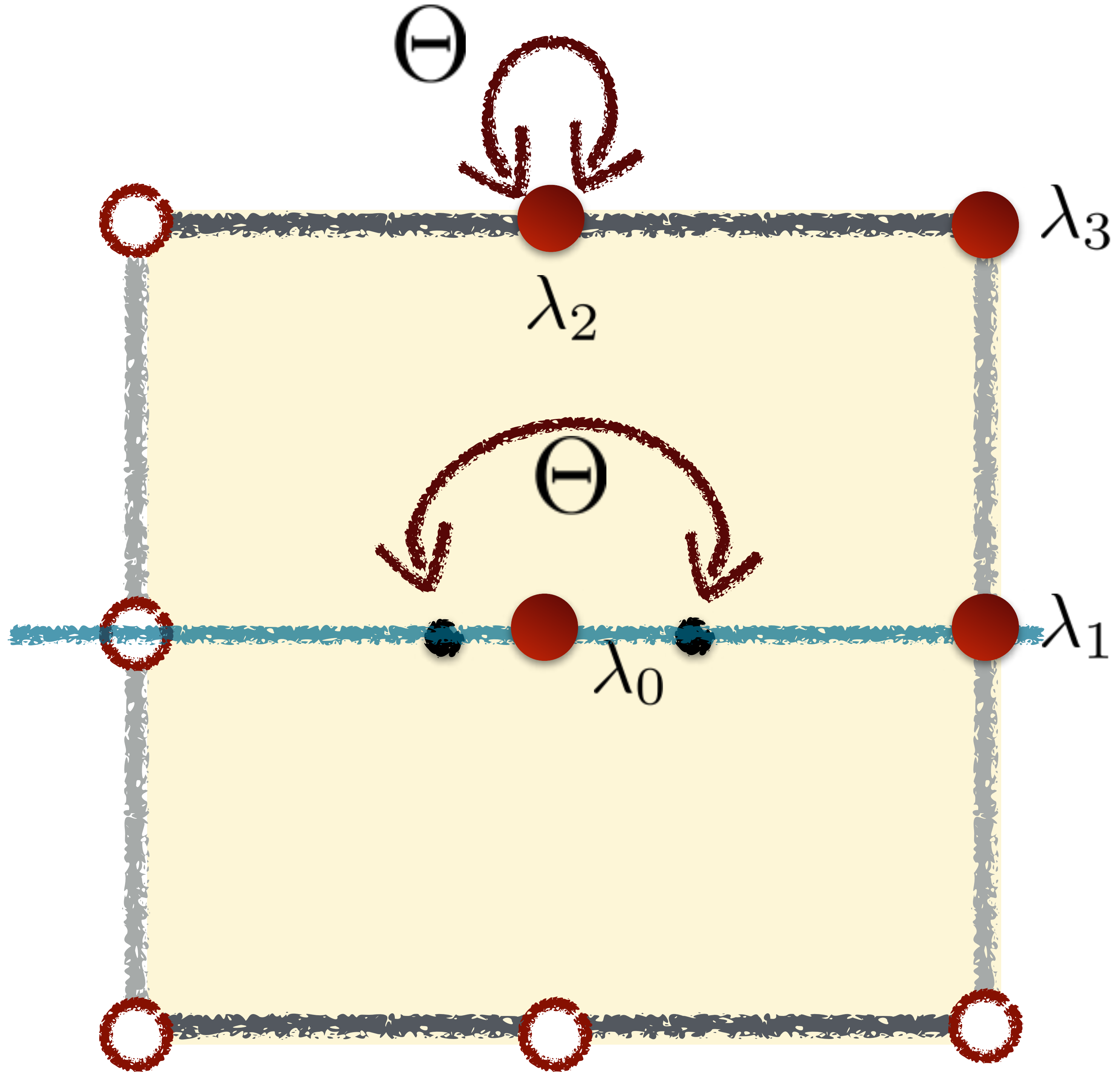
  $\Theta|\psi_{k,\sigma}\rangle = |\psi_{-k,-\sigma}\rangle$

- Special points in Brillouin zone : Time Reversal Invariant Momenta λ_i (●) where $-\lambda_i = \lambda_i + G$

⇒ imposes degeneracy:

$E_{\lambda_i,\sigma} = E_{\lambda_i,-\sigma}$ $\Theta|\psi_{\lambda_i,\sigma}\rangle = |\psi_{\lambda_i,-\sigma}\rangle$



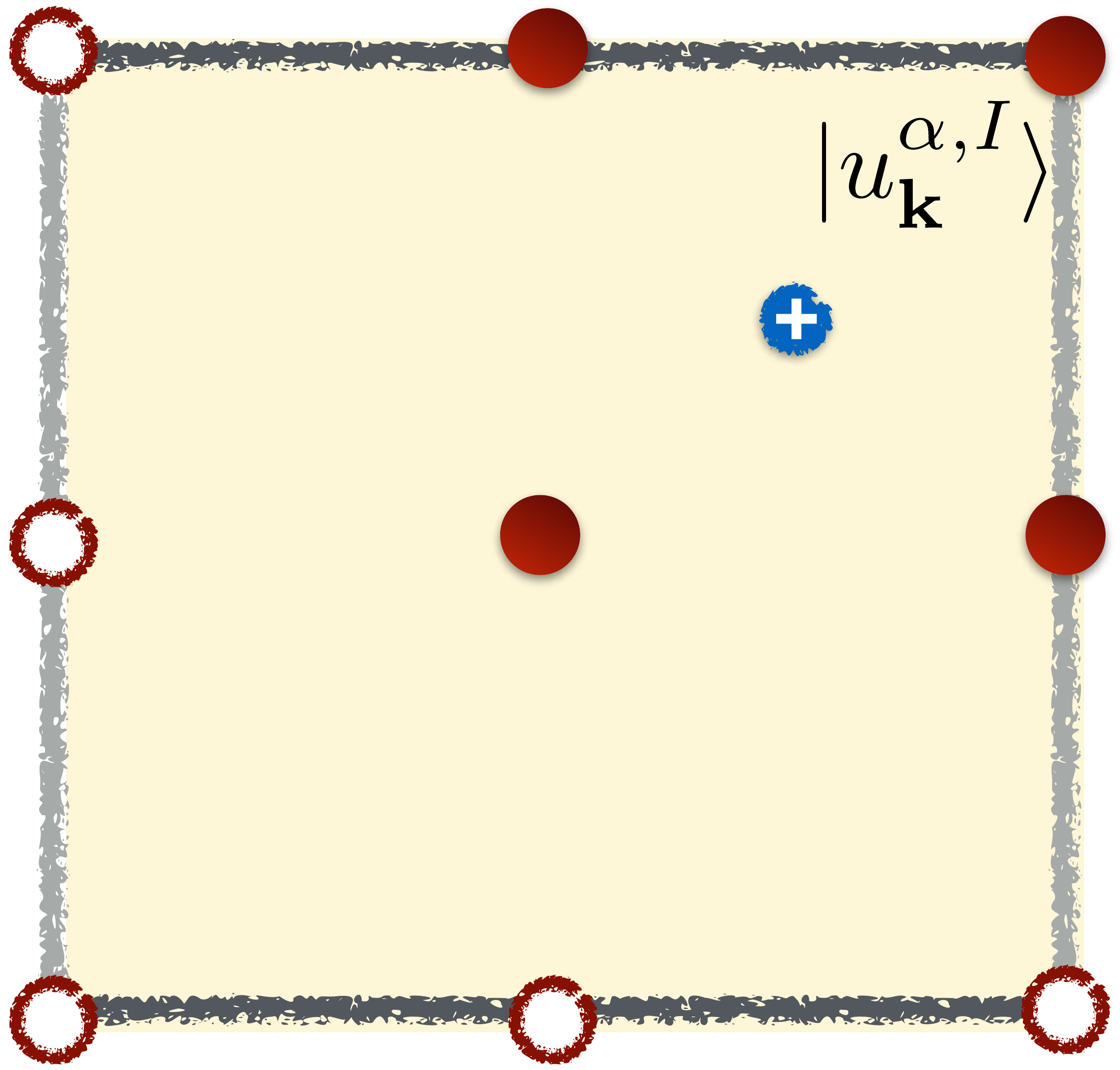


Brillouin Zone

Kane-Mele topological invariant

Kane and Mele (2005)

review : Fruchart and Carpentier (2013)



Brillouin Zone

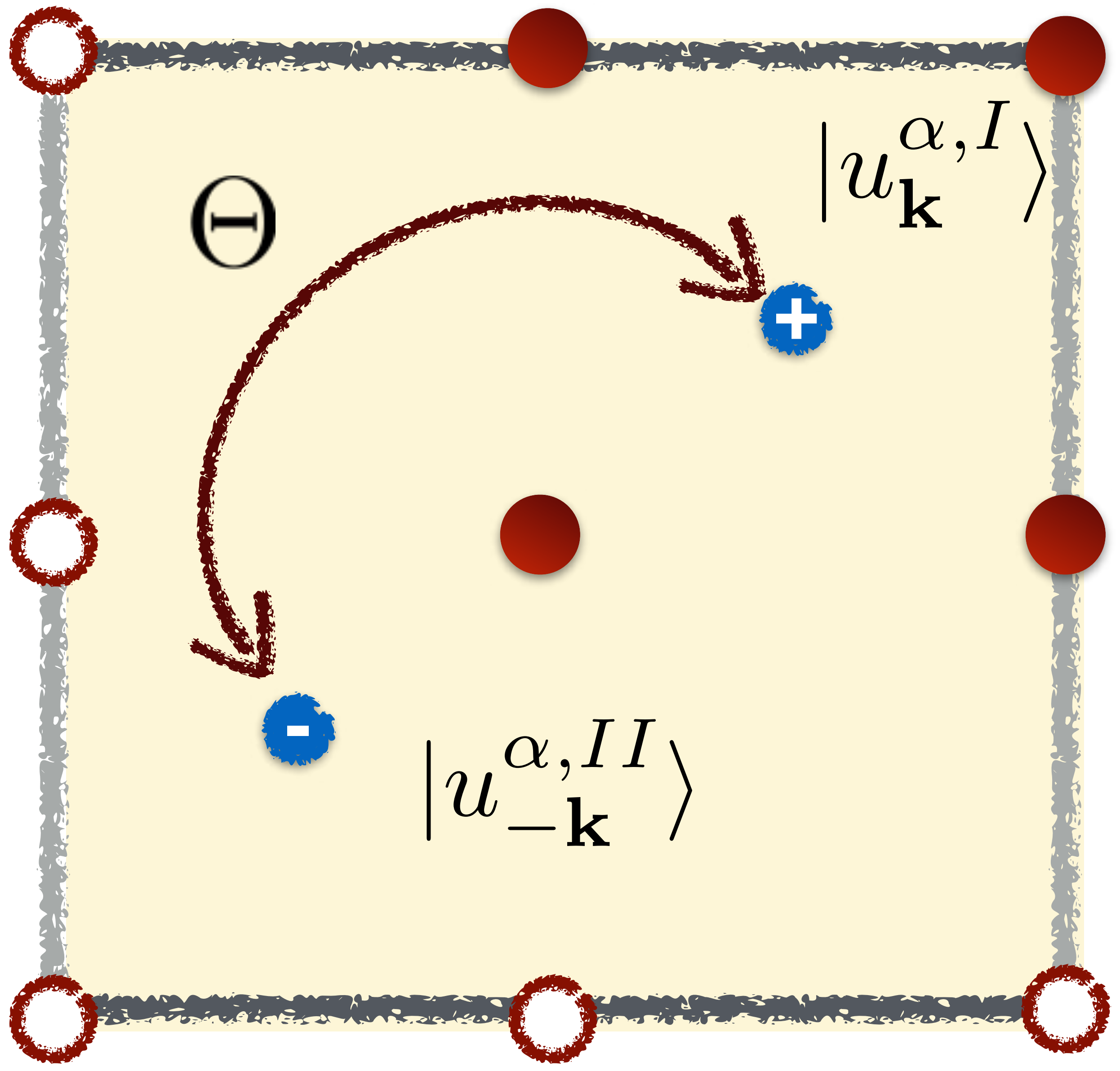
Singularities of wavefunctions

Idea : identify singularities of eigenstates

Kane-Mele topological invariant

Kane and Mele (2005)

review : Fruchart and Carpentier (2013)



Brillouin Zone

Singularities of wavefunctions

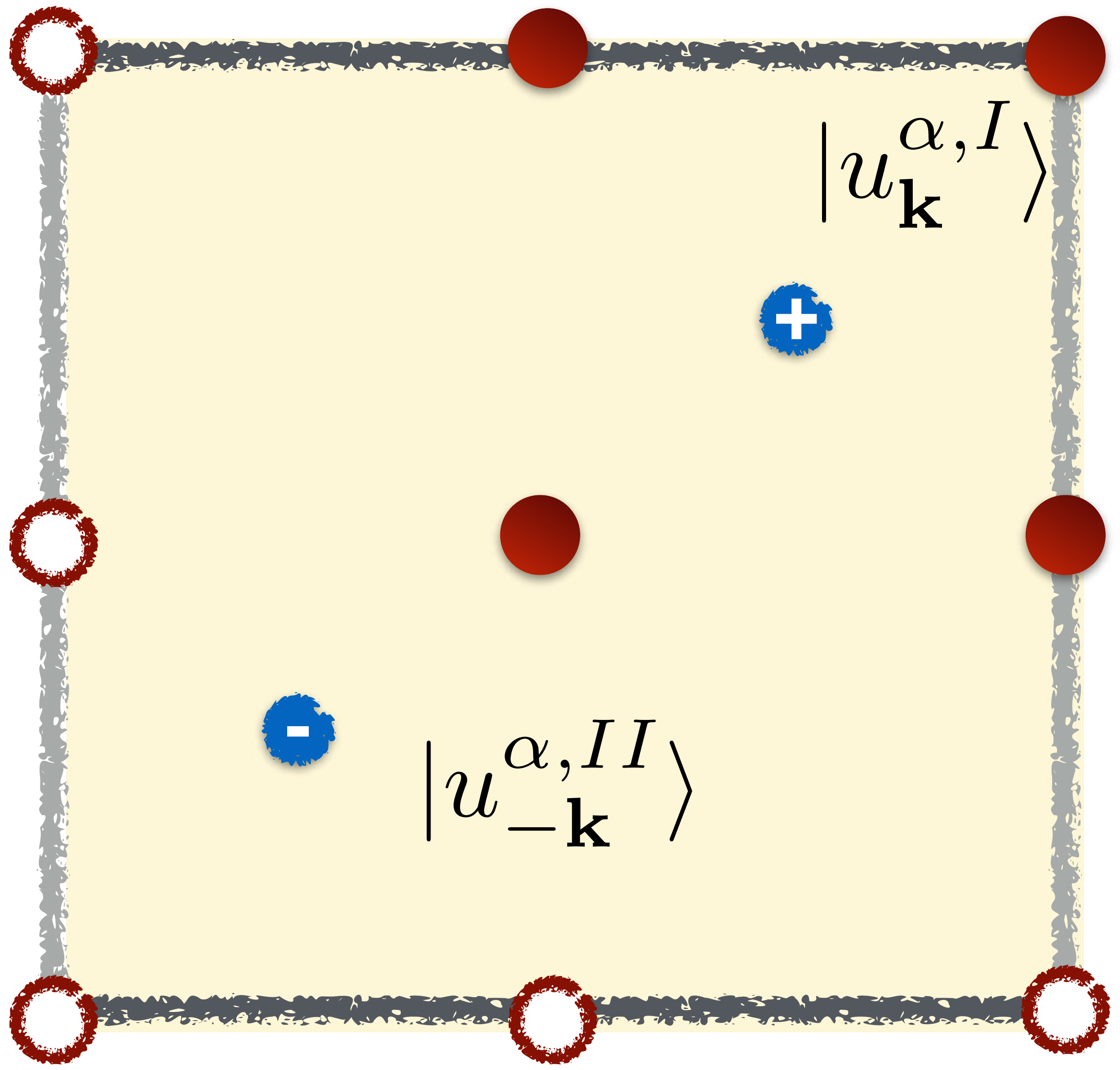
Idea : identify singularities of eigenstates

- Time Reversal symmetry : they come by pairs + / -
- Chern number vanishes

Kane-Mele topological invariant

Kane and Mele (2005)

review : Fruchart and Carpentier (2013)



Brillouin Zone

Singularities of wavefunctions

(Kramers pair)

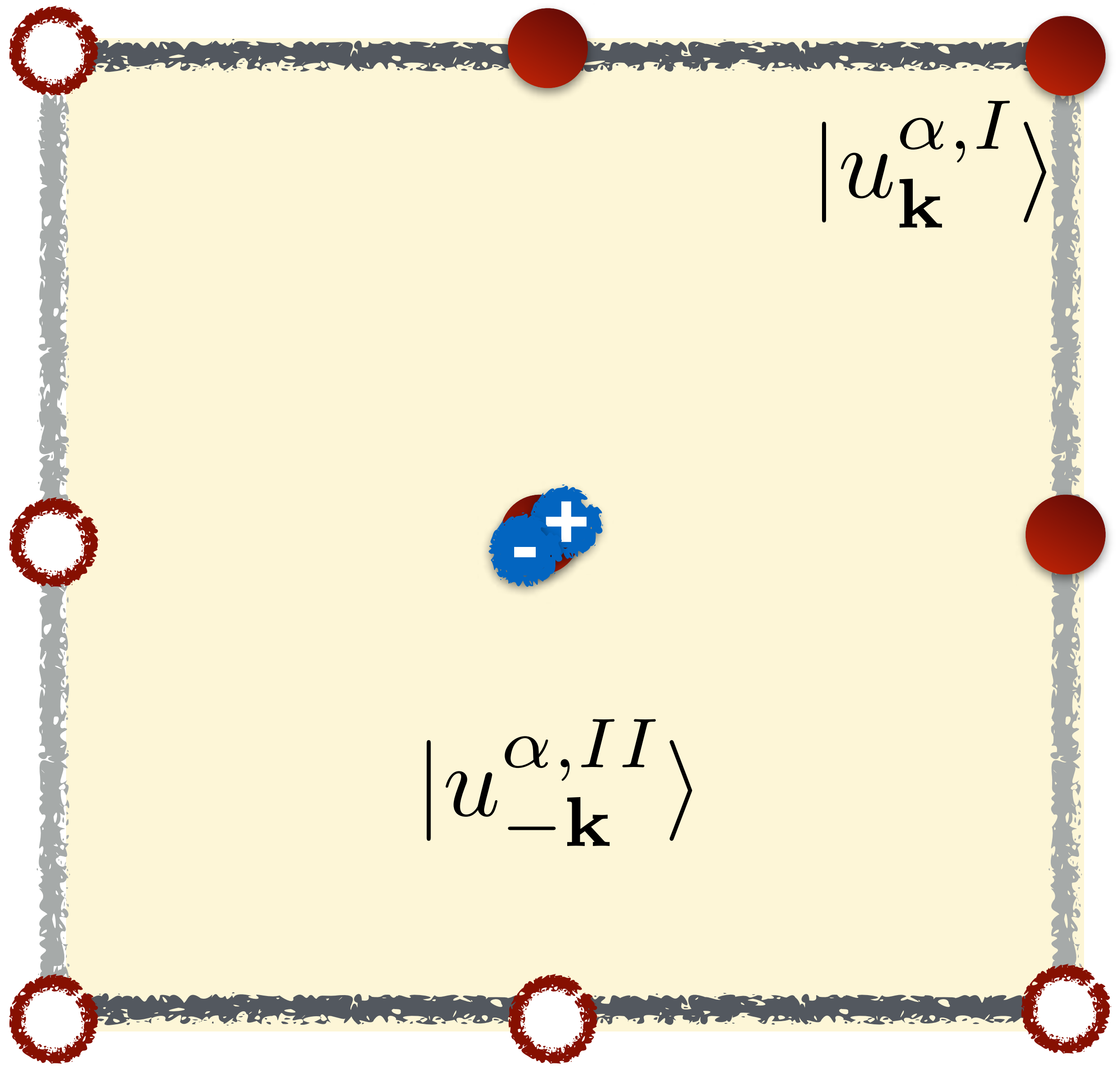
Idea : identify singularities of eigenstates

- Time Reversal symmetry : they come by pairs + / -
- Chern number vanishes
- but **topological property (robust) !**

Kane-Mele topological invariant

Kane and Mele (2005)

review : Fruchart and Carpentier (2013)



Brillouin Zone

Singularities of wavefunctions

a single pair cannot be annihilated

(Kramers pair)

Idea : identify singularities of eigenstates

- Time Reversal symmetry : they come by pairs + / -
- Chern number vanishes
- but **topological property (robust) !**

Kane-Mele topological invariant

Kane and Mele (2005)

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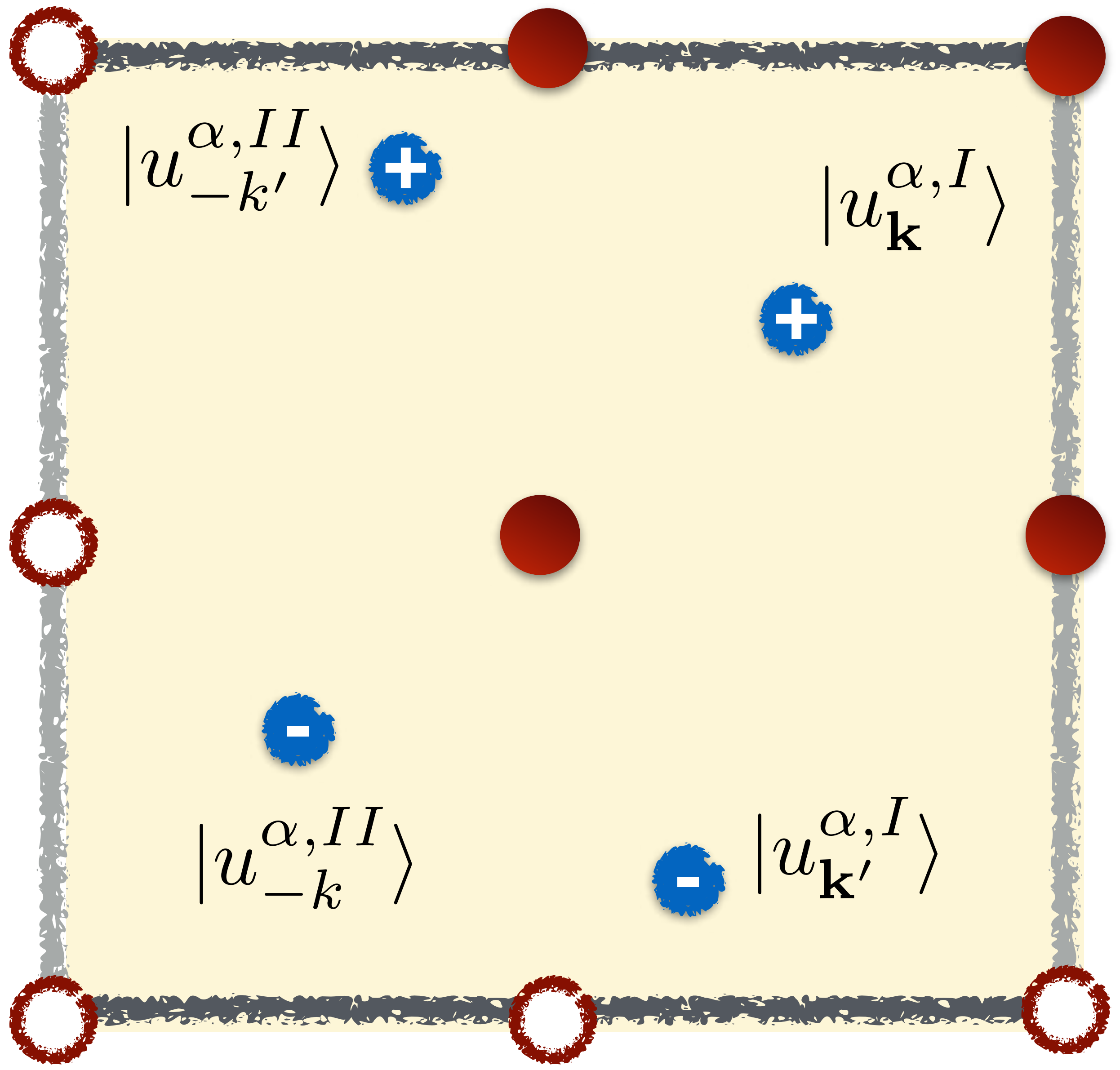


Brillouin Zone

Singularities of wavefunctions

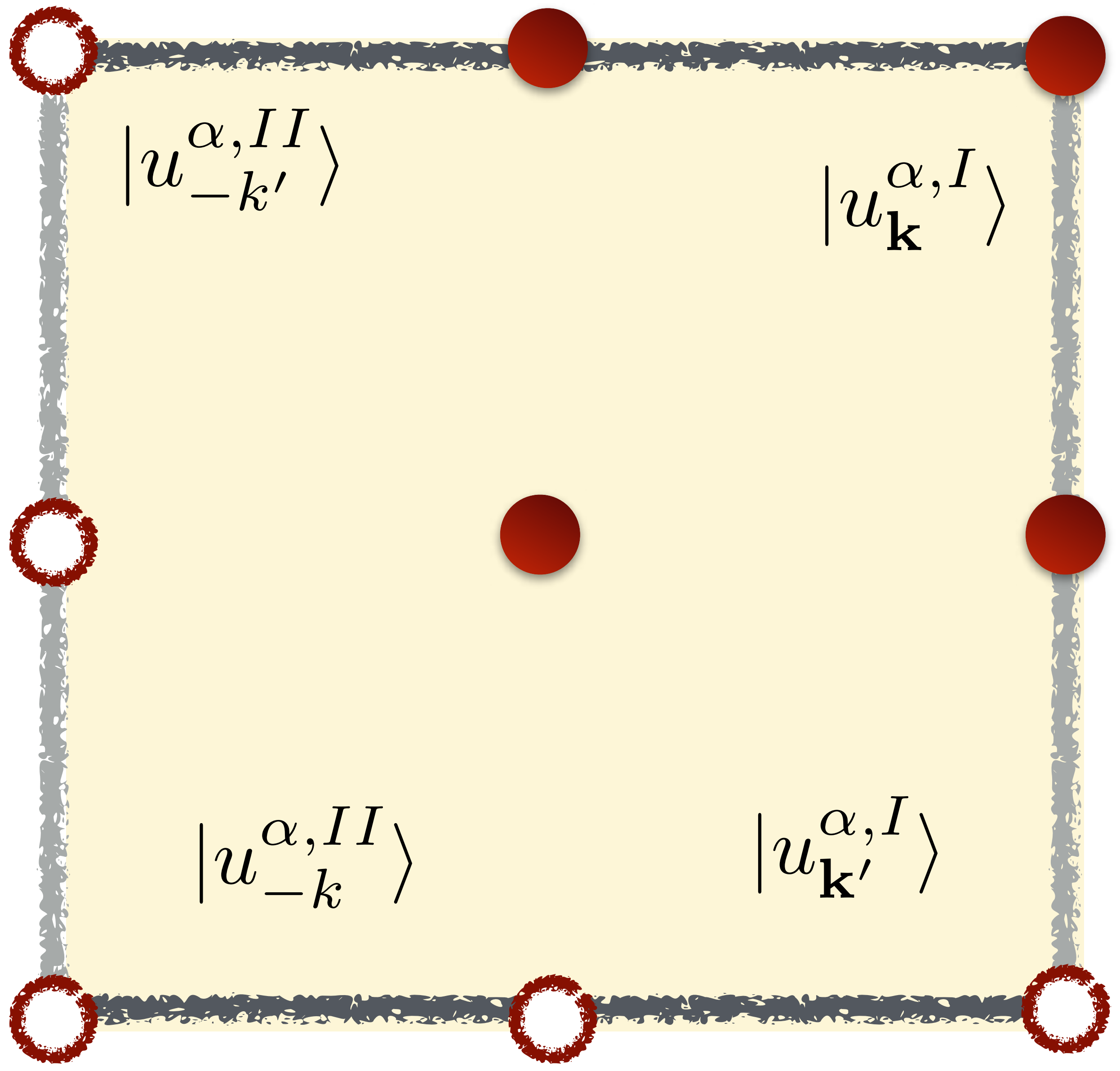
Idea : identify singularities of eigenstates

- Time Reversal symmetry : they come by pairs + / -
- Chern number vanishes
- but **topological property (robust) !**

Kane-Mele topological invariant

Kane and Mele (2005)

review : Fruchart and Carpentier (2013)



Brillouin Zone

Singularities of wavefunctions

two pairs can be annihilated

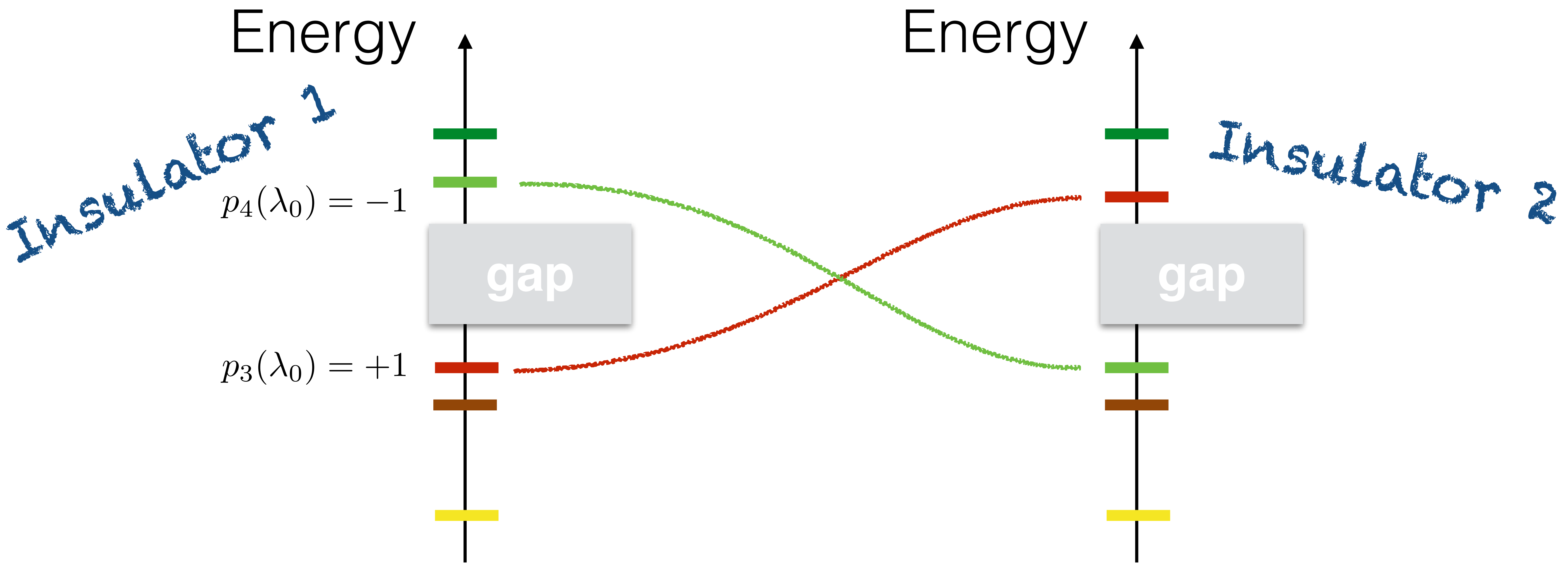
Idea : identify singularities of eigenstates

- Time Reversal symmetry : they come by pairs + / -
- Chern number vanishes
- but **topological property (robust) !**
- **new Z_2 index :** parity of number of pairs of singularities !!!

Kane-Mele invariant and Band Inversion

Fu and Kane (2007)

$$\prod_{\substack{\lambda_i \\ E_n<gap}} [p_n(\lambda_i)] = (-1)^\nu$$

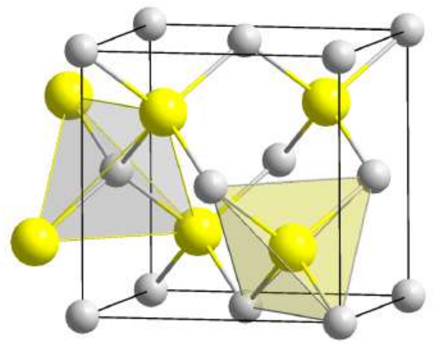


Topological index ν : counts the « inverted bands »

➡ Search for materials with **inverted band order**

(with respect to « standard ordering »)

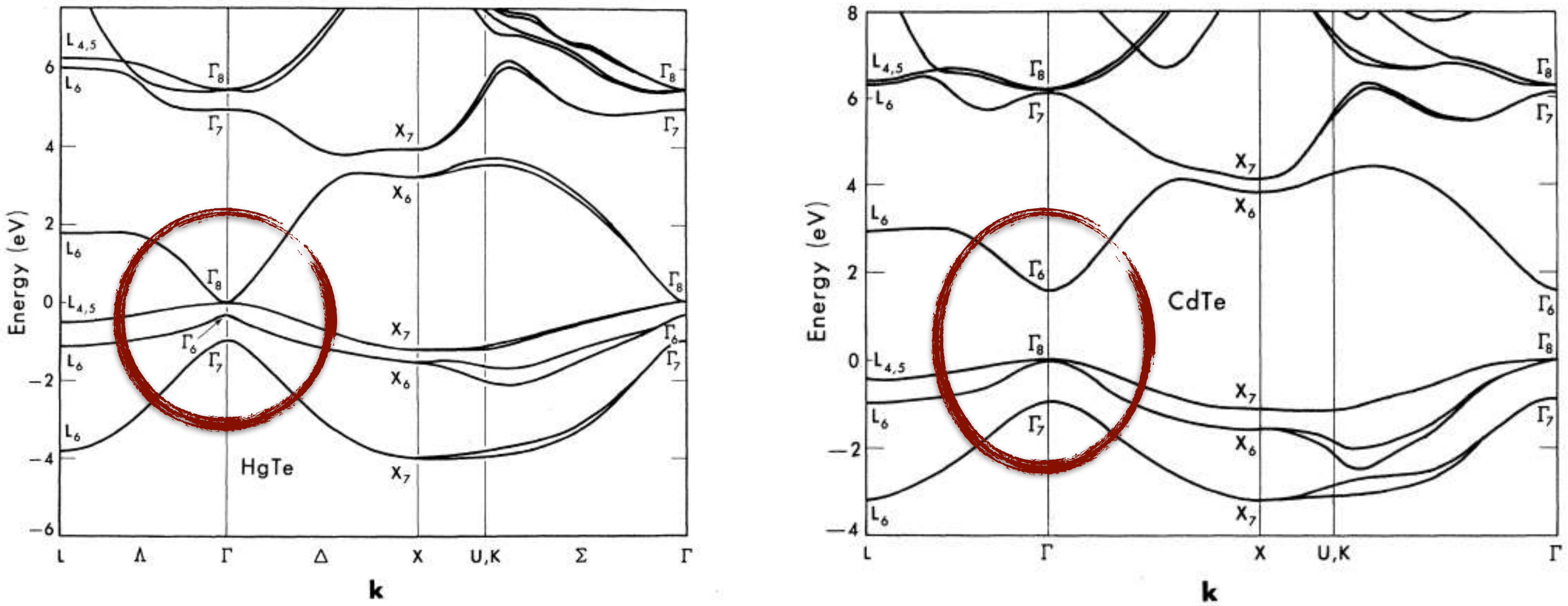
Topology and Band Inversion



➡ Search for materials with **inverted band order**

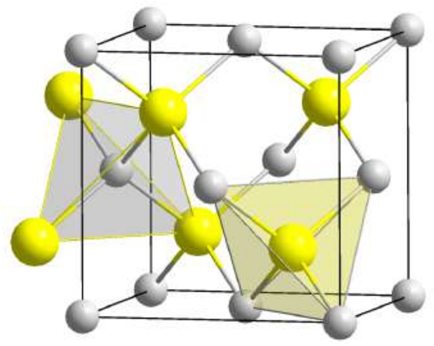
(with respect to « standard ordering »)

HgTe Band Structure CdTe



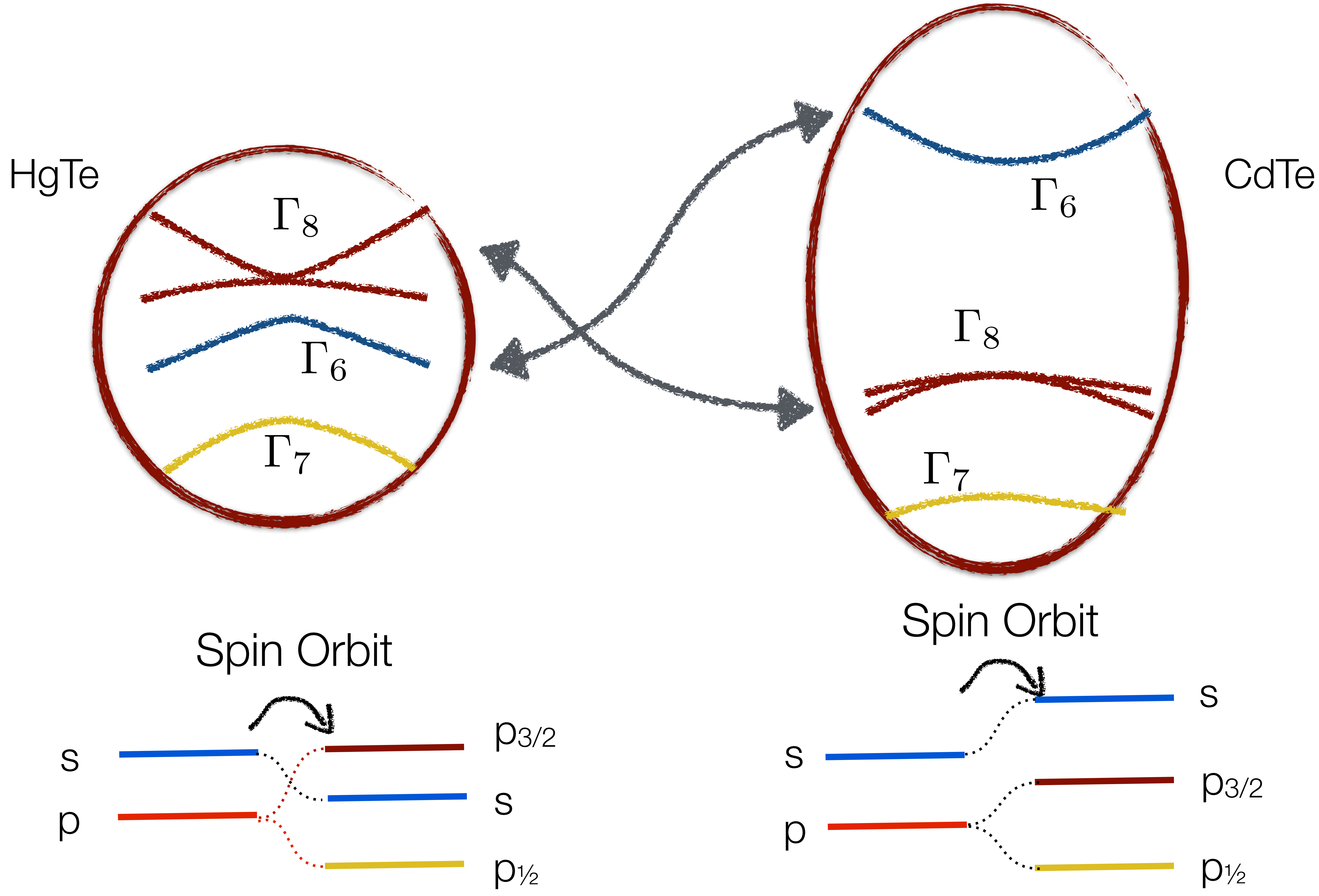
Chadi *et al.*
(2008)

Band Inversion and Topology

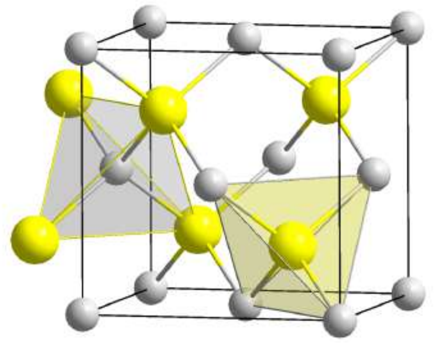


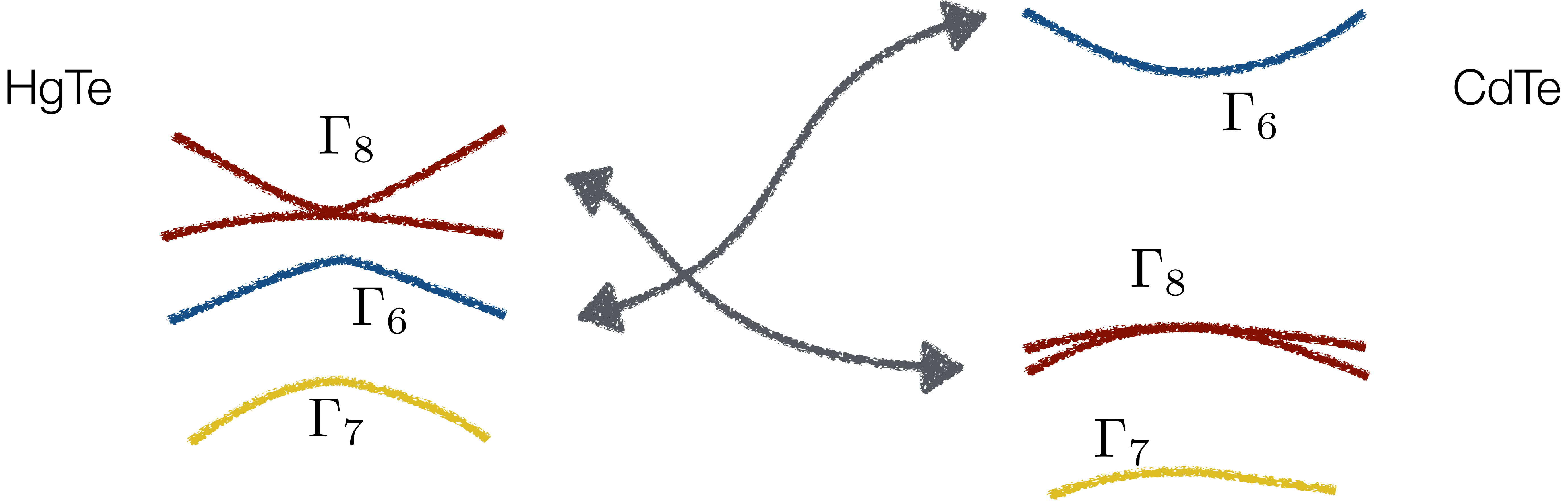
Topological property : parity eigenvalues change sign in the Brillouin zone

↔ band inversion (due to spin-orbit)



HgTe : Topological Insulator

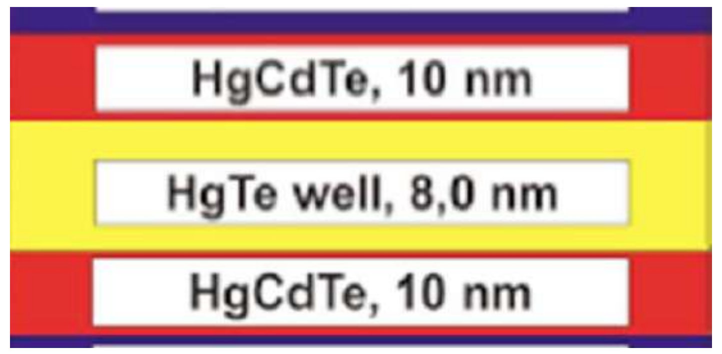




1. Confinement : HgTe / CdTe quantum well

Bernevig, Hugues and Zhang, Science **314** (2006)
König *et al.*, Science **318** (2007)

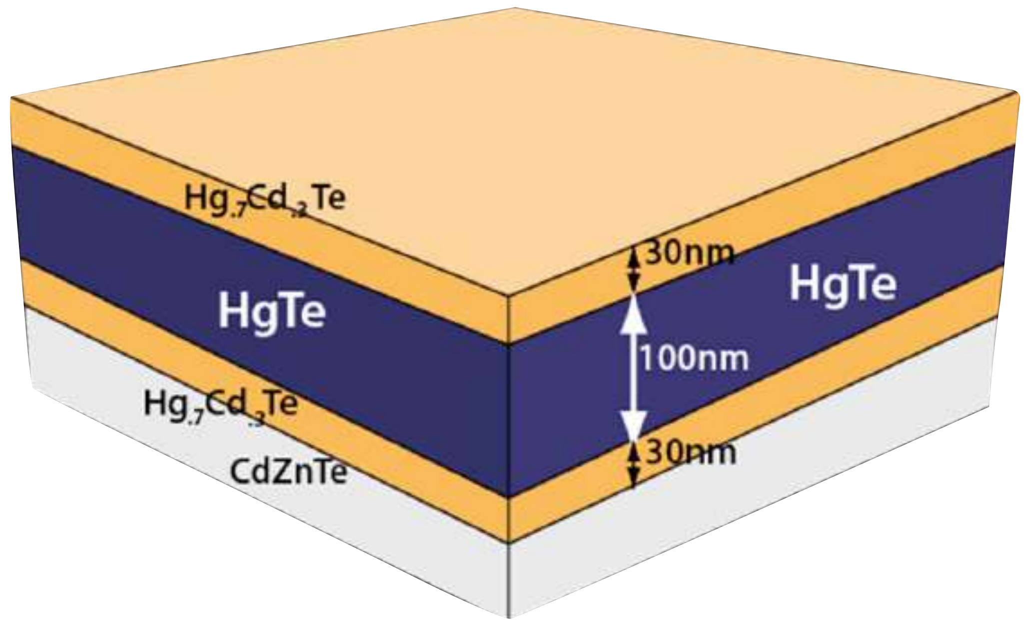
- **2D Topological Insulator** (Quantum Spin Hall Effect)



2. Thick layer of HgTe

L. Molenkamp group, PRL (2011)
P. Ballet, T. Meunier et L. Lévy (Grenoble)

- **3D Topological Insulator**
- gap of ~ 30 meV



Symmetries and topology : classification

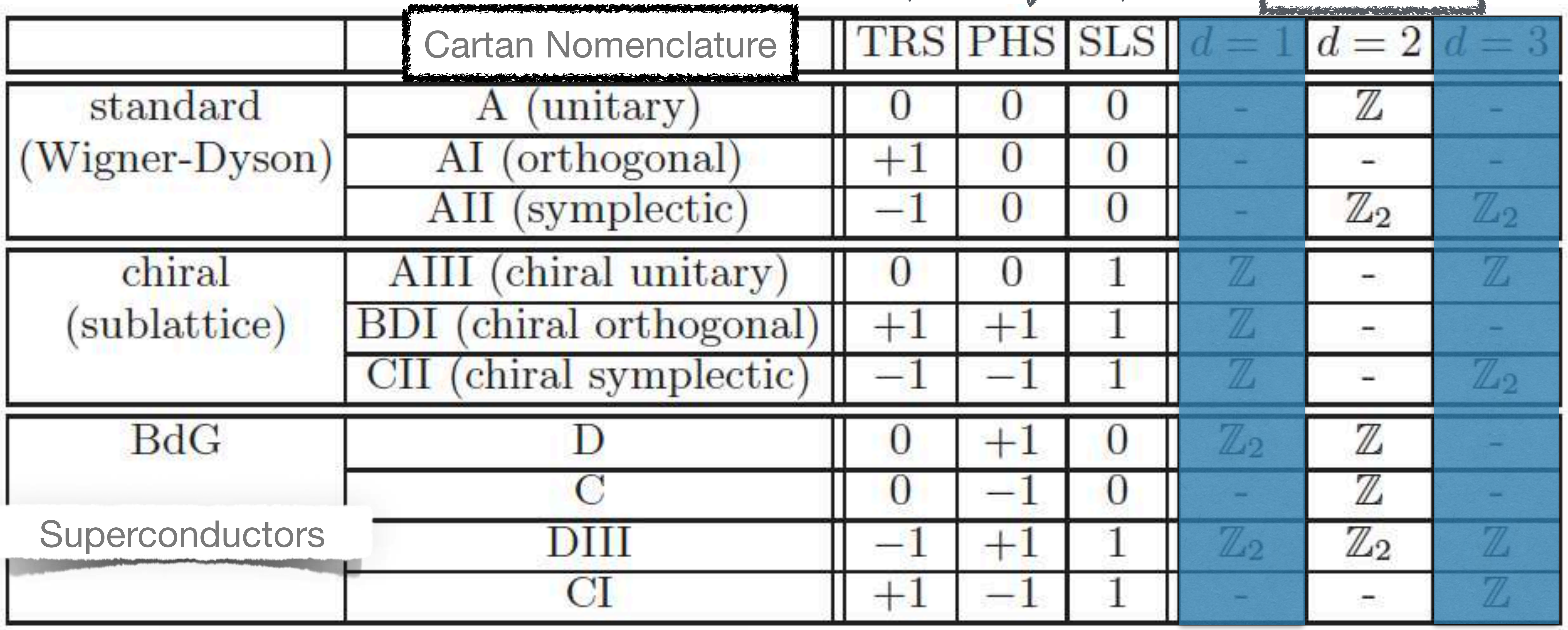
Time Reversal

Particle Hole

(superconductors)

Sub-Lattice (Chiral)

dimension



	Cartan Nomenclature	TRS	PHS	SLS	$d=1$	$d=2$	$d=3$
standard (Wigner-Dyson)	A (unitary)	0	0	0	-	$\mathbb{Z}$	-
	AI (orthogonal)	$+1$	0	0	-	-	-
	AII (symplectic)	-1	0	0	-	$\mathbb{Z}_2$	$\mathbb{Z}_2$
chiral (sublattice)	AIII (chiral unitary)	0	0	1	$\mathbb{Z}$	-	$\mathbb{Z}$
	BDI (chiral orthogonal)	$+1$	$+1$	1	$\mathbb{Z}$	-	-
	CII (chiral symplectic)	-1	-1	1	$\mathbb{Z}$	-	$\mathbb{Z}_2$
BdG	D	0	$+1$	0	$\mathbb{Z}_2$	$\mathbb{Z}$	-
	C	0	-1	0	-	$\mathbb{Z}$	-
Superconductors	DIII	-1	$+1$	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
	CI	$+1$	-1	1	-	-	$\mathbb{Z}$

Symmetry Operator : U

0 : no symmetry

+1 : symmetry with $U^2 = \mathbb{I}$

-1 : symmetry with $U^2 = -\mathbb{I}$

10 classes :

TRS : **x3** (0,+1,-1)

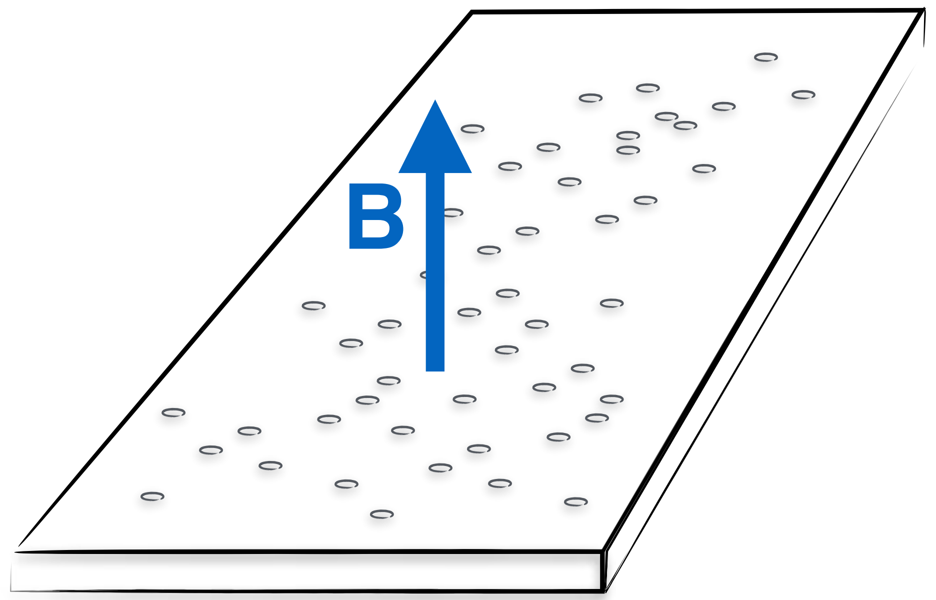
PHS : **x3** (0,+1,-1)

SLS = TRS . PHS (**+1**)

Symmetries and topology : classification

Chern insulators : ex. Quantum Hall Effect

- d=2
- breaks all symmetries (TRS)
- Topological index : Chern number



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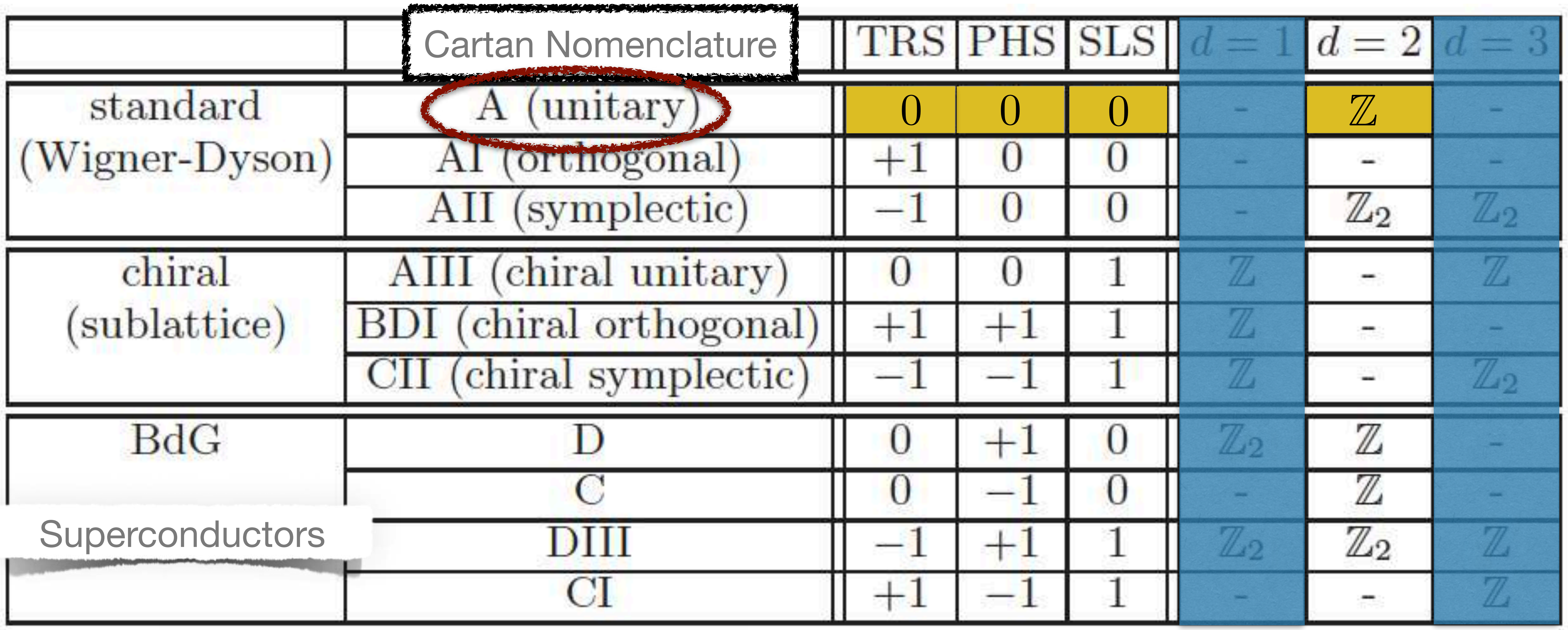

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Symmetries and topology : classification

Topological insulators :

- d=2 and d=3
- TRS with spin 1/2 : spin-orbit
- Topological index : Kane-Mele

Kane and Mele (2005)
Bernevig, Hughes, and Zhang (2006)
Fu, Kane et Mele (2007)
Moore and Balents (2007)
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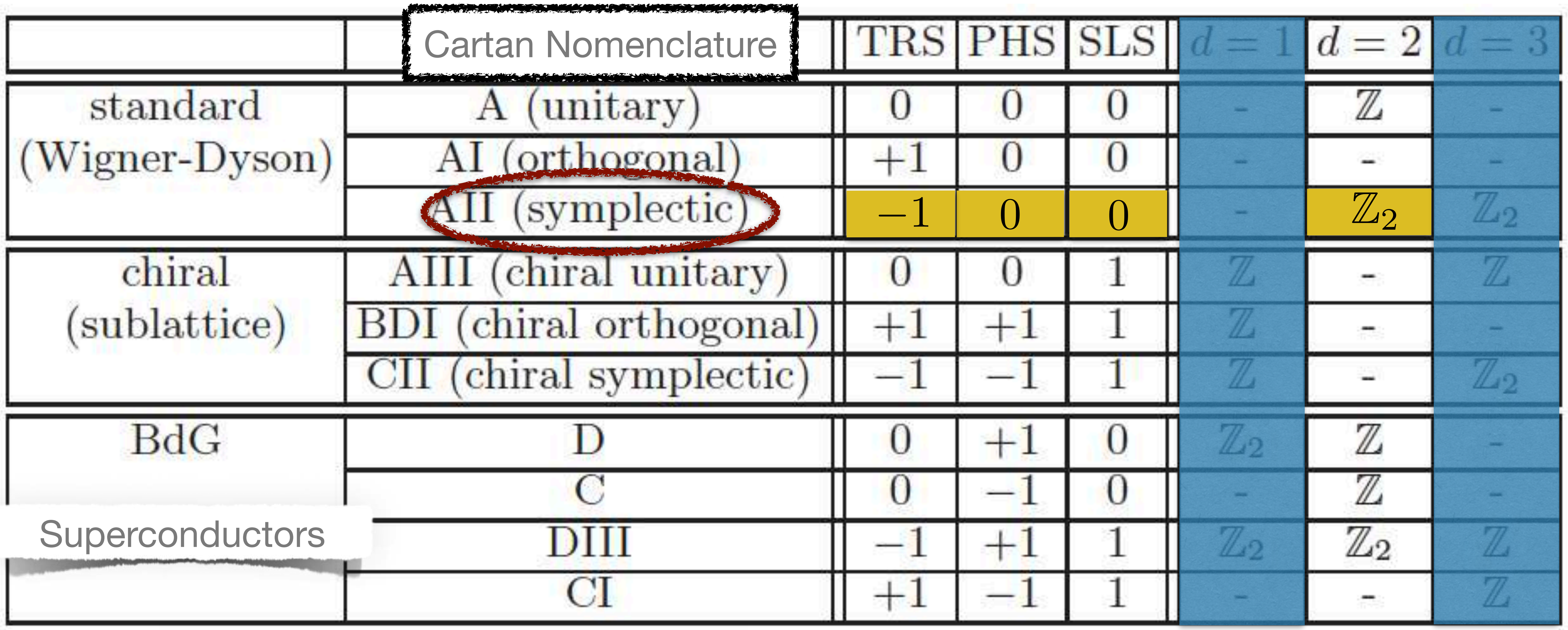
Fu and Kane (2007)



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Topological Insulators

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- time reversal symmetry
- induced by **strong spin-orbit coupling** (material property)
- **New property of band structures !**

Kane and Mele (2005)
Bernevig, Hughes, and Zhang (2006)
Fu, Kane et Mele (2007)
Moore and Balents (2007)
Roy (2009)
Fu and Kane (2007)

2D Materials :

- HgTe / CdTe quantum wells

Bernevig, Hugues and Zhang (2006)
König *et al.* (2007)

3D Materials :

- First proposed candidate : $Bi_{1-x}Sb_x$
- « canonical » Topological Insulators
  - Bi_2Se_3, Bi_2Te_3, Sb_2Te_3, ...
  - Reference material : Bi_2Se_3
    - single Dirac cone at the surface, stoichiometric, large band gap : 0.3 eV
- Strained HgTe
- Half Heusler compounds : Li_2AgSb, Ag_2Te, ScPtBi
- Skutterudites : $CeOs_4P_{12}$, $CeOs_4As_{12}$

Fu and Kane (2007)
Zhang H. et al. (2009)

...

Topological Quantum Chemistry

... combining symmetry representations and topology

Catalogue of Topological Electronic Materials

Tiantian Zhang, Yi Jiang, Zhida Song, He Huang, Yuqing He, Zhong Fang, Hongming Weng, Chen Fang
Nature, 566, 475 (2019)

Towards ideal topological materials: Comprehensive database searches using symmetry indicators

Feng Tang, Hoi Chun Po, Ashvin Vishwanath, Xiangang Wan
Nature 566, 486 (2019)

The (High Quality) Topological Materials In The World

M. G. Vergniory, L. Elcoro, C. Felser, B. A. Bernevig, Z. Wang
Nature 566, 480 (2019)

Abstract: « Topological Quantum Chemistry (TQC) links the chemical and symmetry structure of a given material with its topological properties.

Out of **26938** stoichiometric materials in our filtered ICSD database, we find **2861** topological insulators (TI) and **2936** topological semimetals.

Remarkably, our exhaustive results show that a large proportion **(~ 24% !)** of all materials in nature are topological

We added an open-source code and end-user button on the Bilbao Crystallographic Server (BCS)

Topological Surface States

- Quantum Hall Insulator (Chern index)
  - d=2
  - breaks Time-Reversal Symmetry

  ➡ **Chiral edge states**

- Quantum Spin Hall Insulator (Kane-Mele Z_2 index)
  - d=2
  - Time-Reversal Symmetry + spins 1/2

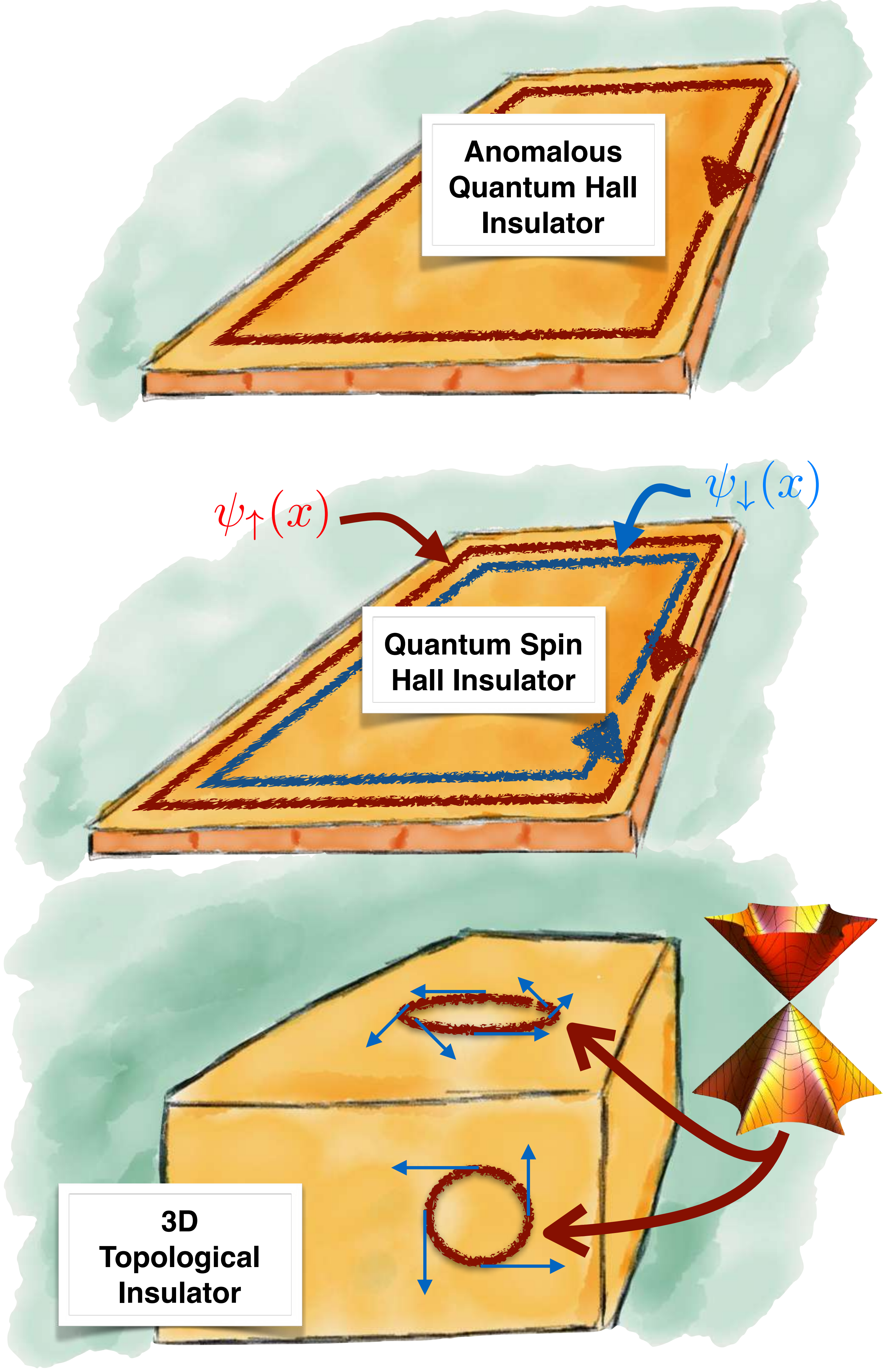
  ➡ **Helical edge states : Kramers pair**

- 3D Topological Insulators (Kane-Mele Z_2 index)
  - d=3
  - Time-Reversal Symmetry + spins 1/2

  ➡ (odd number of) **Dirac cone**

- Topological Superconductors
  - d=1 (or d=2,3)
  - Particle-Hole Symmetry E <-> -E

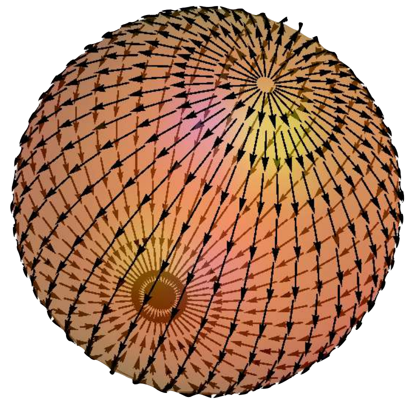
  ➡ **Majorana States** at E=0



Outline

1. Notion of topological number

   Chern number for fields on a manifold

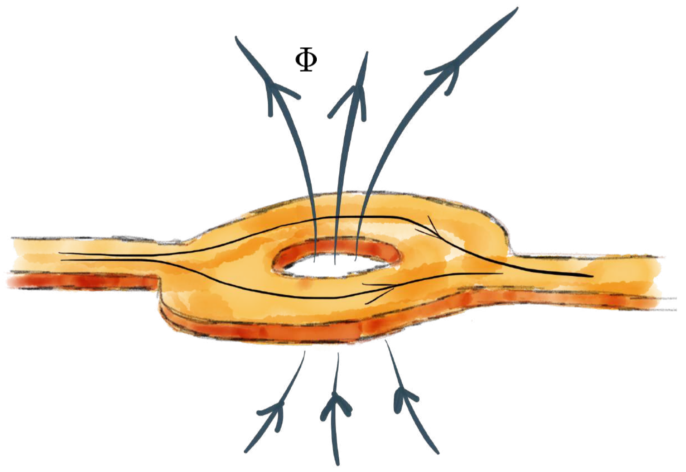


2. Band theory for electrons in solids

   Band : ensemble of Bloch states over the Brillouin zone
   Chern number of a band ↔ topological band ↔ Obstruction to localize Wannier states

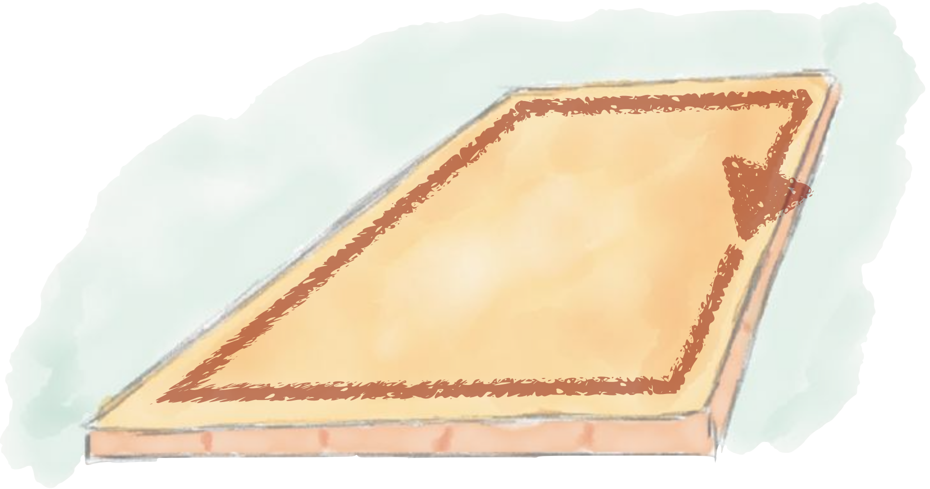
3. How to calculate a topological number ?

   Berry curvature, parallel transport, analogy with Aharonov-Bohm



4. Surface/Interface states

   Between two inequivalent topological band structures :
   interface states



5. Topology and symmetries

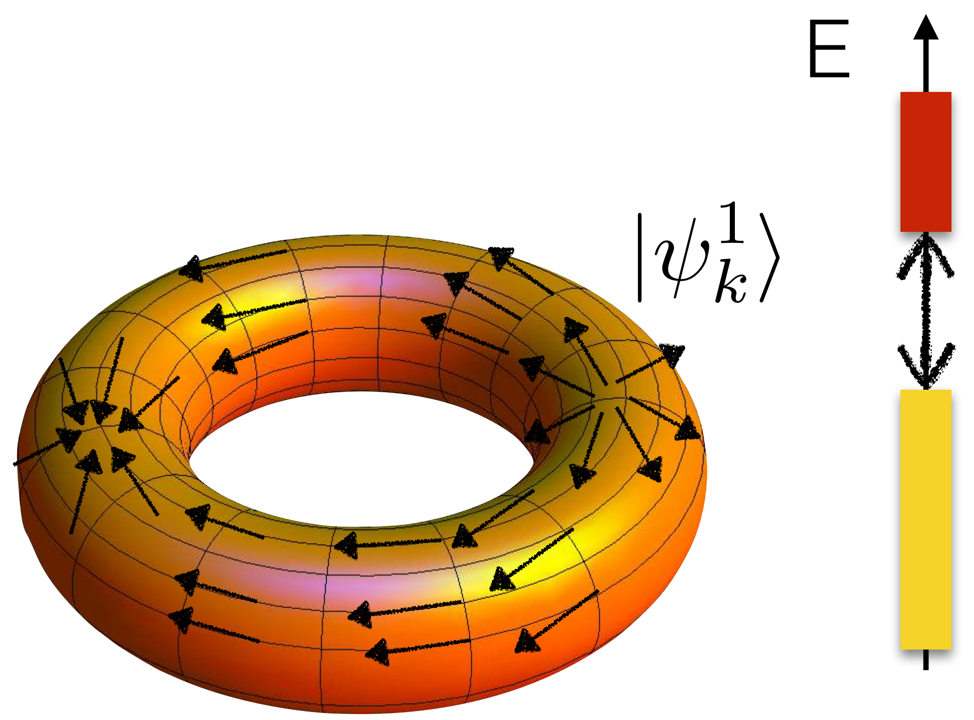
   Time-reversal, chiral symmetry: topological insulators
   Crystalline symmetries: topological quantum chemistry

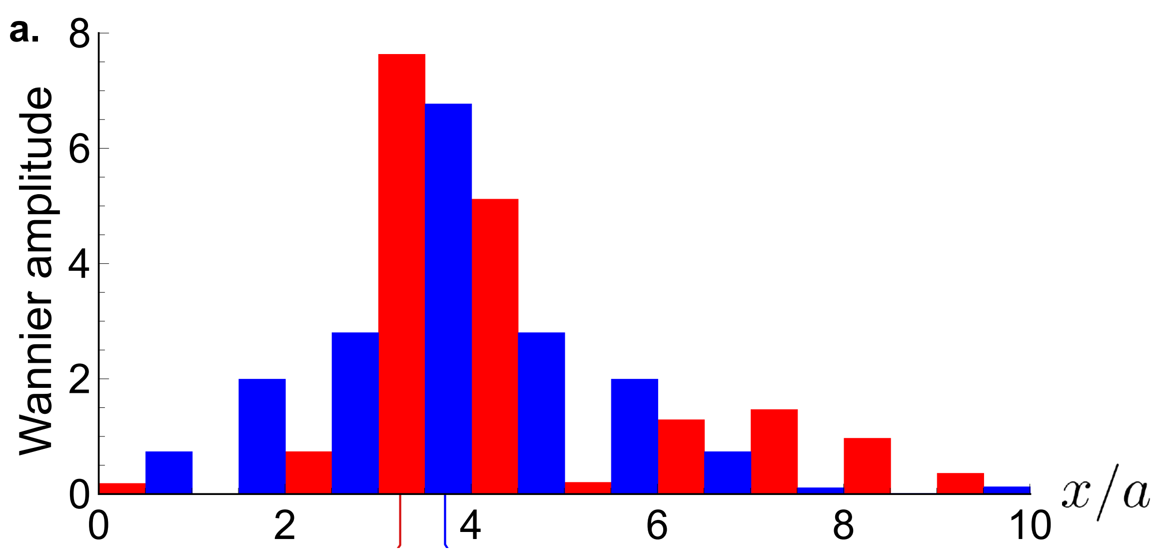
Take home message

What is a topological band ?

Bulk topological property :

- no continuous Bloch states over Brillouin zone



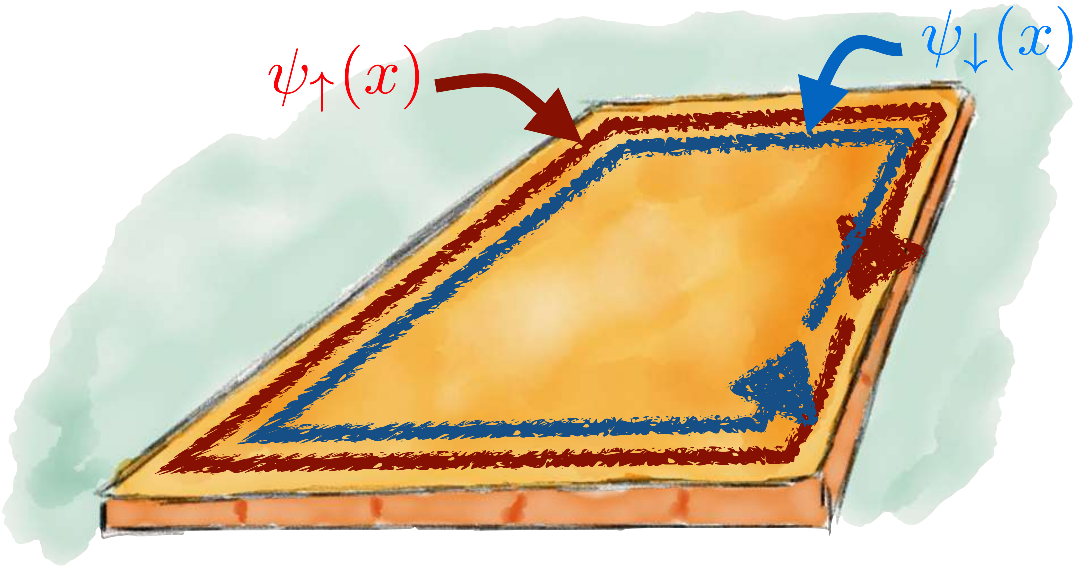


Real space property

- Topological band : obstruction to exponentially-localize Wannier function

Surface / edge states (inside gap)

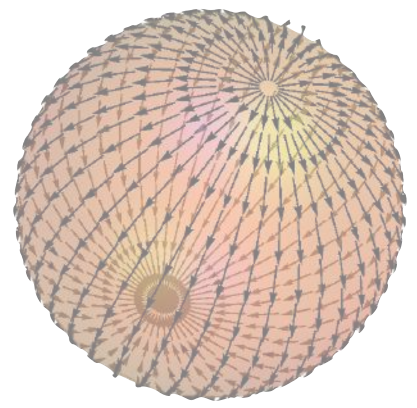
- robust (related to topology)
- unique metals (not conventional)



Outline

1. Notion of topological number

   Chern number for fields on a manifold

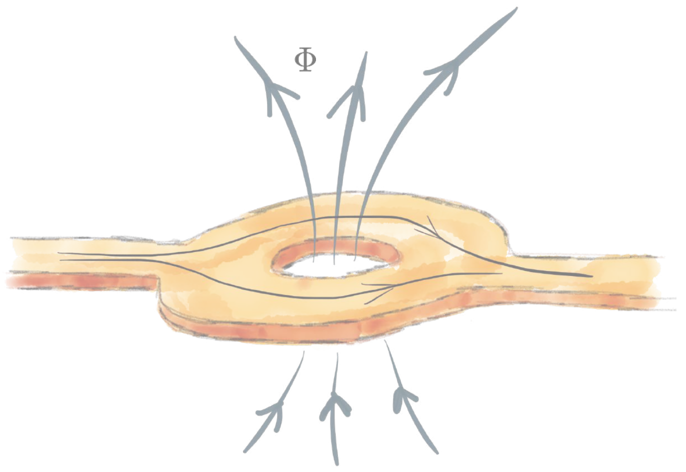


2. Band theory for electrons in solids

   Band : ensemble of Bloch states over the Brillo
   Chern number of a band ↔ topolo on to localize Wannier states

3. How to calculat

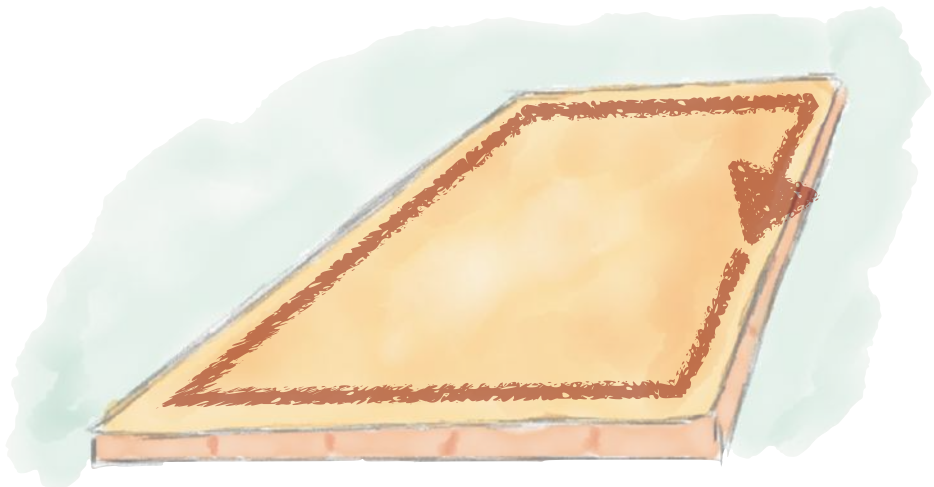
   Berry cur sport, analogy with Aharonov-Bohm



2 recent works

4. Surface/Interface states

   Between two inequivalent topological band structures : interface states



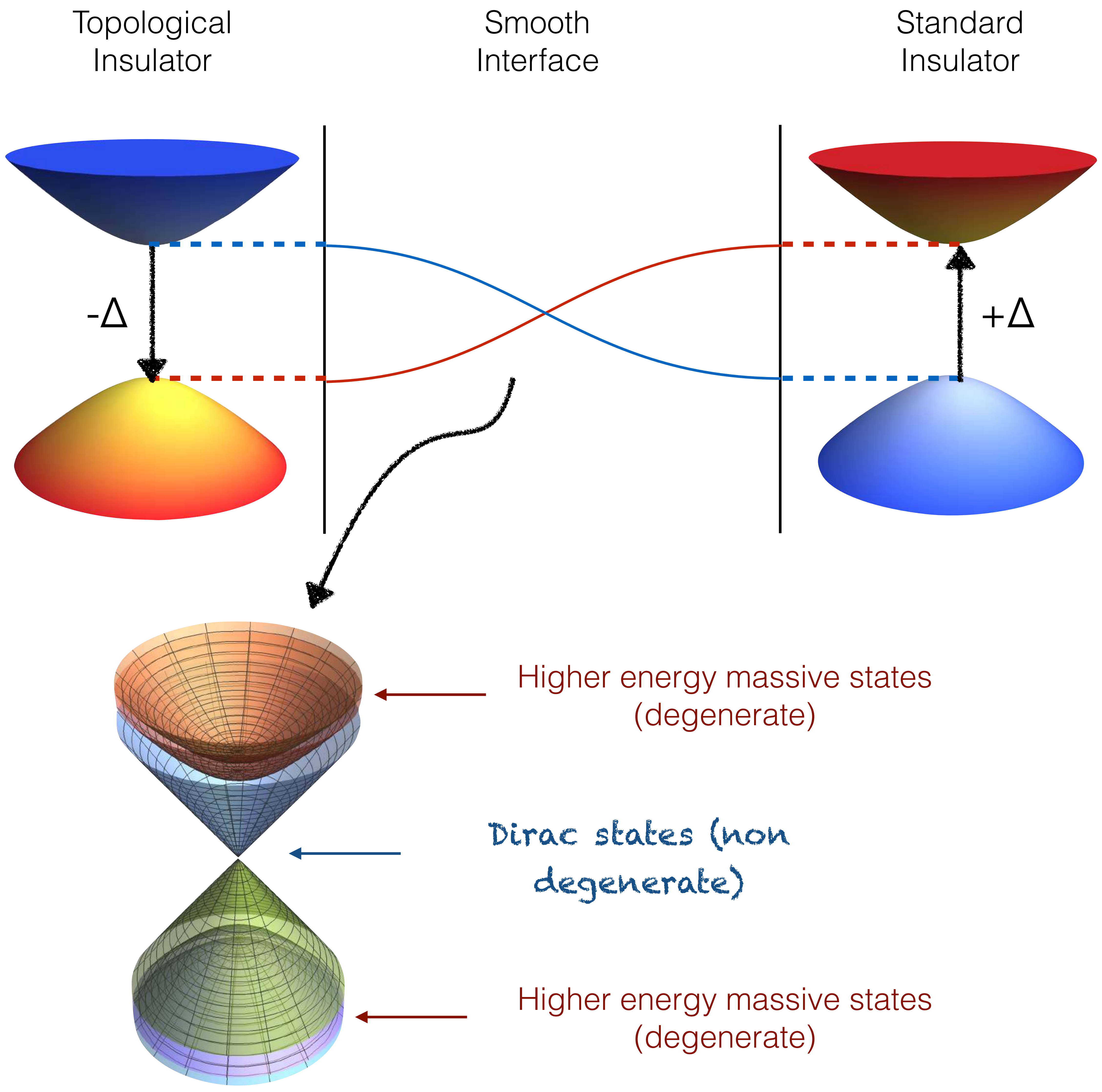
5. Topology and symmetries

   Time-reversal, chiral symmetry: topological insulators
   Crystalline symmetries: topological quantum chemistry

HgTe : Multiple Surface States

ENS Paris / Würzburg / Orsay / ENS-Lyon
B. Plaçais / L. Molenkamp / M. Goerbig / D. Carpentier

A. Inhofer *et al.* , PRB 2017
S. Tchoumakov *et al.* , PRB 2017
see also V. Volkov and O. Pankratov (1985)



Higher energy massive states (degenerate)

Dirac states (non degenerate)

Higher energy massive states (degenerate)

- Smooth interface
  - **Dirac states** (non degenerate)
  - **massive topological surface states** (degenerate)
- Energy controlled by
  - smoothness of interface
  - applied electric field
- Topological nature
  - Dirac + electric field
  - analogous to Landau levels
  - existence **compatible with topological constraint**

HgTe : Multiple Surface States

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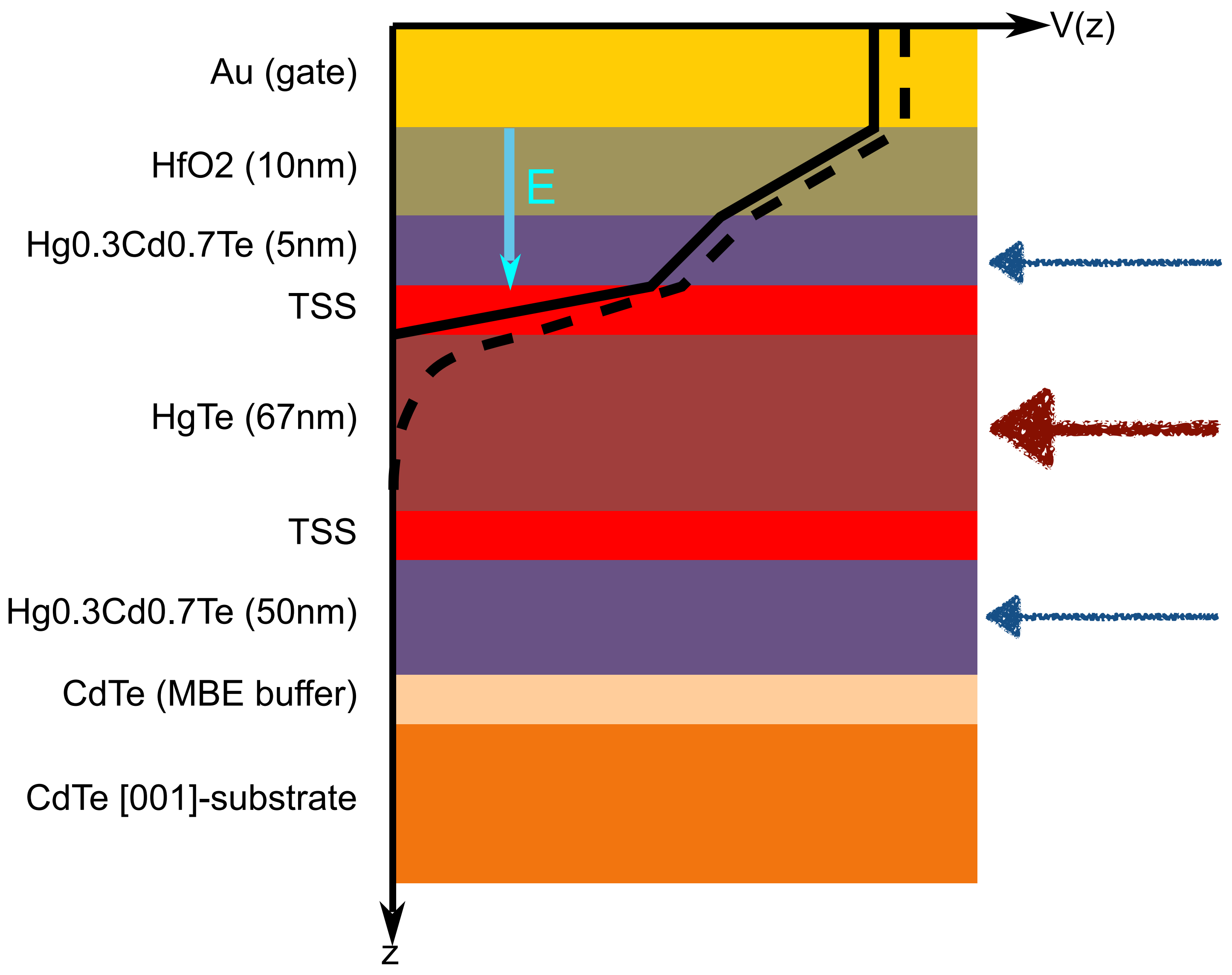
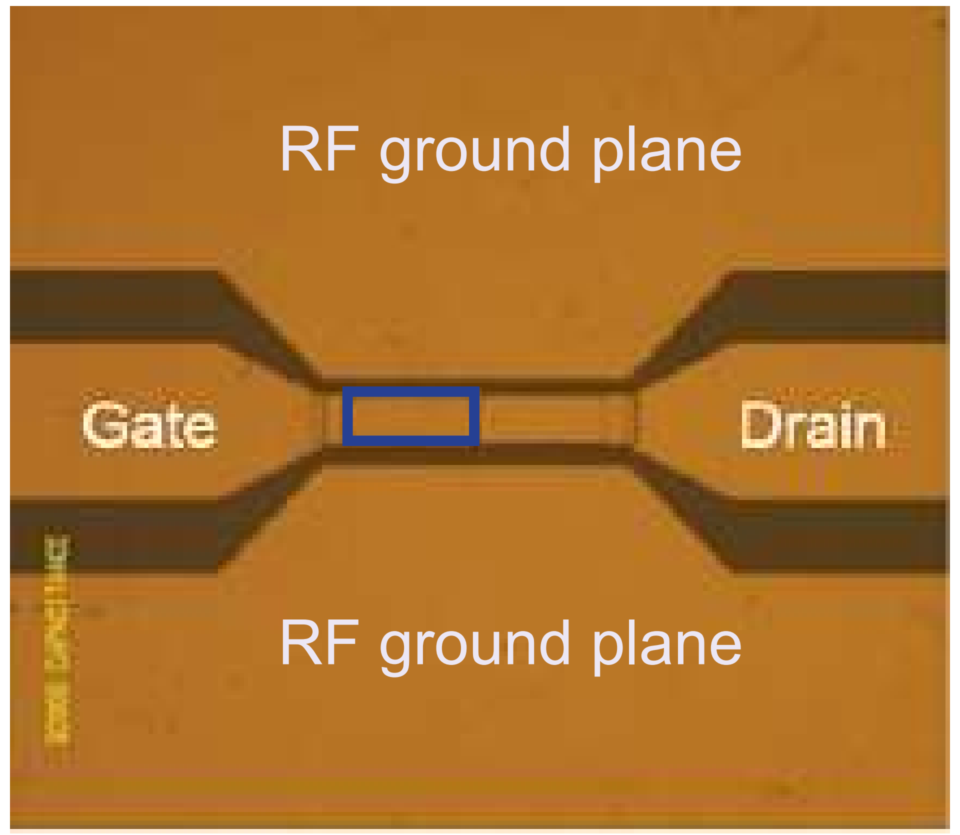
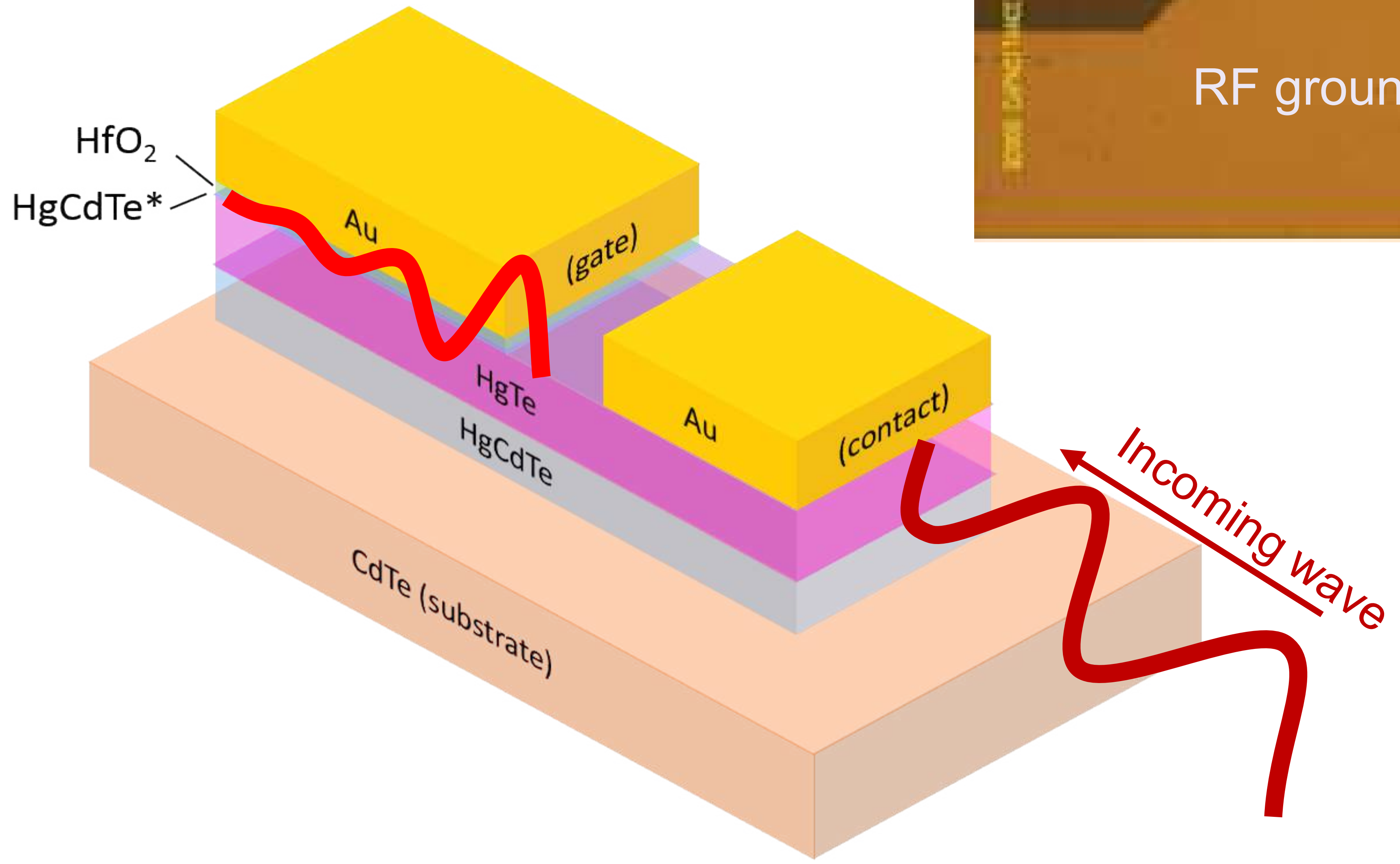


- Bulk 3D Topological Insulator
  - Capping (smooth interface)



- RF capacitor (50 kHz– 8 GHz)
  - probes RF compressibility and resistivity
  - alternative to ARPES
  - allows probe in presence of strong electric field



HgTe : Multiple Surface States

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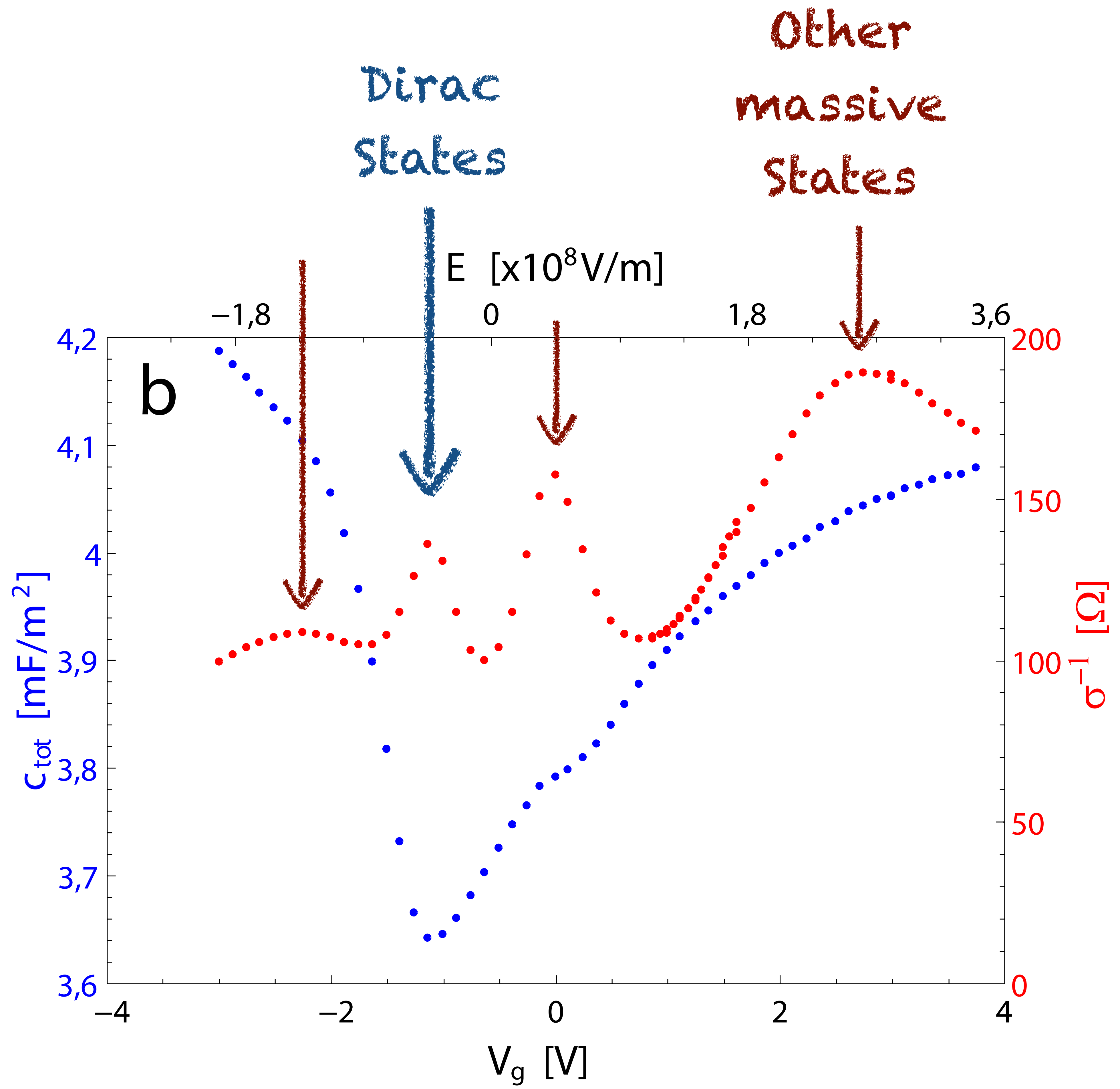


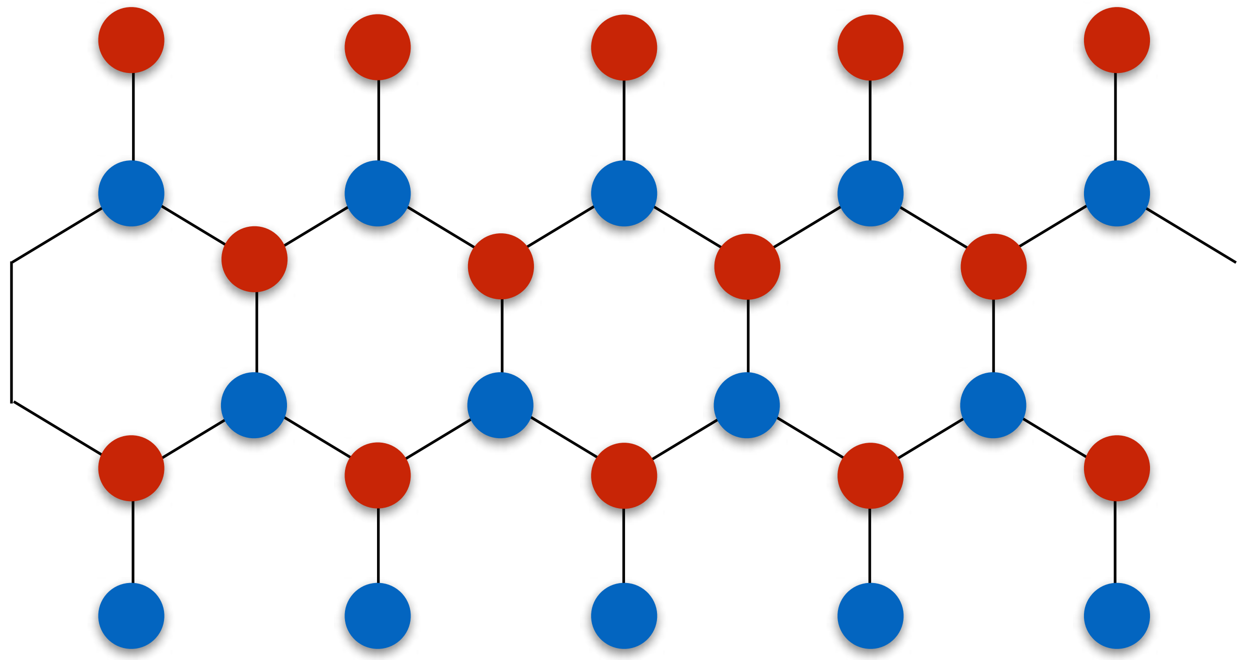
- RF capacitor (50 kHz– 8 GHz)
    - identifies the Dirac cone
    - allows to identify **other massive states**

Chiral / Sublattice Symmetry

ENS-Lyon
M. Guzman / D. Bartolo / D. Carpentier

M. Guzman *et al.* , SciPost (2022)

M. Guzman *et al.* , in preparation (2022)

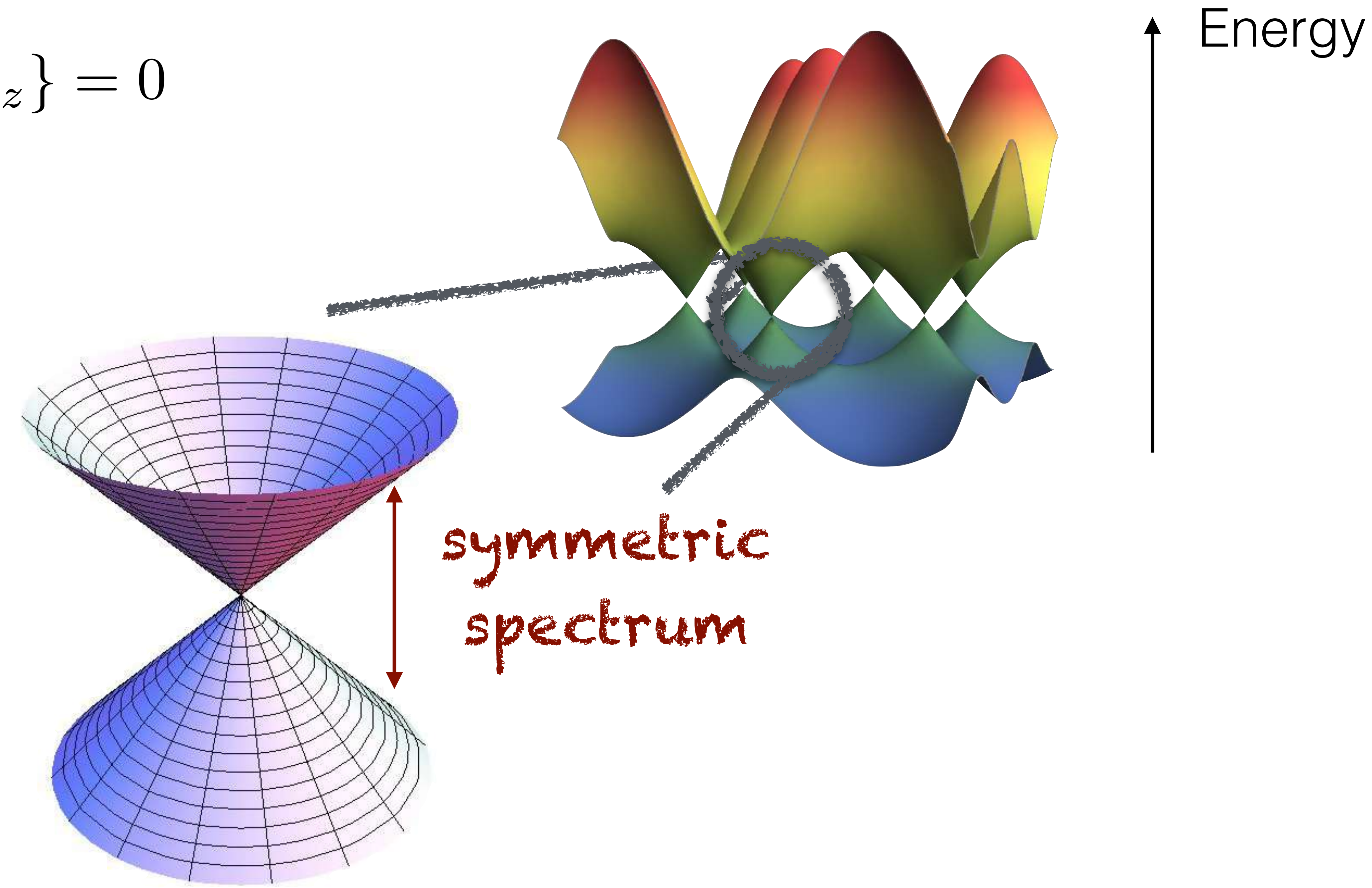


● atome de carbone, sous réseau *A*
● atome de carbone, sous réseau *B*

$$H(\mathbf{k}) = \begin{array}{c} \begin{matrix} \quad A & \qquad B \end{matrix} \\ \begin{pmatrix} \epsilon_0 & t\ \overline{\gamma_{\mathbf{k}}} \\ t\ \gamma_{\mathbf{k}} & \epsilon_0 \end{pmatrix} \end{array} \begin{array}{c} \\ A \\ B \end{array}$$

$$\gamma_{\mathbf{k}} = \left(1 + e^{i\mathbf{k}.\mathbf{a}_2} + e^{i\mathbf{k}.\mathbf{a}_3}\right)$$

$$\{H(\mathbf{k}) - \epsilon_0\mathbb{I}, \sigma_z\} = 0$$



Property of chiral symmetry :

- unitary operator $\mathbb{C}$, which anticommutes with H: $\{H, \mathbb{C}\} = 0$
- if $|\psi\rangle$ is eigenstate of energy E, then $\mathbb{C}|\psi\rangle$ is an eigenstate with energy -E

Chiral / Sublattice Symmetry

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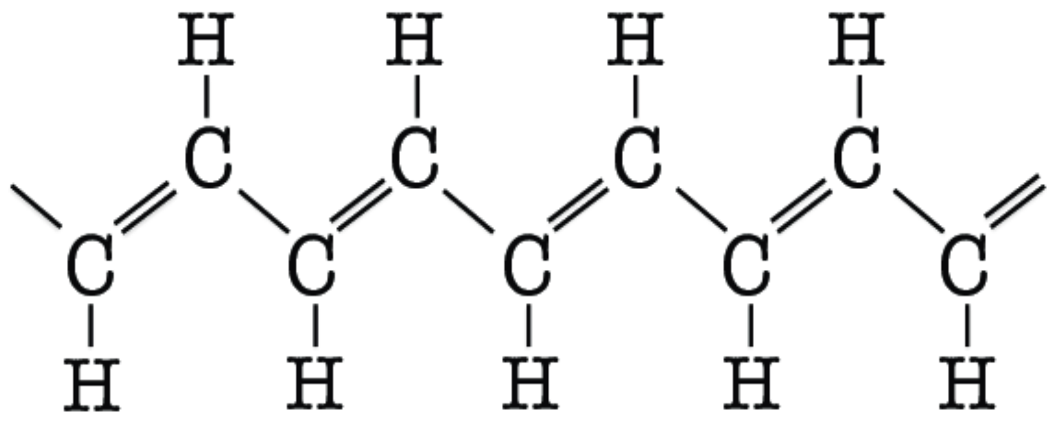
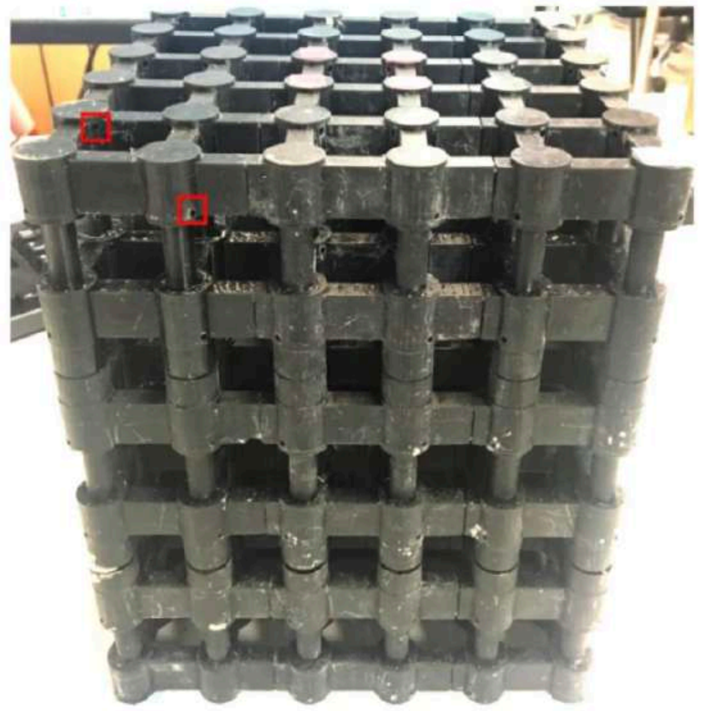
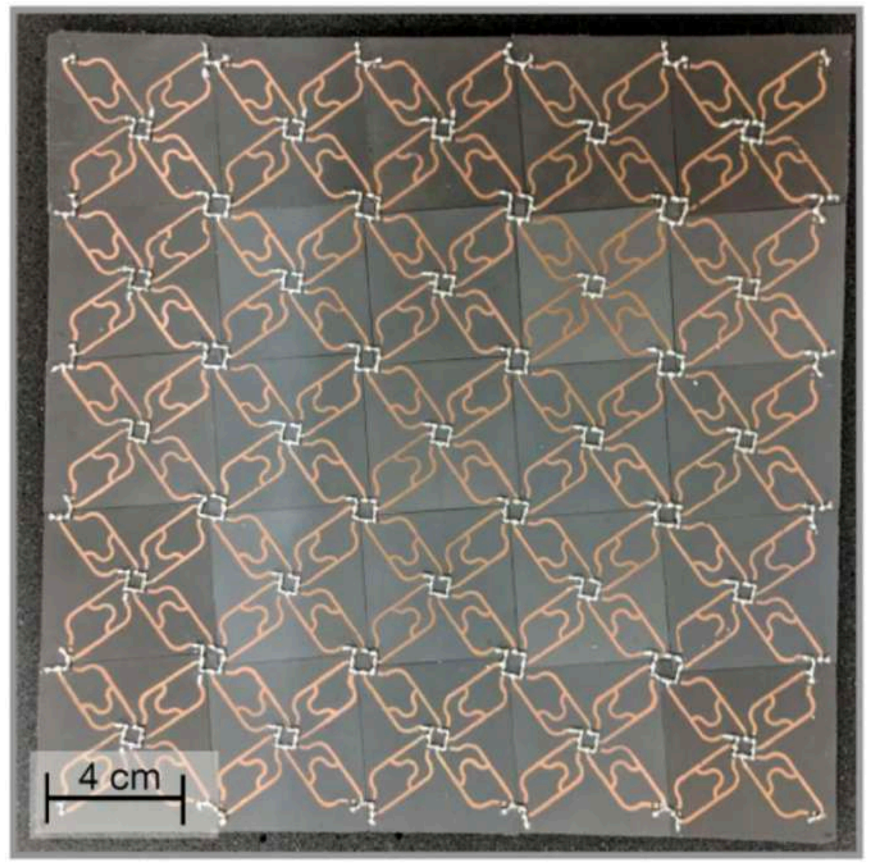
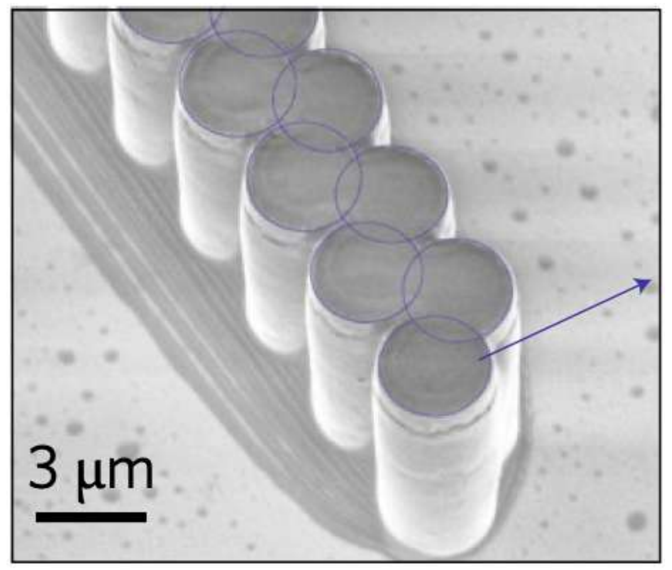




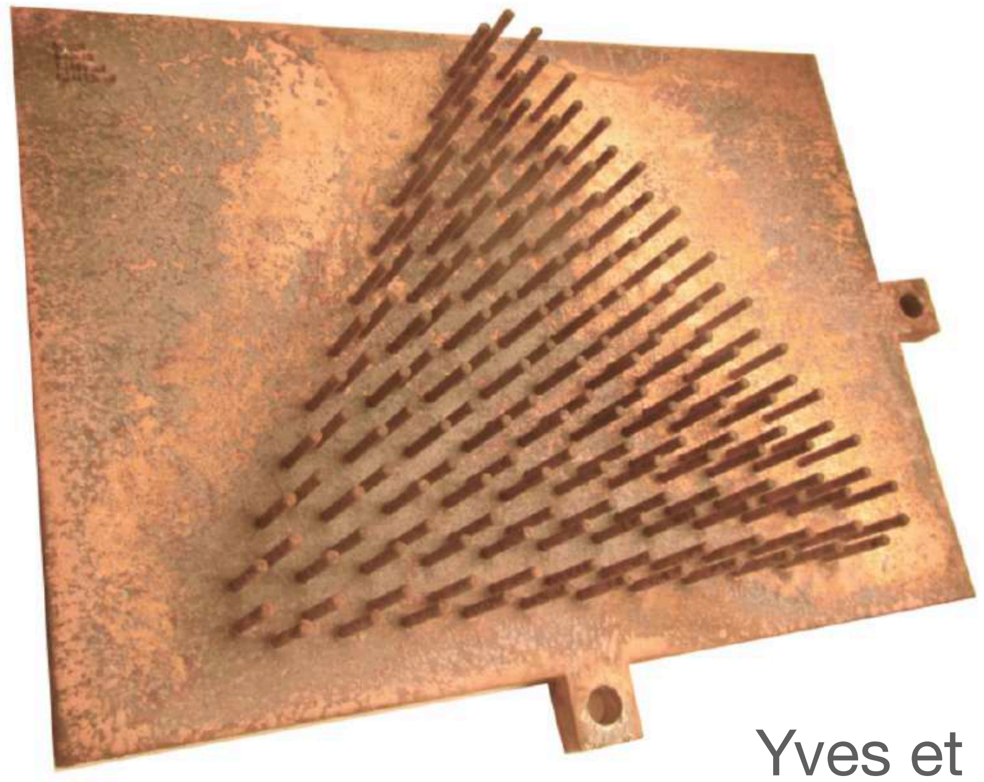
Ni et al.



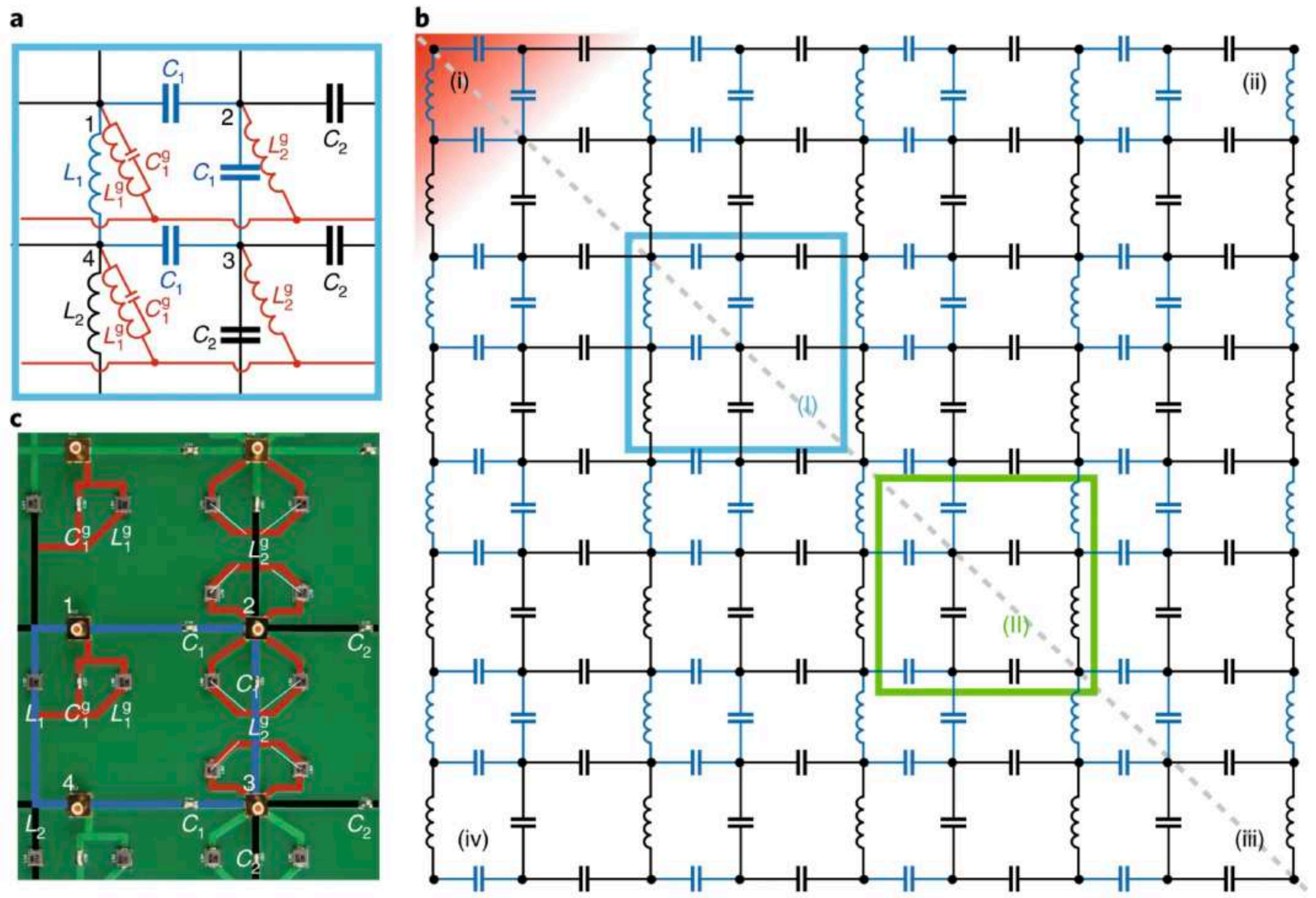
Peterson et al.



St-Jean et al.



Yves et al.



Imhof et al.

Chiral / Sublattice Symmetry: analogy with charges

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Accumulation of charges

Chiral / Sublattice Symmetry: analogy with charges

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Accumulation of charges

→ Equivalent characterization of chiral state : topological chiral polarization

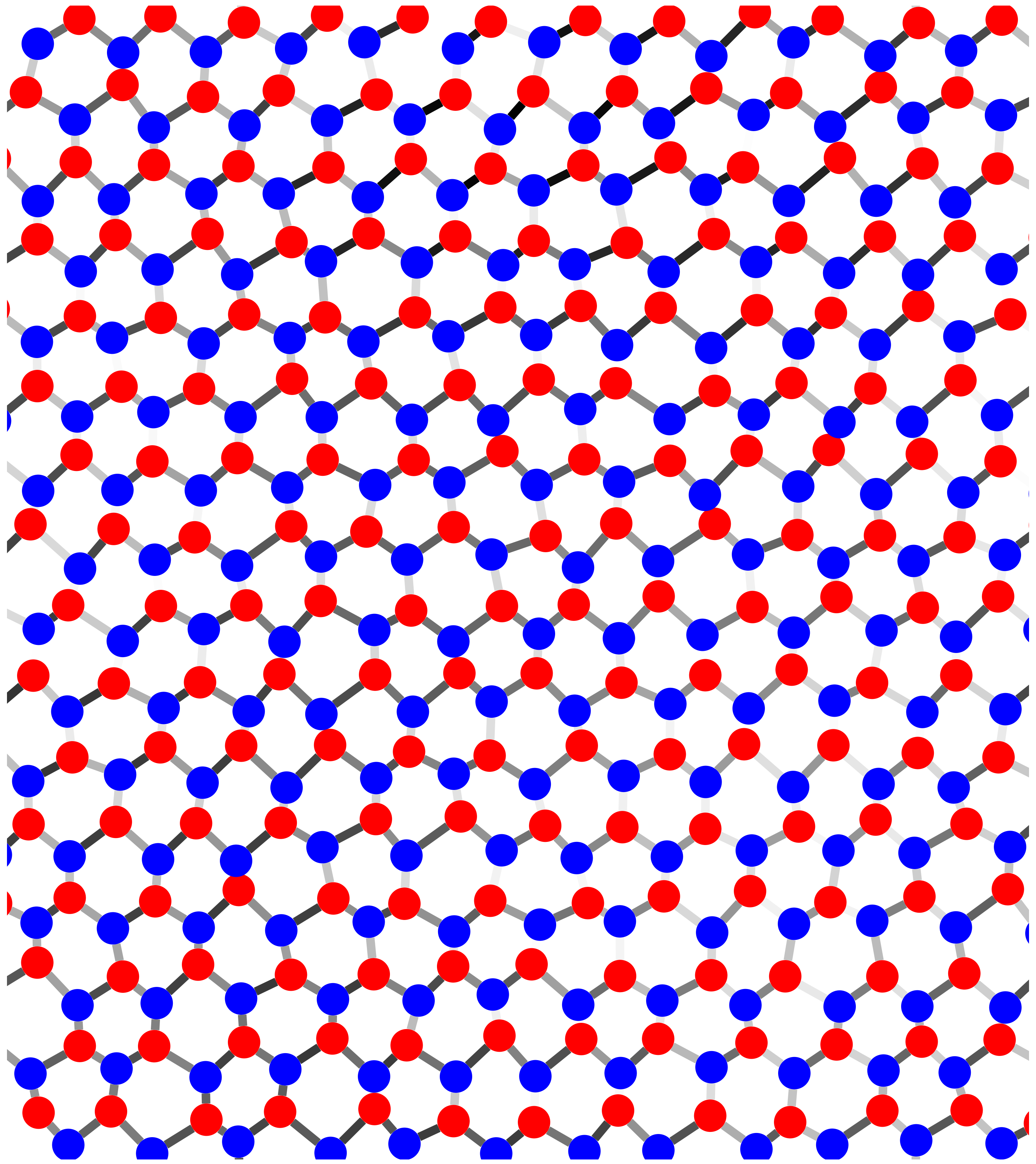
(Disordered) Chiral topological phase

ENS-Lyon
M. Guzman / D. Bartolo / D. Carpentier

M. Guzman *et al.* , SciPost (2022)

M. Guzman *et al.* , in preparation (2022)

Chiral 2D state (graphene) with random positions, random couplings



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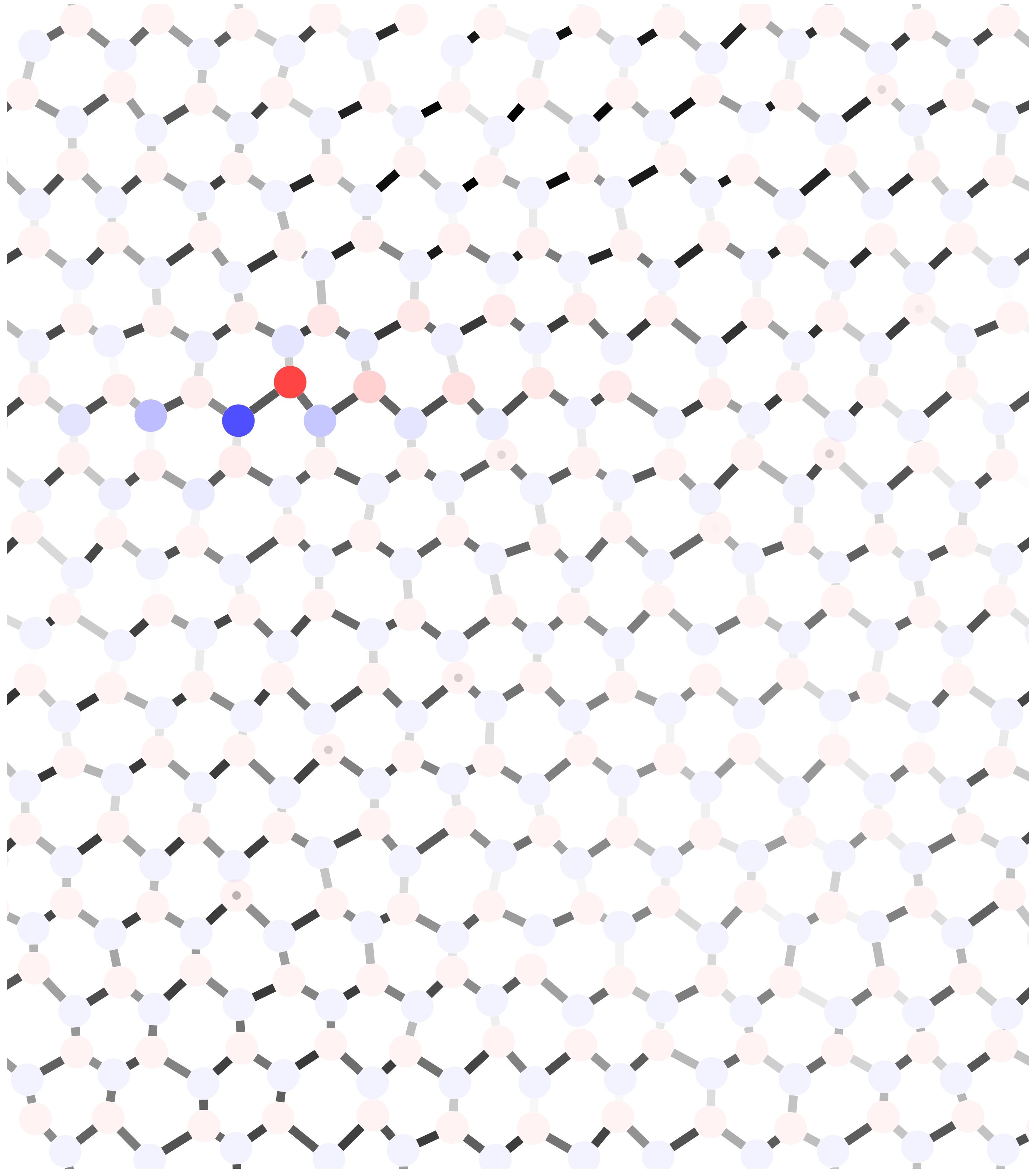
Wannier state W_i



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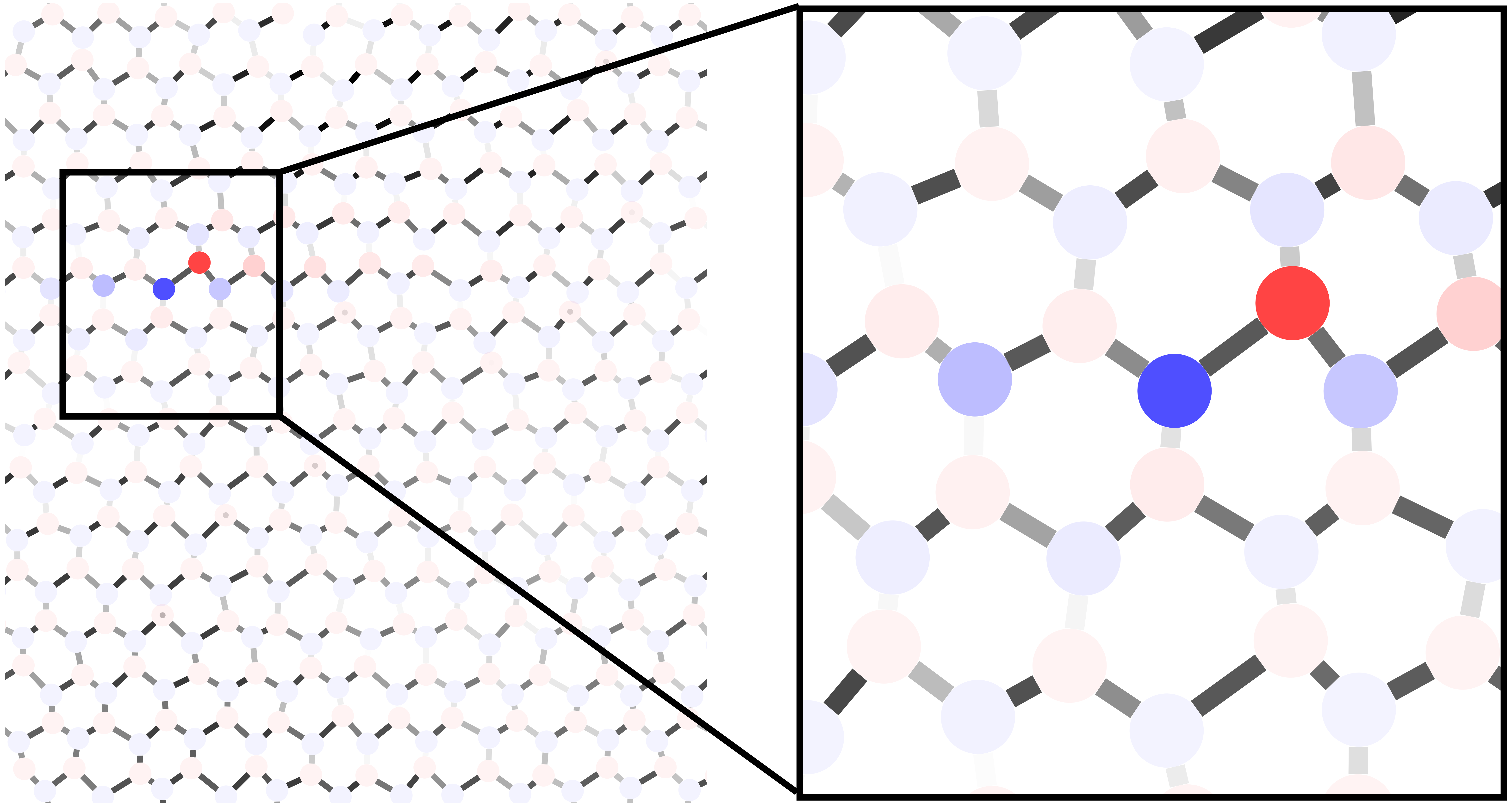

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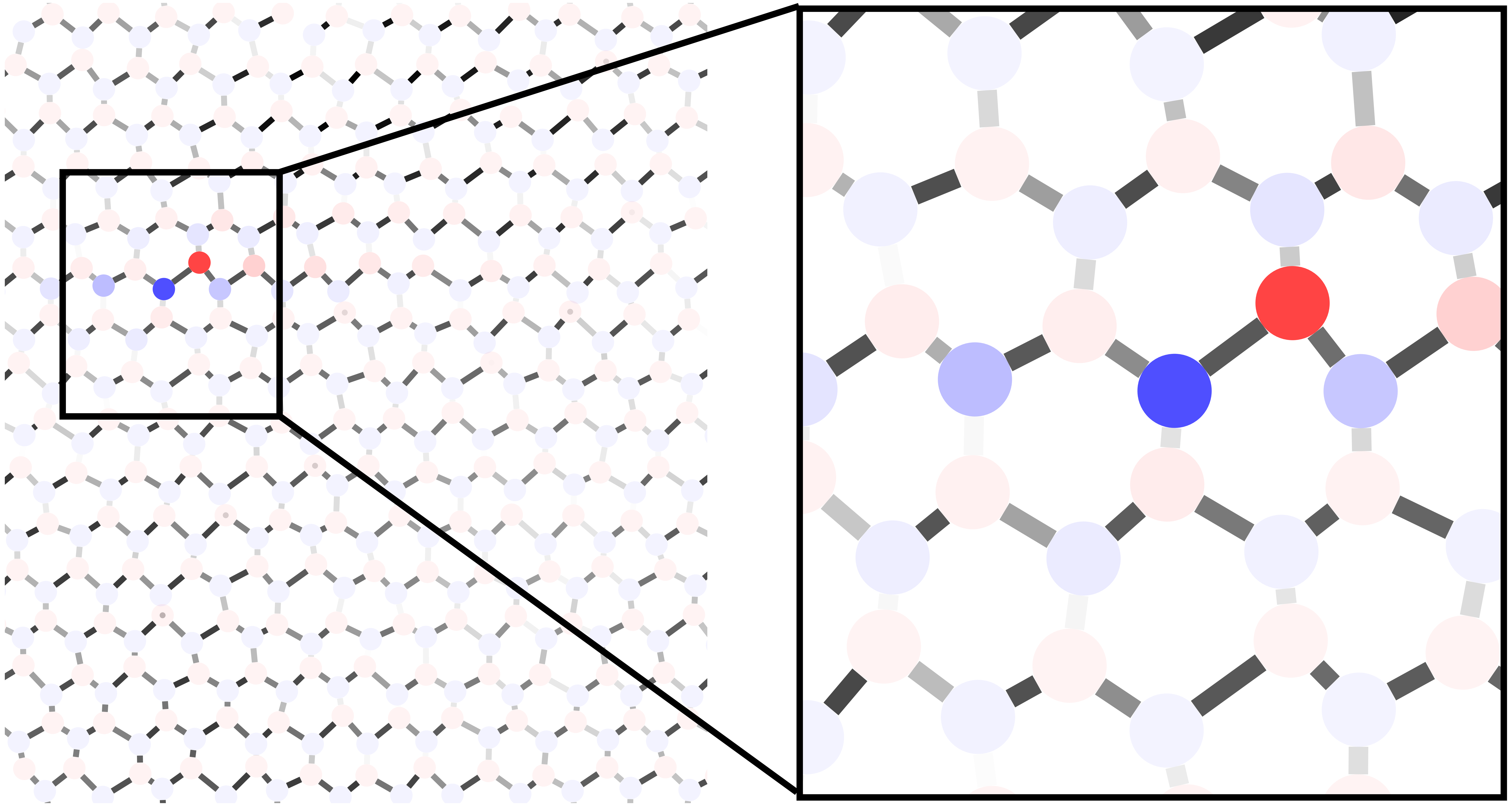
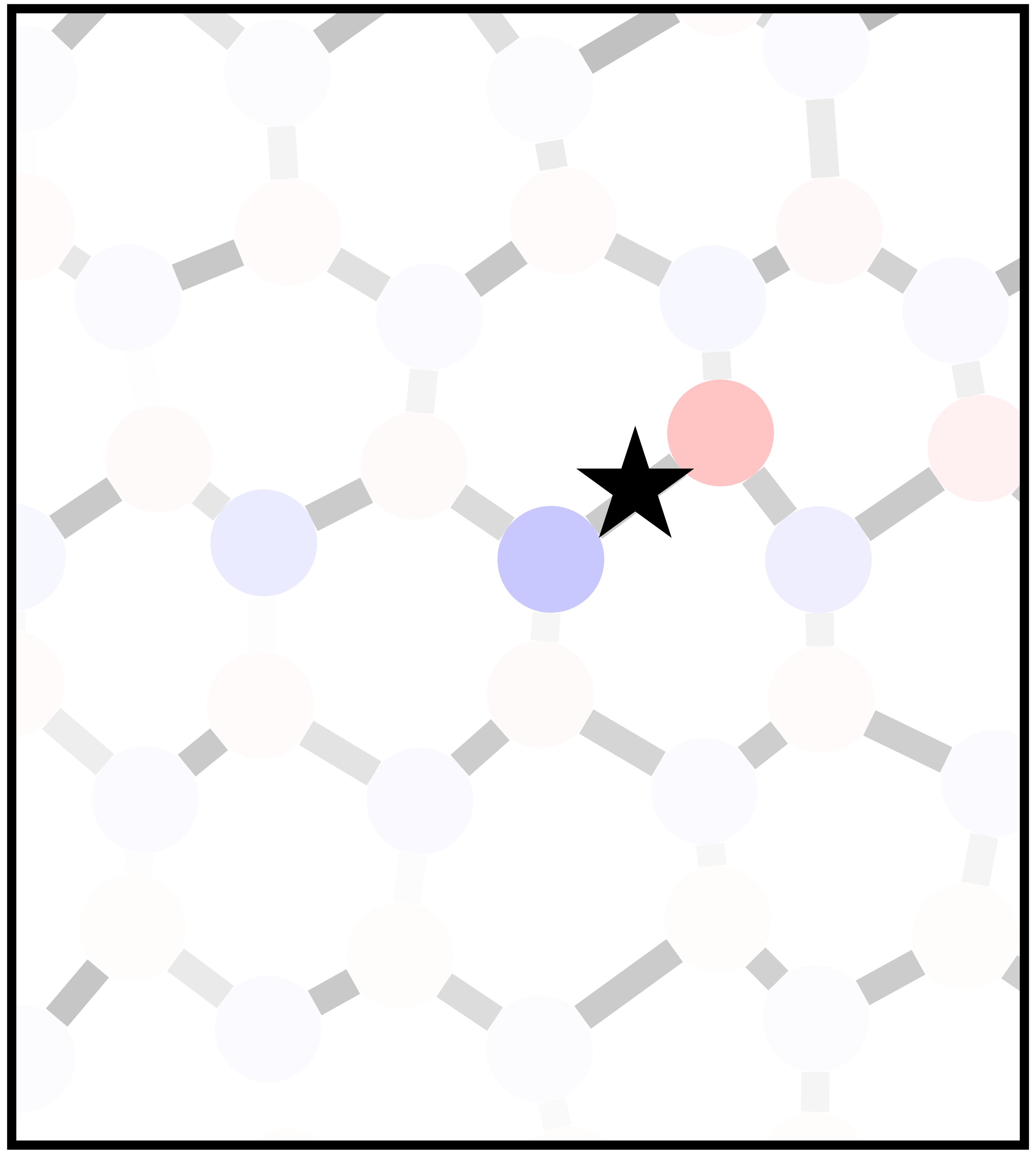


Wannier center $\overline{\mathbf{r}}_i = \langle W_i \,|\, \hat{\mathbf{r}} \,|\, W_i \rangle$



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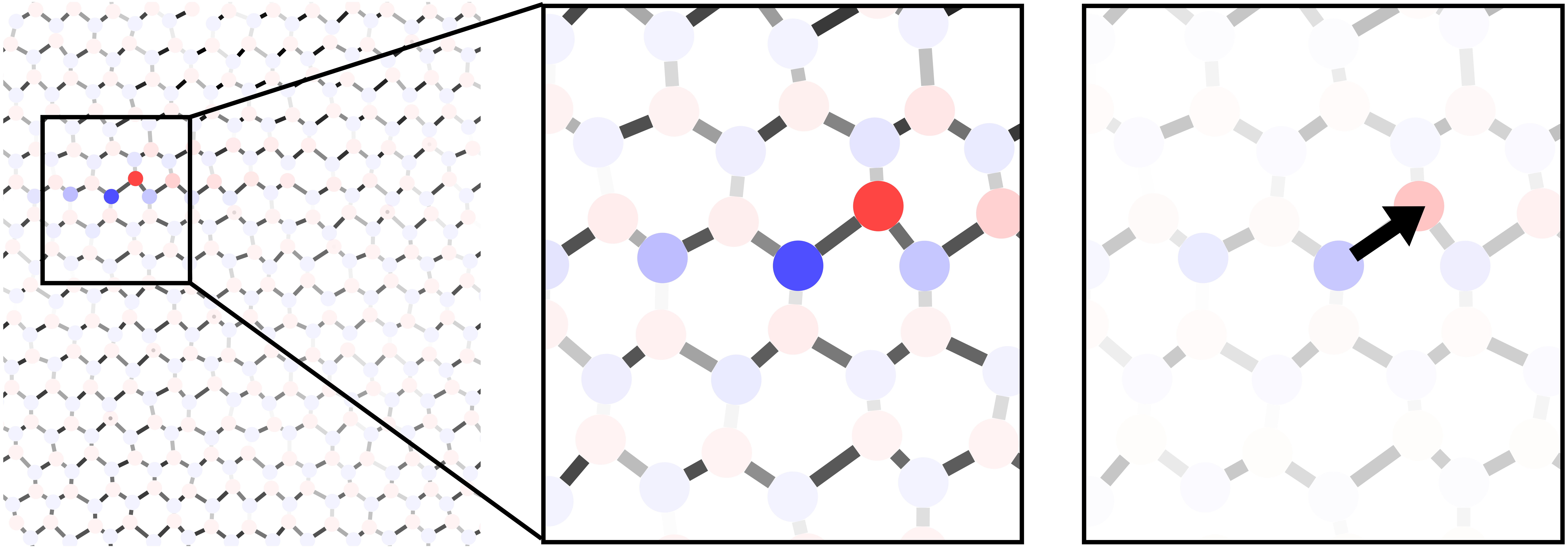
Wannier state W_i

Topological indicator: Chiral polarization $\mathbf{\Pi}_i = 2\langle W_i | \mathbb{C}\hat{\mathbf{r}} | W_i \rangle$



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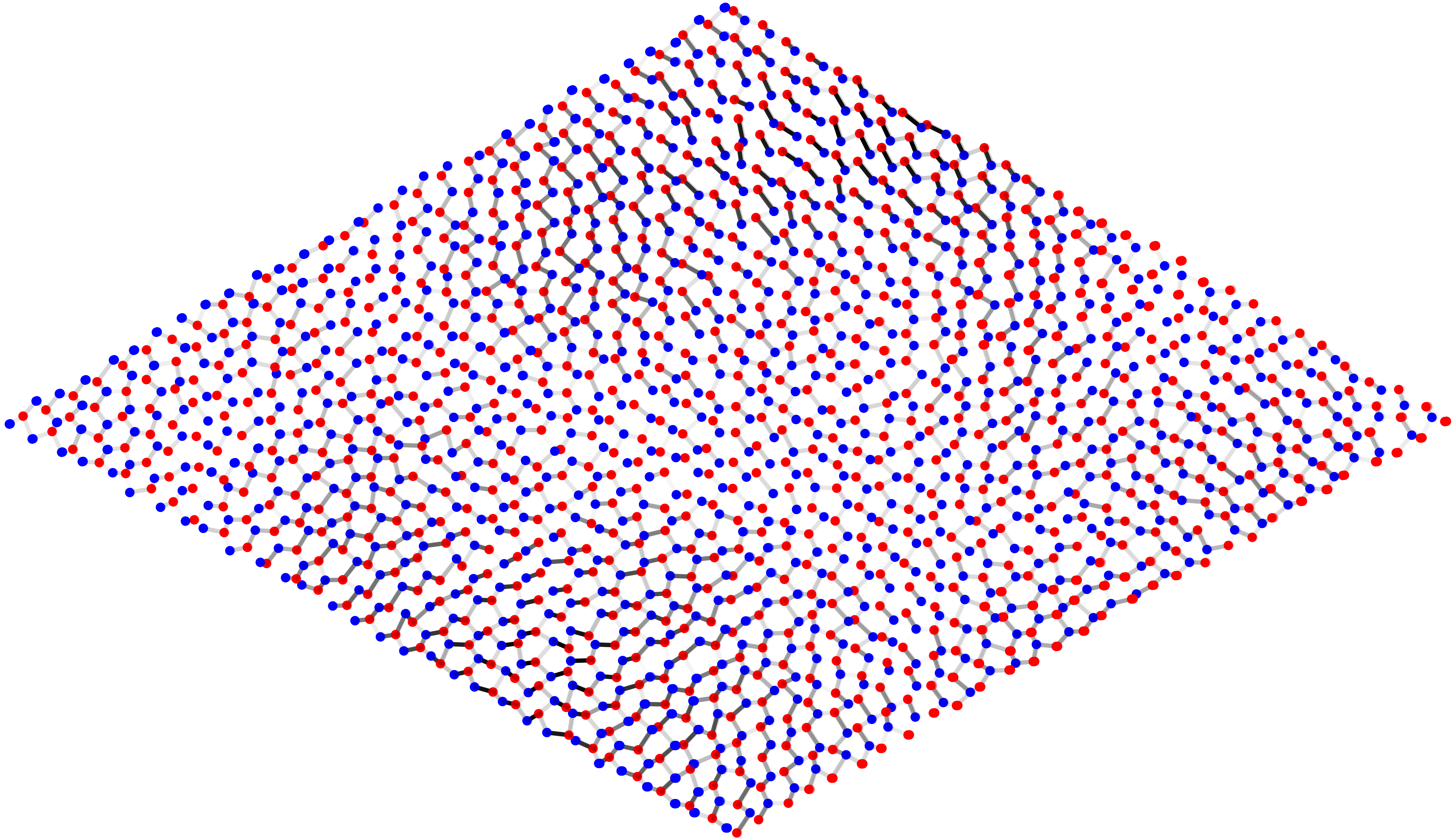

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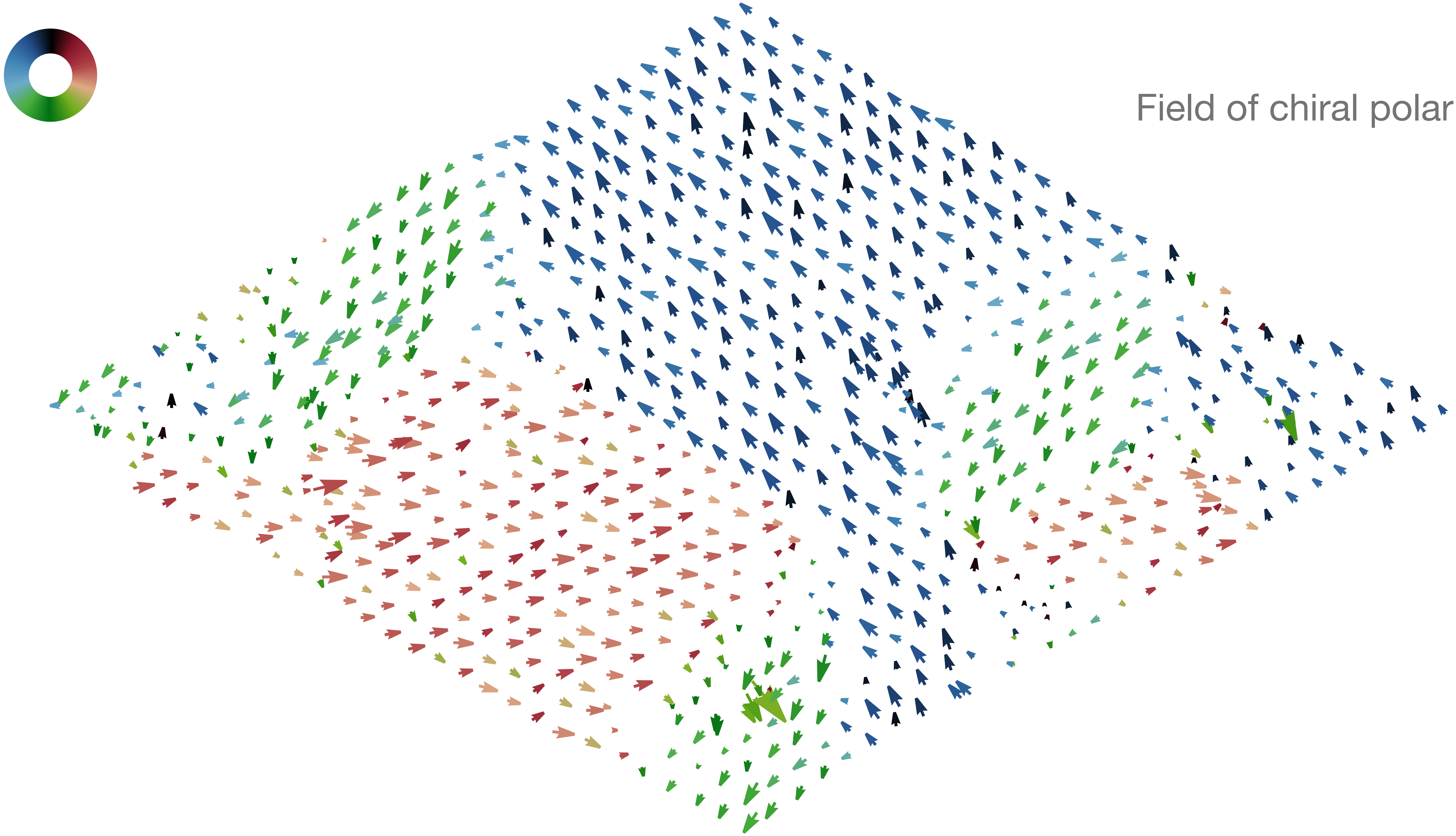

Field of chiral polarization $\mathbf{\Pi}$

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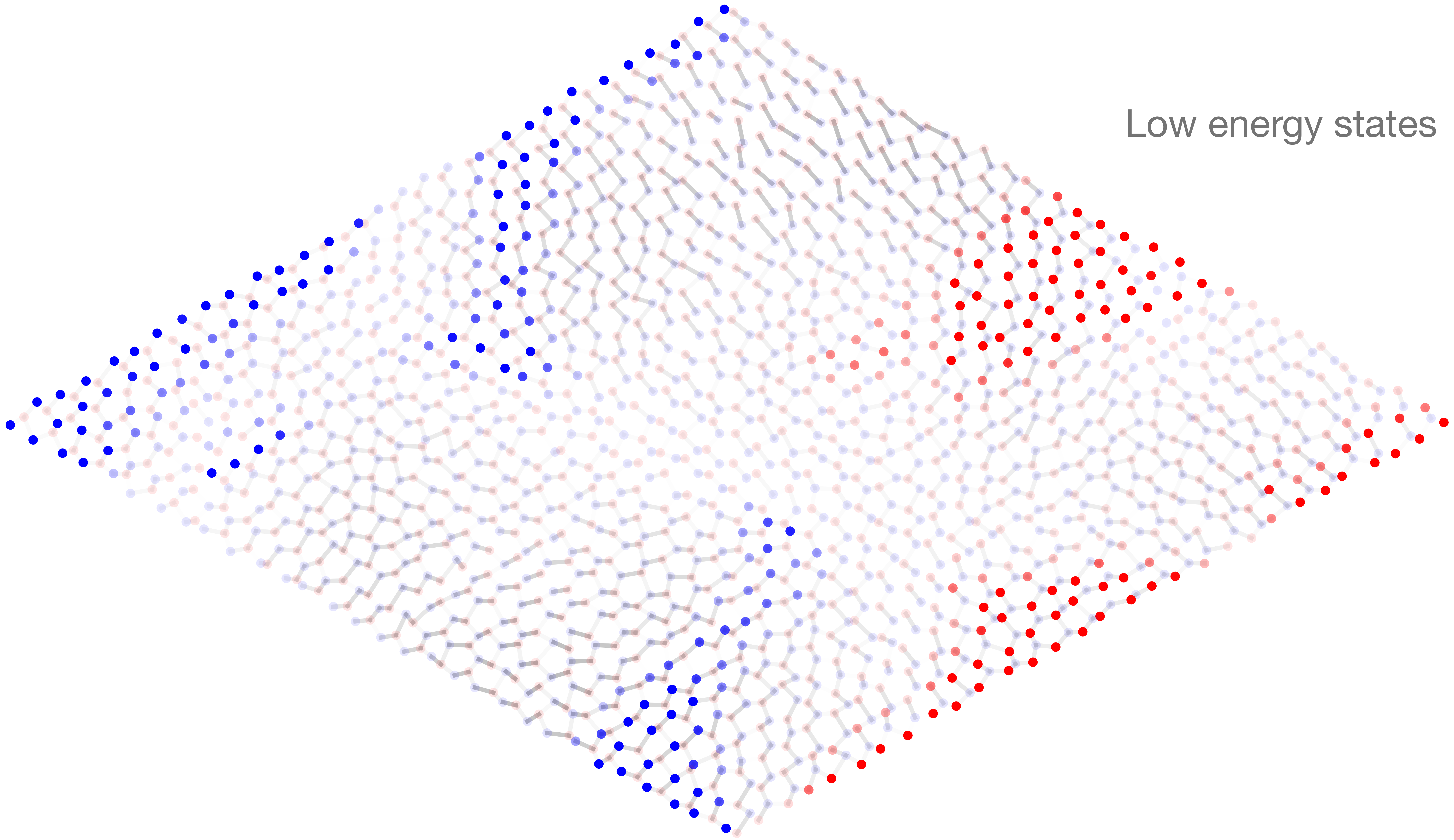

Low energy states

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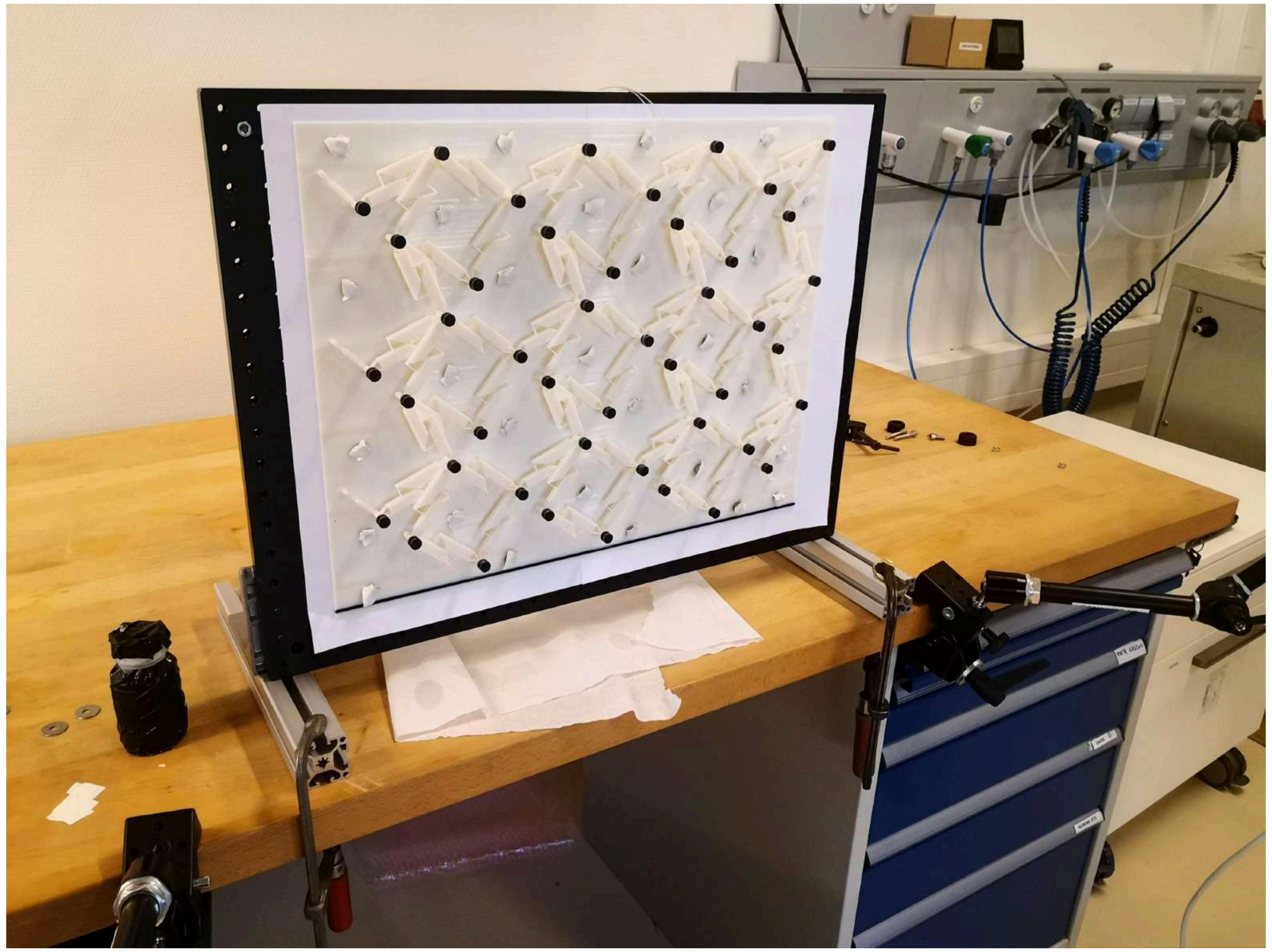

Mechanical metamaterial

- A sites : beads, B sites : springs
- Hit the system: excite deformations
- Dynamical study of chiral polarization and low energy topological states

(Disordered) Chiral topological phase

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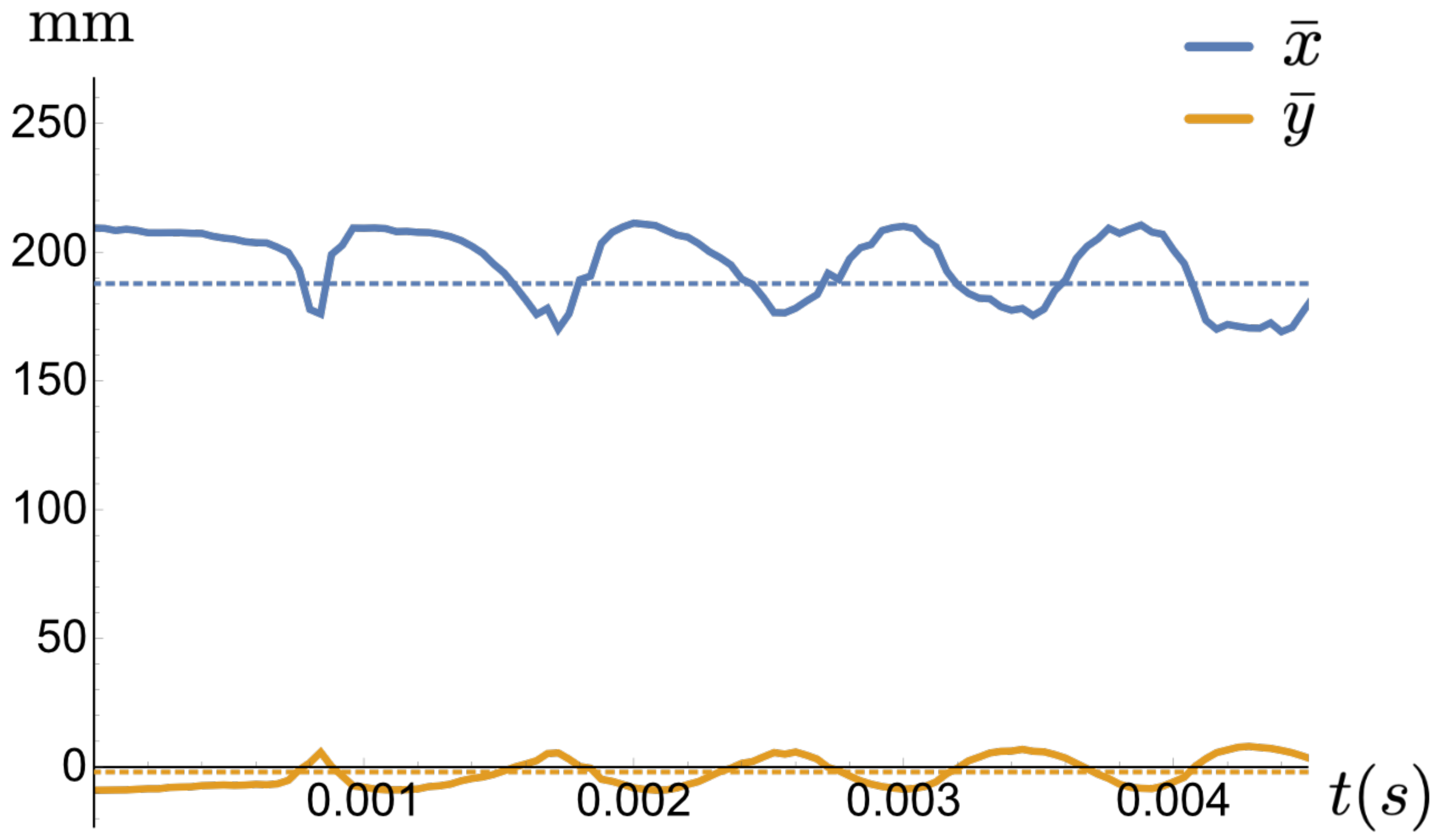
M. Guzman *et al.* , SciPost (2022)

M. Guzman *et al.* , in preparation (2022)

Wannier center

$$\bar{\boldsymbol{x}} = \langle \Psi | \hat{\boldsymbol{x}} | \Psi \rangle$$



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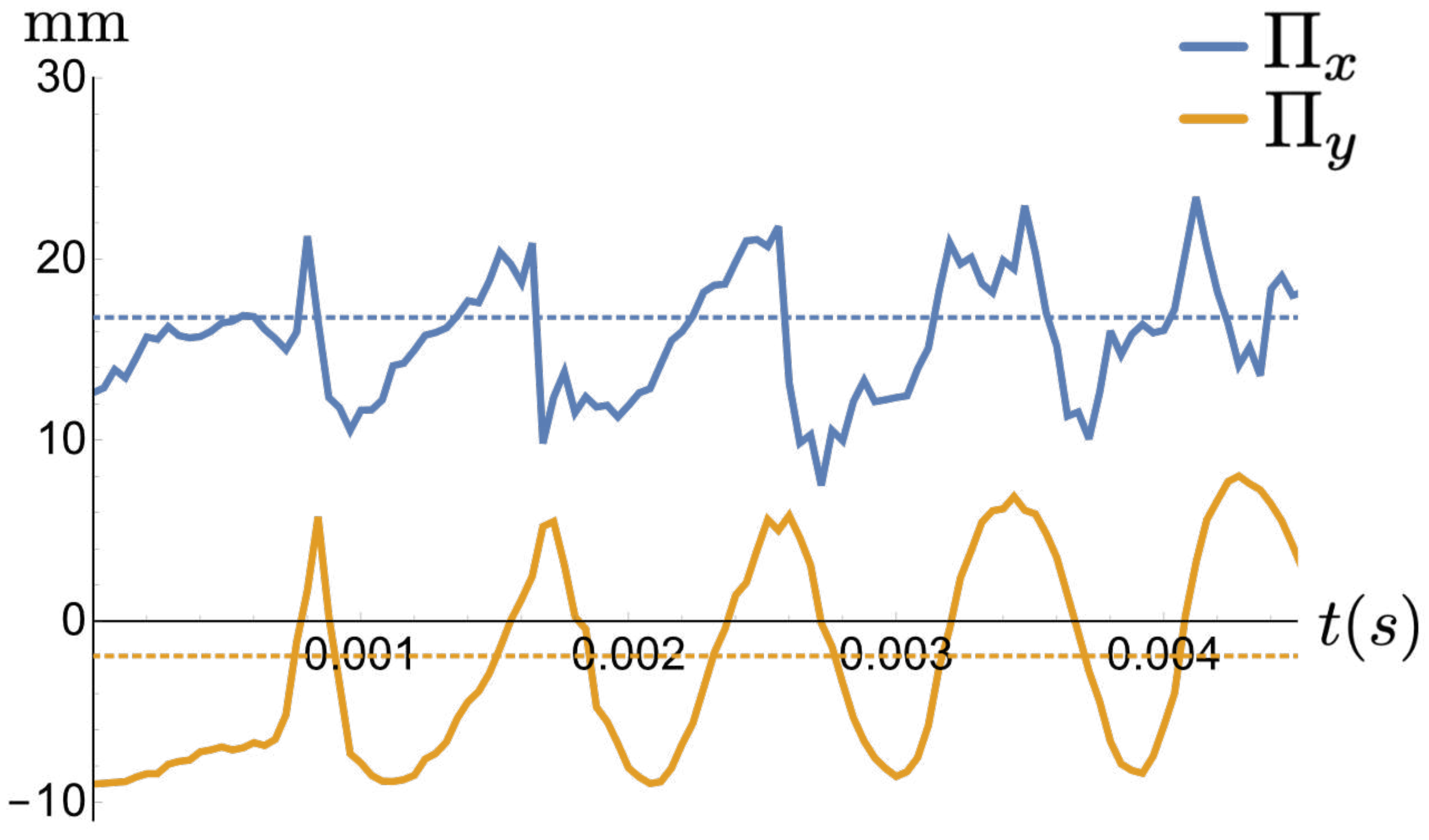

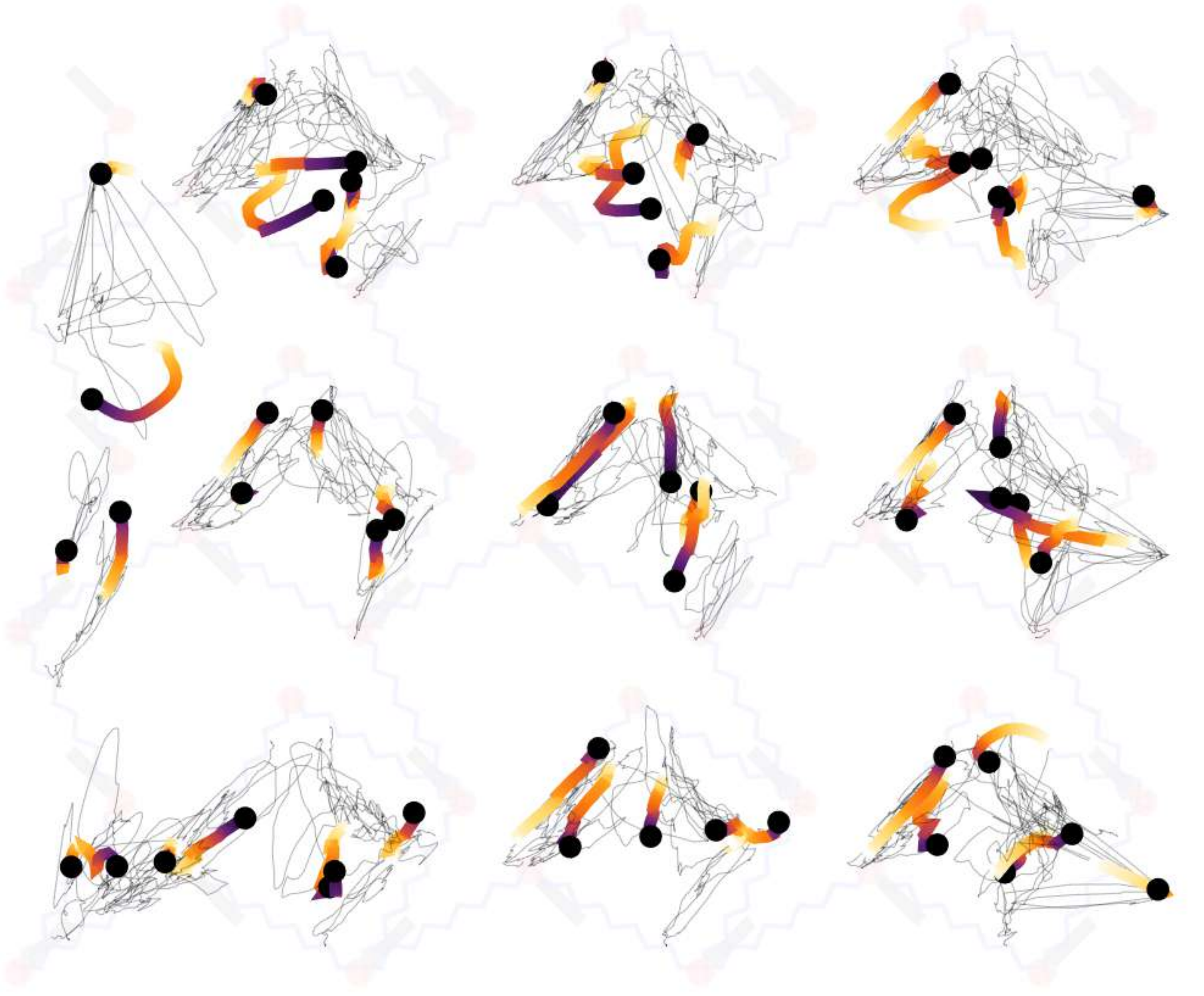

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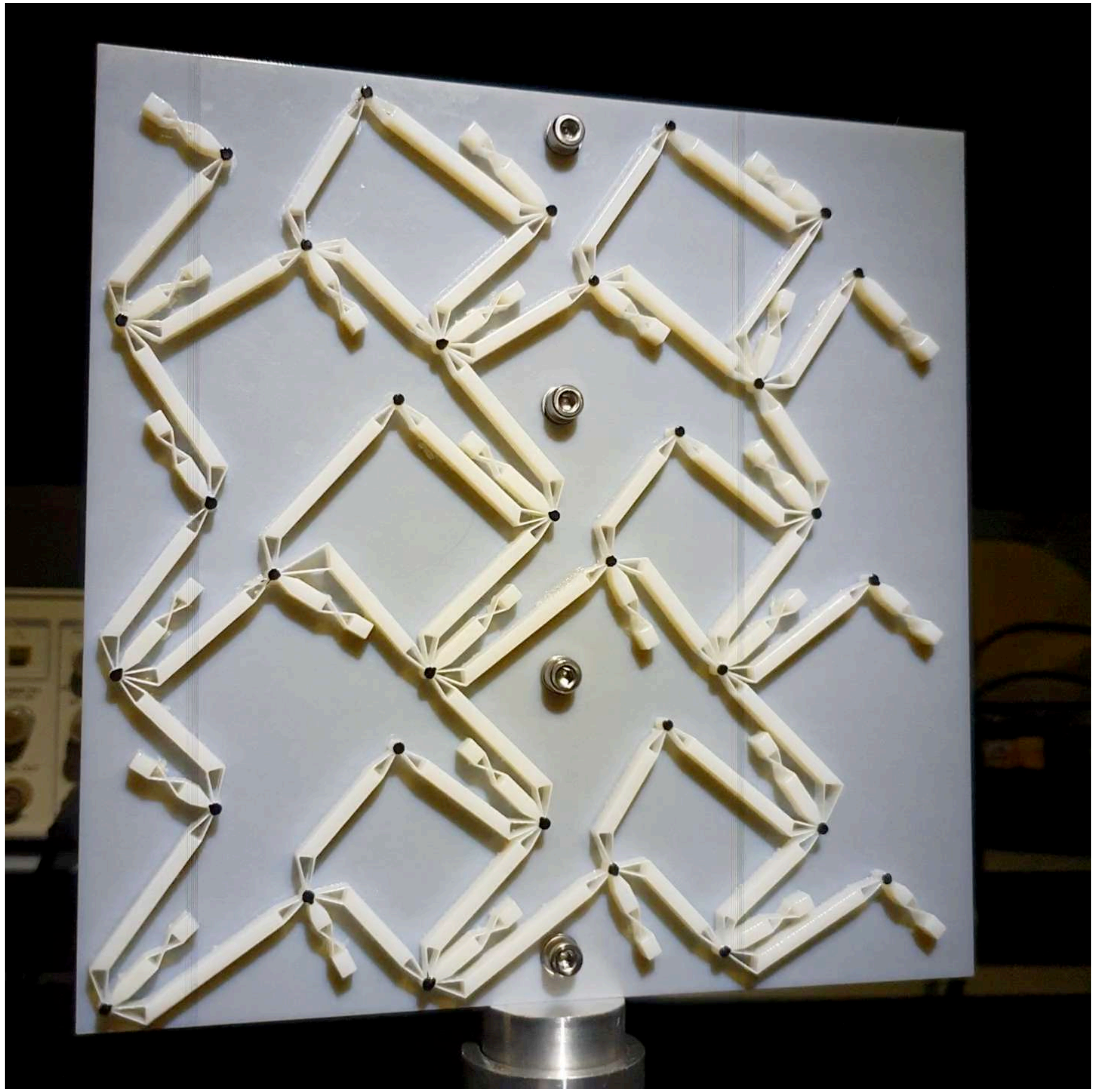

Prediction of corner / edge states

(Disordered) Chiral topological phase

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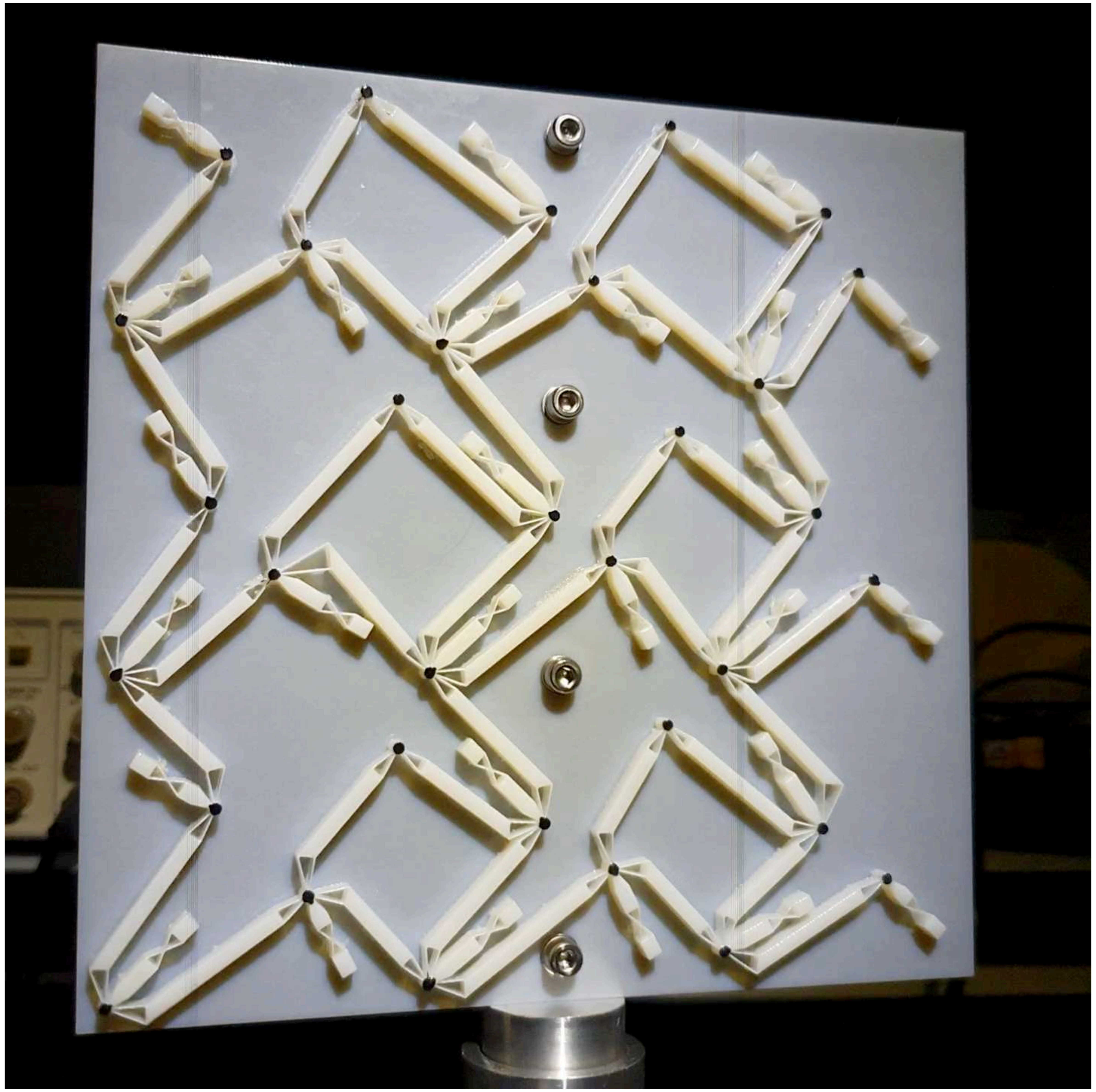

Prediction of corner / edge states

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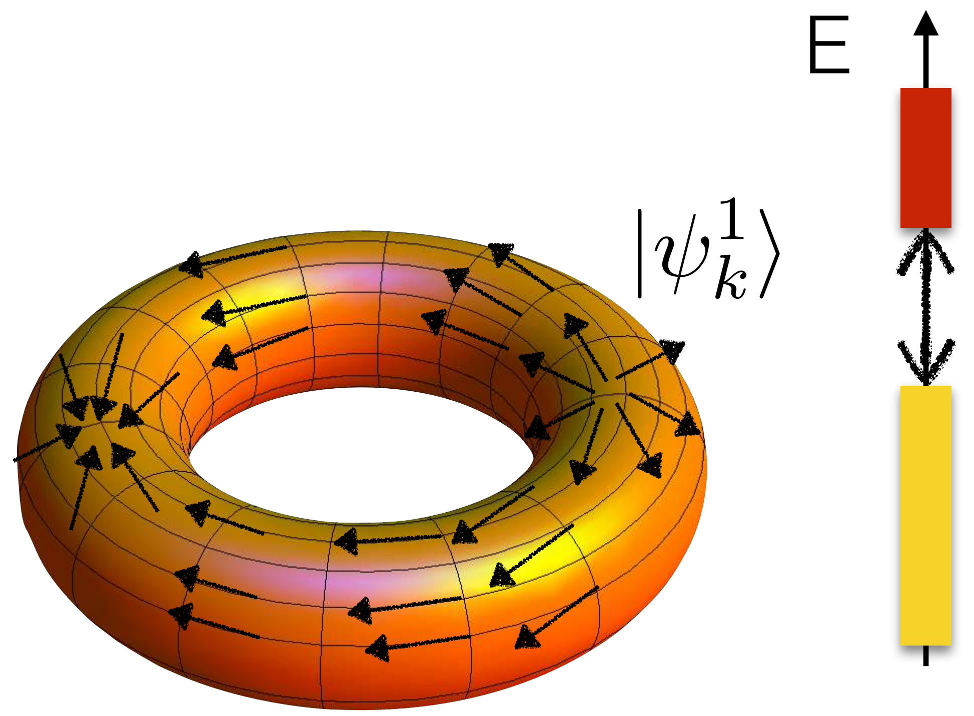

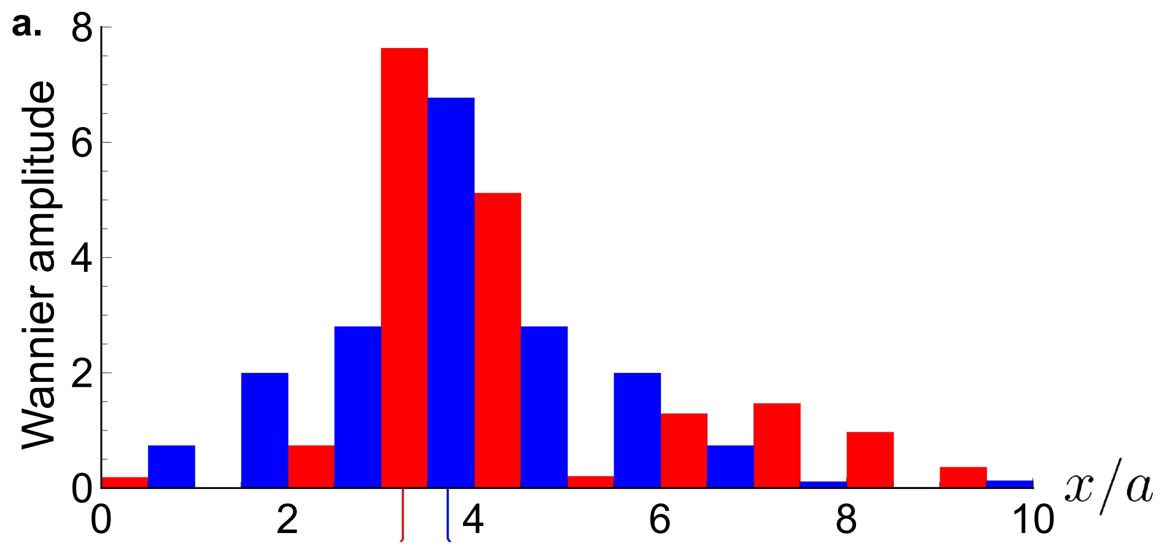

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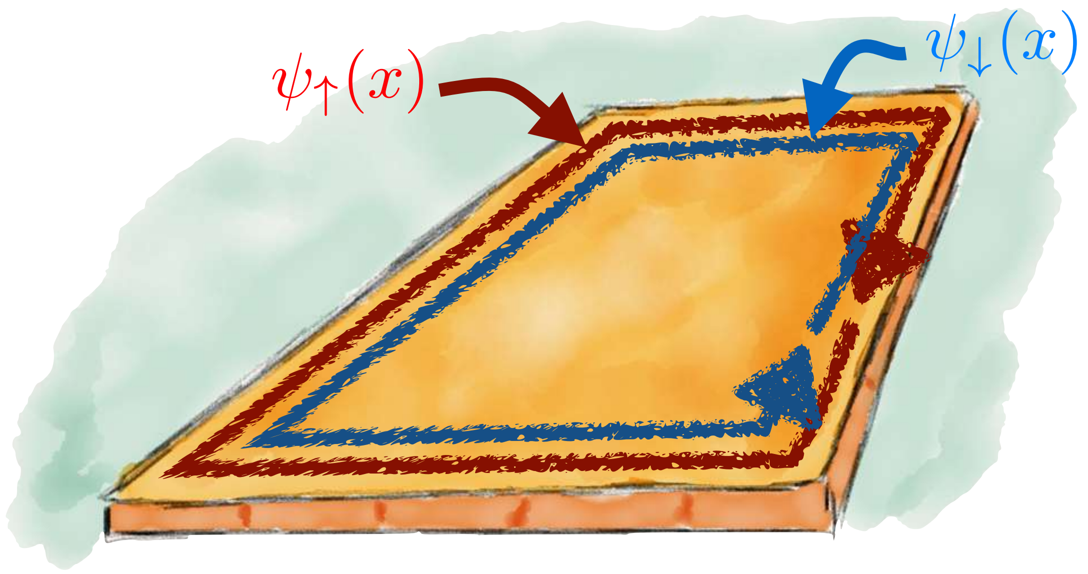

III. Measurements: by time evolution

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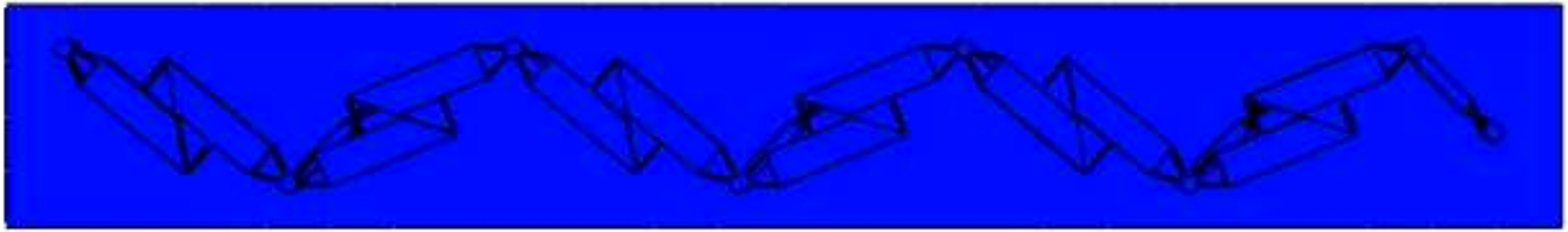

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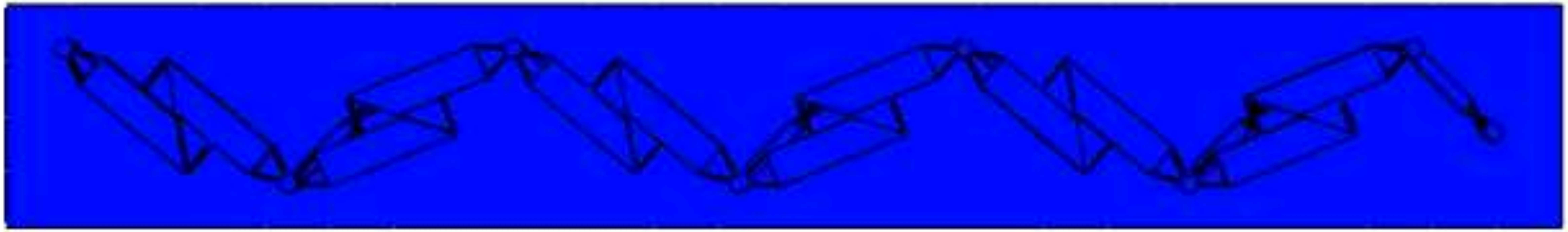

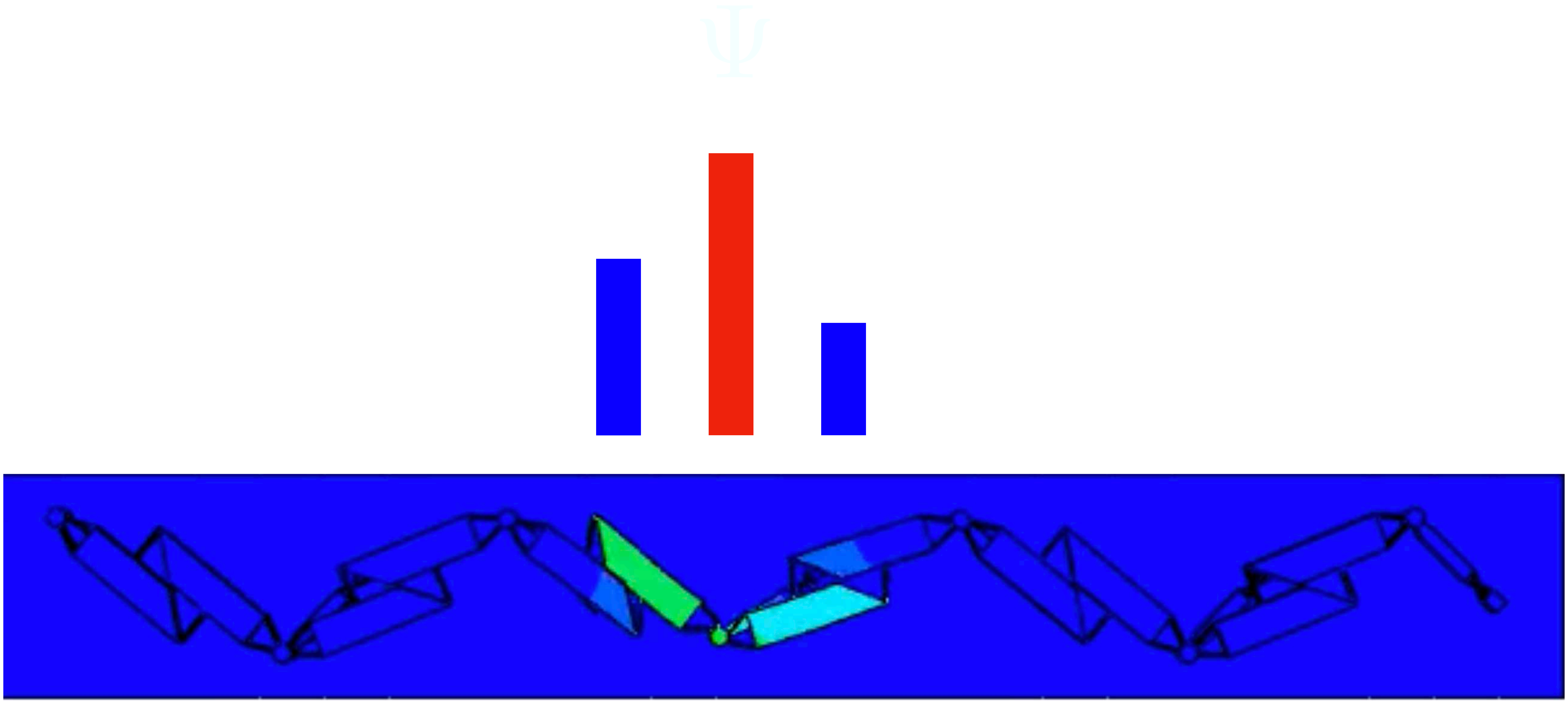
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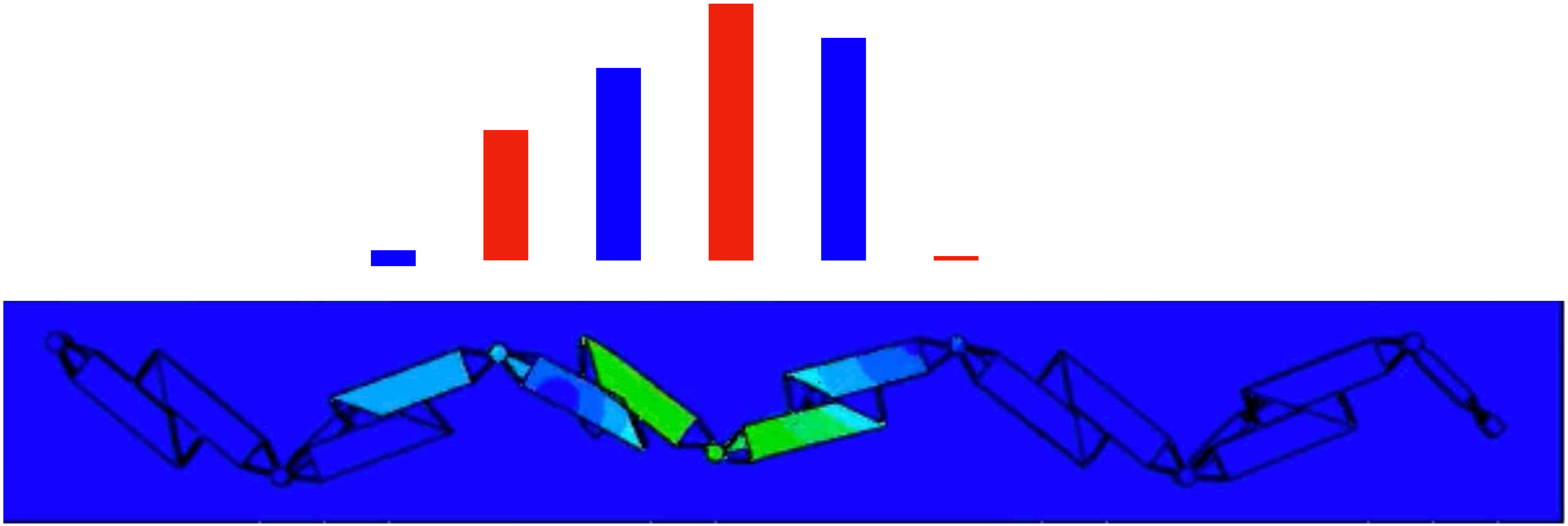

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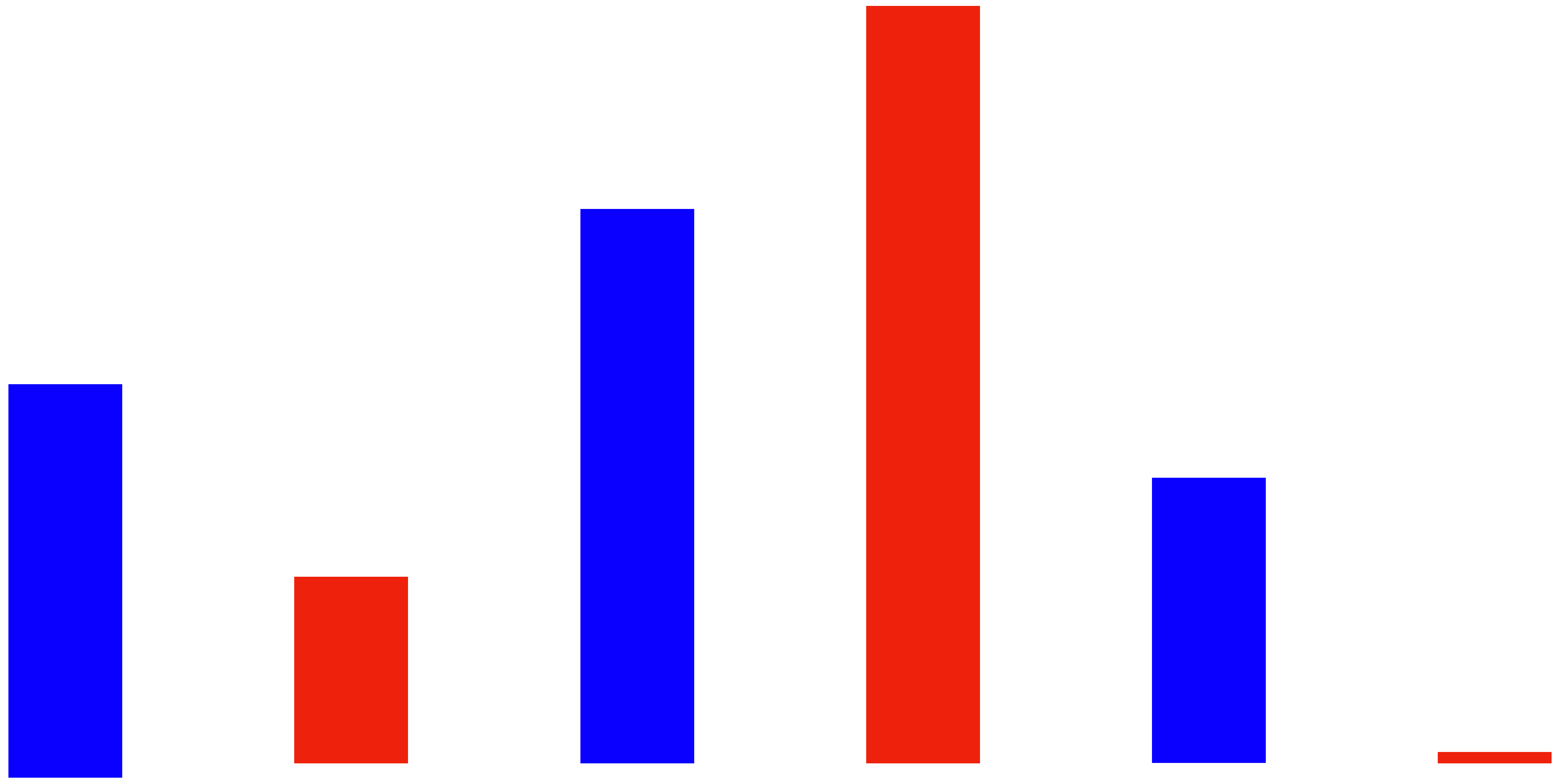

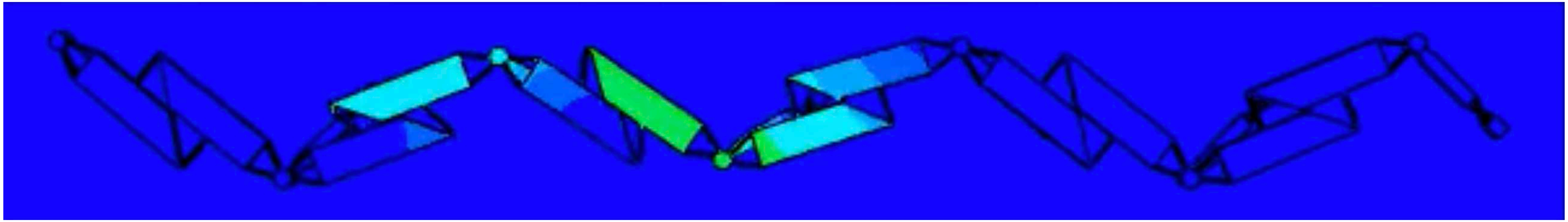

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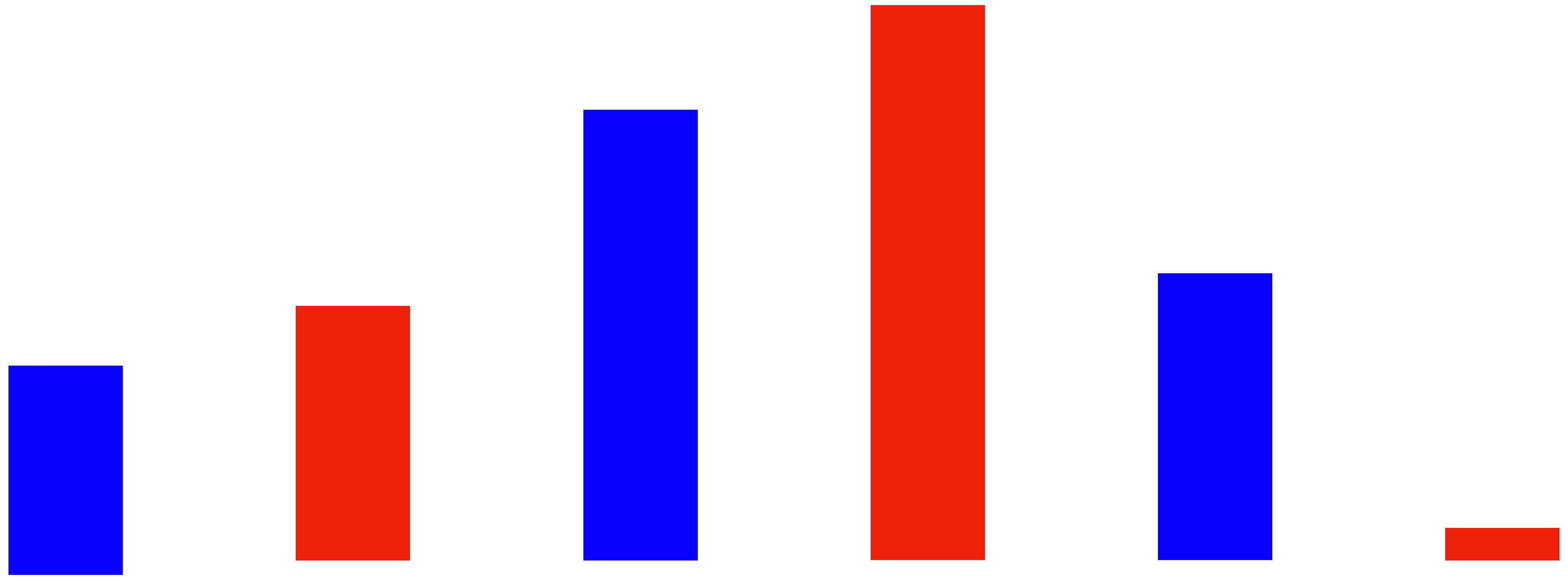
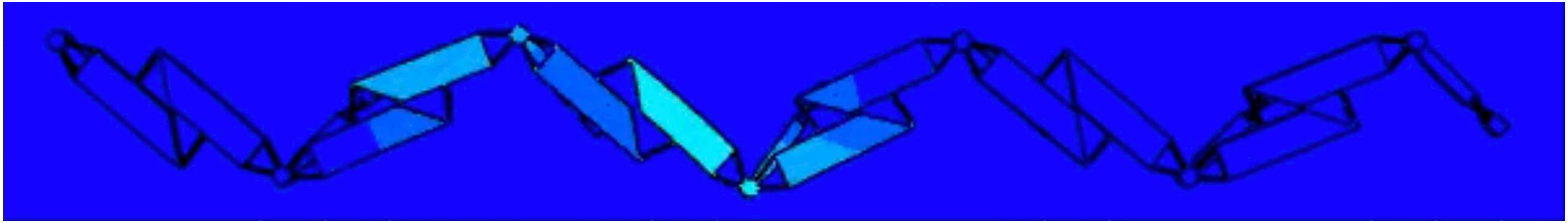
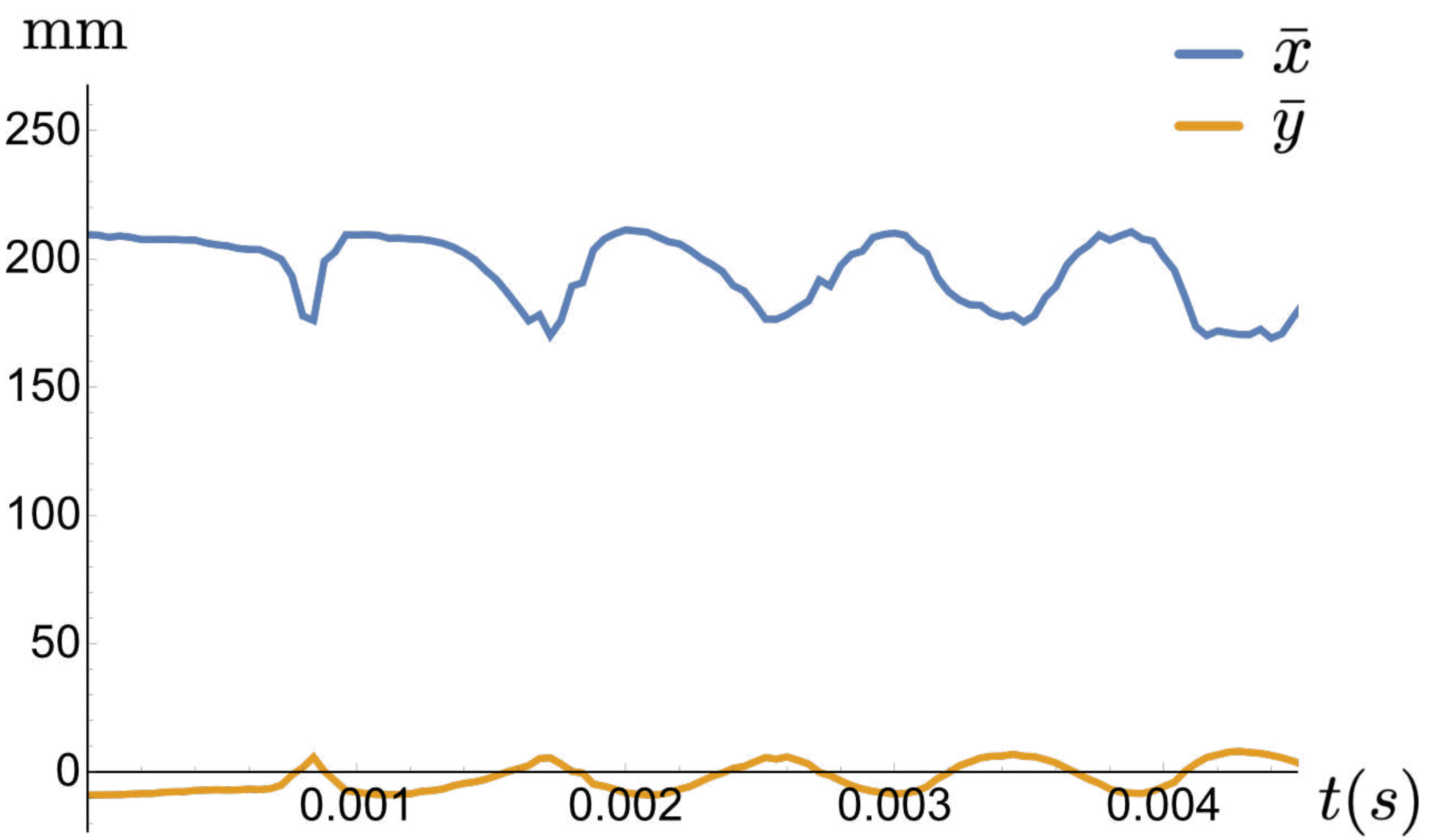




Center of perturbation

$$\bar{\boldsymbol{x}} = \langle \Psi | \hat{\boldsymbol{x}} | \Psi \rangle$$



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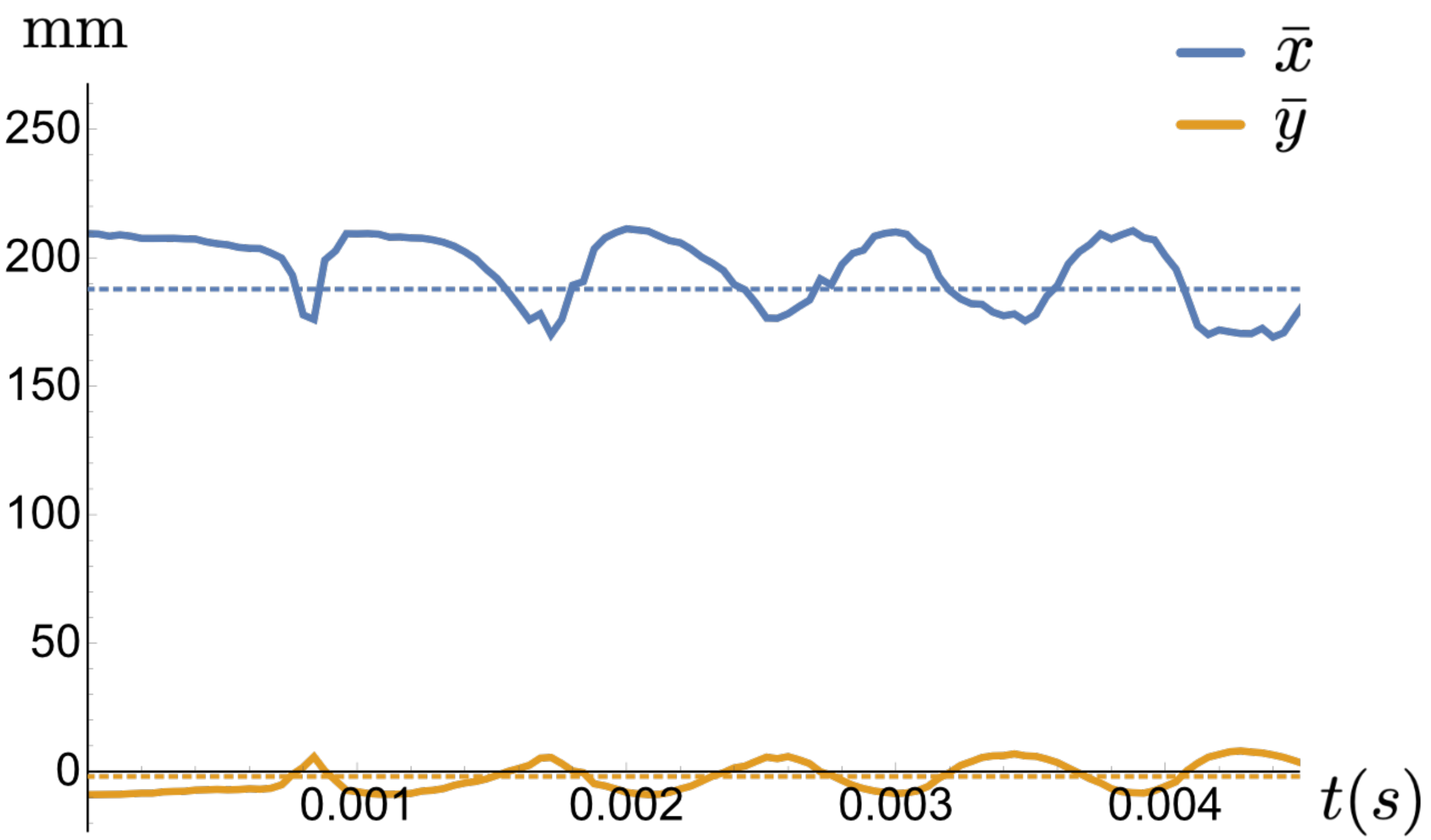

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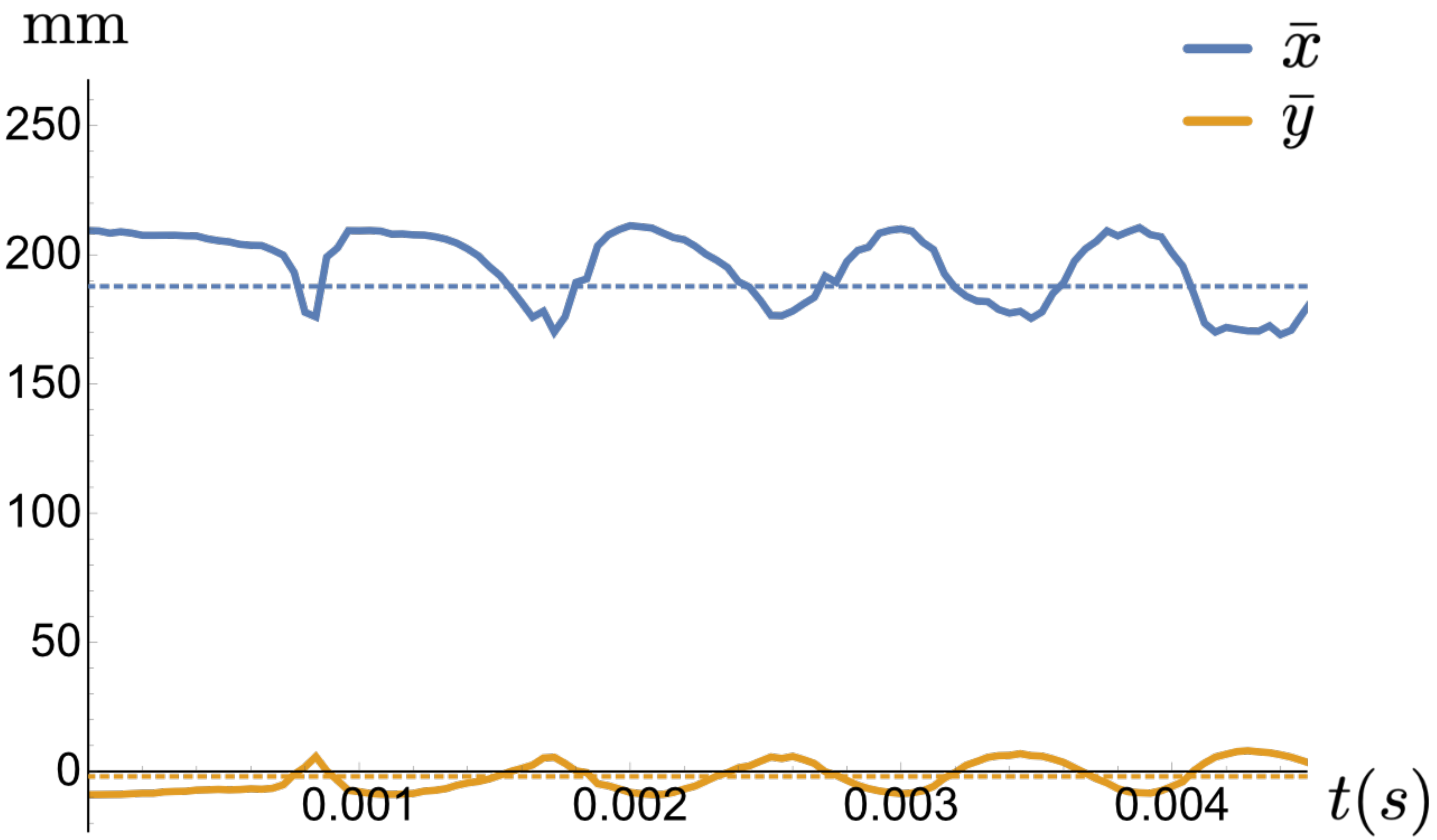
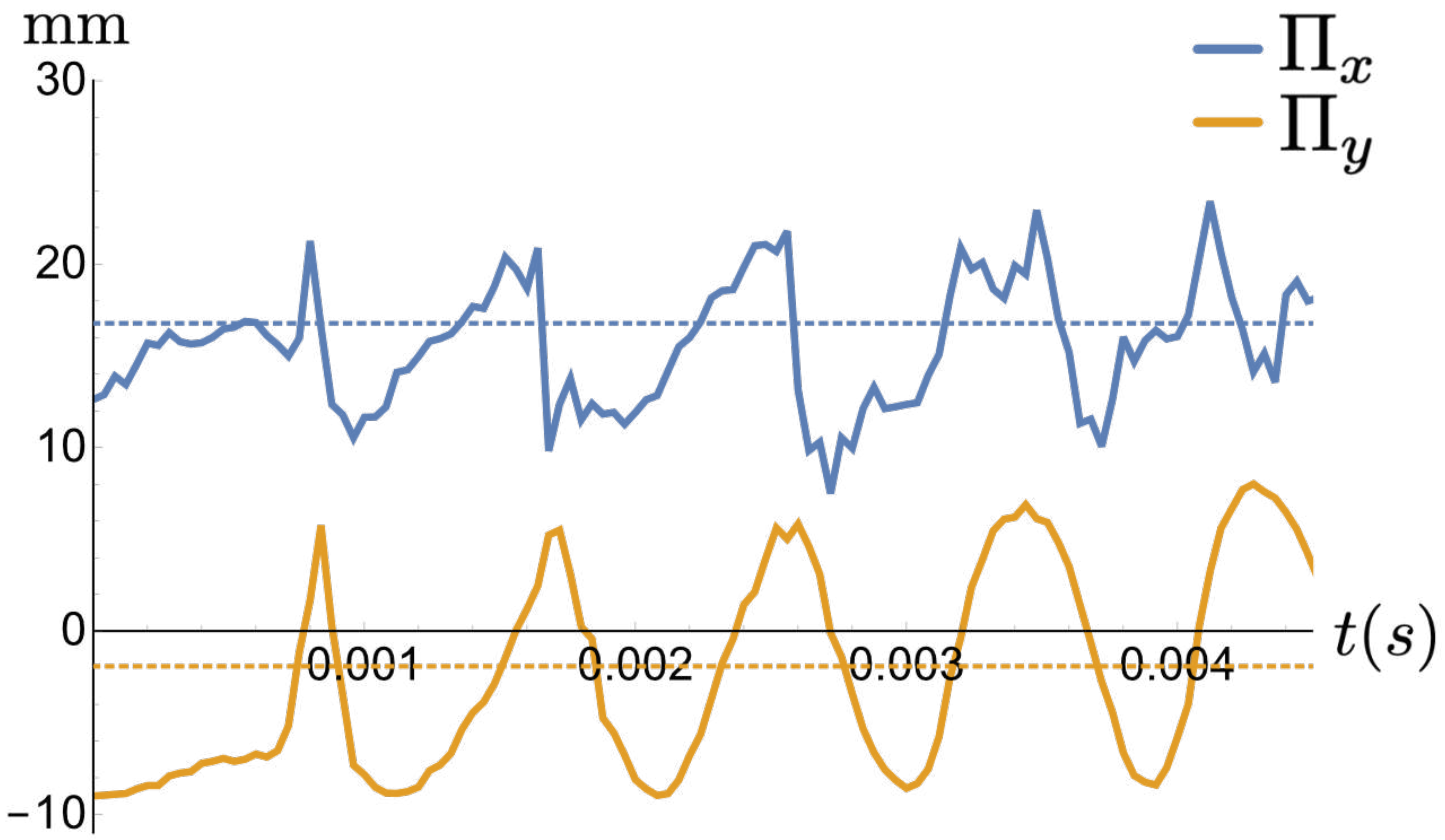
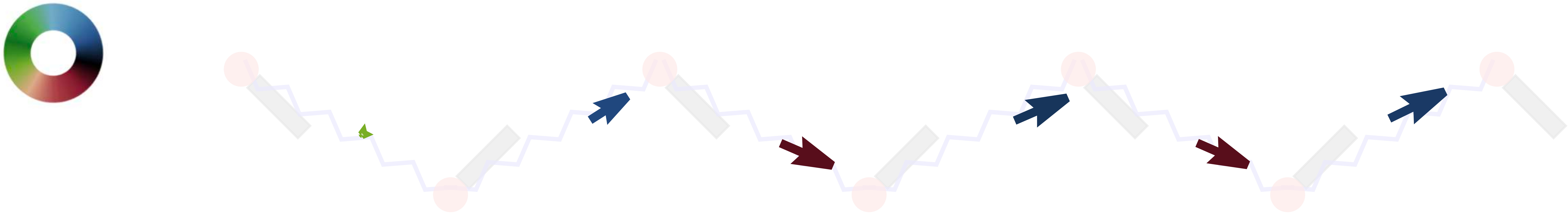
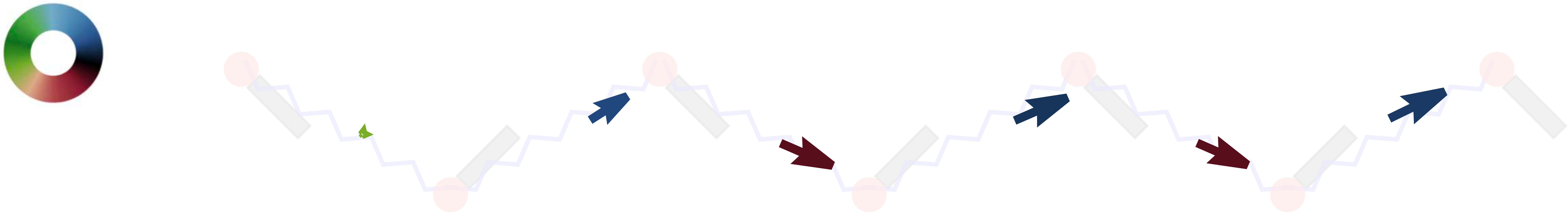


Chiral polarization

$$\boldsymbol{\Pi} = \langle \Psi | \mathbb{C} \hat{\boldsymbol{x}} | \Psi \rangle$$







Model-free characterization of a chiral insulator