Symmetries in Solid-State Systems

European School of Magnetism 2025, Liège, Belgium - 30 Jun to 11 July

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UNIVERSITY of York

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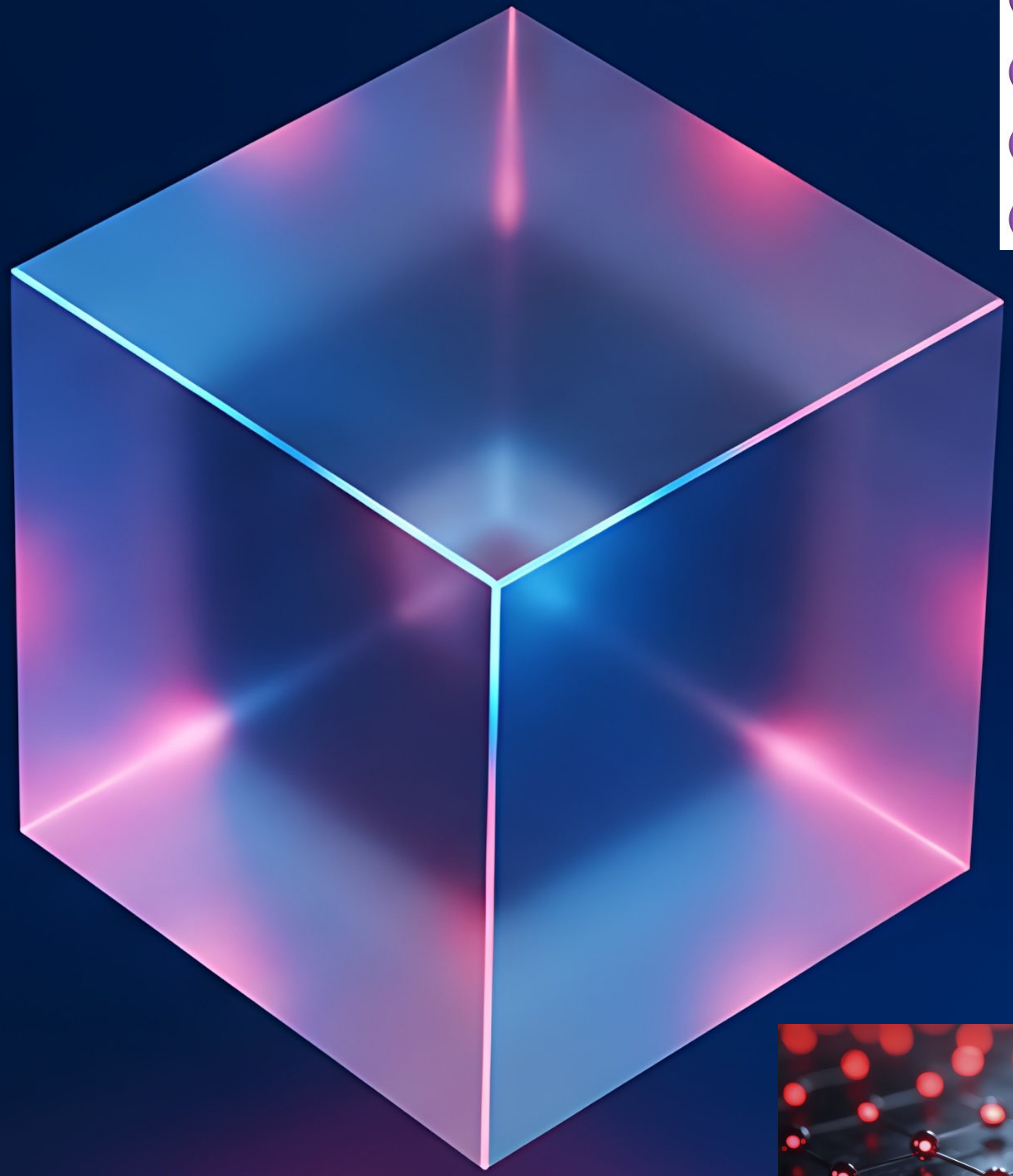
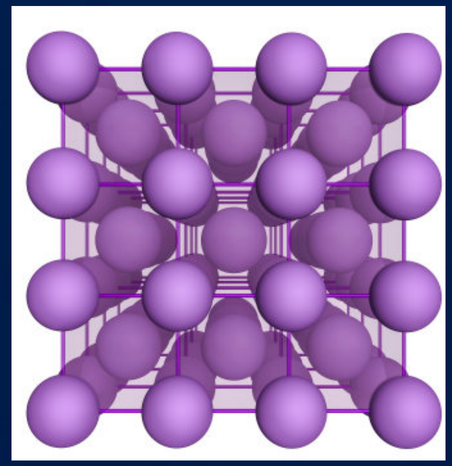
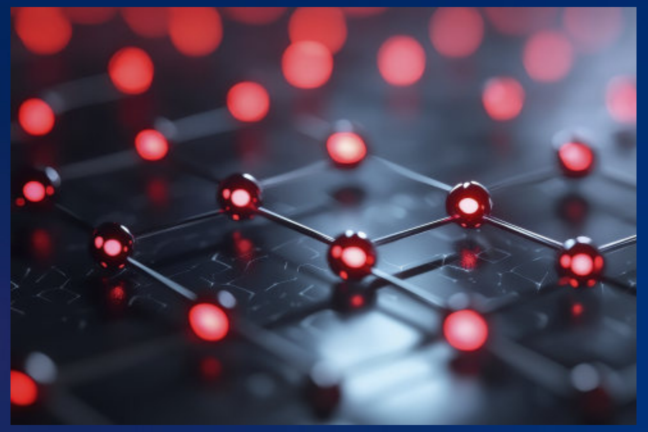
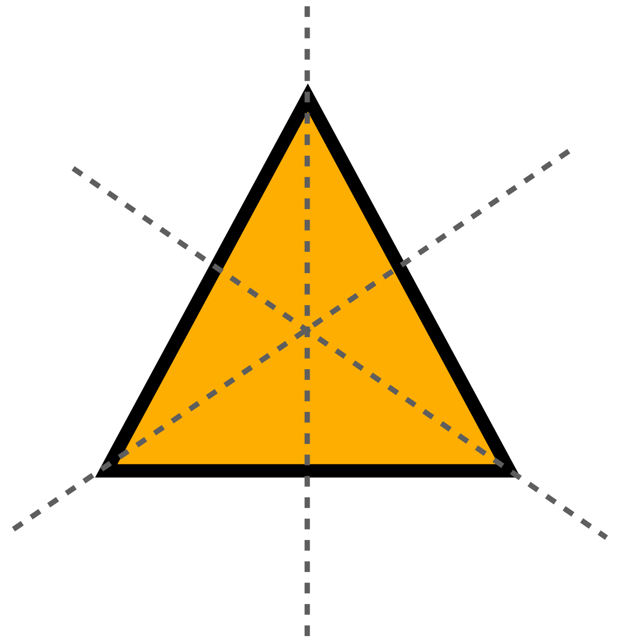






Outline

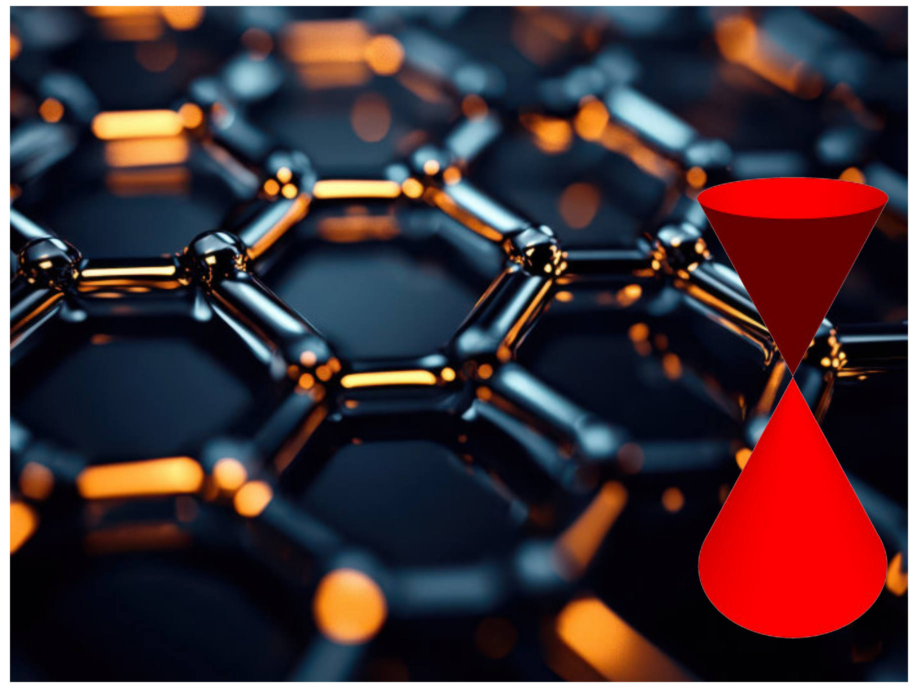
Part 1: Symmetries (ground rules)



➡ Symmetries in quantum mechanics, a recap

➡ Spatial symmetries: relation between symmetries and energy bands

Part 2: Modern Applications



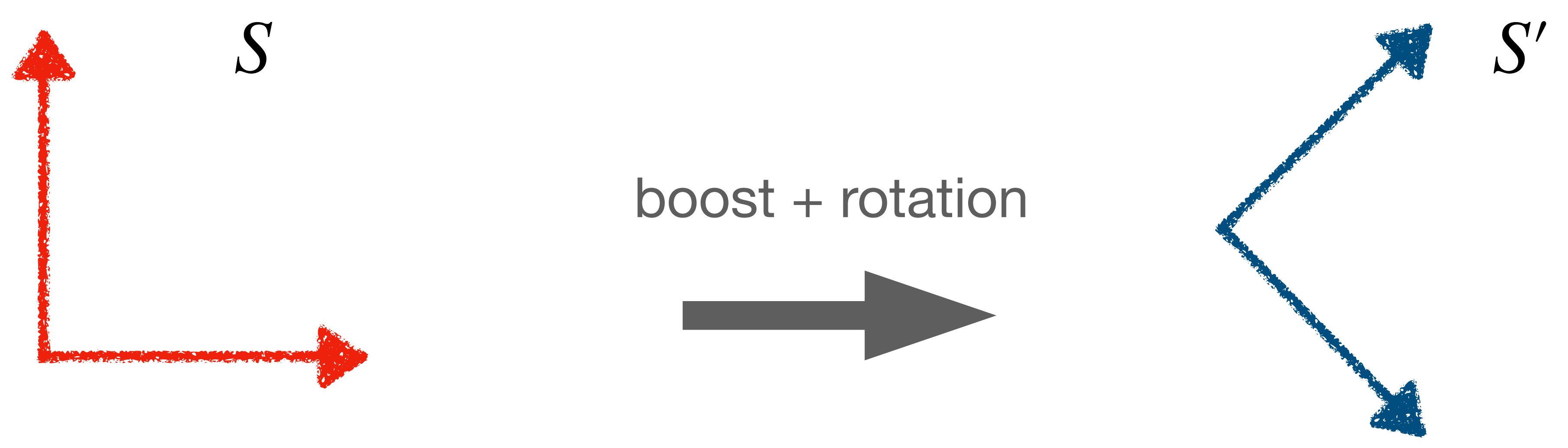
➡ Gapped topological phases: non-spatial symmetries

➡ Topological semi-metals protected by symmetry

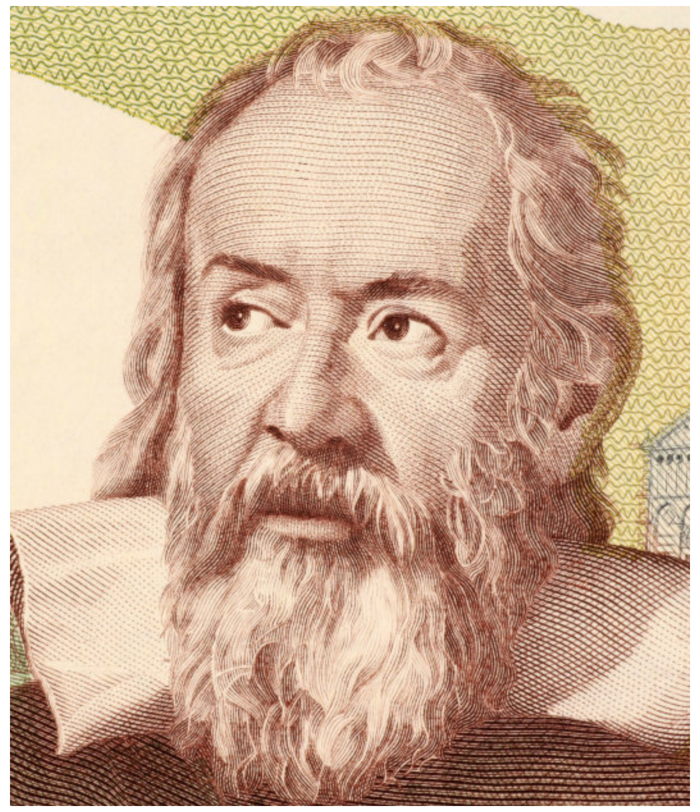
Part 1: Introduction I Symmetry transformations in QM

Invariance of the laws of nature: *lessons from classical physics*

The fundamental laws of nature preserve their form under space-time transformations such as rotations, temporal shifts, etc.

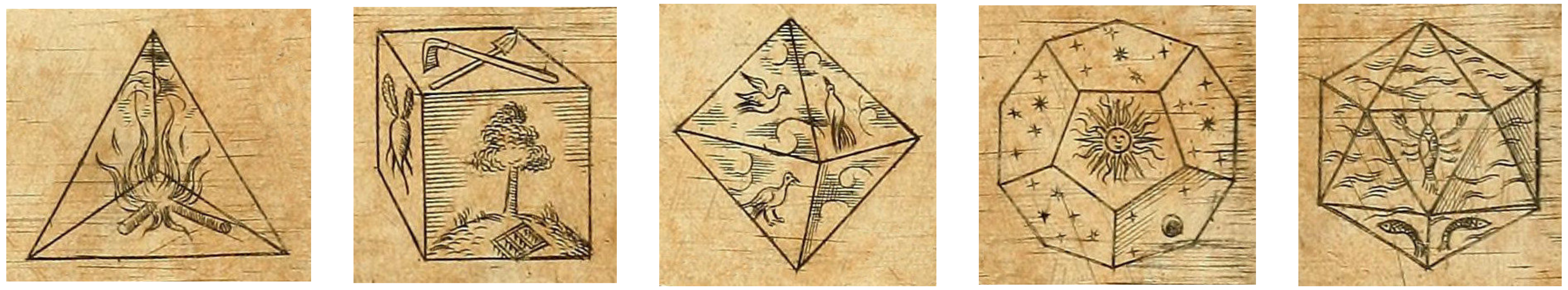


$$m\frac{d^2\mathbf{r}}{dt^2} = \mathbf{F} \qquad\qquad m\frac{d^2\mathbf{r}'}{dt^2} = \mathbf{F}$$



Galileo Galilei
(1564-1642)

All inertial frames are equivalent: *free space is homogenous and isotropic*



Harmonices Mundi (The Harmony of the World, 1619) Johannes Kepler

Symmetry operations form a group (such as the SO(3) rotation group):

- Identity (**1**) is the trivial symmetry
- g_1 and g_2 are symmetries (i.e. elements of the group), then $g_1 g_2$ is also a symmetry
- g^{-1} exists (and is also a symmetry)
- In general, $g_1 g_2 \neq g_2 g_1$

Symmetry transformations in QM

Assume that a given symmetry group G is specified (e.g., 3D rotation) transforming the system S into S', as in a reference frame change.

S: observables A, B, … and states $|\psi\rangle$, $|\phi\rangle$, …

will be described by

S': observables A', B', … and states $|\psi'\rangle$, $|\phi'\rangle$, …

$$|\langle\psi|A|\phi\rangle|^2 = |\langle\psi'|A'|\phi'\rangle|^2$$

If $S \leftrightarrow S'$ is a symmetry,
<u>no observable effect can be produced</u>

Symmetry transformations in QM

Postulating a unitary linear operator U is one way to guarantee the invariance of the quantum laws under symmetry operations

$$|\psi\rangle \rightarrow |\psi'\rangle = U|\psi\rangle$$

$$|\langle\phi|\psi\rangle|^2 = |\langle\phi'|\psi'\rangle|^2 = |\langle U\phi|U\psi\rangle|^2$$

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$$|\psi\rangle \to |\psi'\rangle = U|\psi\rangle$$

$$|\langle\phi|\psi\rangle|^2 = |\langle\phi'|\psi'\rangle|^2 = |\langle U\phi|U\psi\rangle|^2 = |\langle\phi|U^\dagger U|\psi\rangle|^2 \longrightarrow U^\dagger = U^{-1}$$

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Likewise, $$A \rightarrow A' = UAU^{-1}$$

$$|\langle\phi'|A'|\psi'\rangle|^2 = |\langle\phi|U^\dagger UAU^{-1}U|\psi\rangle|^2 = |\langle\phi|A|\psi\rangle|^2$$

Symmetry transformations in QM

Wigner's theorem *states that there are only two ways of preserving the modulus of inner products, namely:*

- *Unitary transformations,* U
- *Anti-unitary transformations,* $U^* := KU$ → *needed to represent certain discrete symmetries*

K = *complex conjugation operation*

$$\langle \phi' | \psi' \rangle = \langle U^* \phi | U^* \psi \rangle \underset{U^* = KU}{=} \langle U\phi | U\psi \rangle^* = \langle \phi | \psi \rangle^*$$

Eugene P. Wigner
(1902-1995)

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Eugene P. Wigner
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Example: Time-reversal symmetry (motion reversal) $\mathscr{T}$

Free particle

$\mathscr{T}$-symmetry is enacted by $U^* = K$

$$\Psi'_{0\mathbf{k}}(\mathbf{r}) = K\,\Psi_{0\mathbf{k}}(\mathbf{r}) = K e^{i\mathbf{k}\cdot\mathbf{r}} = e^{-i\mathbf{k}\cdot\mathbf{r}} \longrightarrow \mathbf{k} \to -\mathbf{k}$$

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Spin 1/2

$$U^* = i\sigma_y K \longrightarrow U^*\sigma_i U^{*\dagger} = -\sigma_i\,, (i = x, y, z) \longrightarrow \mathbf{S} \to -\mathbf{S}$$

$$\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$$

Part 1: Introduction I Continuous symmetries & conservation laws

continuous (differentiable) symmetries ⟷ conservation laws

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$$U^{-1}\, H\, U = H$$

$$[H, U] = 0$$

Symmetry

$$U(a) = e^{iaG}$$

Generator

continuous (differentiable) symmetries ⟷ conservation laws

$$U^{-1}\,H\,U = H$$

$$[H,U] = 0$$

← Symmetry → $U(a) = e^{iaG}$ ← Generator

space shift $U(a)\,\psi(x) = \psi(x+a)$

$$G = -\frac{p}{\hbar} = i\frac{d}{dx} \quad \Rightarrow \quad U(a) = e^{-iap/\hbar}$$

continuous (differentiable) symmetries ⟷ conservation laws

$$U^{-1}\,H\,U = H$$

$$[H, U] = 0$$

⇐ Symmetry → $U(a) = e^{iaG}$ ← Generator

space shift $U(a)\,\psi(x) = \psi(x+a)$

$$G = -\frac{p}{\hbar} = i\frac{d}{dx} \Rightarrow U(a) = e^{-iap/\hbar}$$

time shift $U(t)\,\psi(0) = \psi(t)$

$$G = -\frac{H}{\hbar} \Rightarrow U(t) = e^{-iHt/\hbar}$$

Part 1: Introduction I Continuous symmetries & conservation laws

continuous (differentiable) symmetries ⟷ conservation laws

Amalie Emmy Noether
(1882-1935)

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continuous (differentiable) symmetries ⟷ conservation laws

$U = e^{iaG}$ *is a symmetry of H, i.e.* $[U, H] = 0$

$$[G, H] = 0 \quad \Rightarrow \quad \textit{G is constant of motion*}$$

Amalie Emmy Noether (1882-1935)

(*) This results from the equation of motion for operators (Heisenberg equation): $\partial_t G = (i/\hbar)[H, G] = 0$

continuous (differentiable) symmetries ⟷ conservation laws

$U = e^{iaG}$ *is a symmetry of H, i.e.* $[U, H] = 0$

$$[G, H] = 0$$ ⟶ *G is constant of motion**

Amalie Emmy Noether (1882-1935)

Noether's theorem: Every continuous symmetry of the dynamics has a corresponding conservation law

Free particle **(translation symmetry,** $G = -p/\hbar$**)**

$$[\hat{H}, \hat{\mathbf{p}}] = 0$$ **conservation of momentum**

(*) This results from the equation of motion for operators (Heisenberg equation): $\partial_t G = (i/\hbar)[H, G] = 0$

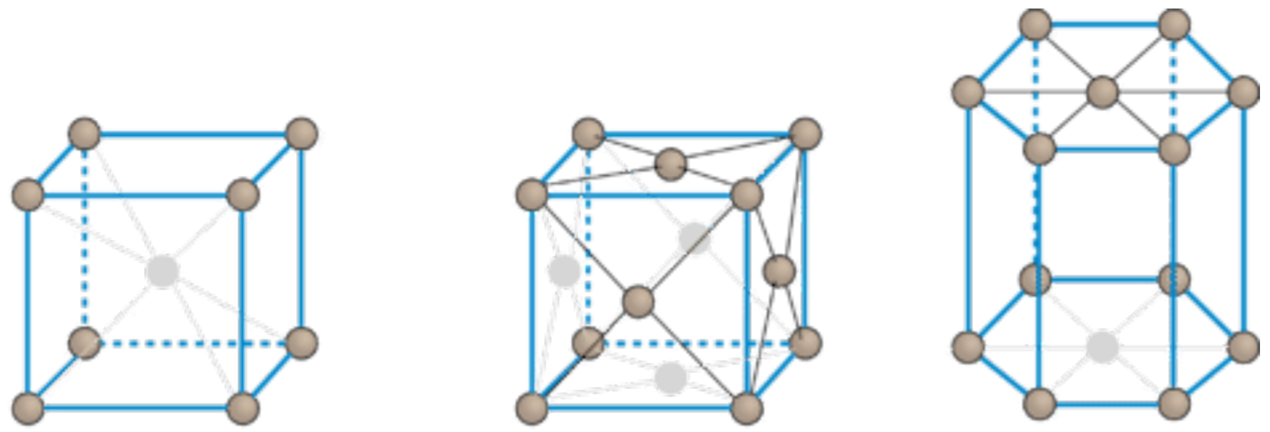
Discrete symmetries

Infinite group — Discrete translation group $\mathbb{Z}^d$ of a regular d-dimensional lattice

Finite group (of order n) — **Example:** C_n of rotation symmetries of a regular n-sided polygon

→ **Both types are crucial in the study of crystalline structures**

Spatial symmetries in solids



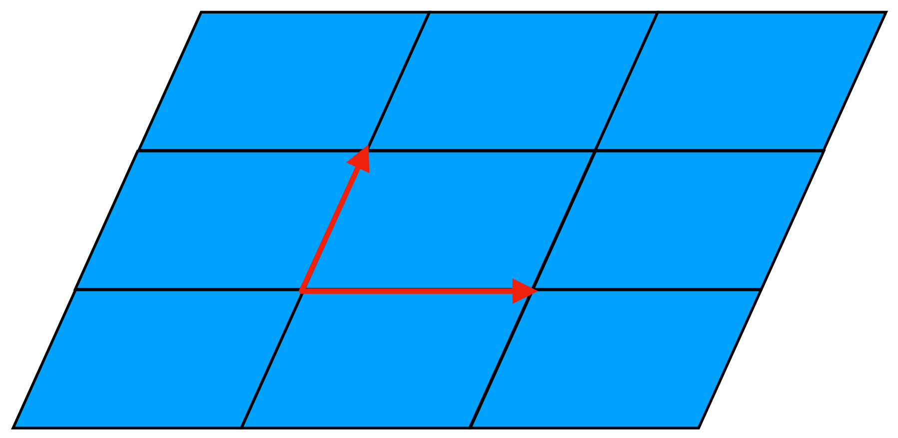
Each crystallographic lattice possesses a certain **symmetry group**

230 Space Groups

Sets of symmetry operations that completely describe the spatial arrangement of crystalline systems

Bravais lattices

Bravais lattices



Array of points generated by discrete translation operations:

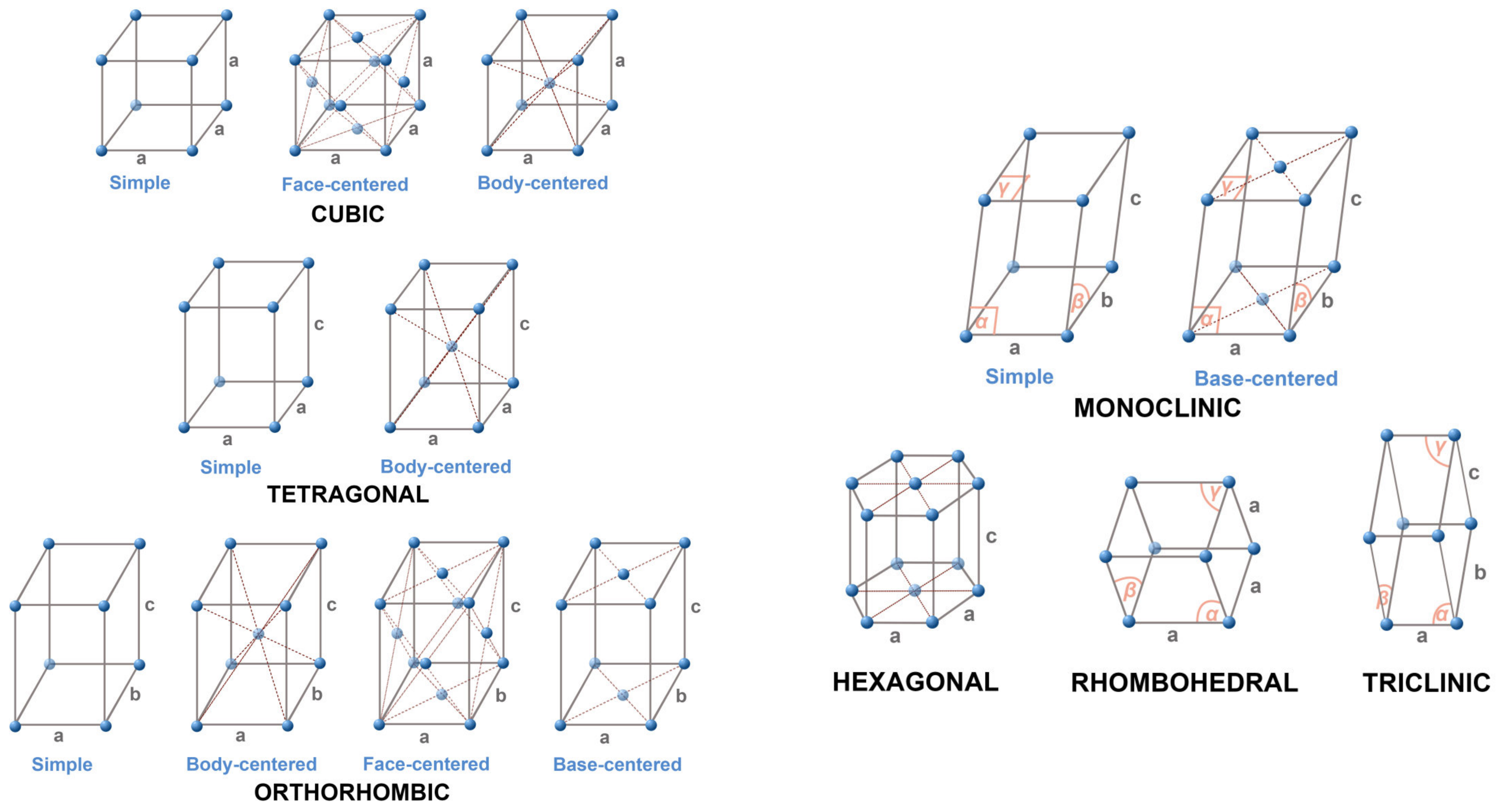
$$\mathbf{R}_{ijk} = i\,\mathbf{a}_1 + j\mathbf{a}_2 + k\mathbf{a}_3 \quad i, j, k \in \mathbb{Z}$$

Bravais lattices

14 possibilities (in 3D)

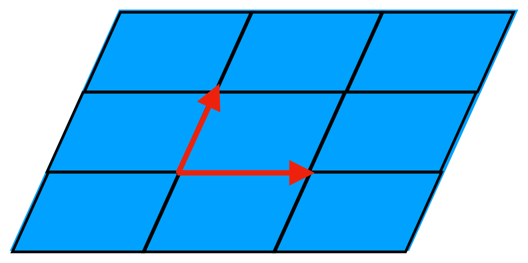
➡ 7 basic crystal systems

➡ 4 lattice centerings

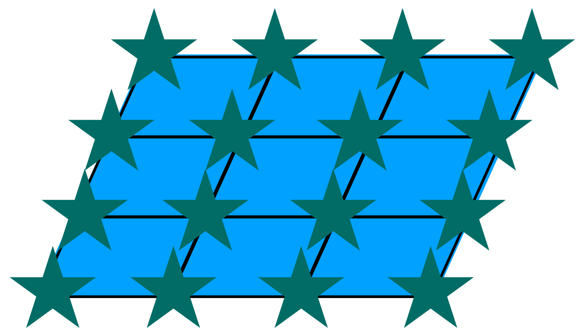


Crystal structure = lattice + motif

lattice



+ basis (or motif) = crystal structure



Crystal structure = lattice + motif

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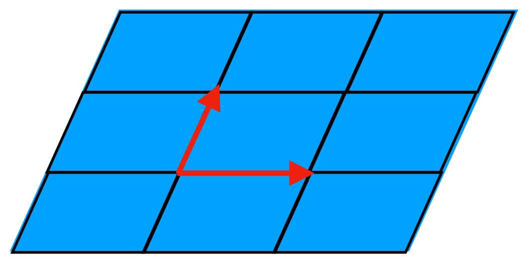
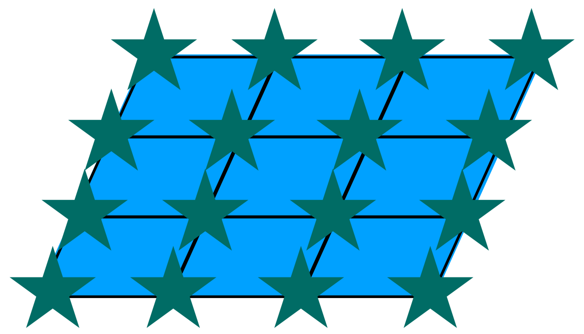
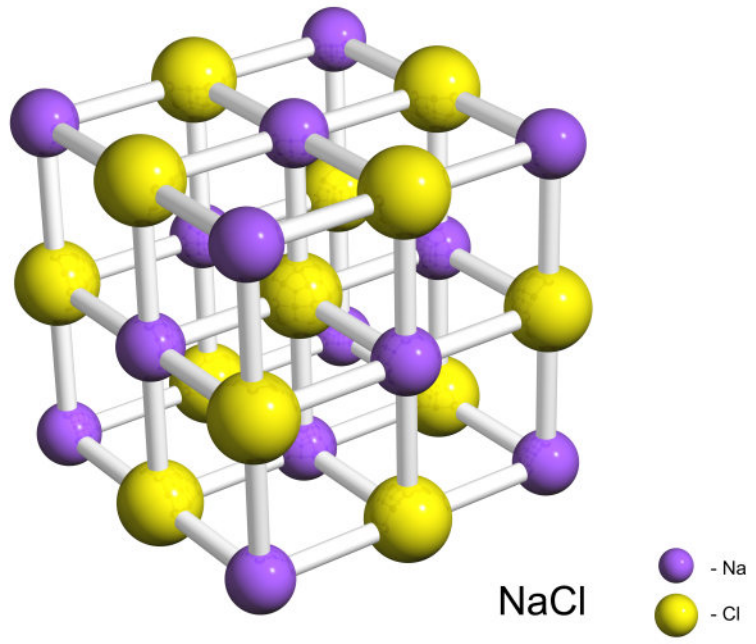


+ basis
(or motif)
= crystal structure



Example: *rock salt*



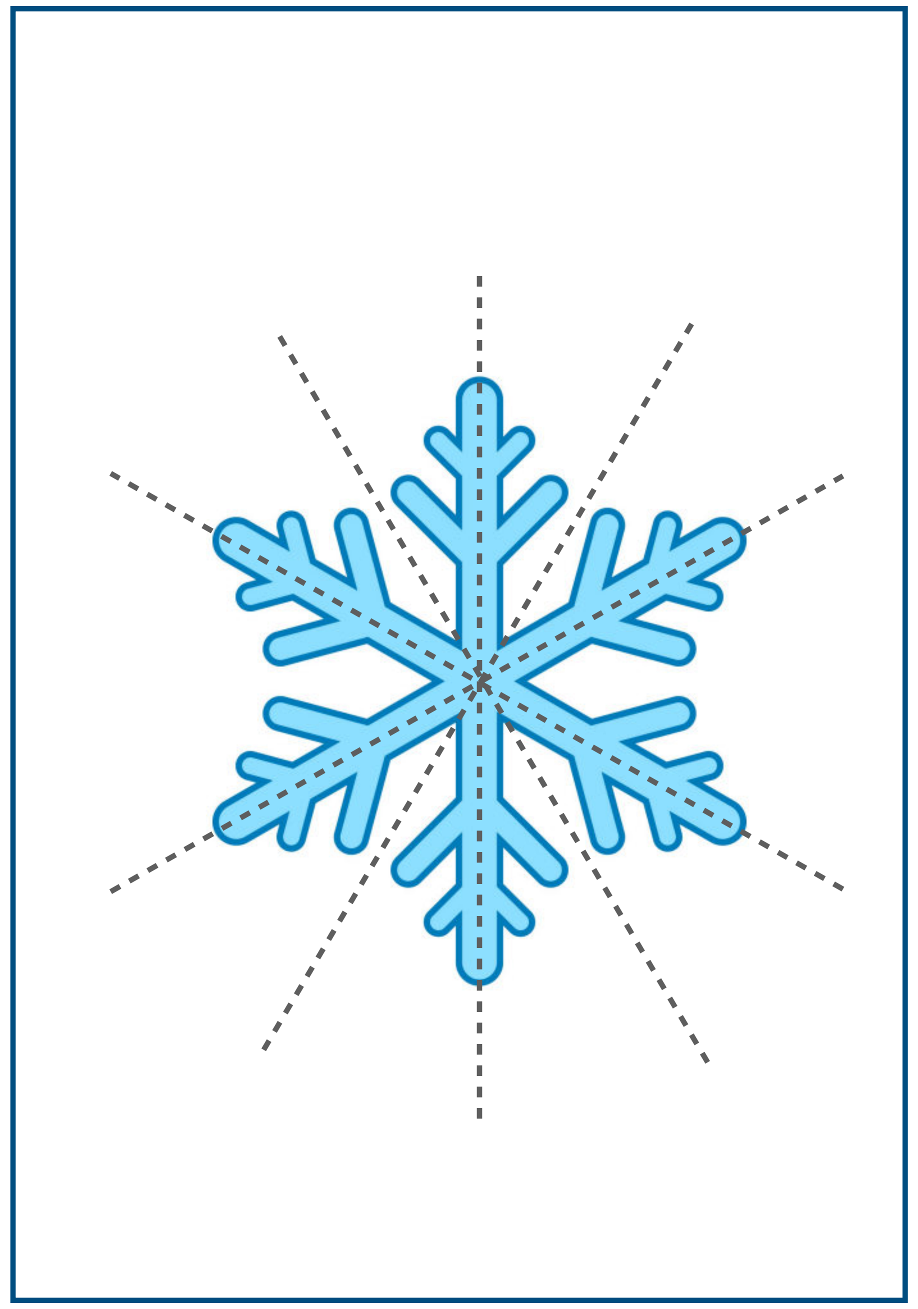
FCC with a two-atom basis

or

2 interpenetrating FCC lattices

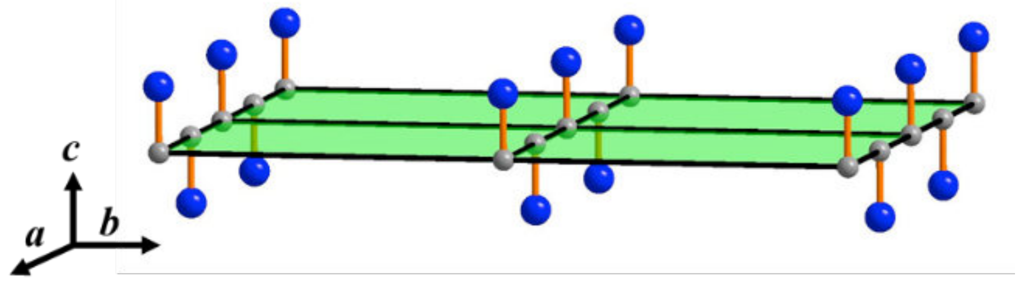
Point group symmetries

PG operations (in 2D): identity, mirror reflections, rotations and glide reflections



mirror + rotation C_6

Point group symmetries



glide reflection with $\tau \parallel \mathbf{a}$

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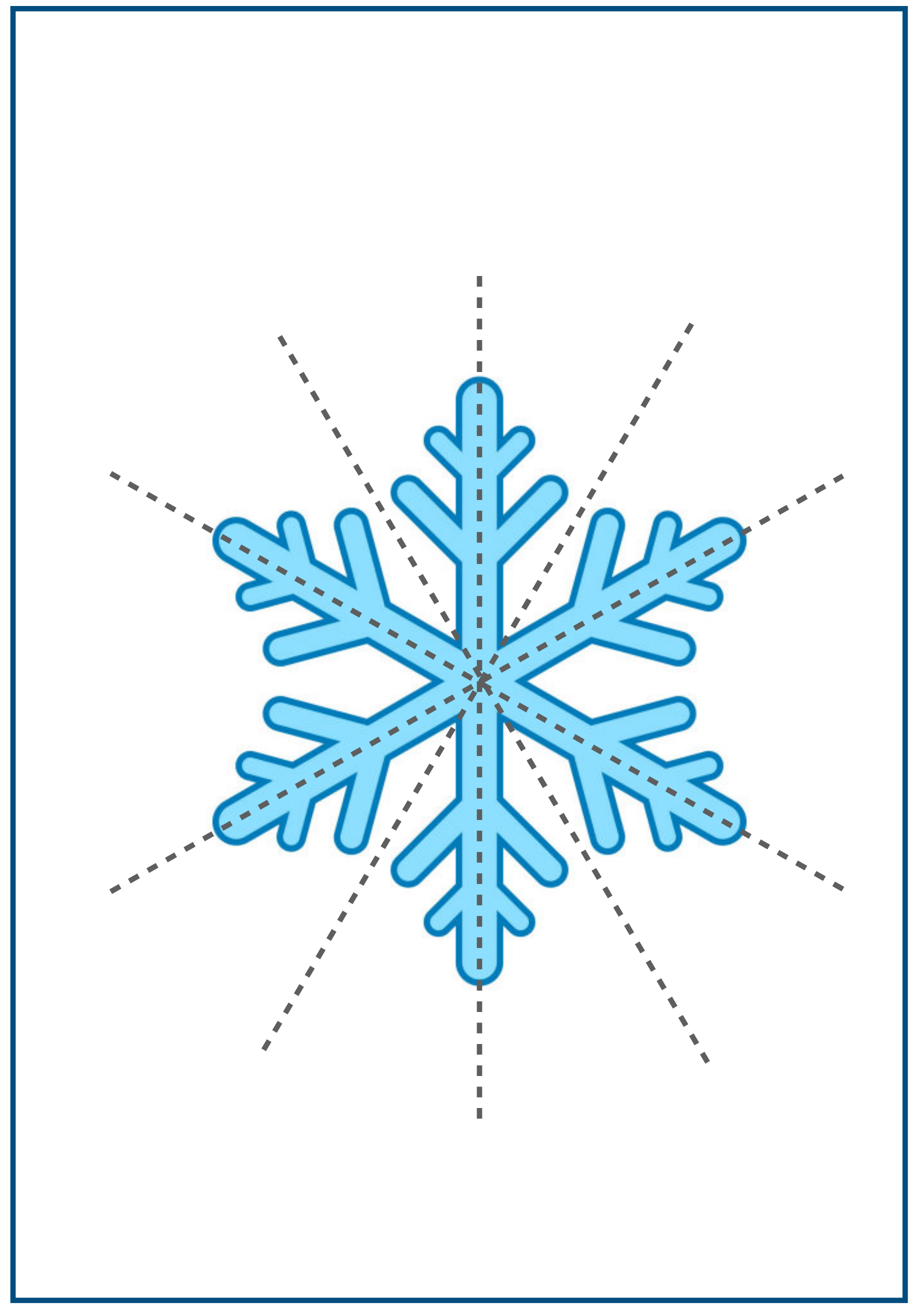

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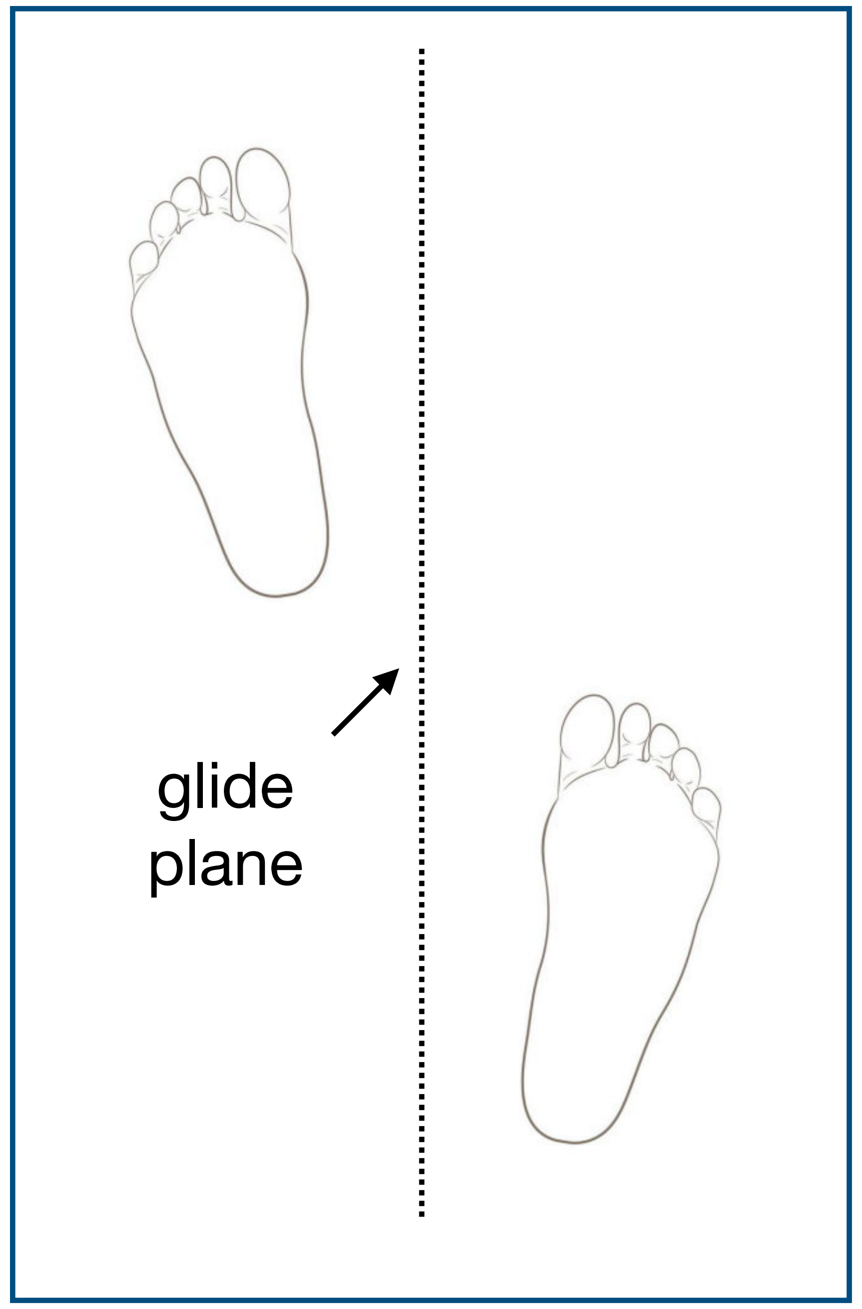


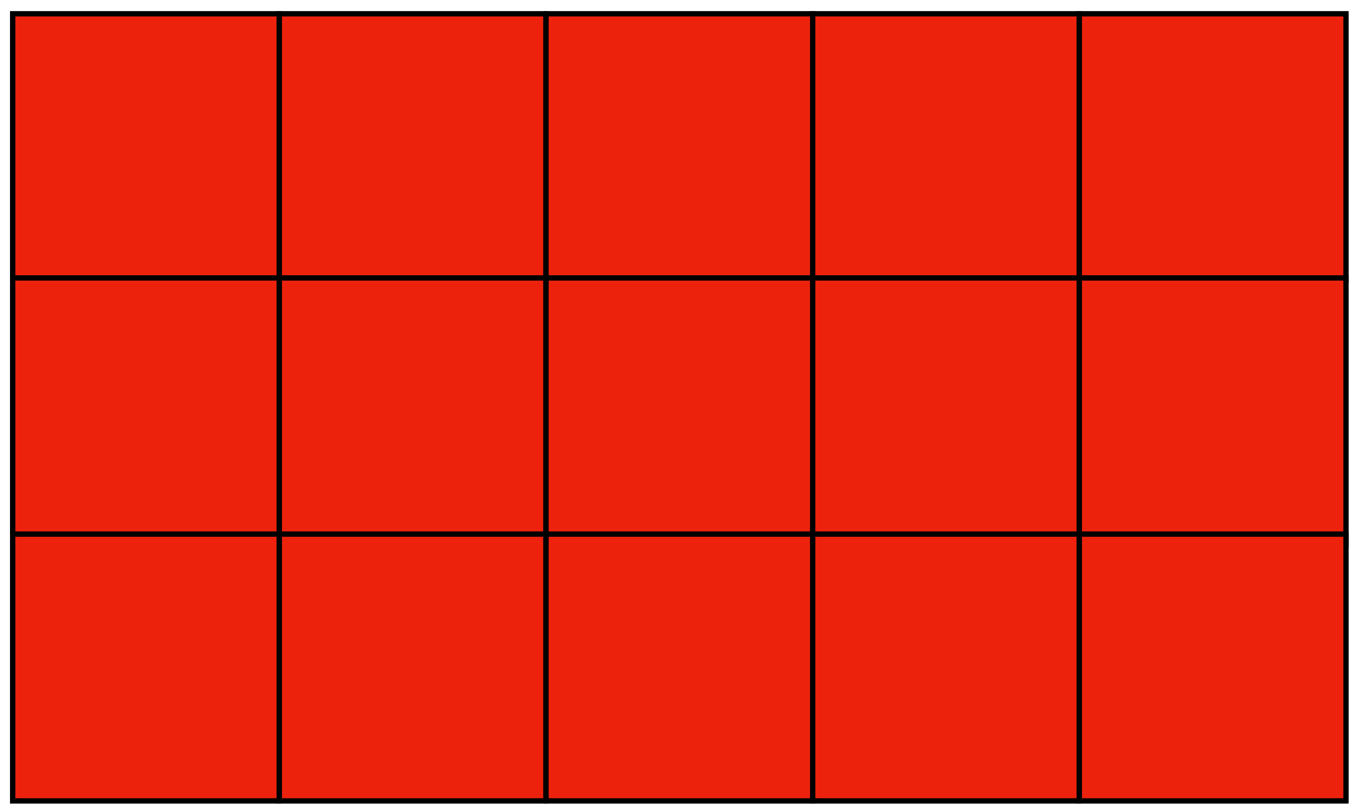
glide

(reflection + $1/2$ translation)

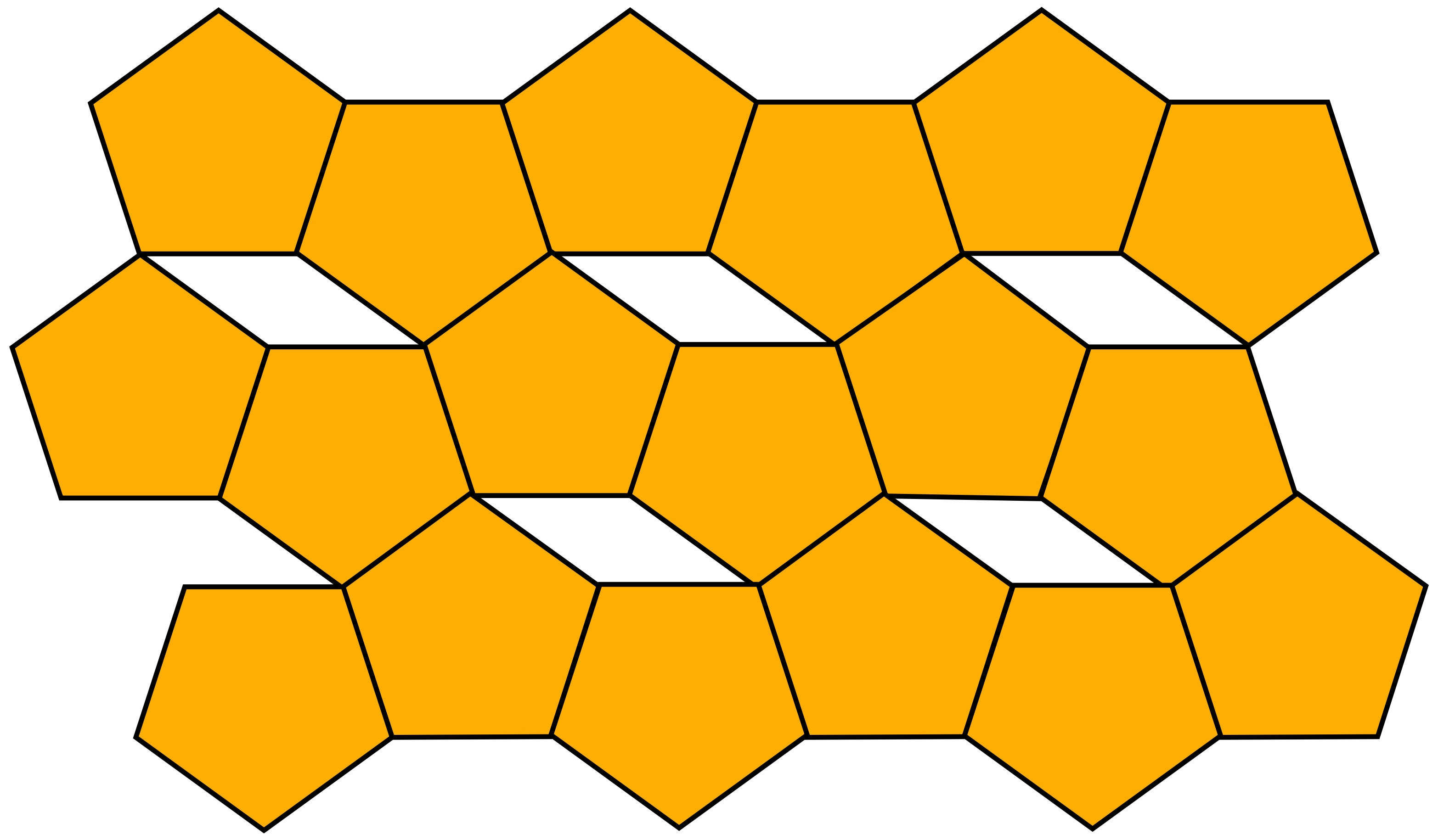
Point group symmetries

Point symmetries like *n*-fold rotations must be compatible with translations

Square lattice (4-fold rotations) - ***this works***



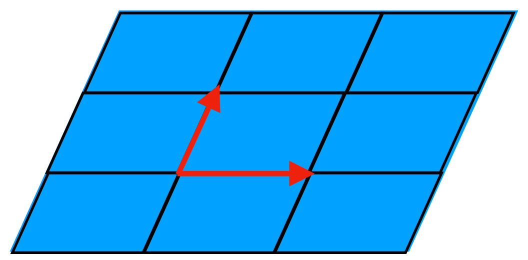
Pentagonal lattice (5-fold rotations) - ***this doesn't***



Part 1: Introduction I Spatial symmetries (Crystals)

Bravais lattices → **Point group symmetries**

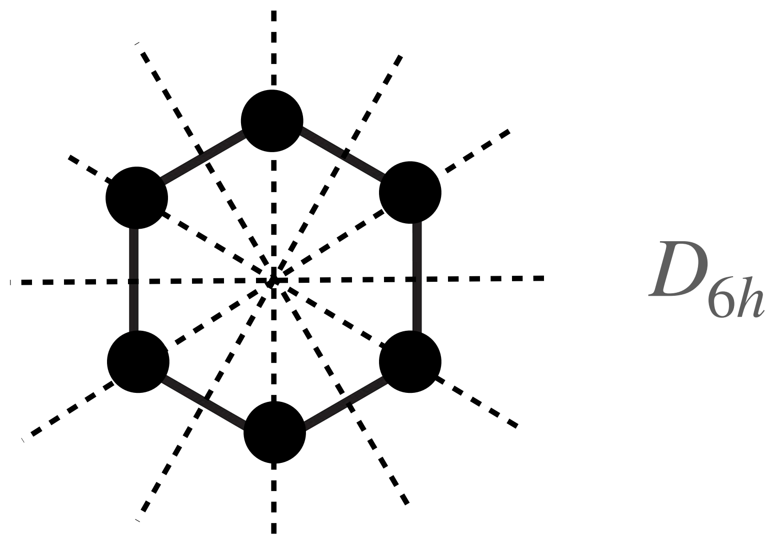
Bravais lattices



Translation + Centering
=
14 possibilities

+

32 point groups
(compatible with crystalline periodicity)



- ✦ ***n*-fold rotations (*n* = 2, 3, 4, 6)**
- ✦ **inversion at a point**
- ✦ **reflection at mirror planes**
- ✦ **rotoinversions (3D)**

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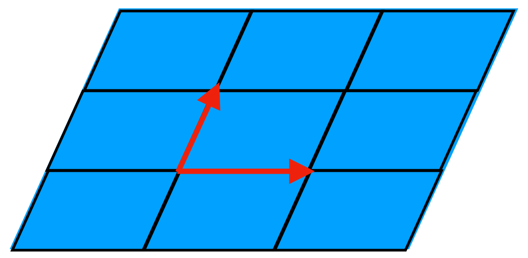
Bravais lattices → **Point group symmetries**

Bravais lattices



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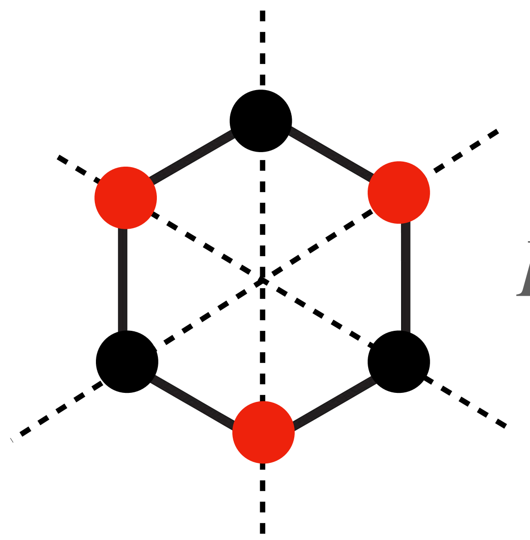

$D_{6h} \rightarrow D_{3h}$

✦ ***n*-fold rotations (*n* = 2, 3, 4, 6)**

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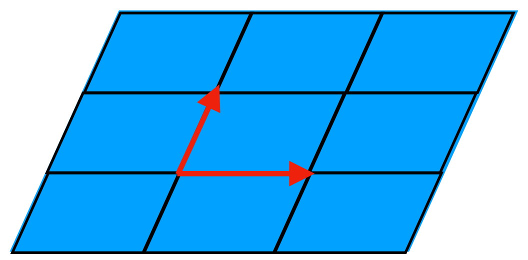
Part 1: Introduction I Spatial symmetries (Crystals)

Bravais lattices → **Point group symmetries** → **Space groups**

Bravais lattices



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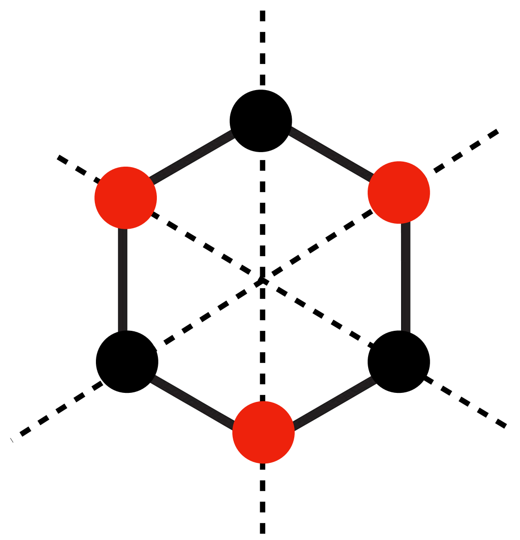

- ✦ ***n*-fold rotations (*n* = 2, 3, 4, 6)**
- ✦ **inversion at a point**
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- ✦ **rotoinversions (3D)**

=

73 simple space groups

+

non-symmorphic symmetry elements
(screw axes & glide planes)

=

230 space groups

Relation between symmetries and energy bands

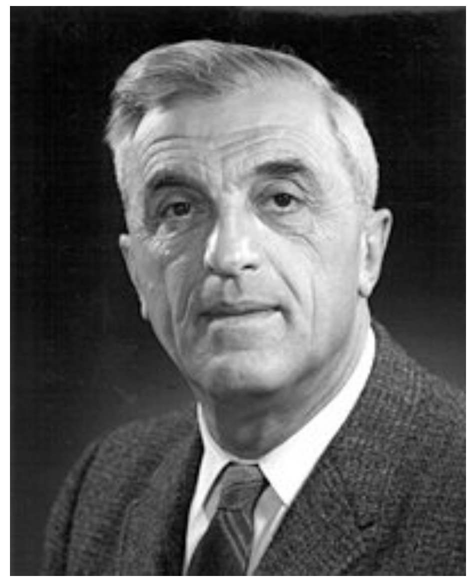
Relation between symmetries and energy bands

Translation invariance: Bloch's theorem

Translation operator

$$\hat{T}_{\mathbf{R}}\,\Psi(\mathbf{r}) = \Psi(\mathbf{r}+\mathbf{R})$$

$\mathbf{R}$ is a direct lattice vector



Felix Bloch
(1905-1983)

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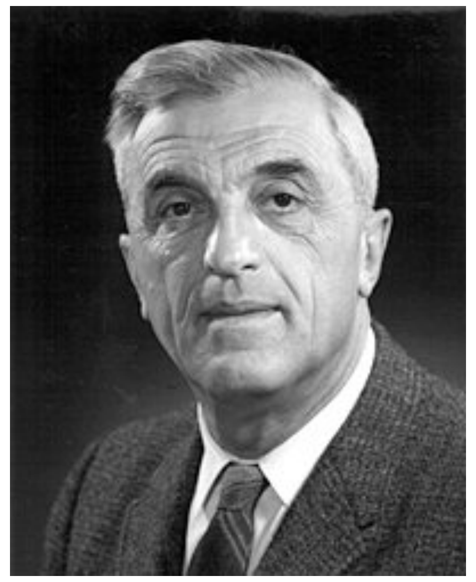

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$\hat{T}_{\mathbf{R}}$ is an unitary operator (as seen earlier), so $\hat{T}_{\mathbf{R}}\Psi(\mathbf{r}) = e^{i\theta(\mathbf{R})}\Psi(\mathbf{r})$

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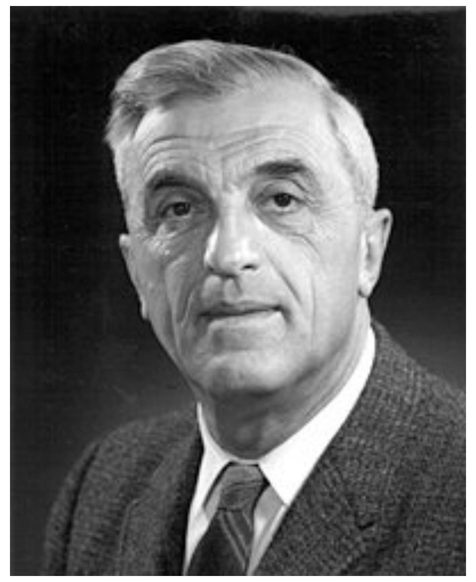

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group structure

$$\hat{T}_{\mathbf{R}_1}\hat{T}_{\mathbf{R}_2} = \hat{T}_{\mathbf{R}_1+\mathbf{R}_2}$$

Relation between symmetries and energy bands

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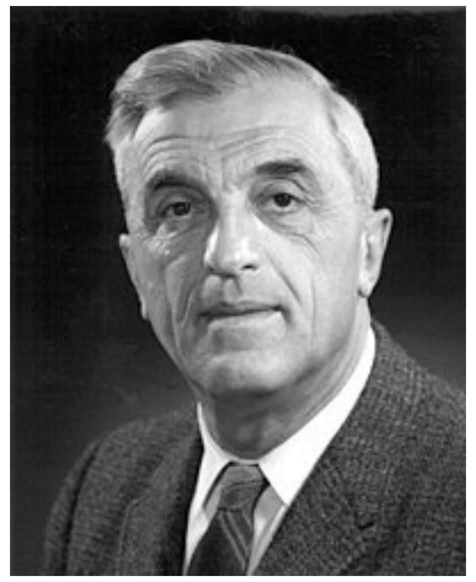

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$\theta(\mathbf{R}) = \mathbf{k}\cdot\mathbf{R}$ [with $\mathbf{k} \in \mathbb{R}^d$]

crystal momentum

Relation between symmetries and energy bands

Translation operator

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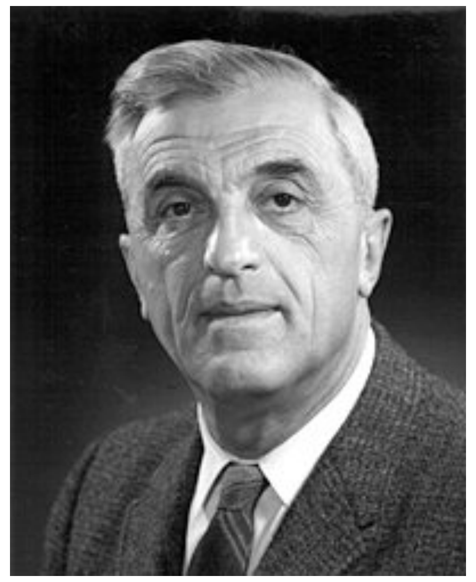

Felix Bloch
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Translation invariance: Bloch's theorem

periodic crystal Hamiltonian

$$[\hat{T}_{\mathbf{R}}, \hat{H}] = 0$$

Energy eigenstates can be labelled by the eigenvalues of $\hat{T}_{\mathbf{R}}$

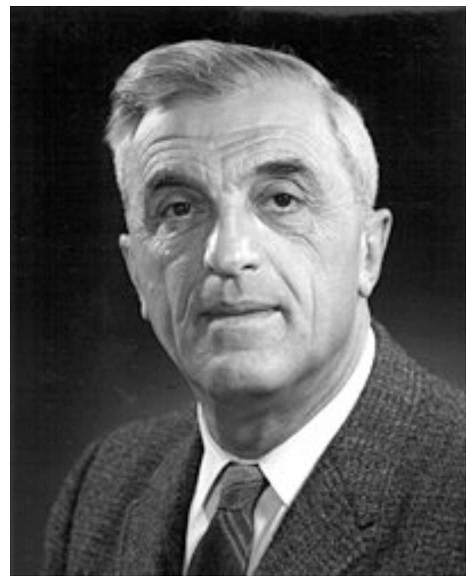
Part 1: Spatial Symmetries I Band structure

Relation between symmetries and energy bands

Translation operator

$$\hat{T}_{\mathbf{R}}\Psi(\mathbf{r}) = \Psi(\mathbf{r}+\mathbf{R})$$

$\mathbf{R}$ is a direct lattice vector



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Translation invariance: Bloch's theorem

$$\hat{T}_{\mathbf{R}}\Psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{R}}\Psi_{\mathbf{k}}(\mathbf{r})$$

energy eigenstate
($\mathbf{k}$ labelling)

Relation between symmetries and energy bands

Translation operator

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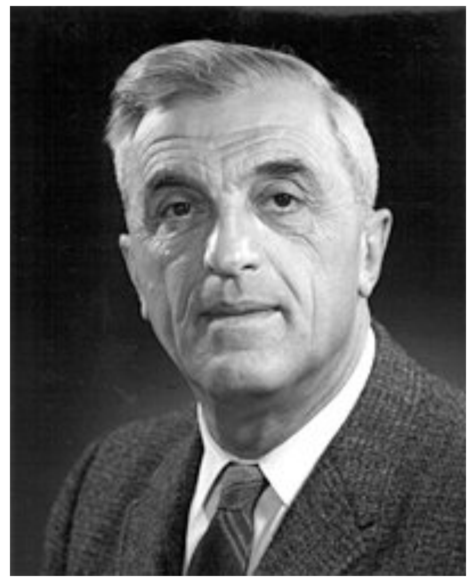

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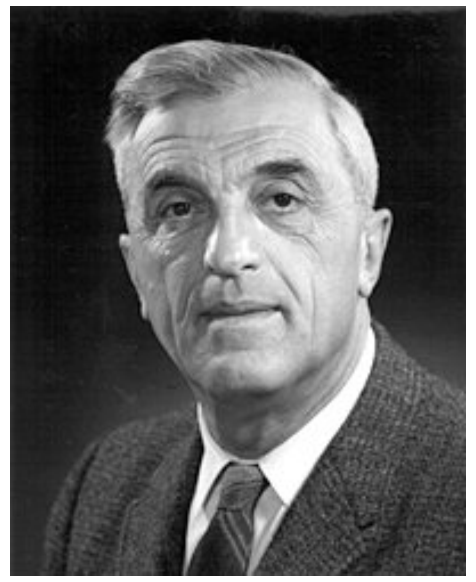
energy eigenstate
($\mathbf{k}$ labelling)

arbitrariness (!) since $e^{i\mathbf{k}\cdot\mathbf{R}} = e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{R}}$,
with $\mathbf{G}$ a reciprocal lattice vector ($\mathbf{G}\cdot\mathbf{R} = 2\pi\mathbb{Z}$)

This is dealt with by restricting $\mathbf{k}$ to a Brillouin zone

E.g. for a simple cubic lattice $\mathbf{k} \in]-\pi/a, \pi/a]^3$

Relation between symmetries and energy bands



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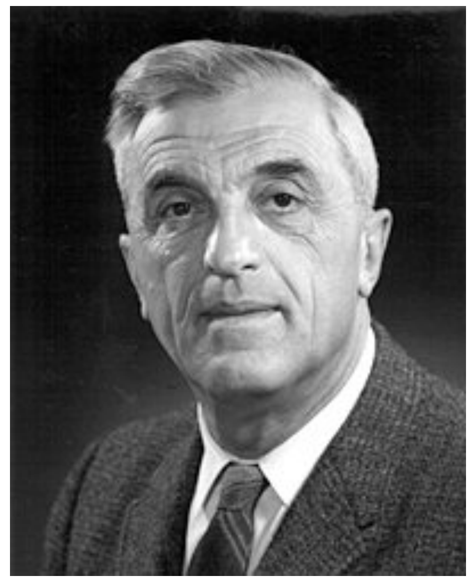
Translation invariance: Bloch's theorem

$$\hat{T}_{\mathbf{R}}\Psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{R}}\Psi_{\mathbf{k}}(\mathbf{r}) \quad \Rightarrow \quad \Psi_{\mathbf{k}}(\mathbf{r}) = u(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$$

Bloch's theorem

Bloch (lattice-periodic) function

Relation between symmetries and energy bands



Felix Bloch
(1905-1983)

Eigenvalue problem for $u_{\mathbf{k}}(\mathbf{r})$:

$$H_{\mathbf{k}}\, u_{\mathbf{k}}(\mathbf{r}) = \left[-\frac{\hbar^2}{2m} (i\mathbf{k} + \nabla)^2 + V(\mathbf{r}) \right] u_{\mathbf{k}} = \varepsilon(\mathbf{k})\, u_{\mathbf{k}}(\mathbf{r})$$

➡ Family of solutions $\varepsilon_n(\mathbf{k})$ ($n \in \mathbb{Z}$) with discretely spaced eigenvalues: energy bands!

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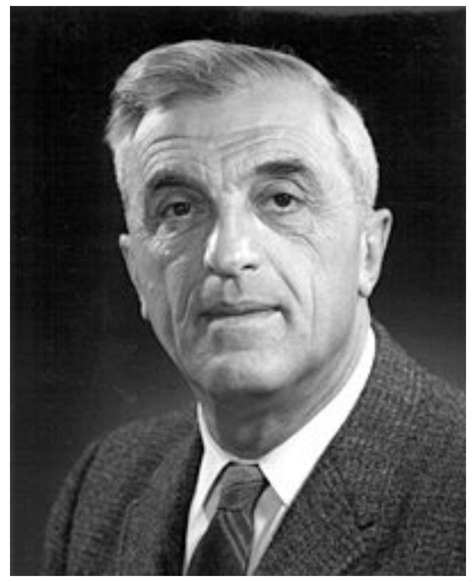

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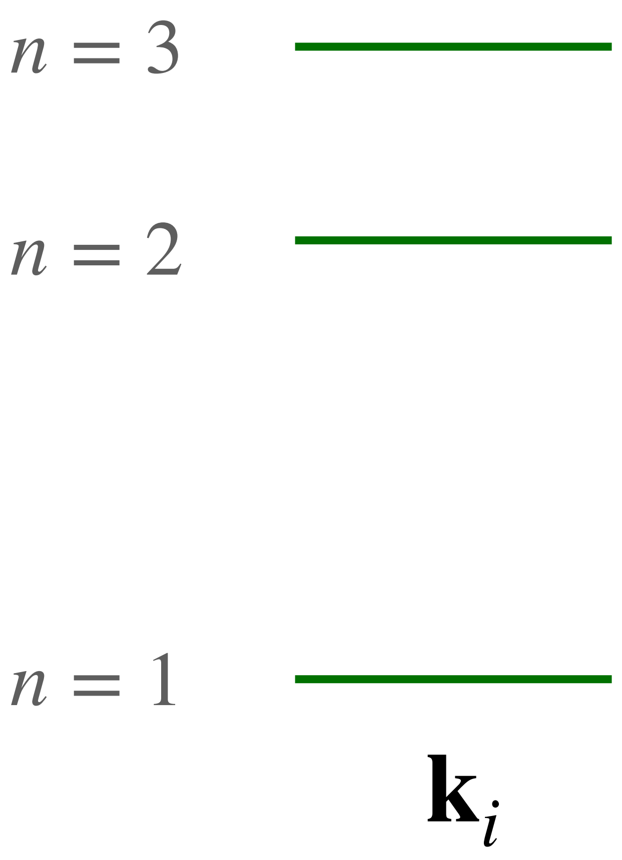
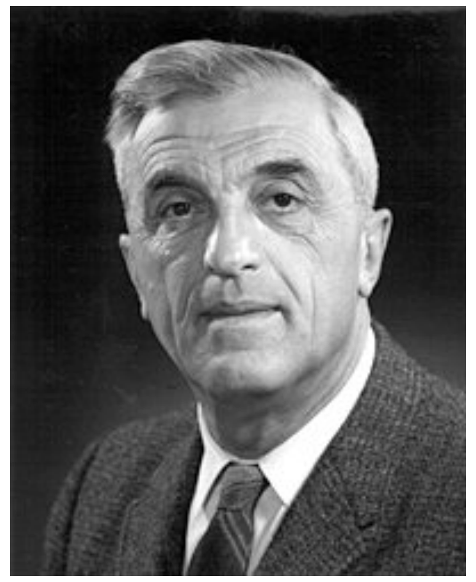


Part 1: Spatial Symmetries I Band structure

Relation between symmetries and energy bands



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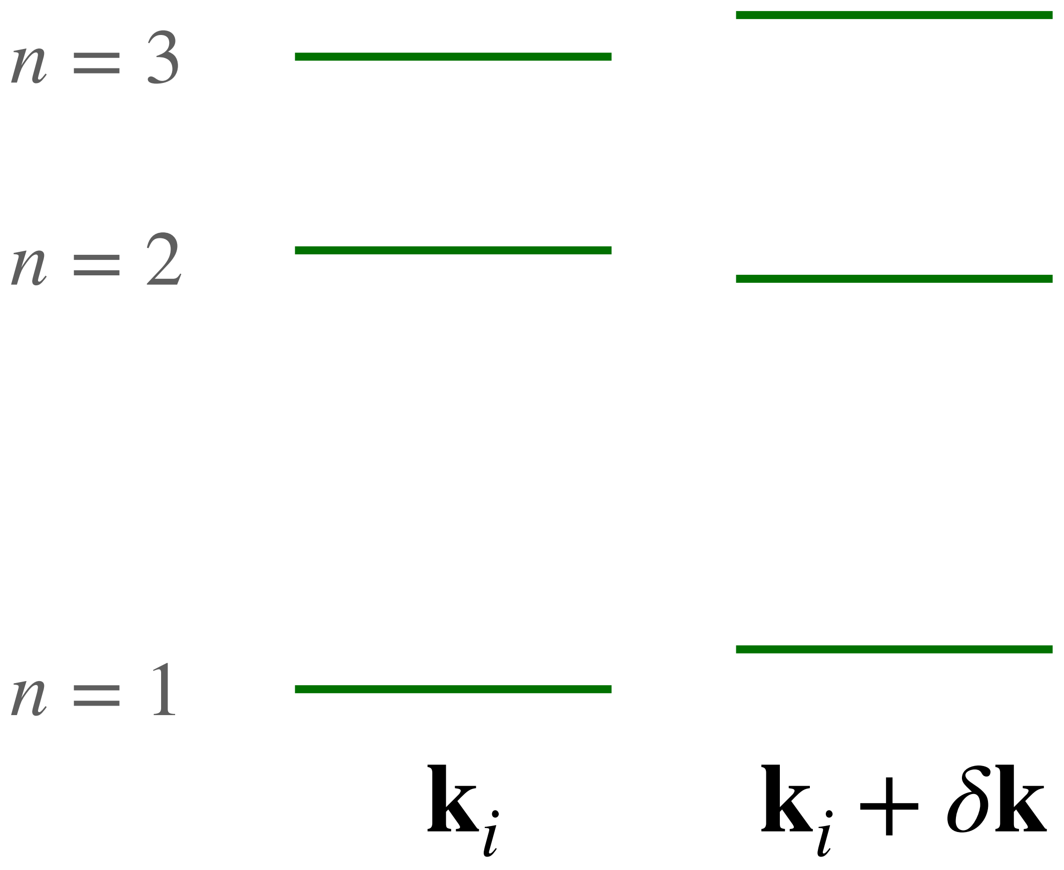

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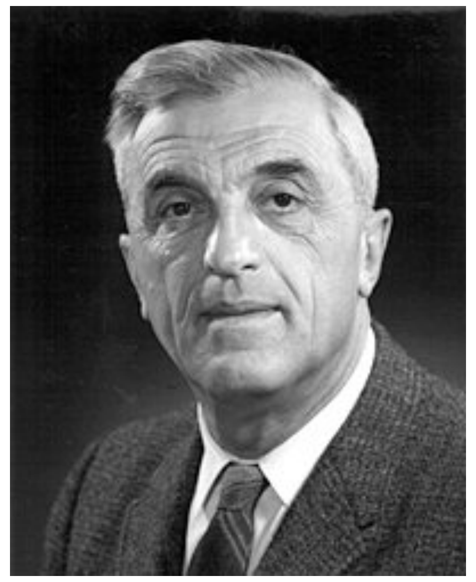

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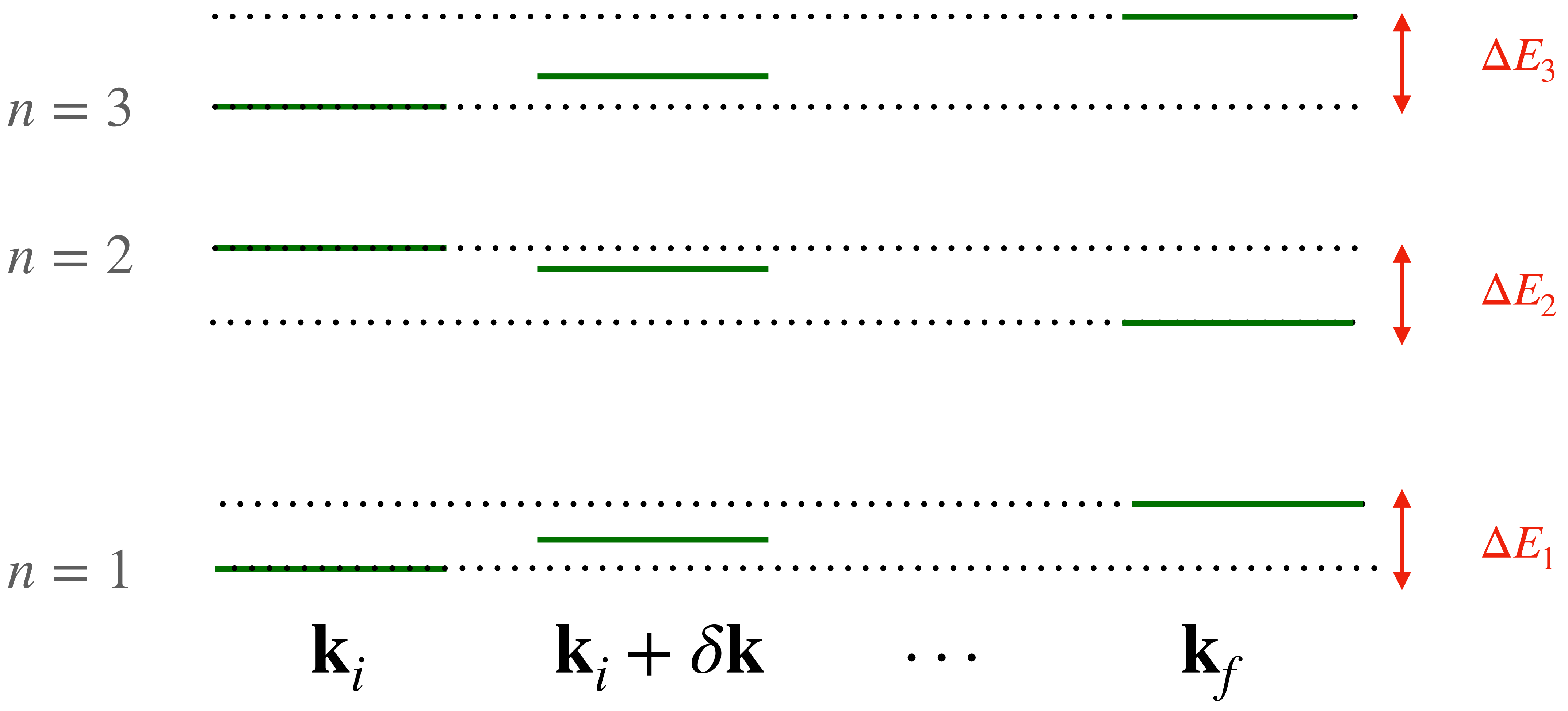
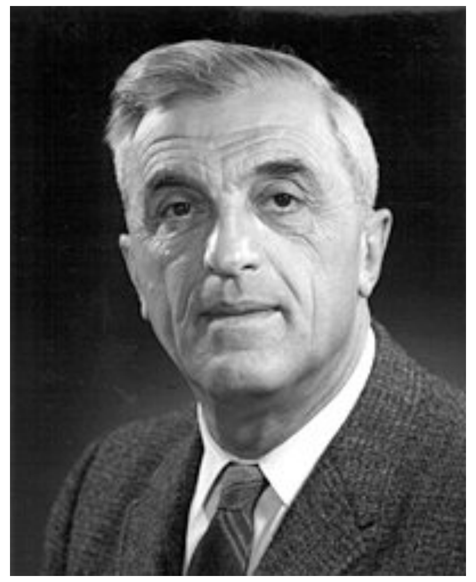


Translation symmetry leads to energy bands

Relation between symmetries and energy bands



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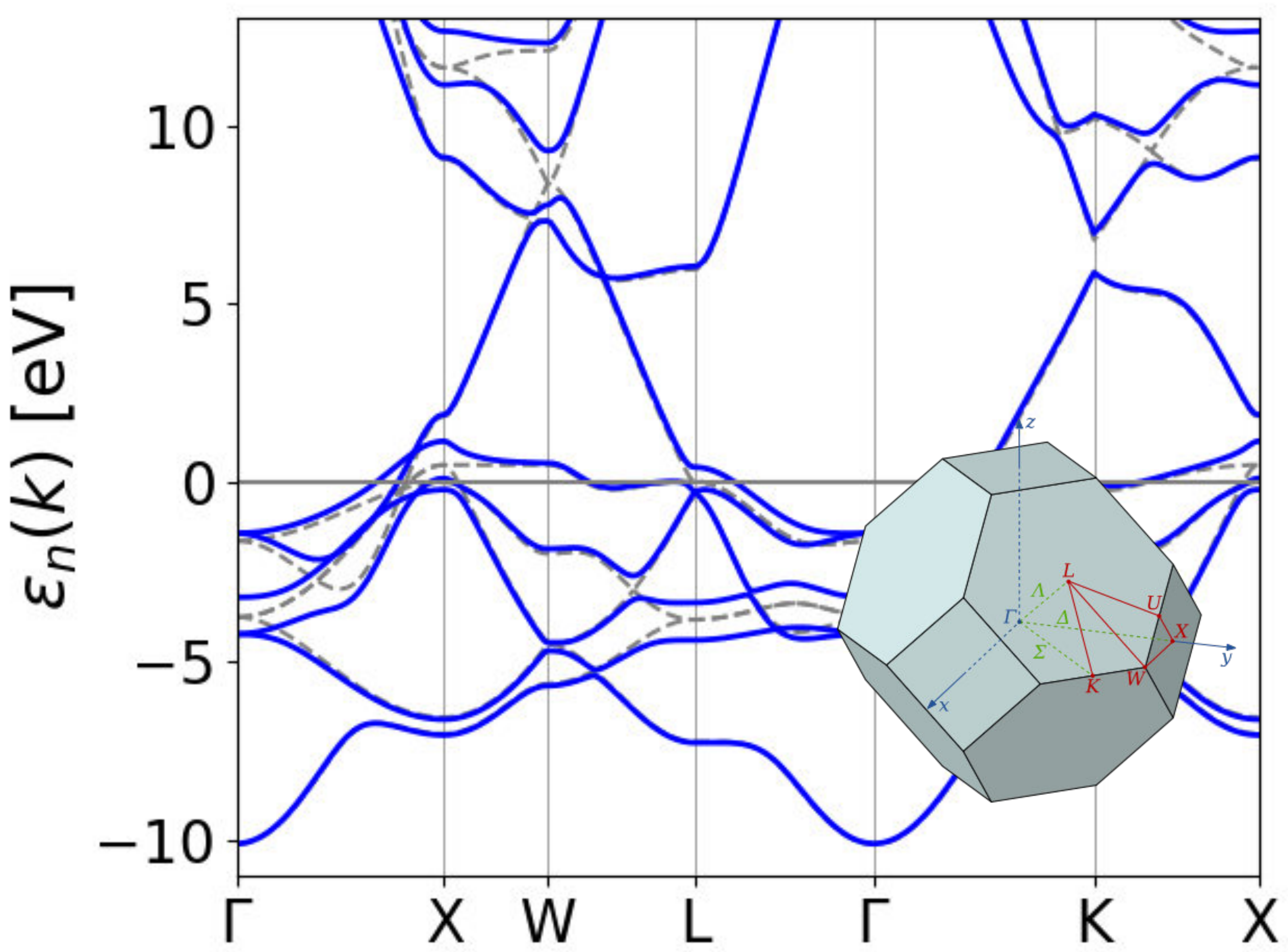
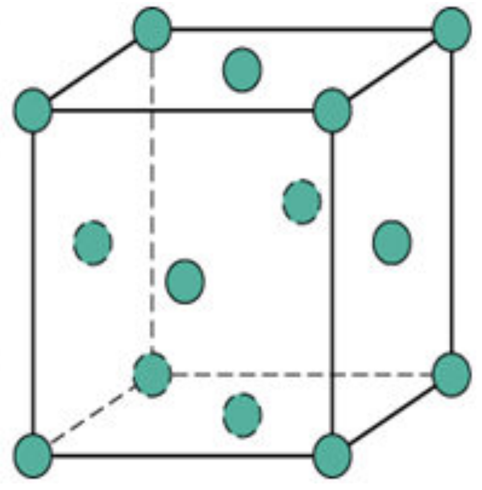
→ Family of solutions $\varepsilon_n(\mathbf{k})$ ($n \in \mathbb{Z}$) with discretely spaced eigenvalues: energy bands!

$$\Psi_{n\mathbf{k}}(\mathbf{r}) = u_n(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}$$

Band index

Energy bands $\{\varepsilon_n(\mathbf{k})\}$ reflect crystal symmetries



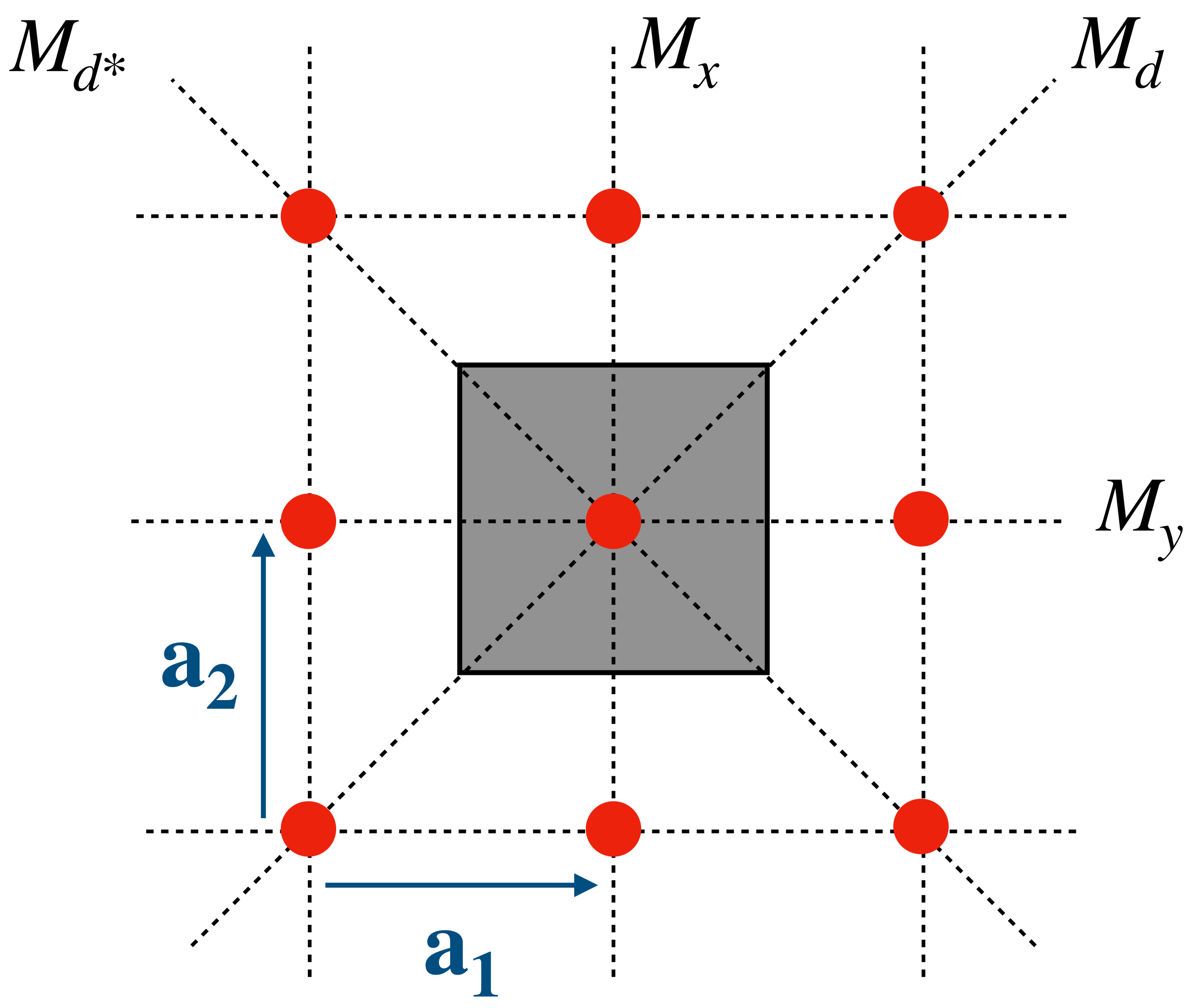


Relation between symmetries and energy bands

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r}), \qquad V(\mathbf{r}) = V(\mathbf{r} + \mathbf{R})$$

$V(\mathbf{r})$ denotes the crystal potential

$\mathbf{R}$ is a direct lattice vector



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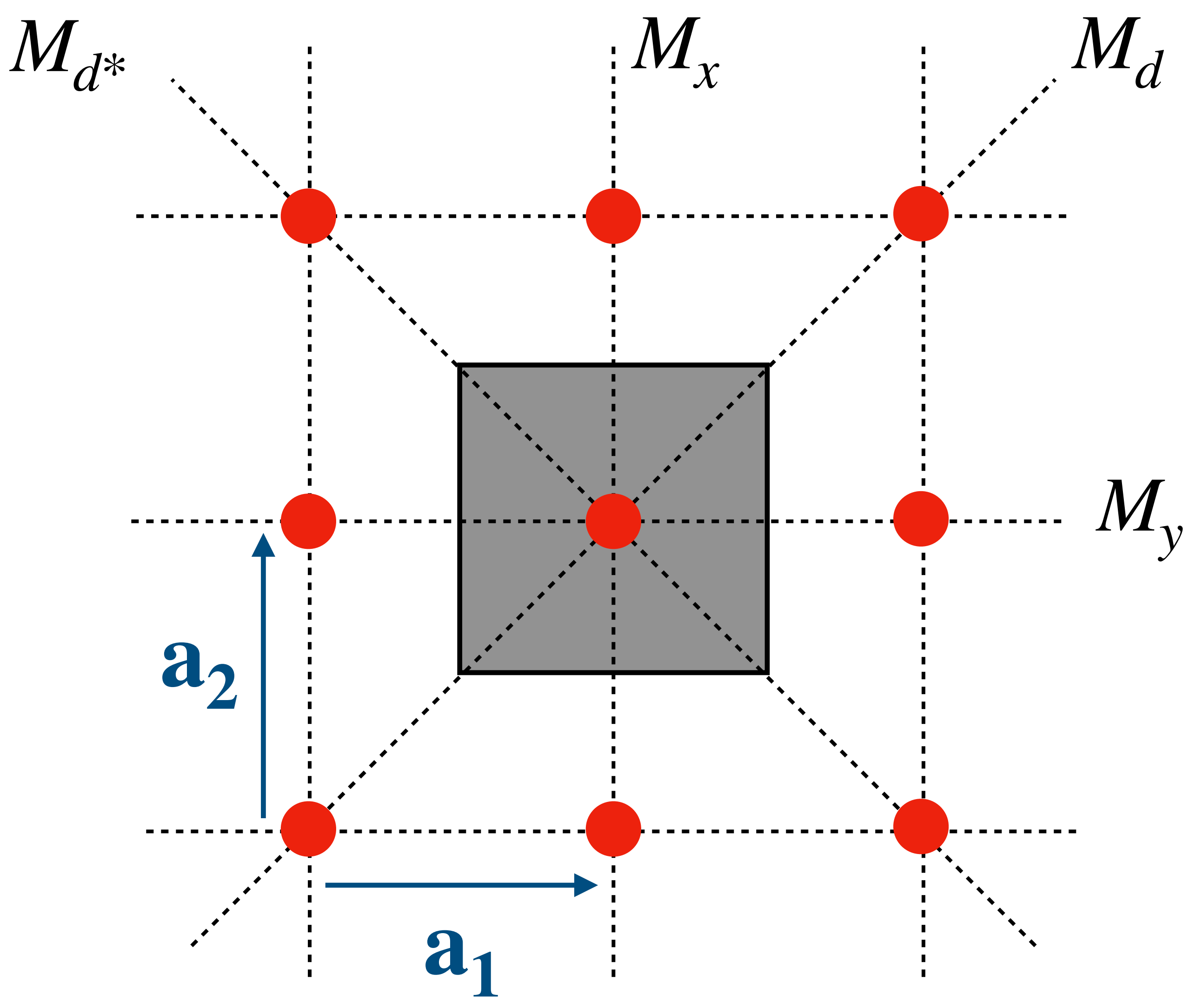

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Beyond translation, $V(\mathbf{r})$ has discrete, point-group symmetries:

➡ 4-fold rotations (90°, 180° & 270°) with a rotation axis || $\mathbf{a}_1 \times \mathbf{a}_2$

➡ mirrors: M_x, M_y, M_d, M_{d*}

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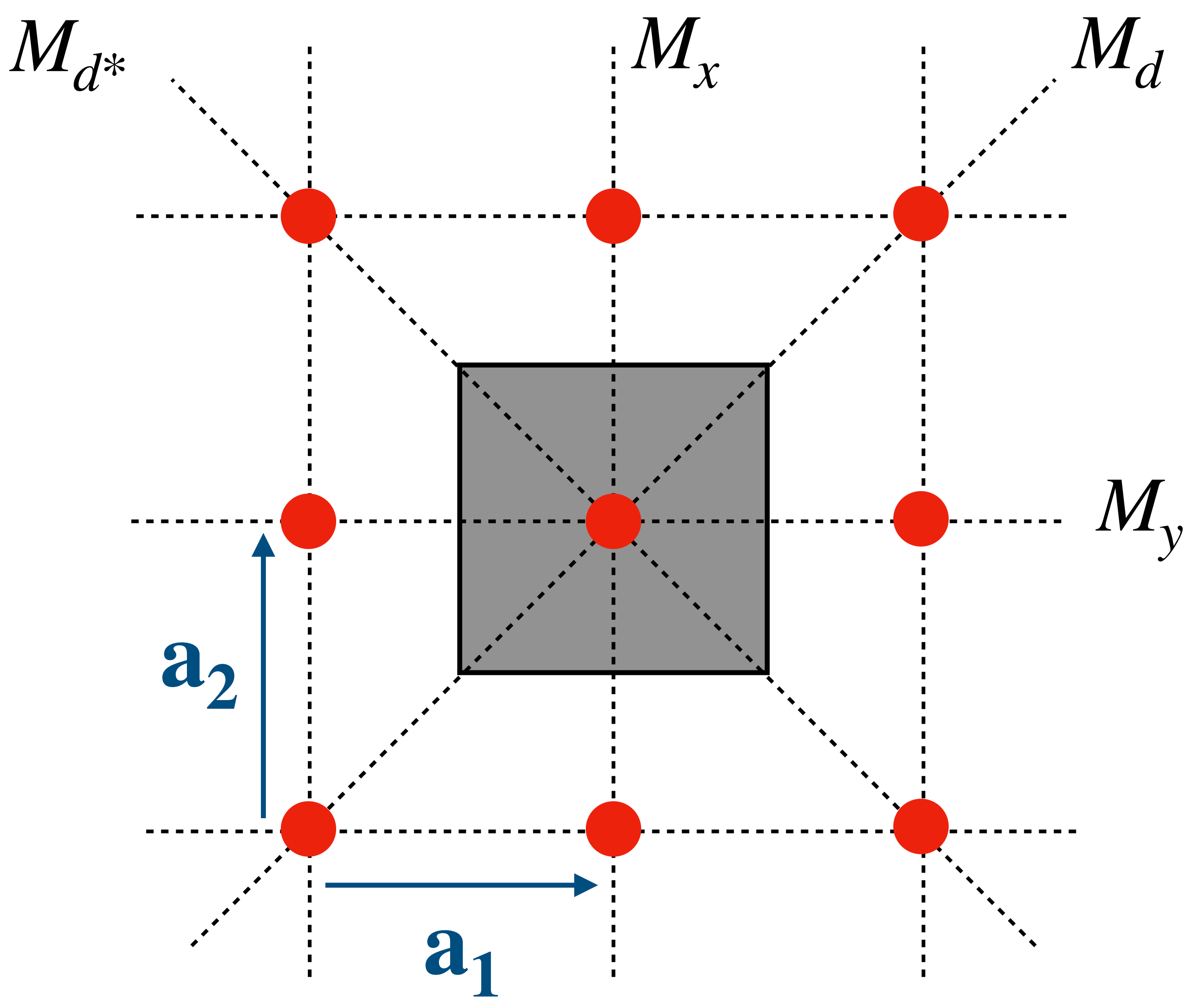

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$$\mathbf{r}' = U\,\mathbf{r} \quad \Rightarrow \quad V(U\,\mathbf{r}) = V(\mathbf{r})$$

any unitary (spatial) symmetry

Relation between symmetries and energy bands

Suppose a solution $(n, \mathbf{k})$ was found

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\Psi_{n\mathbf{k}}(\mathbf{r}) = \varepsilon_n(\mathbf{k})\Psi_{n\mathbf{k}}(\mathbf{r})$$

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symmetry transformation

Laplacian is invariant under Euclidean transformations: $\nabla^2_{U\mathbf{r}} = \nabla^2_{\mathbf{r}}$

$$\left[-\frac{\hbar^2}{2m}\nabla^2_{U\mathbf{r}} + V(U\mathbf{r})\right]\Psi_{n\mathbf{k}}(U\mathbf{r}) = \varepsilon_n(\mathbf{k})\Psi_{n\mathbf{k}}(U\mathbf{r})$$

Symmetric by construction

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New solutions $\Psi_{n\mathbf{k}}(U\mathbf{r})$ with energy $\varepsilon_n(\mathbf{k})$ are obtained!

Relation between symmetries and energy bands

What are the quantum numbers of the symmetry-related solutions $\Psi_{n\mathbf{k}}(U\mathbf{r})$?

Relation between symmetries and energy bands

$$\Psi_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\Psi_{\mathbf{k}}(\mathbf{r})$$

What are the quantum numbers of the symmetry-related solutions $\Psi_{n\mathbf{k}}(U\mathbf{r})$?

Bloch's theorem:

$$\Psi_{n\mathbf{k}}(U\mathbf{r}+U\mathbf{R}) = e^{i\mathbf{k}\cdot U\mathbf{R}}\,\Psi_{n\mathbf{k}}(U\mathbf{r}) \overset{(*)}{\Leftrightarrow} \Psi_{n\mathbf{k}}(U\mathbf{r}+U\mathbf{R}) = e^{i(U^{-1}\mathbf{k})\cdot\mathbf{R}}\,\Psi_{n\mathbf{k}}(U\mathbf{r})$$

(*) Note that $U\mathbf{R}$ is just another lattice vector and $\mathbf{k}\cdot U\mathbf{R} = (U^{-1}\mathbf{k})\cdot\mathbf{R}$

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$\Psi_{n\mathbf{k}}(U\mathbf{r})$ is a Bloch eigenstate with wavevector $U^{-1}\mathbf{k}$ and energy $\varepsilon_n(\mathbf{k})$. That is, $\Psi_{n\mathbf{k}}(U\mathbf{r}) = \Psi_{n,U^{-1}\mathbf{k}}(\mathbf{r})$.

(*) Note that $U\mathbf{R}$ is just another lattice vector and $\mathbf{k}\cdot U\mathbf{R} = (U^{-1}\mathbf{k})\cdot\mathbf{R}$

Relation between symmetries and energy bands

$$\varepsilon_n(\mathbf{k}) = \varepsilon_n(U\mathbf{k})$$

Energy bands inherit symmetries of the crystal potential

Example: centro-symmetric systems like Pt

$$\varepsilon_n(\mathbf{k}) = \varepsilon_n(-\mathbf{k})$$

Relation between symmetries and energy bands

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Energy bands inherit symmetries of the crystal potential

↓

degeneracies therefore emerge from spatial symmetries like inversion

We shall see shortly that spatial symmetries are important for ***band crossings*** in topological materials

Relation between symmetries and energy bands

Time-reversal symmetry

In the absence of internal degrees of freedom (DOF), like spin, TRS is enacted by the anti-unitary operator $U^* = K \equiv \mathcal{T}$

$$\mathcal{T}^{-1}\hat{H}\mathcal{T} = \hat{H}$$

$\Rightarrow$ $\mathcal{T}\Psi_{n\mathbf{k}}(\mathbf{r}) = \Psi^*_{n\mathbf{k}}(\mathbf{r})$ is a solution with the same energy than $\Psi_{n\mathbf{k}}(\mathbf{r})$

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$\Psi_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\Psi_{n\mathbf{k}}(\mathbf{r})$ ➡ $[\Psi_{n\mathbf{k}}(\mathbf{r}+\mathbf{R})]^* = e^{-i\mathbf{k}\cdot\mathbf{R}}[\Psi_{n\mathbf{k}}(\mathbf{r})]^*$

➡ $[\Psi_{n\mathbf{k}}(\mathbf{r})]^*$ is a Bloch eigenfunction with wavevector $-\mathbf{k}$

Relation between symmetries and energy bands

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$$\varepsilon_n(\mathbf{k}) = \varepsilon_n(-\mathbf{k})$$

General property of TR invariant systems

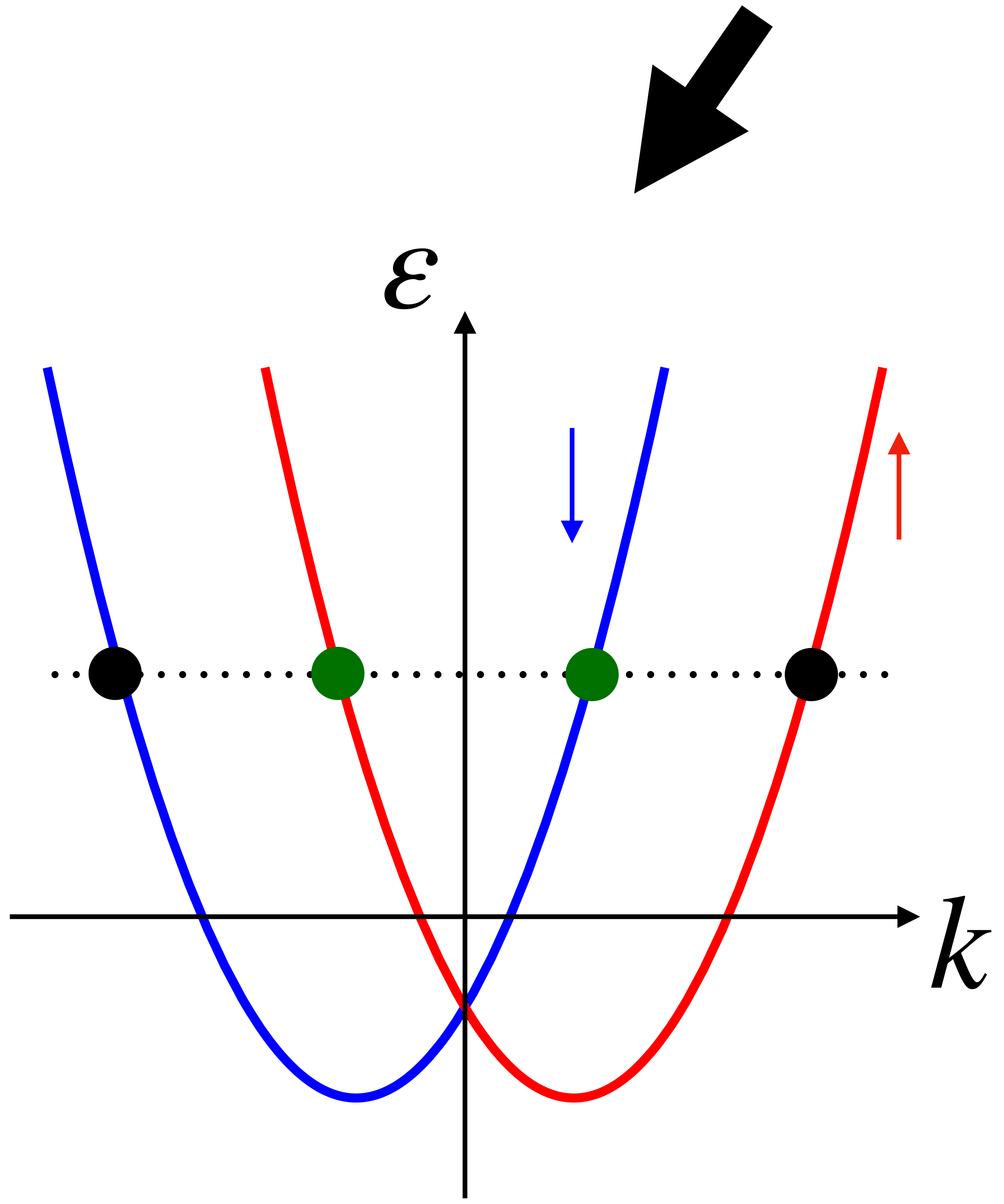
(even if they lack spatial inversion symmetry, such as GaAs)

Relation between symmetries and energy bands

The spin degree of freedom: Kramers degeneracy

time-reversal symmetry $\mathscr{T}$

$$\varepsilon_{\uparrow}(\mathbf{k}) = \varepsilon_{\downarrow}(-\mathbf{k})$$



2 Kramers' pairs

Part 1: Time-reversal symmetry I Band structure

Relation between symmetries and energy bands

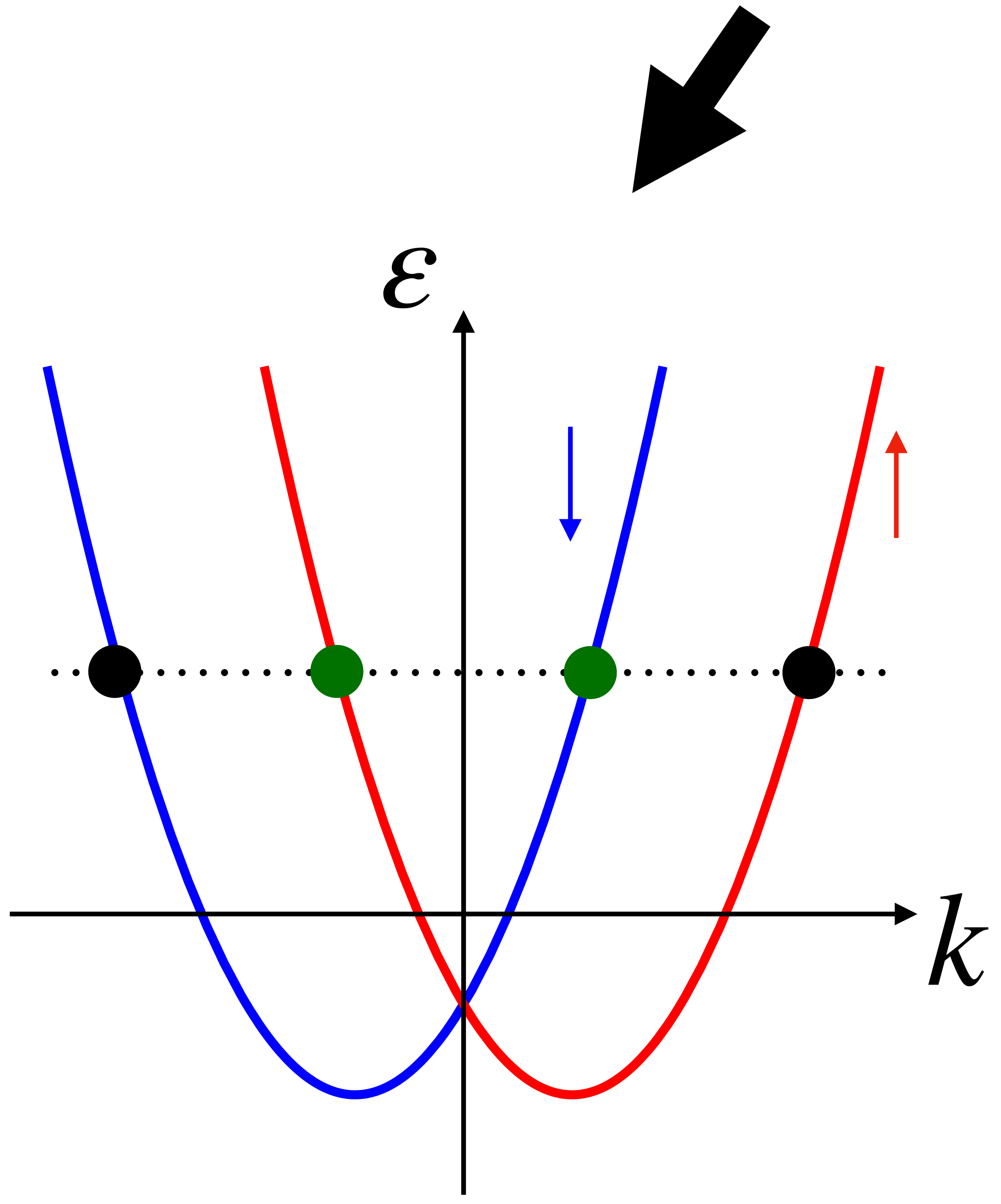
The spin degree of freedom: Kramers degeneracy

time-reversal symmetry $\mathscr{T}$	inversion symmetry I
$\varepsilon_\uparrow(\mathbf{k}) = \varepsilon_\downarrow(-\mathbf{k})$	$\varepsilon_{\downarrow(\uparrow)}(\mathbf{k}) = \varepsilon_{\downarrow(\uparrow)}(-\mathbf{k})$

$I\mathscr{T}$ **symmetry**

$$\varepsilon_\uparrow(\mathbf{k}) = \varepsilon_\downarrow(\mathbf{k})$$

spin-degenerate bands



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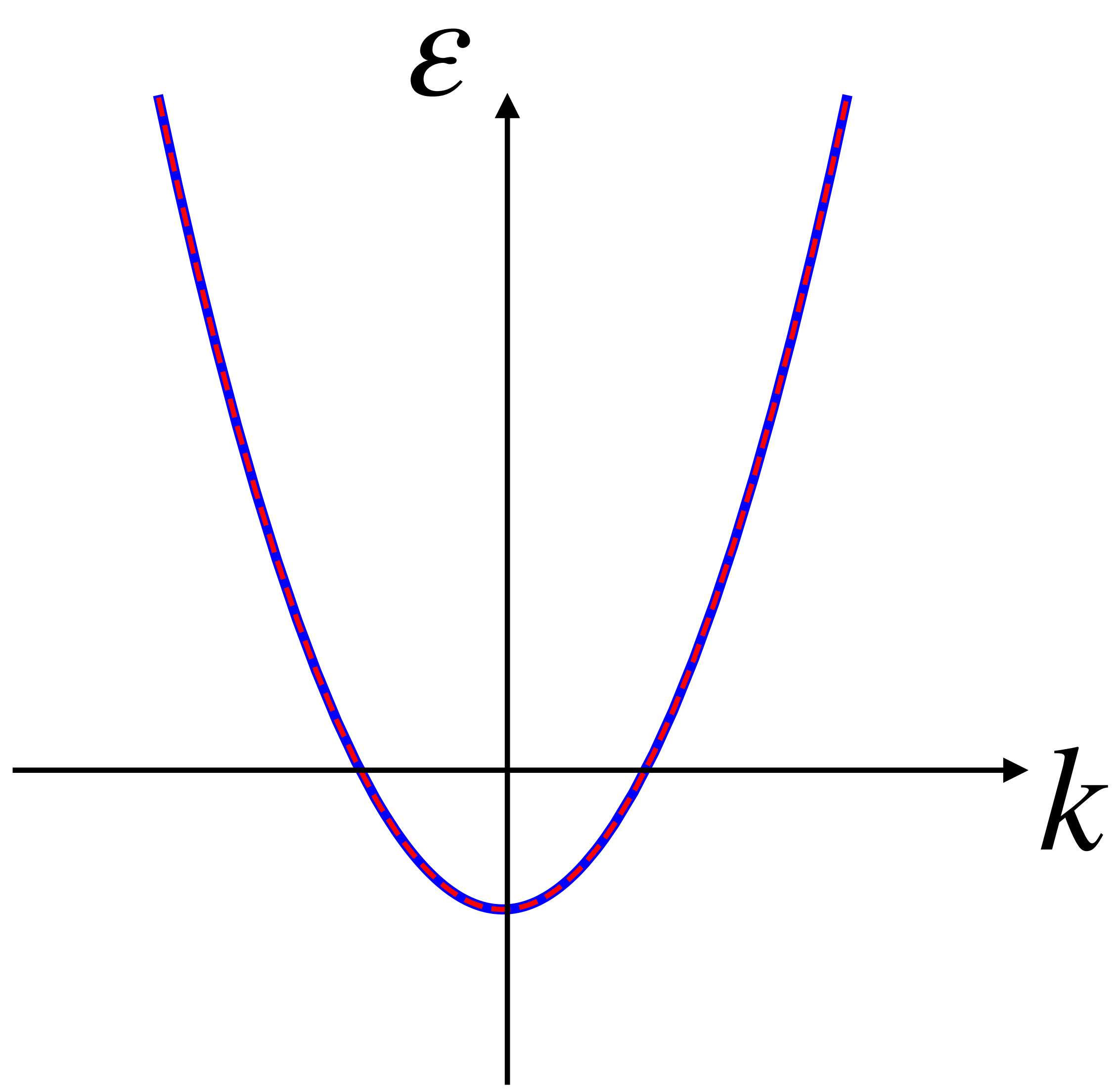


Relation between symmetries and energy bands

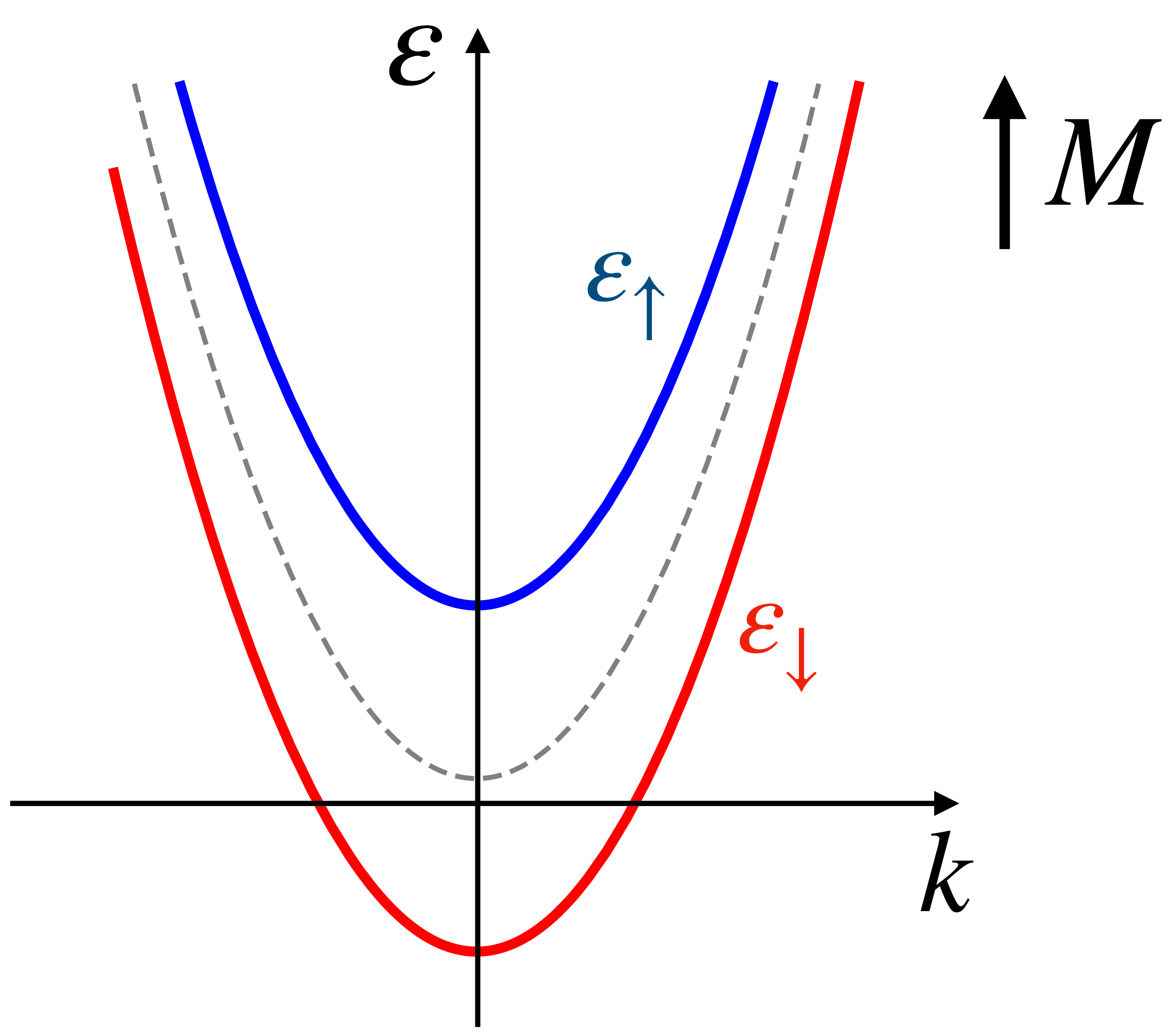
Magnetic materials

spin-degeneracy lifting (FMs) → broken $\mathscr{T}$ symmetry

$\mathbf{M} \neq 0$

Think of a Stoner instability,

$U\rho(\varepsilon_F) \geq 1$



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TR symmetry is effectively restored if $\mathscr{T}$ **+** spatial operation
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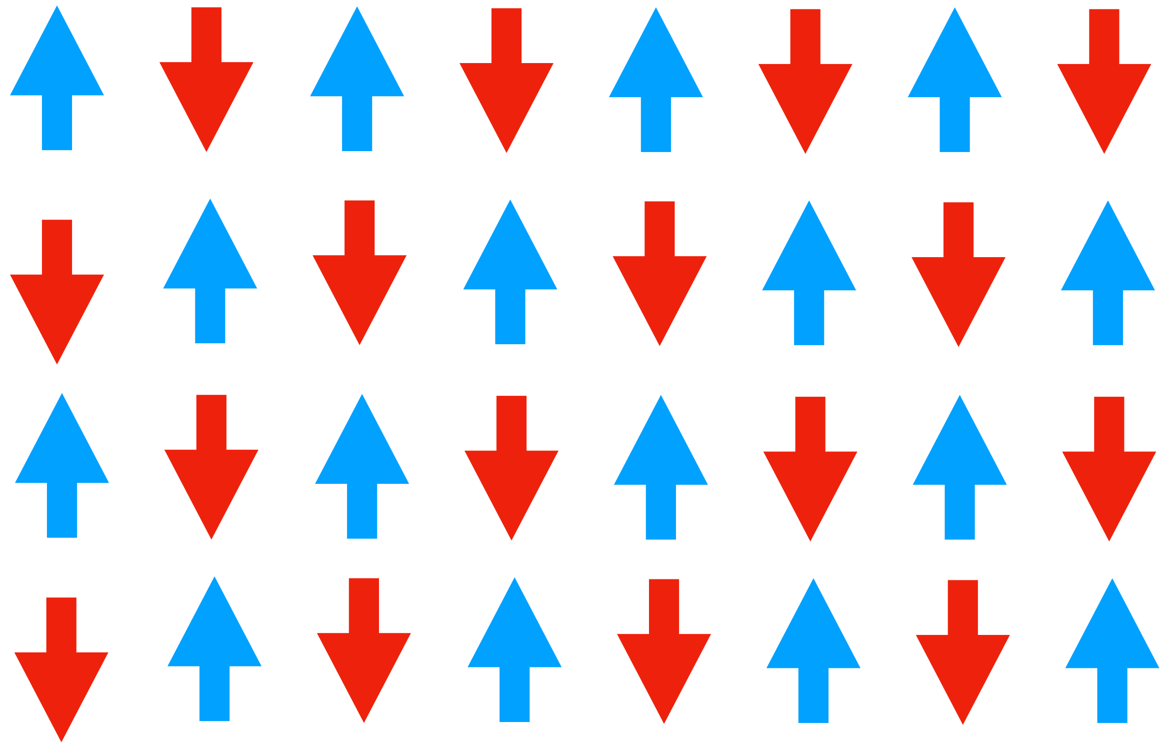
Bipartite antiferromagnetic lattice



Part 1: Time-reversal symmetry I Band structure

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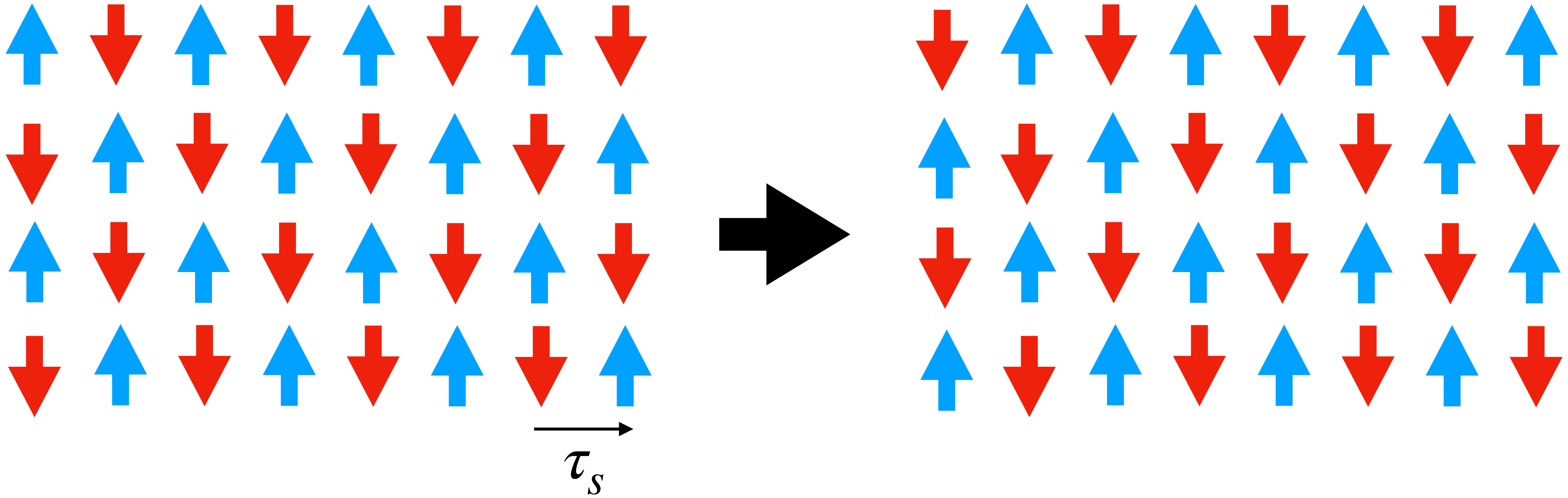

Sublattice translation

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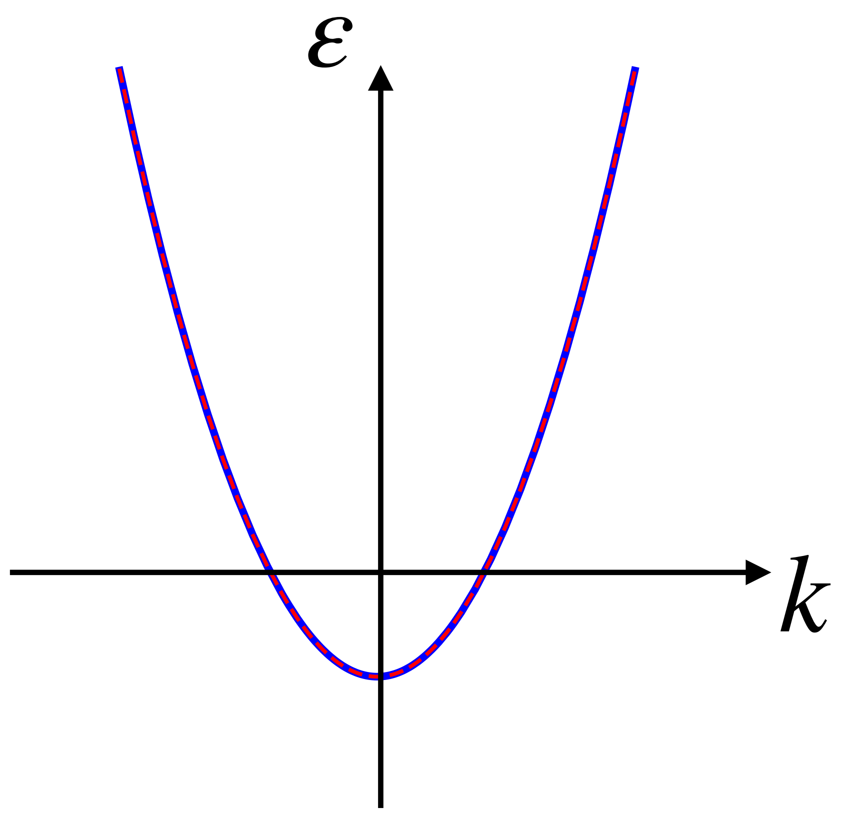
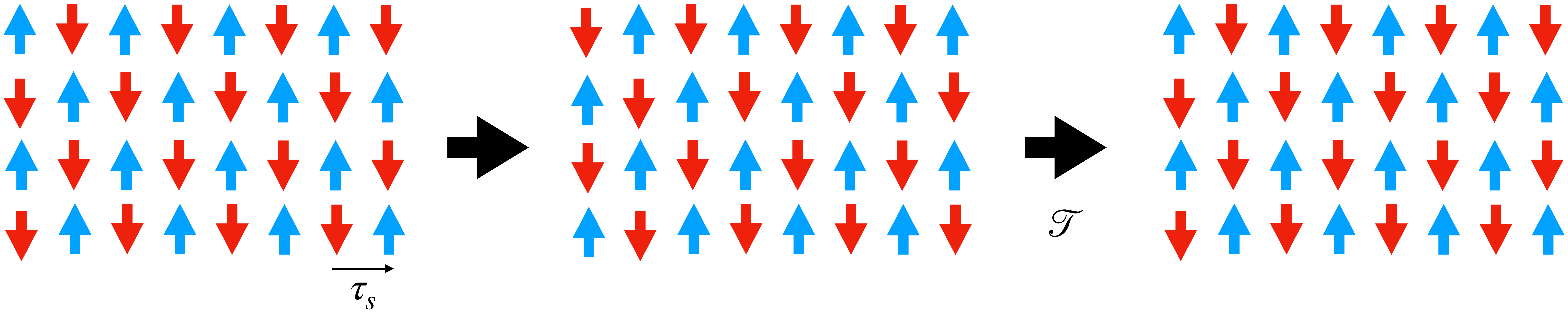
Kramers antiferromagnetism



$\mathscr{T}\tau_s$ **symmetry**

Bipartite antiferromagnetic lattice

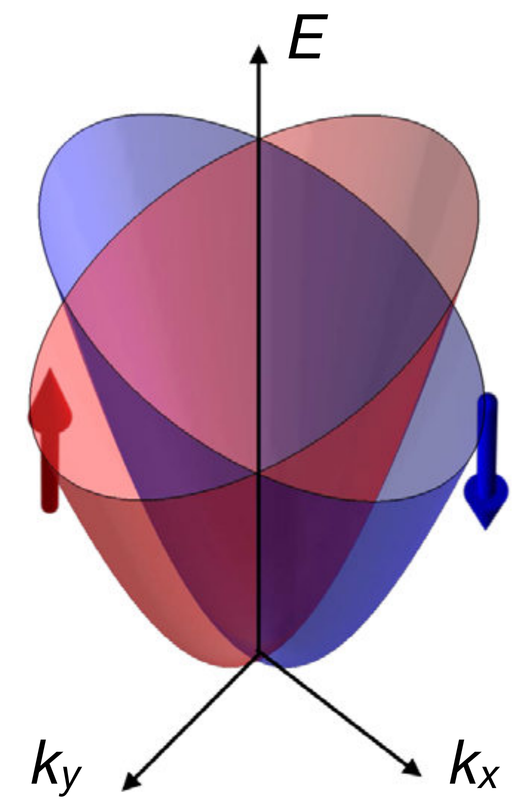


Sublattice translation

Relation between symmetries and energy bands

Altermagnets combine unique properties of ferromagnets and antiferromagnets

staggered magnetic order *both in* ***real space*** *(like AFMs) and in* ***$\mathbf{k}$-space*** *(like FMs)*



Šmejkal, Sinova & Jungwirth (2022)

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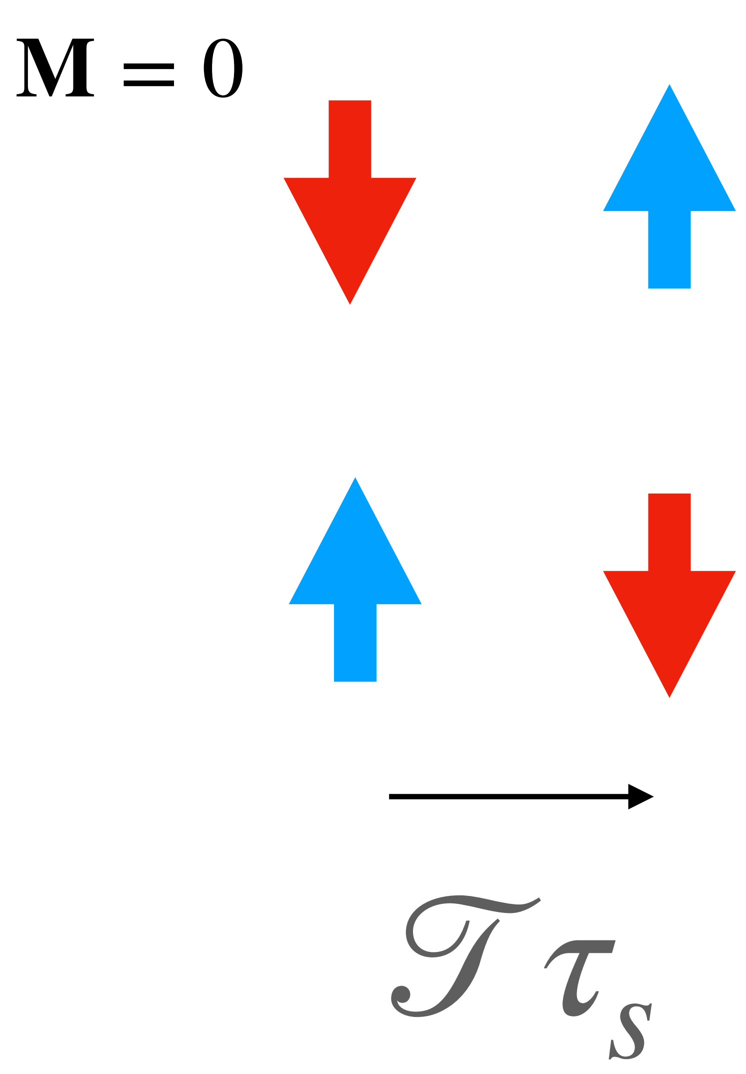
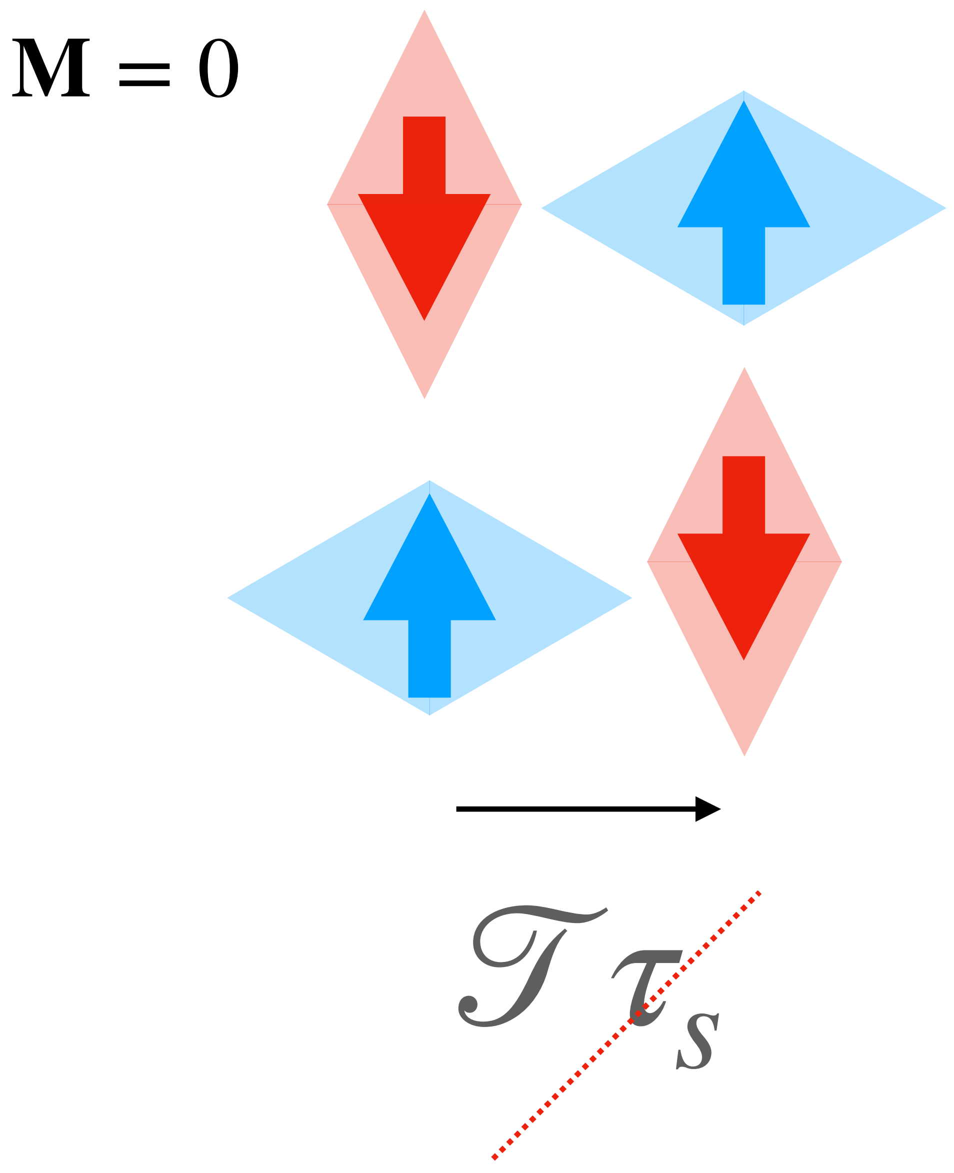
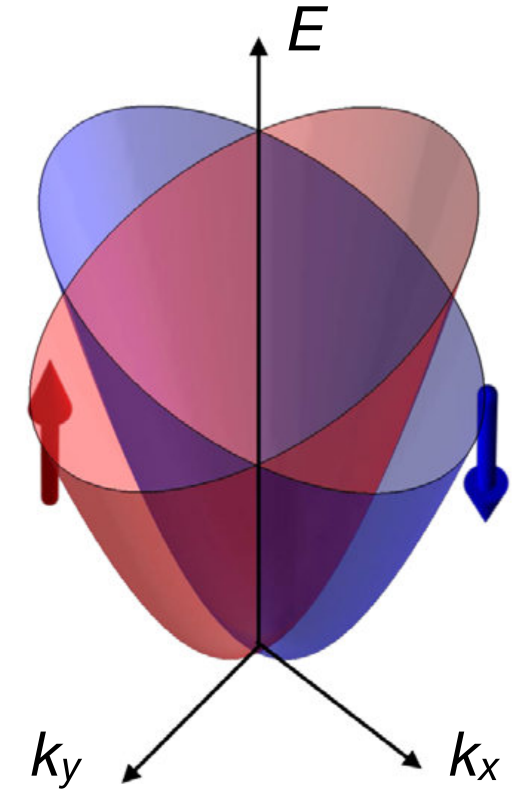


Antiferromagnet



Altermagnet



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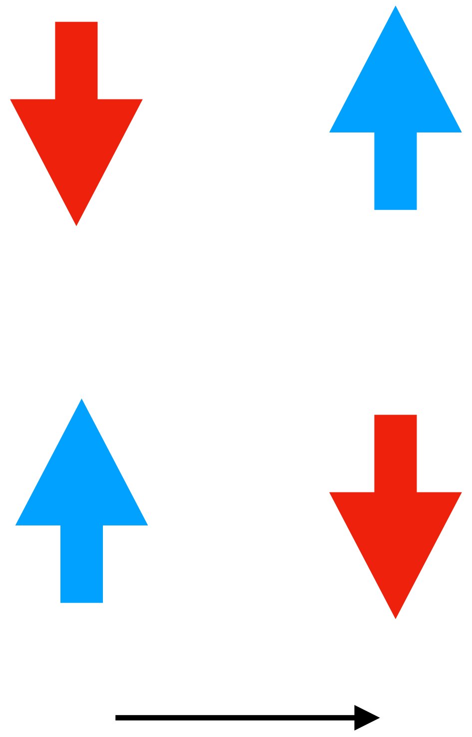

$\mathcal{T}\tau_s$

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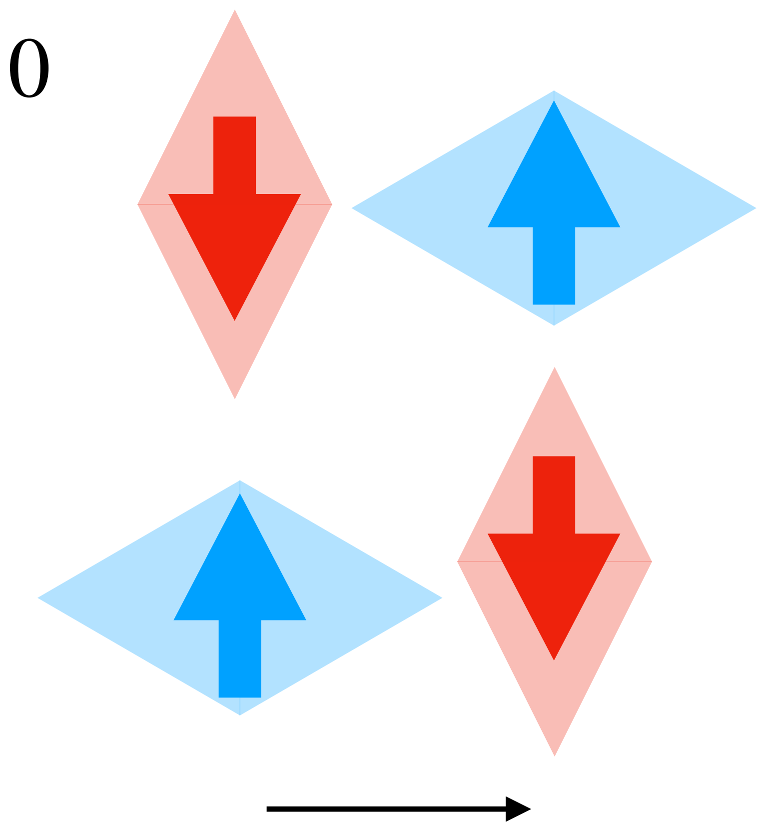


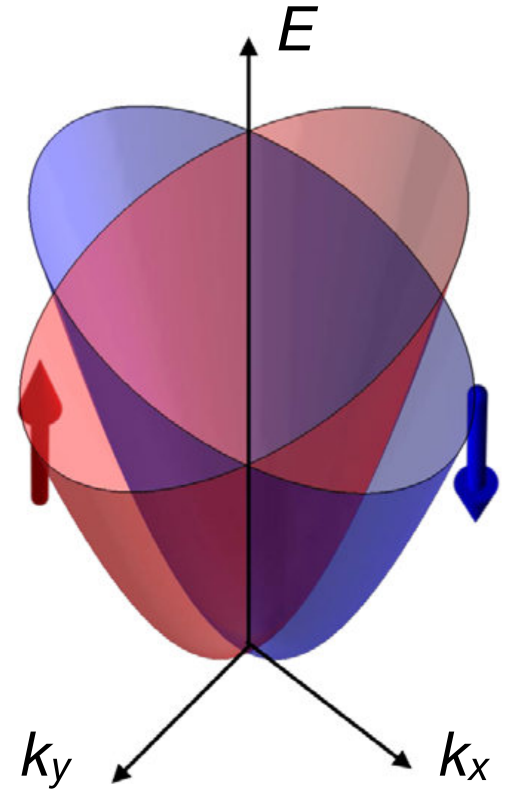
~~$\mathcal{T}\tau_s$~~

Altermagnet

Sublattices connected by rotation:

$$[C_2 || C_4\tau_s]$$

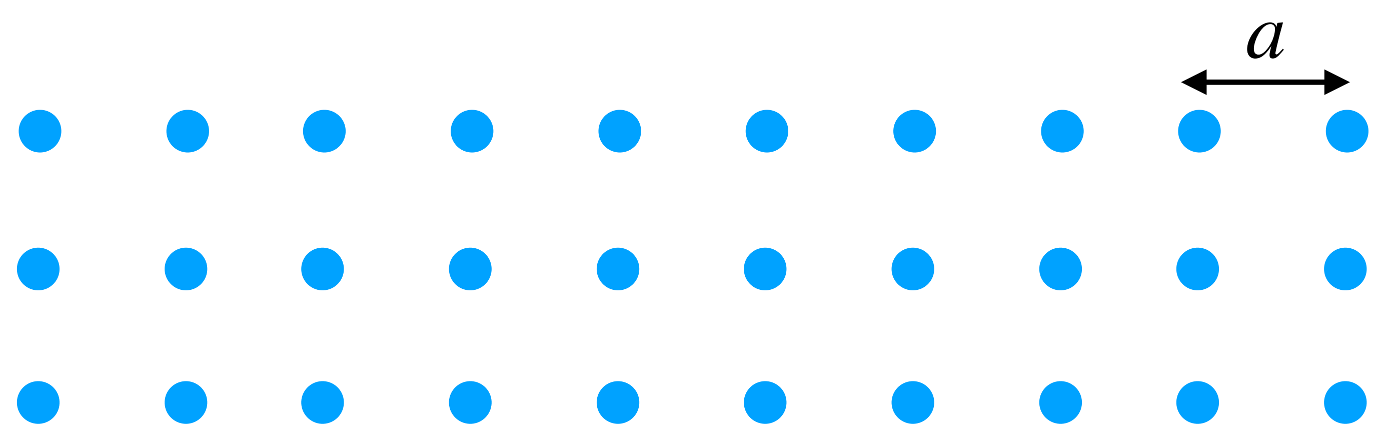
non-relativistic spin-group symmetry

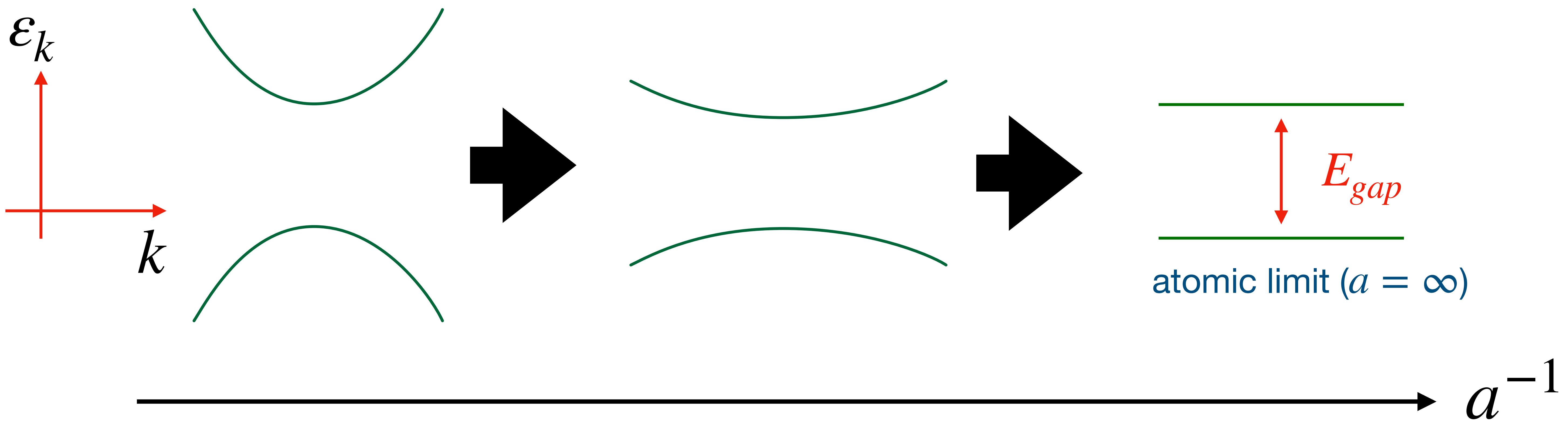


Šmejkal, Sinova & Jungwirth (2022)

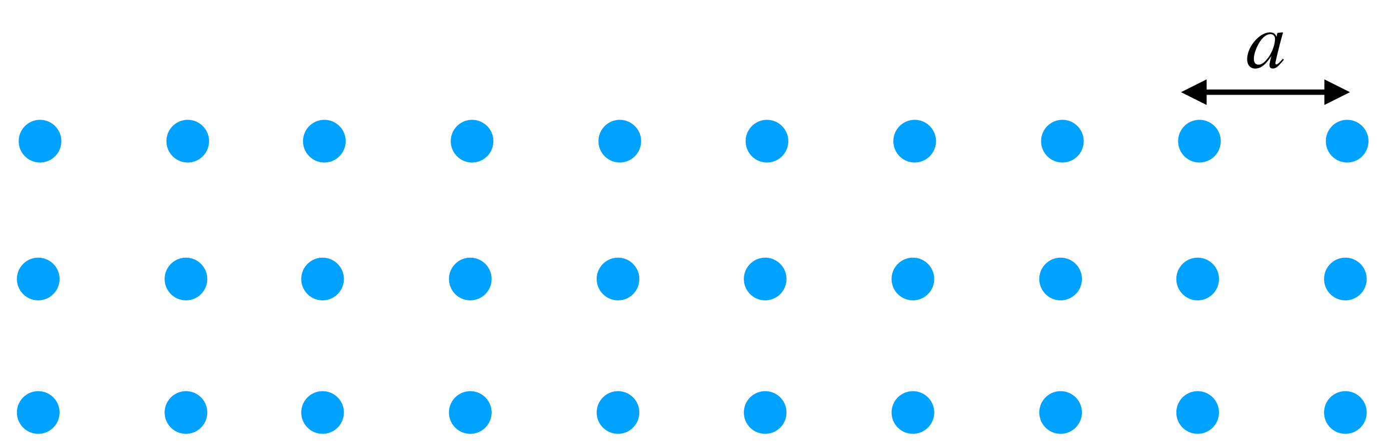
Gapped topological matter

Trivial insulator as an atomic limit

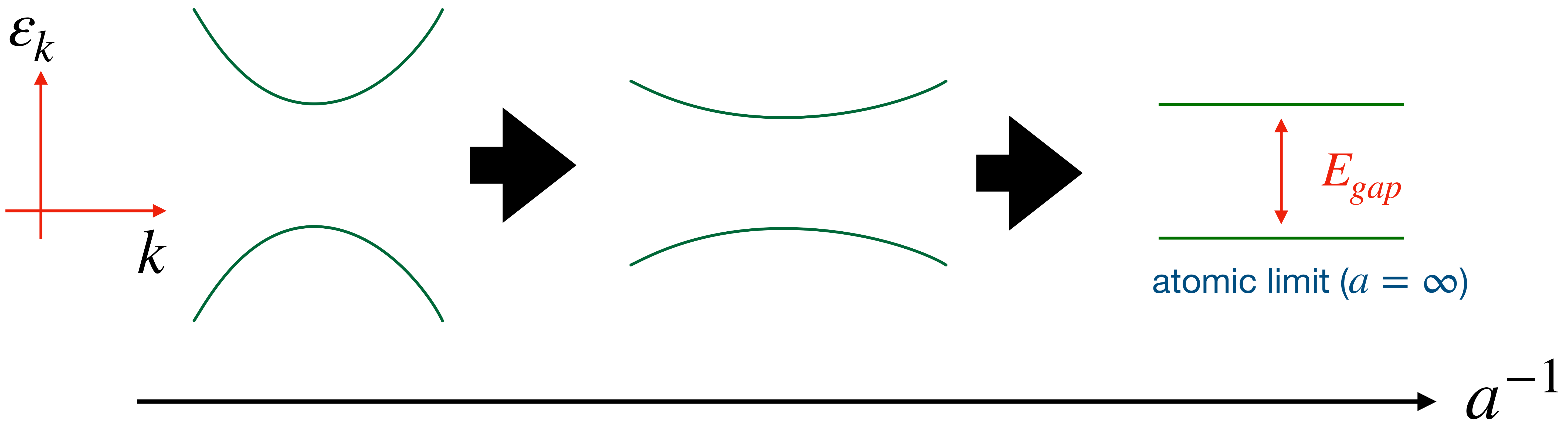




Gapped topological matter



Trivial insulator as an atomic limit



➡ Band structure admits smooth ψ_n with $|\psi_{n,\mathbf{k}+\mathbf{G}}\rangle = |\psi_{n,\mathbf{k}}\rangle$

(Bloch functions $u_n(\mathbf{k})$ are smooth on the BZ torus $\mathbf{T}$)

Berry connection, $\mathscr{A}_n(\mathbf{k}) = i\langle u_n(\mathbf{k}) | \nabla_{\mathbf{k}} u_n(\mathbf{k})\rangle$, is smooth on $\mathbf{T}$

trivial topology

Part 2: Non-Spatial Symmetries I 10-fold classification of topological matter

Gapped topological matter

For 2D:

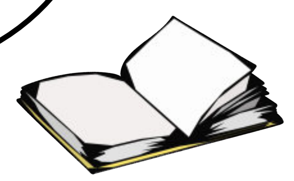
$$C_n = \frac{1}{2\pi} \oint_{\partial BZ} d\mathbf{k} \cdot \mathscr{A}_n(\mathbf{k})$$

No. of vortices of the vector field $\mathscr{A}(\mathbf{k})$

Vortices emerge from phase discontinuities in $\psi_n(\mathbf{k})$ *(so-called topological obstructions)*

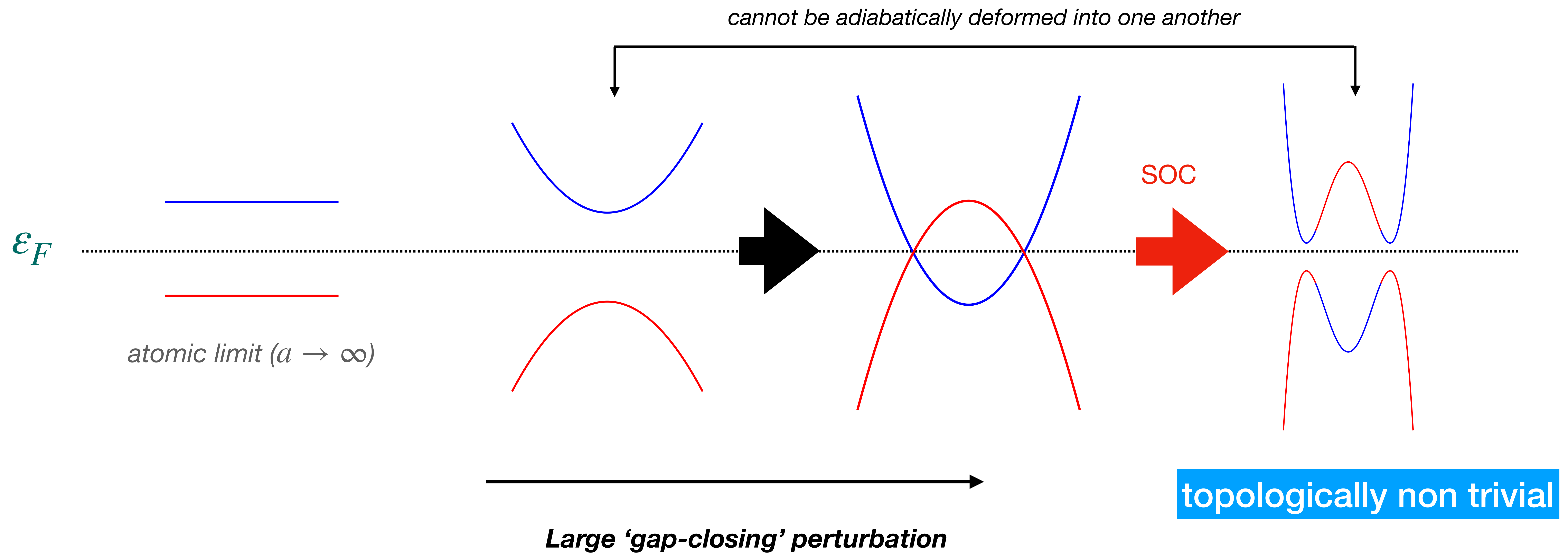
For smooth $u_n(\mathbf{k})$, $C_n = 0$ *due to Stokes theorem applied to a closed manifold:*

$$\iint_{\mathbf{T}^2} \nabla \times \boldsymbol{f} \cdot d\mathbf{S} = 0$$



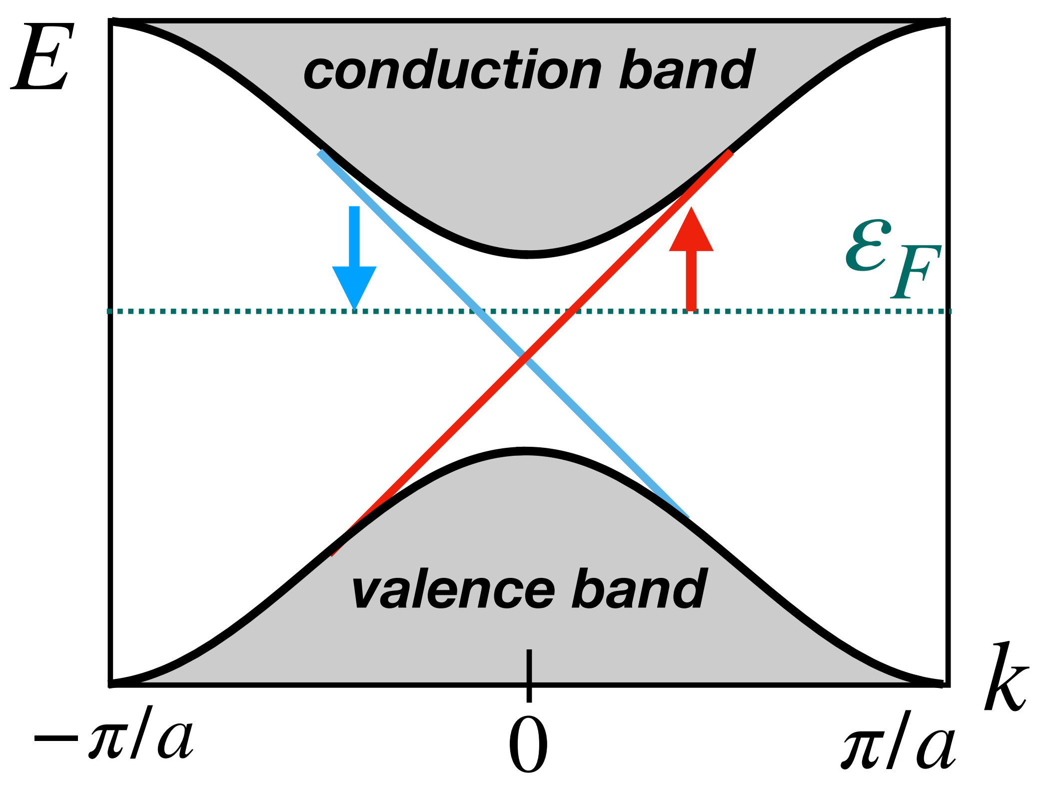
Gapped topological matter

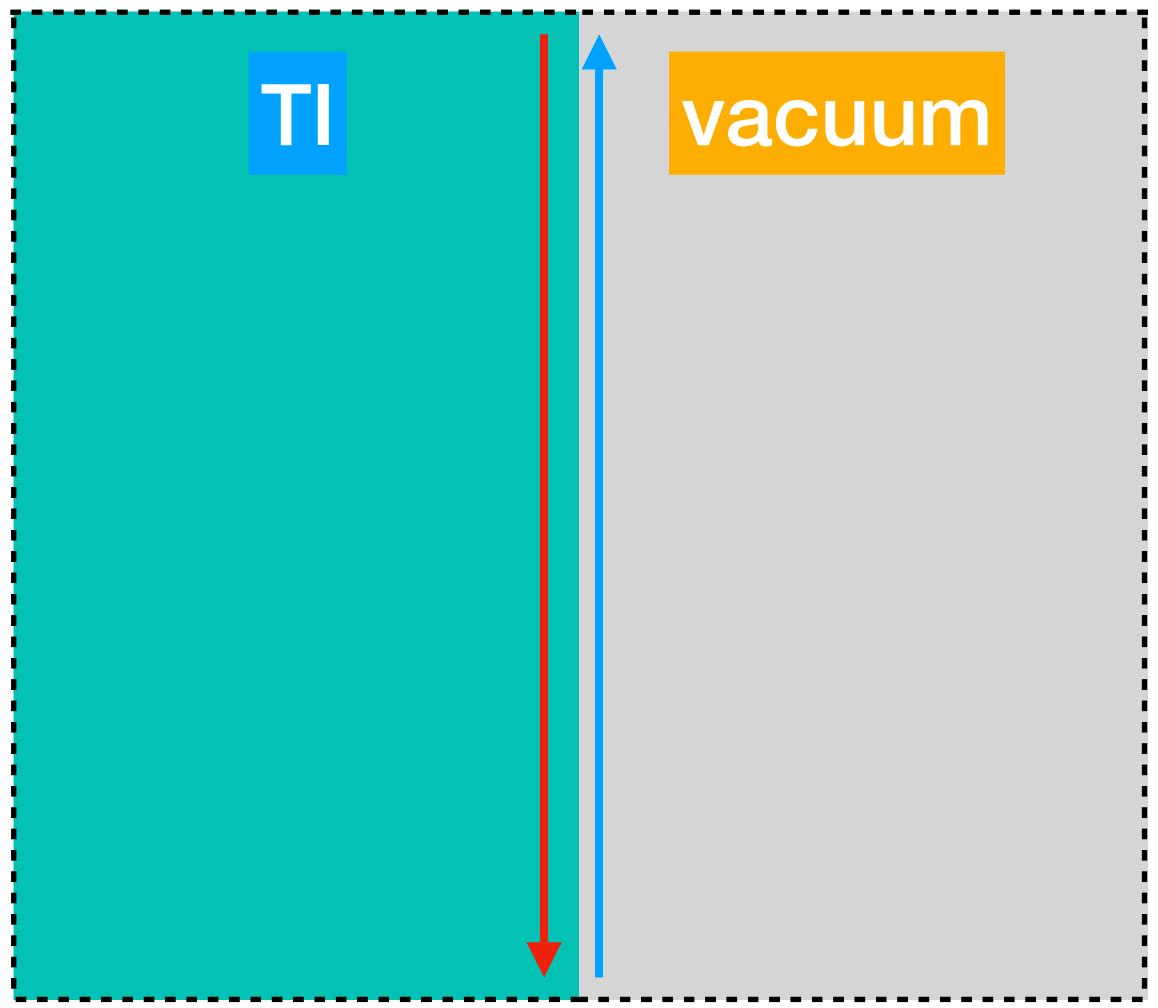
<u>*Topological insulators **vs** trivial insulators*</u>



Part 2: Non-Spatial Symmetries I 10-fold classification of topological matter

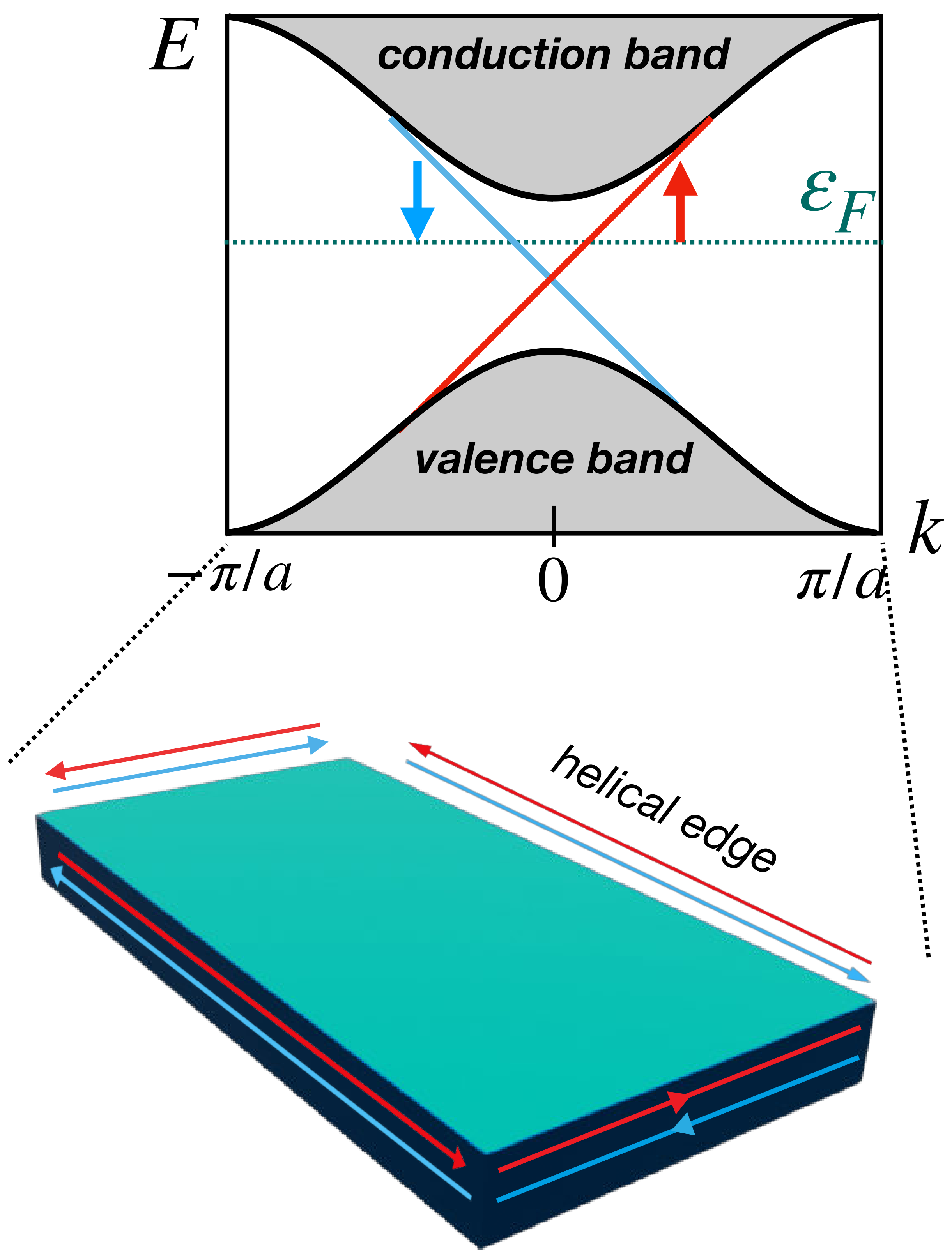
spin up
spin down

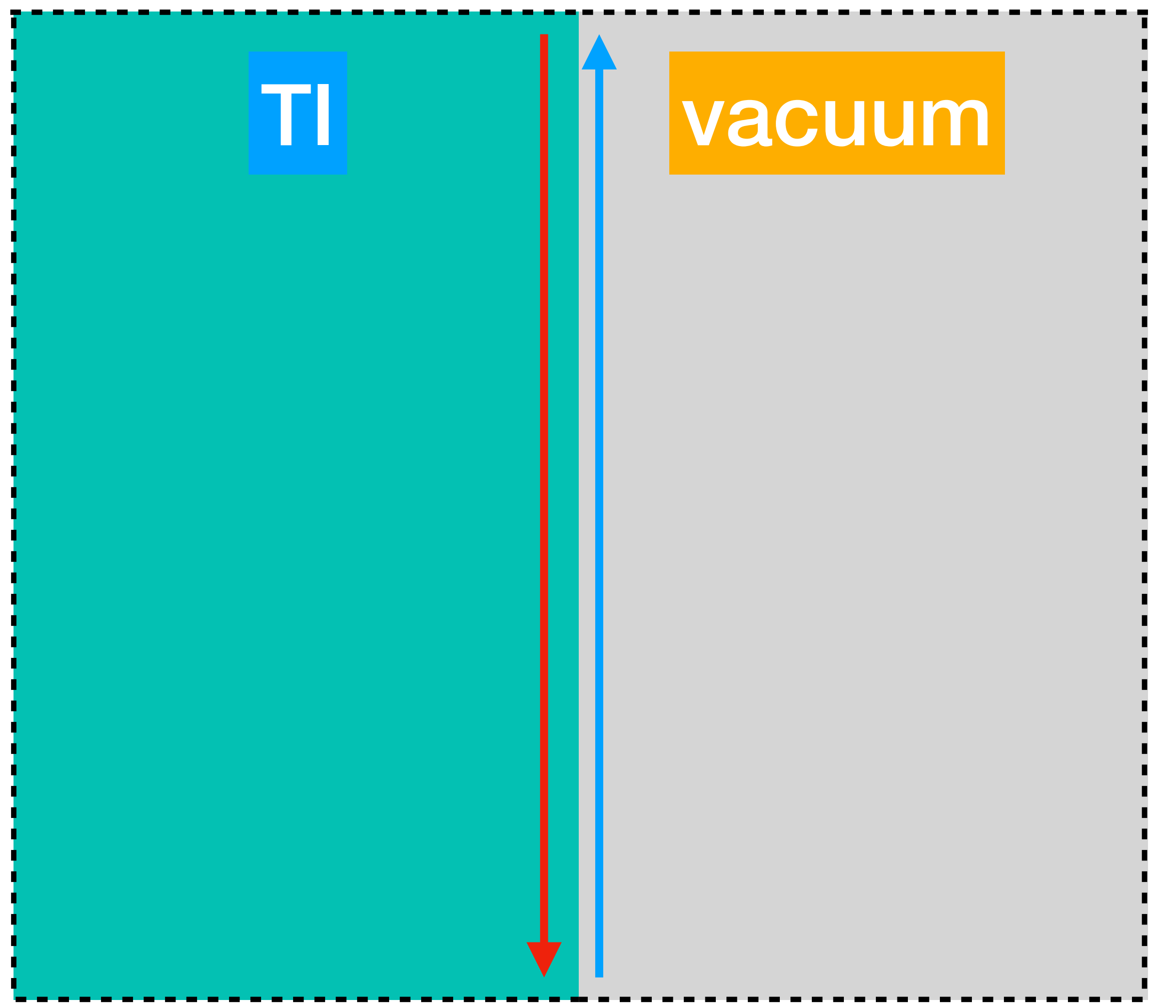




Part 2: Non-Spatial Symmetries I 10-fold classification of topological matter

spin up
spin down





Quantum spin Hall insulator

$$C_s = (C_\uparrow - C_\downarrow)/2, \quad \sigma^s_{yx} = (e/2\pi)\, C_s$$

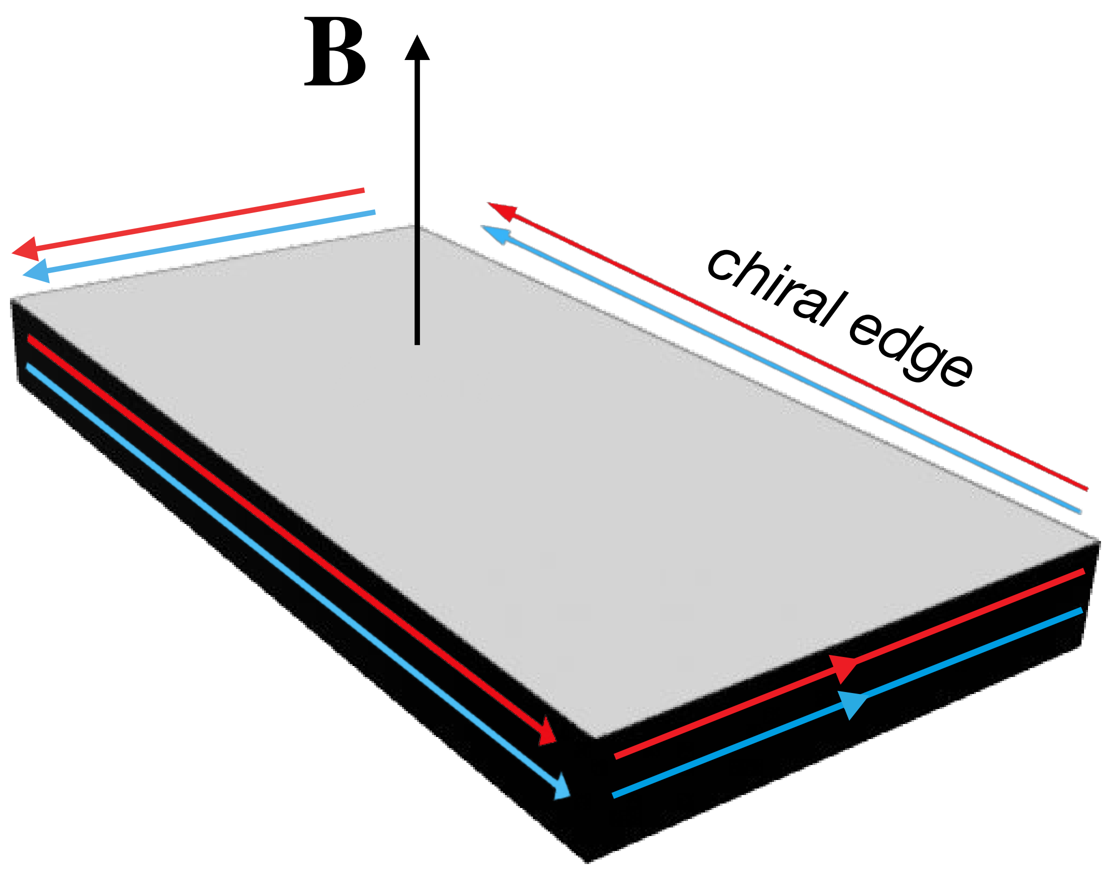
$$\mathbb{Z}_2 = C_s \bmod 2$$

$\mathcal{T}$ symmetry protected

Part 2: Non-Spatial Symmetries | 10-fold classification of topological matter

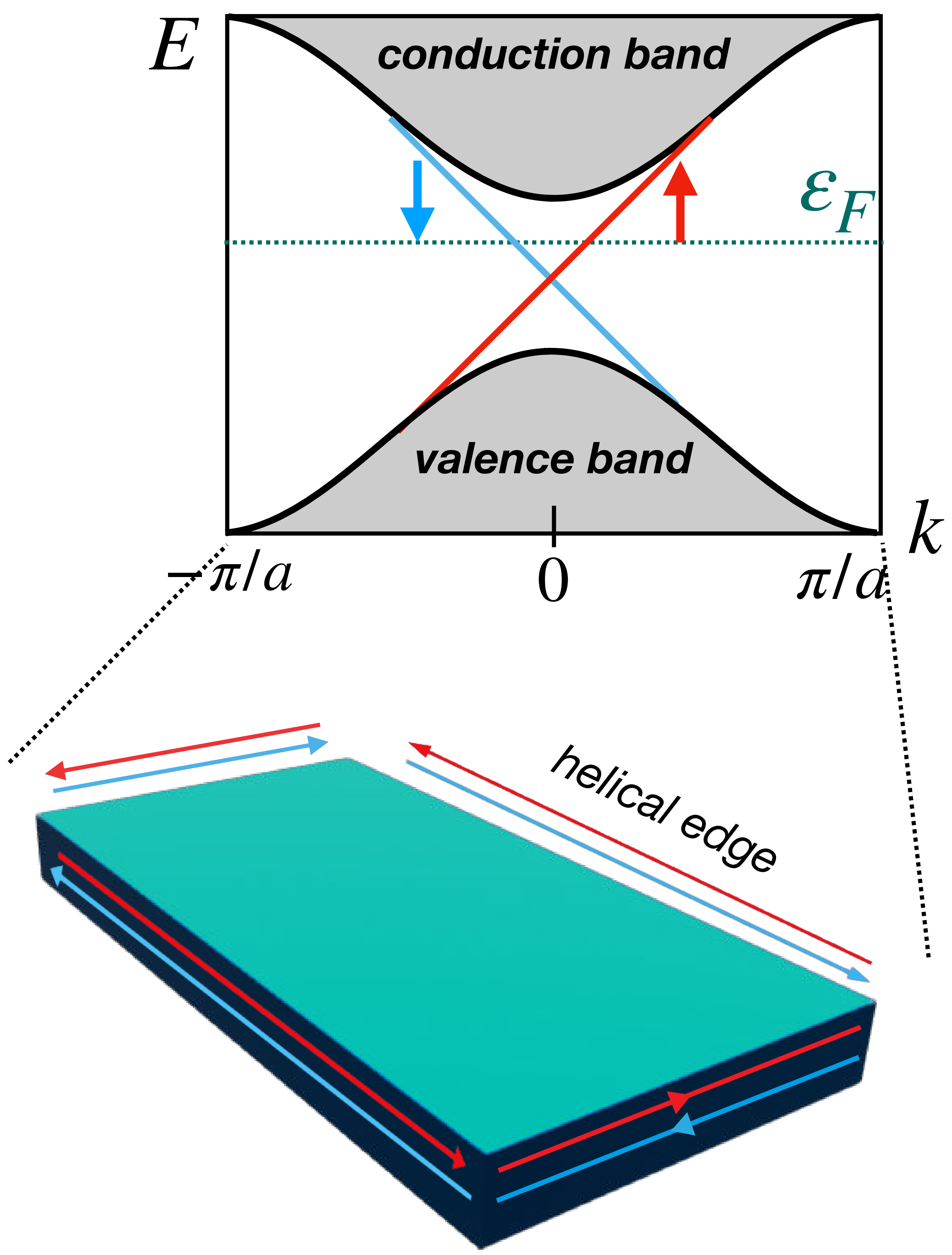
spin up
spin down

Broken $\mathscr{T}$



Quantum Hall insulator

$$C = C_\uparrow + C_\downarrow \in \mathbb{Z}, \quad \sigma_{yx} = (e^2/h)\, C$$



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Part 2: Non-Spatial Symmetries I 10-fold classification of topological matter

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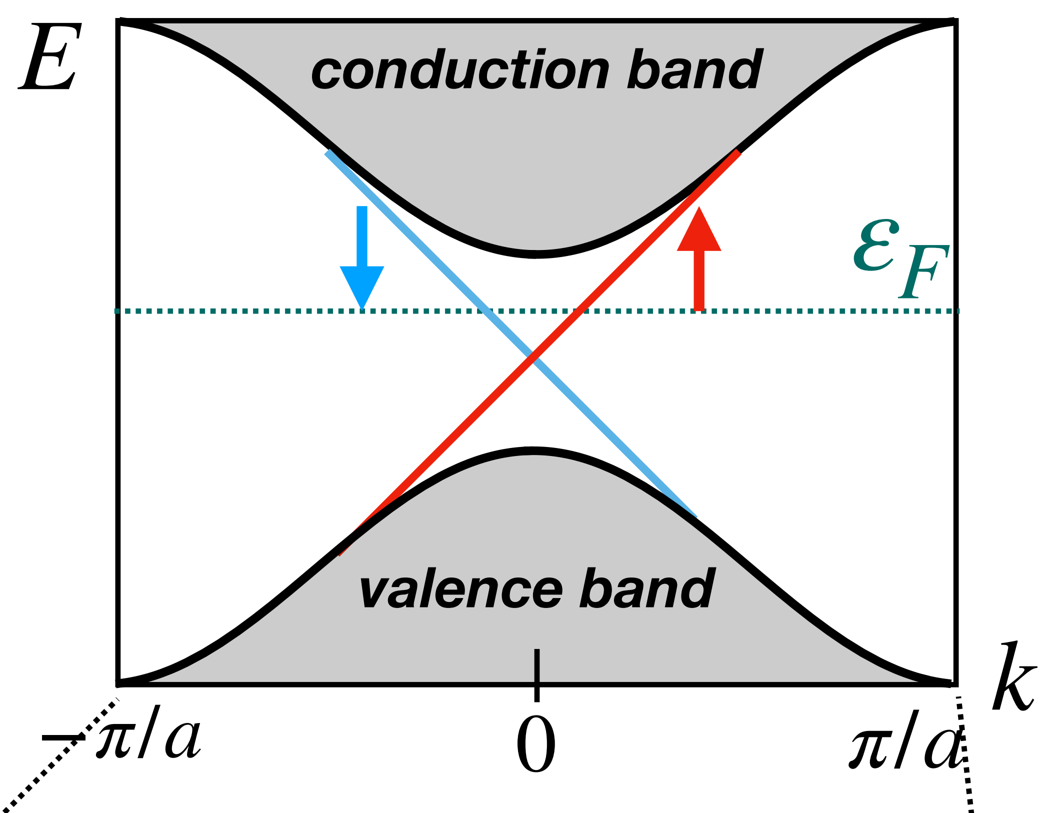

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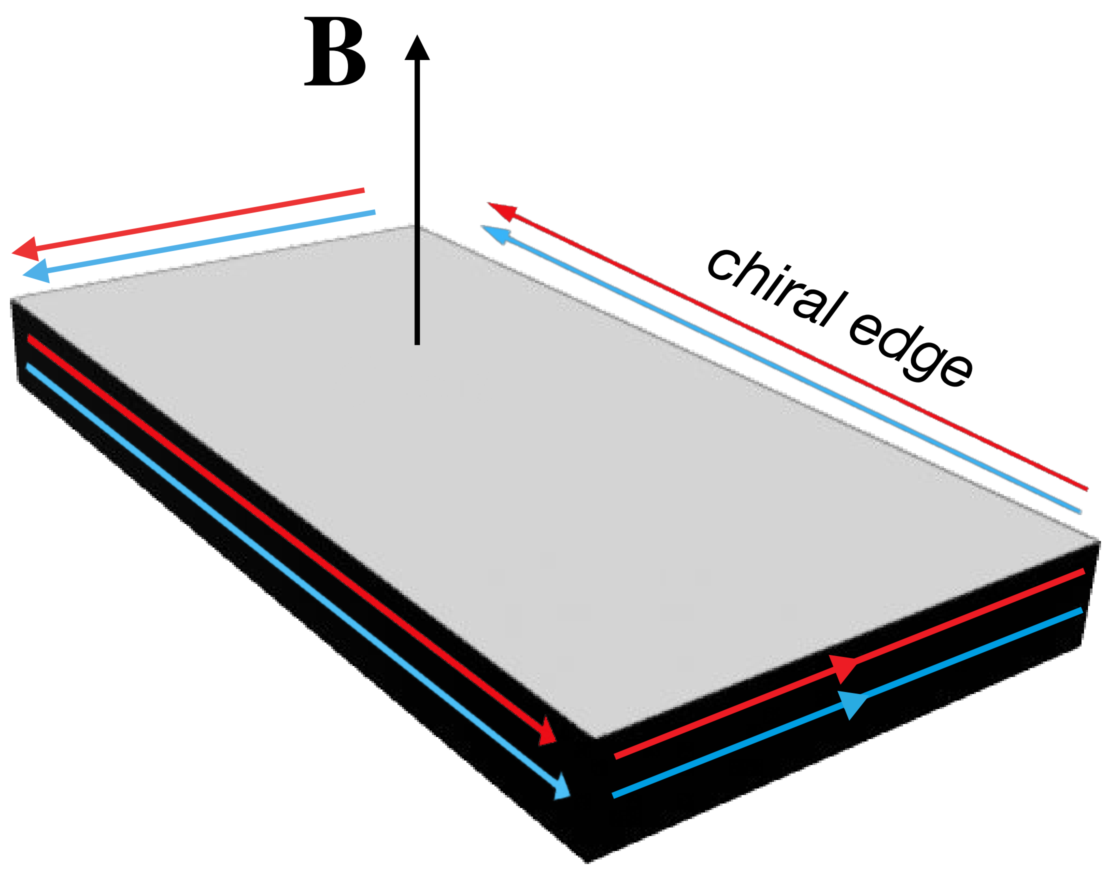

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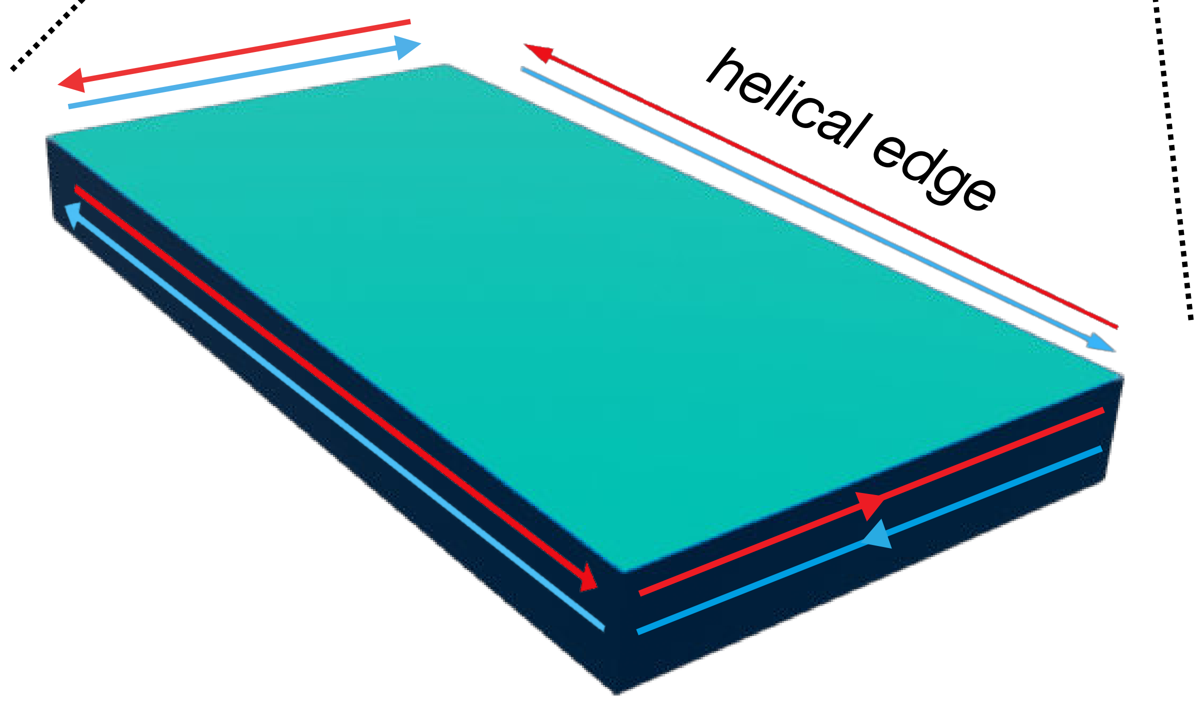

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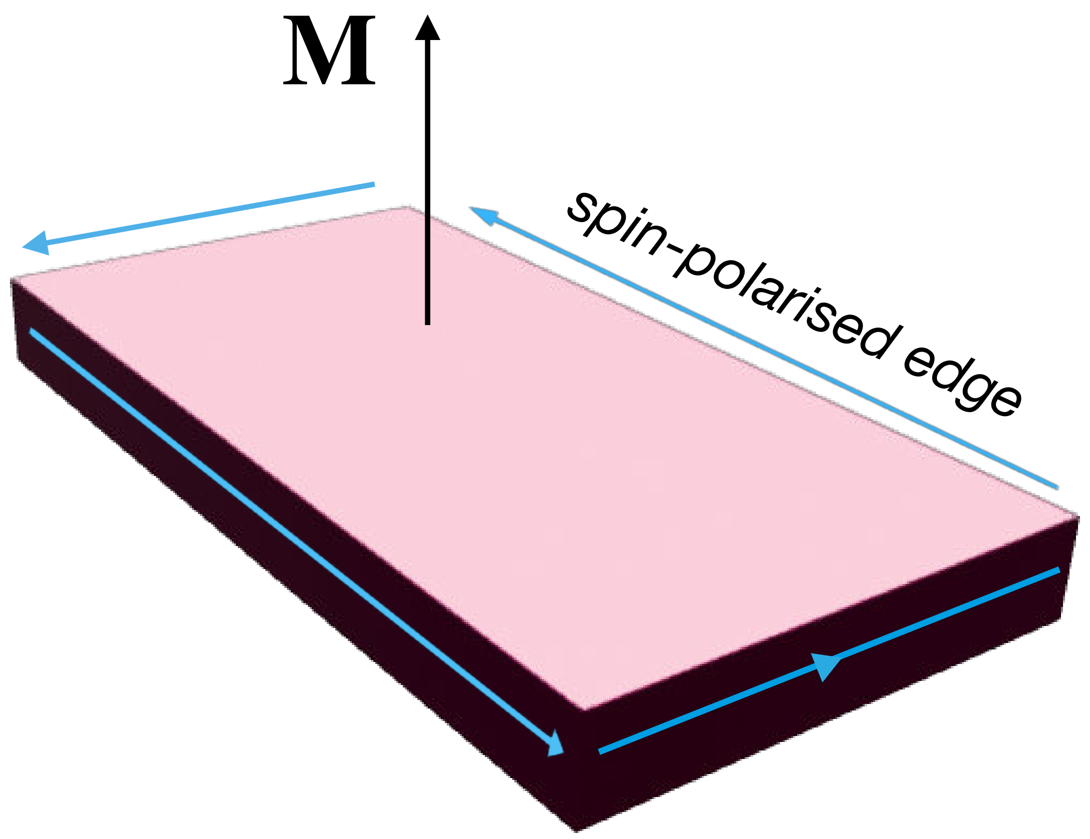

Quantum anomalous Hall / Chern insulator

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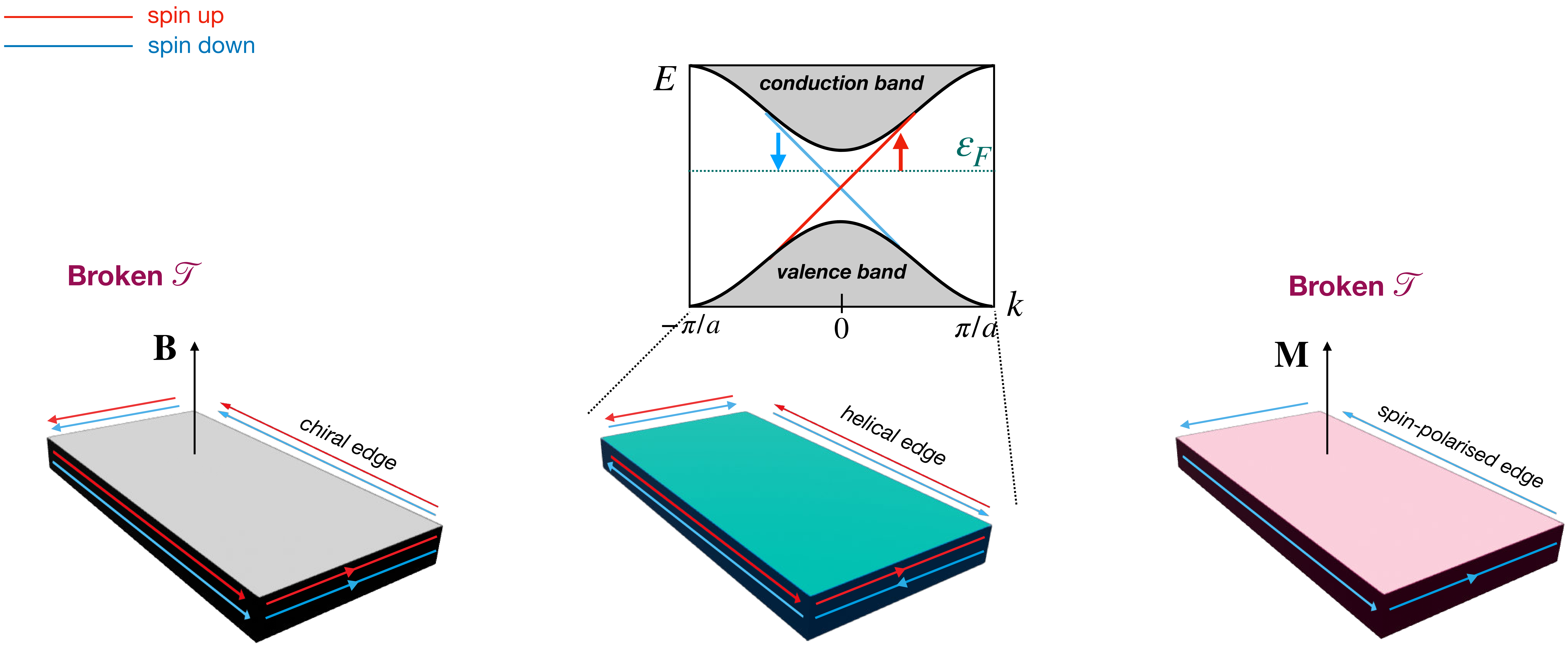
Part 2: Non-Spatial Symmetries I 10-fold classification of topological matter



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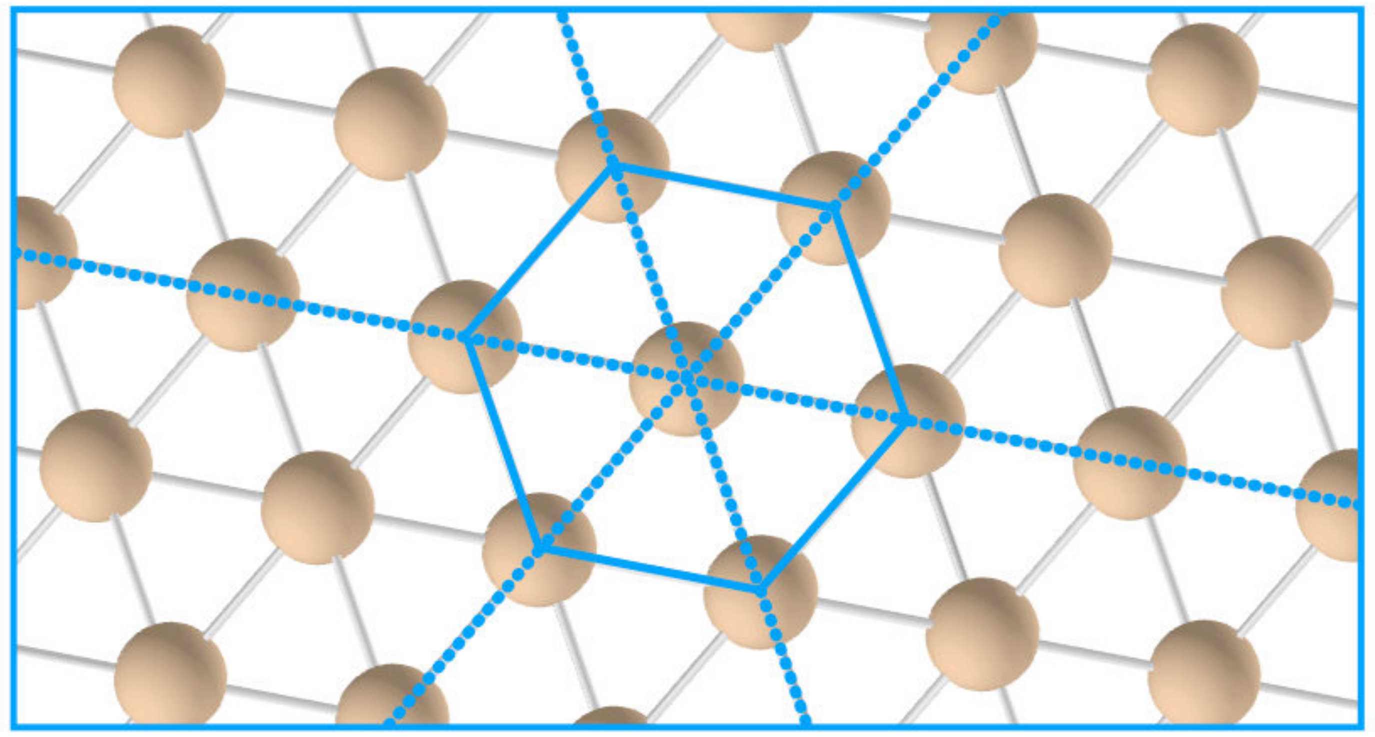
Non-spatial symmetries play a key role in the classification of gapped topological phases of matter!

Part 2: Non-Spatial Symmetries I 10-fold classification of topological matter

Gapped topological phases call for a classification based upon **generic quantum-mechanical symmetries**, such as **TR symmetry (TRS)** (*)

Spatial symmetries
(act non-locally in real space)



Credit: Sebastian Kokott

Non-spatial symmetries
(act locally in real space)

(*) Translation and typical point-group symmetries are not generic enough in this context due to being easily broken by impurities, defects, etc.

Starting point: Wigner-Dyson classification of random matrices

- **No TR invariance** (as in the IQHE)
- **TR invariance with** $\mathscr{T}^2 = -1$ (as in the QSHE)
- **TR invariance with** $\mathscr{T}^2 = +1$ (integer angular momentum)

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

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Another generic symmetry: **particle-hole symmetry (PHS)**

- **No PHS** ($\mathscr{C} = 0$)
- **PHS with** $\mathscr{C}^2 = -1$
- **PHS with** $\mathscr{C}^2 = +1$

$$\mathscr{C}^{-1} H(\mathbf{k})\, \mathscr{C} = -H(-\mathbf{k})$$

These non-spatial symmetries combined offer $\underline{9 = 3 \times 3 \text{ possibilities}}$, **but there is one more!**

$$\mathscr{C}, \mathscr{T} = \{0, 1, -1\}$$

Chiral ('sublattice') symmetry: $\mathscr{S} = \mathscr{T} \cdot \mathscr{C}$

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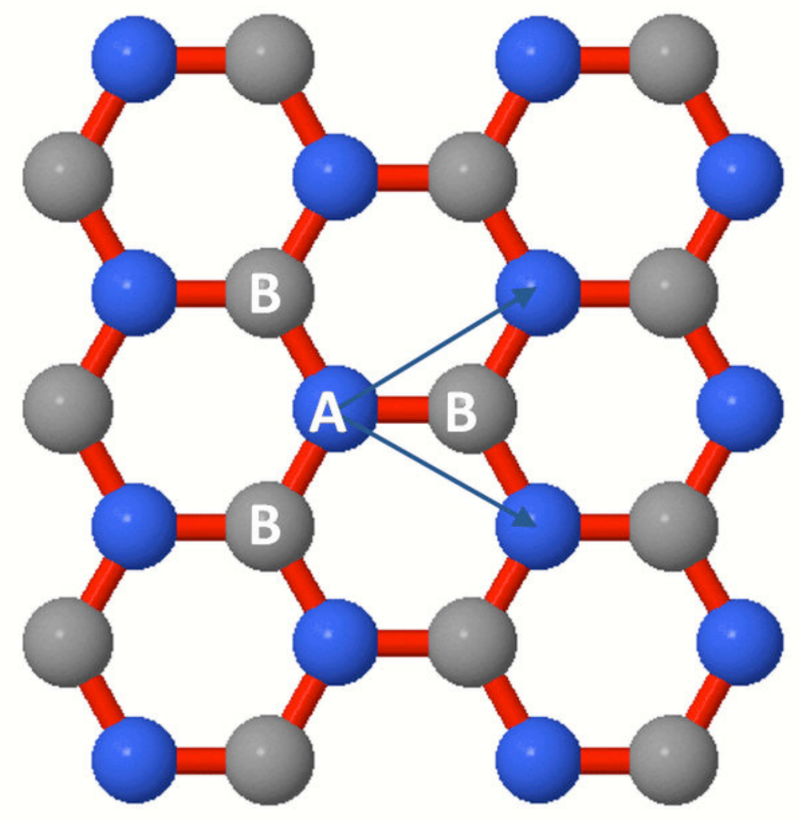
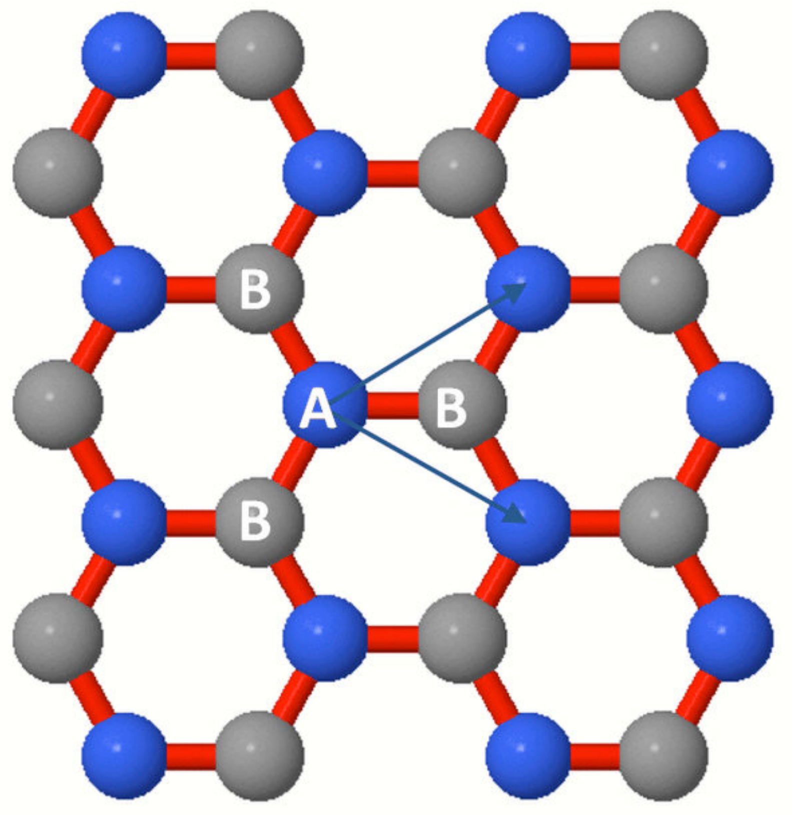


$$H = \begin{bmatrix} 0 & H_{AB} \\ H_{AB}^{\dagger} & 0 \end{bmatrix}$$

Part 2: Non-Spatial Symmetries I 10-fold classification of topological matter

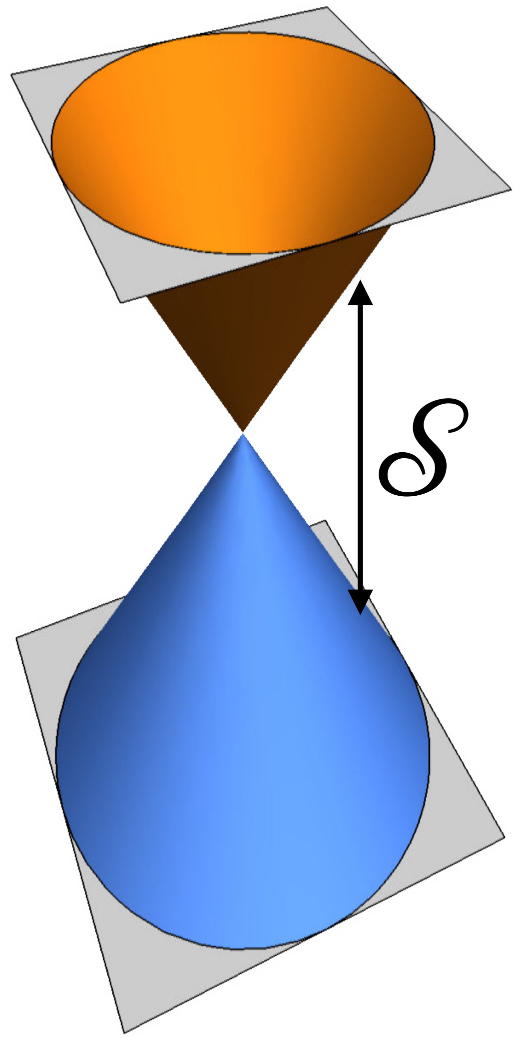
Chiral ('sublattice') symmetry: $\mathcal{S} = \mathcal{T} \cdot \mathcal{C}$ → $\mathcal{S}^{-1} H(\mathbf{k})\, \mathcal{S} = -H(\mathbf{k})$ *unitary symmetry* ($\mathcal{S} = 0{,}1$)

$$\mathcal{S} = \sigma_z$$



$$H = \begin{bmatrix} 0 & H_{AB} \\ H^{\dagger}_{AB} & 0 \end{bmatrix}$$

$$\sigma_z H \sigma_z = -H$$



Example: graphene

States with energy $\pm E$ are connected via $\mathcal{S}$

$\mathscr{S} = \mathscr{T} \cdot \mathscr{C}$ is uniquely fixed by TRS and PHS **except when** $\mathscr{T}, \mathscr{C} = 0 \implies$ **2 choices** $\mathscr{S} = 0$ **or** $\mathscr{S} = 1$

All together, we have $(9-1)+2 = 10$ distinct choices

10-fold way (Altland & Zirnbaeur, 1997)

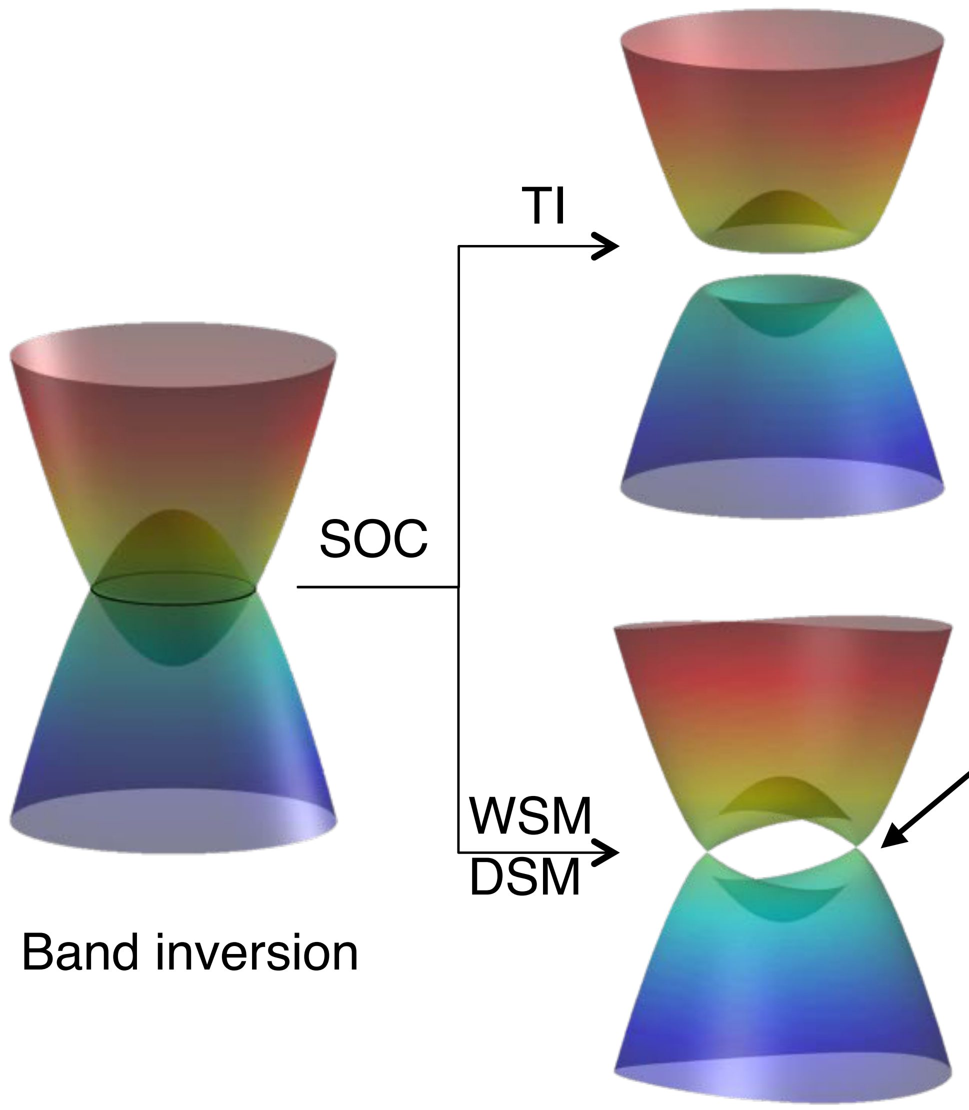
Part 2: Non-Spatial Symmetries I 10-fold classification of topological matter

	Class	$\mathcal{T}$	$\mathcal{C}$	$\mathcal{S}$	d = 2	d = 3	Some examples
Wigner-Dyson	**A** (unitary)	0	0	0	$\mathbb{Z}$	–	*2D IQHE, 2D Chern insulator, broken-$\mathcal{T}$ metal*
	AI (orthogonal)	+1	0	0	–	–	
	AII (symplectic)	-1	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	*$\mathbb{Z}_2$ topological insulators (bismuth-antimony alloys) & QSH insulators (2d)*
Chiral	**AIII** (chiral unit.)	0	0	1	–	$\mathbb{Z}$	
	BDI (chiral ortho.)	+1	+1	1	–	–	*graphene*
	CII (chiral symp.)	-1	-1	1	–	$\mathbb{Z}_2$	
Bogoliubov-de Gennes (Superconductors)	**D**	-1	-1	1	$\mathbb{Z}$	–	
	C	0	-1	0	$\mathbb{Z}$	–	*2D spin quantum Hall fluid in d+id SCs*
	DIII	-1	+1	1	$\mathbb{Z}_2$	$\mathbb{Z}$	
	CI	+1	-1	1	–	$\mathbb{Z}$	

Part 2: Topological semi-metals protected by symmetry

Topological semi-metals

Figure adapted from
B. Yan and C. Felser (2017)



Topological band crossings near Fermi level

interesting physics

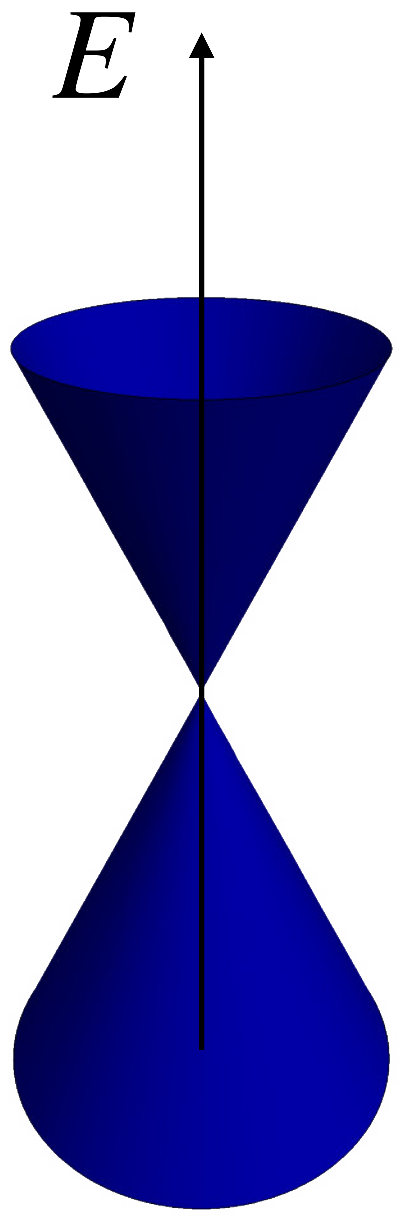
- ➡ Fermi Arcs
- ➡ Unconventional magneto-optical response
- ➡ Chiral magneto-electric response
- ➡ Spin-momentum locking

Experimental evidence:

Weyl semi-metal (WSM): TaAs family (2015), NbAs (2015), TaP (2016), …, 2D bismuthene (2024)

Dirac semi-metal (DSM): Cd_3As_2 (2014), $PtSe_2$ (2017) … Au_2Pb (2023), TlBiSSe (2023)

Part 2: Topological semi-metals protected by symmetry



Weyl semimetal

(non-degenerate linearly dispersing bands)

$$E = \pm \hbar v \sqrt{k_x^2 + k_y^2 + k_z^2}$$

Requires broken $\mathscr{T}$ or broken inversion symmetry

(recall Kramers' theorem)

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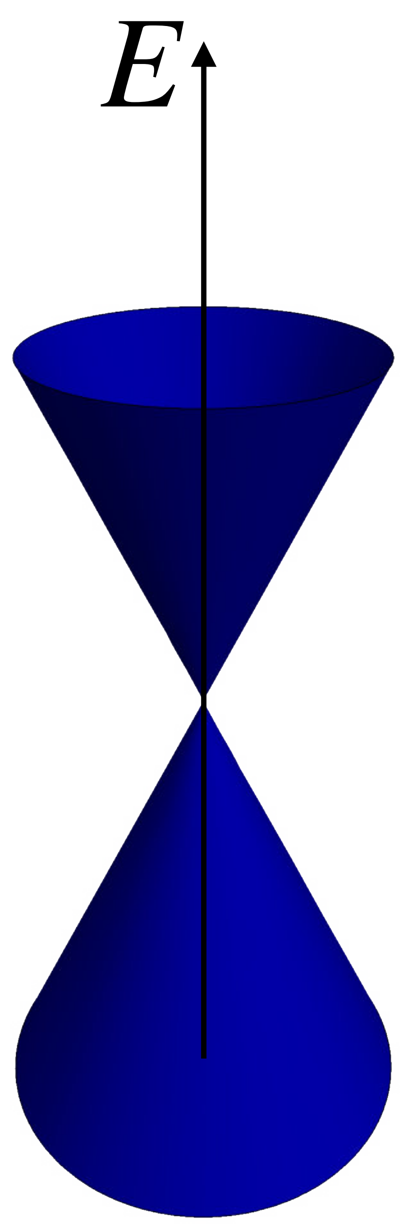


Weyl semimetal

(non-degenerate linearly dispersing bands)

$$E = \pm \hbar v \sqrt{k_x^2 + k_y^2 + k_z^2}$$

Inspection of the eigenstate hints at a topological charge

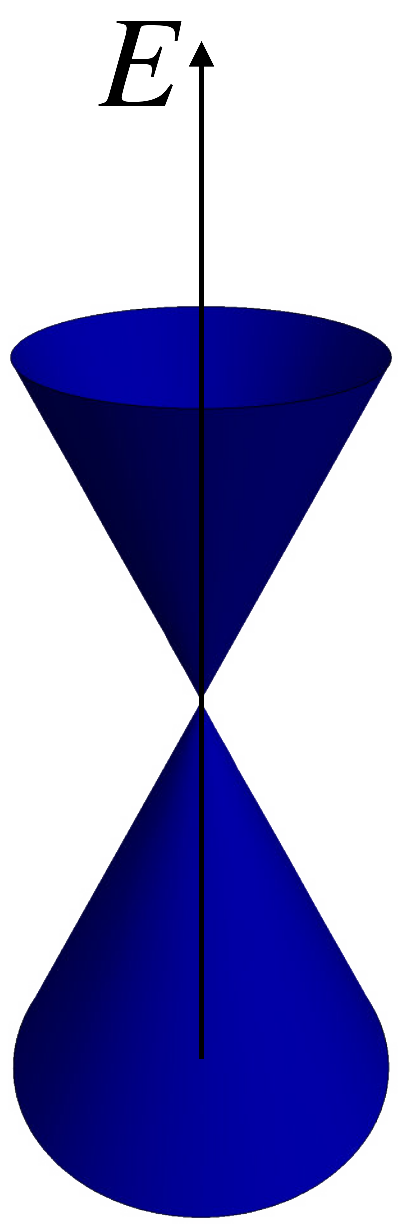
$$|\, u_+(\theta,\phi)\rangle = e^{-i\phi} \cos\frac{\theta}{2} |\uparrow\rangle + \sin\frac{\theta}{2} |\downarrow\rangle$$

→ $|u_+\rangle$ is single valued except at the "north pole" **($\theta = 0, \phi = ?$)**

Other choice of gauge will merely move the singularity to another location on the 2-sphere

The singularity acts as a <u>source/drain of Berry curvature</u>

Part 2: Topological semi-metals protected by symmetry

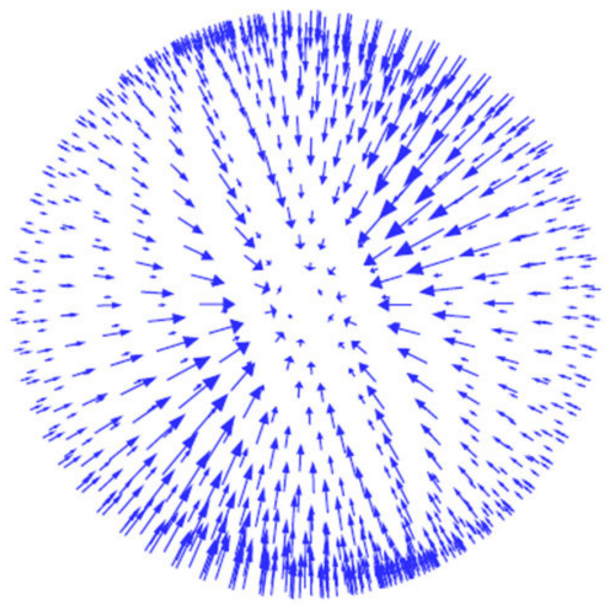


Weyl semimetal

(non-degenerate linearly dispersing bands)

$$E = \pm \hbar v \sqrt{k_x^2 + k_y^2 + k_z^2}$$

$$\mathscr{B}(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathscr{A}(\mathbf{k})$$



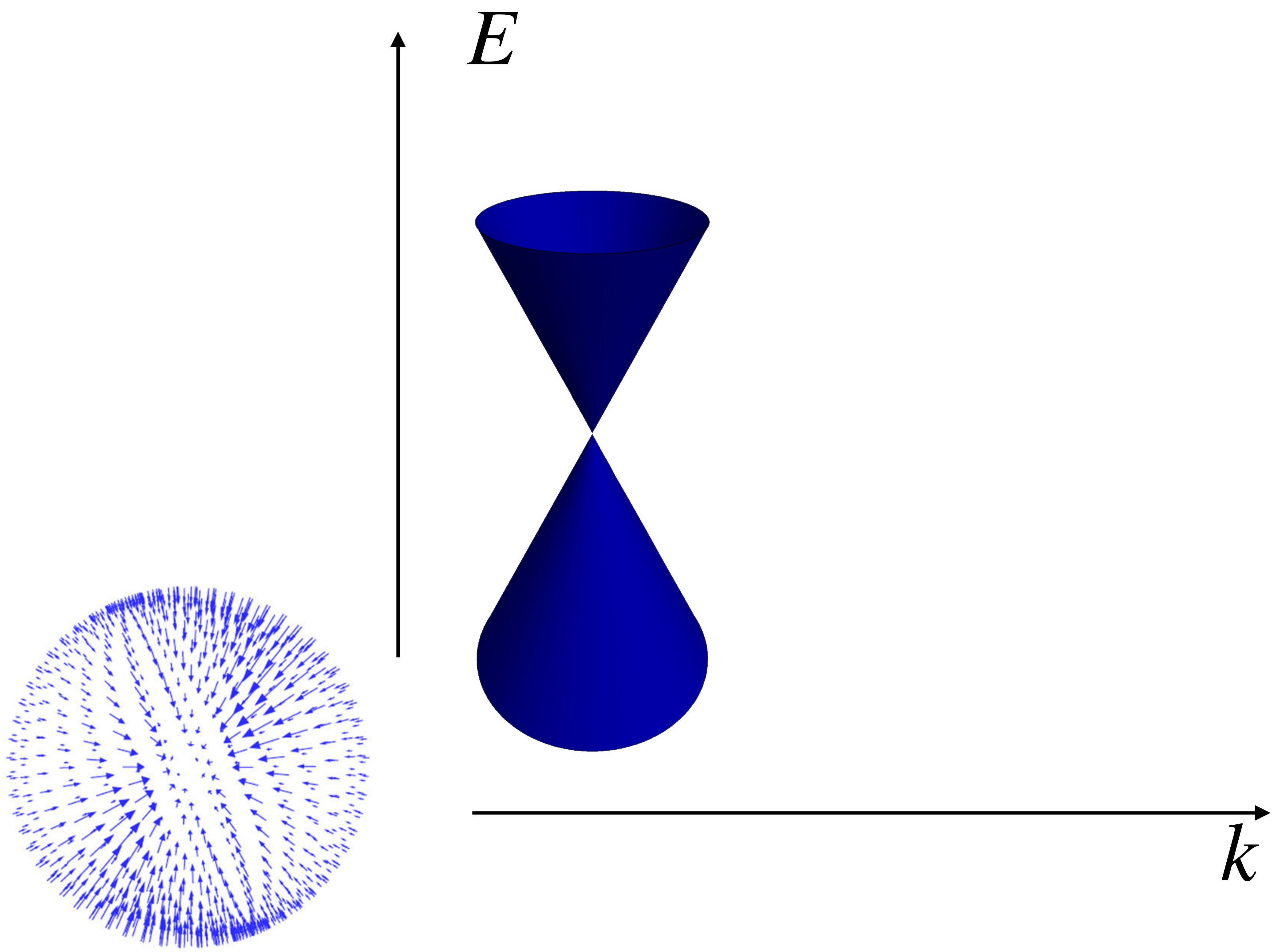
non-zero topological charge (monopole)

$$|+E\rangle \qquad \mathscr{B}_{+}(\mathbf{k}) = -\frac{1}{2}\frac{\mathbf{k}}{|\mathbf{k}|^3}$$

$$\frac{1}{2\pi}\oint_{\text{node}} \mathscr{B}(\mathbf{k}) \cdot d\mathbf{S}_{\mathbf{k}} = \pm 1$$

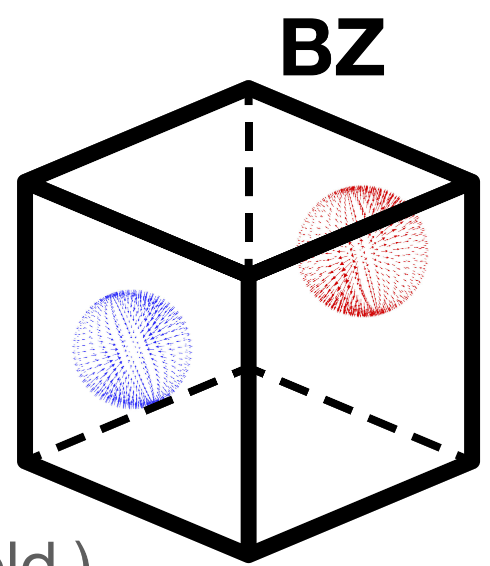
Quantised topological charge (Chern number)

Part 2: Topological semi-metals protected by symmetry

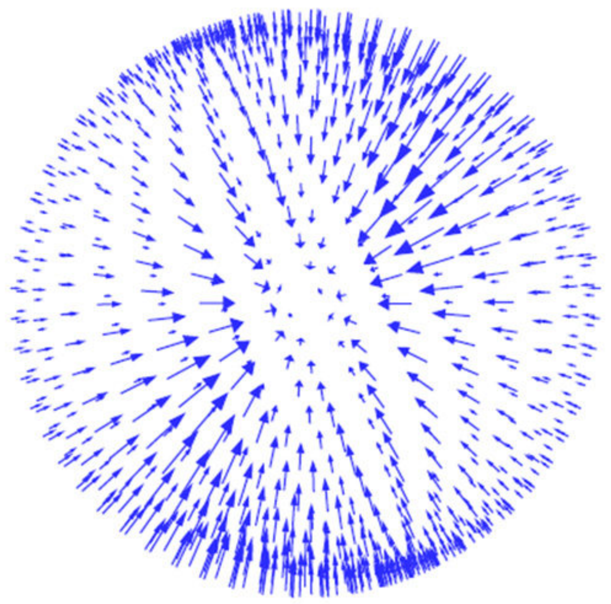


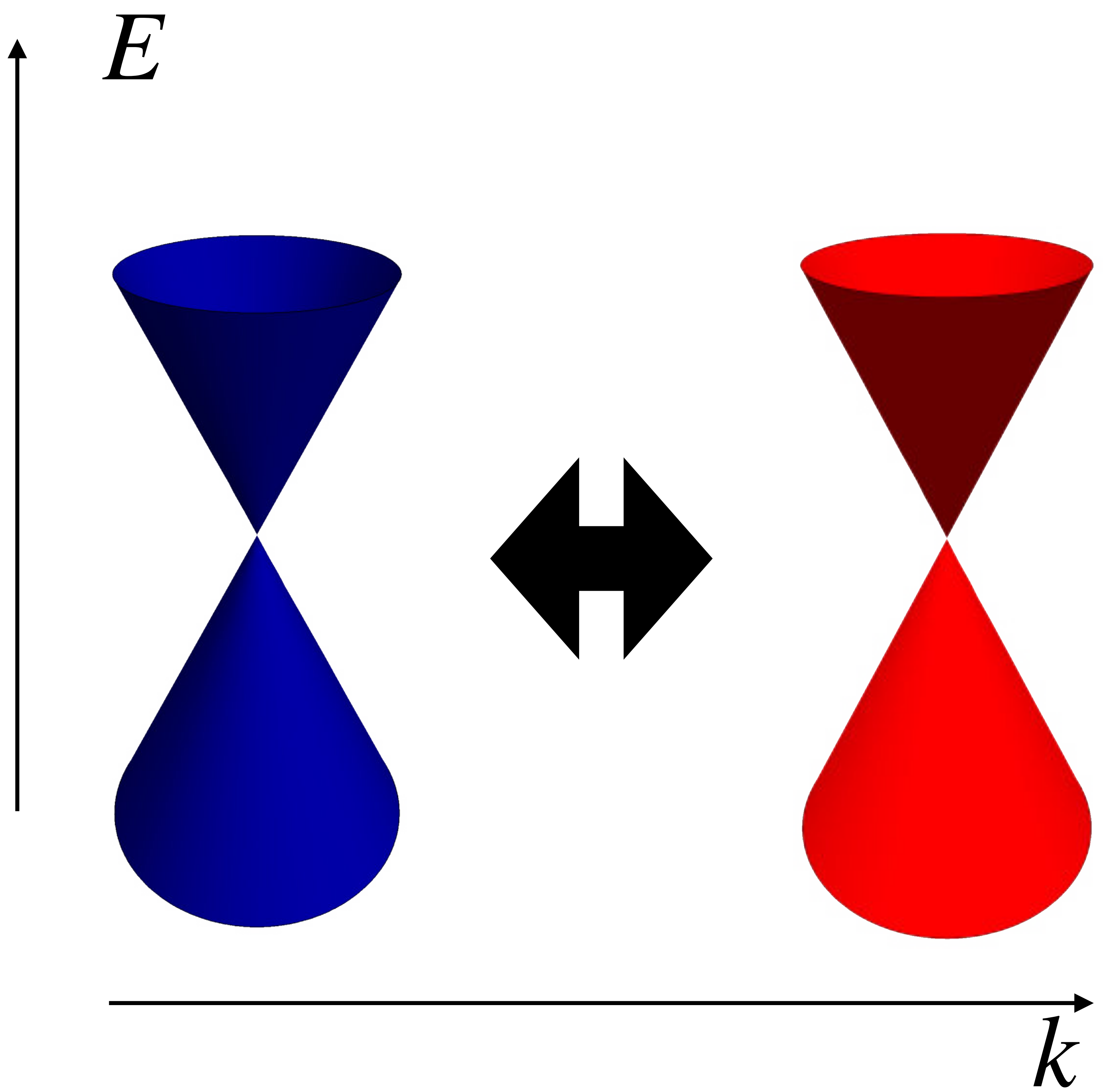
Total Berry flux penetrating the whole BZ is **zero**.

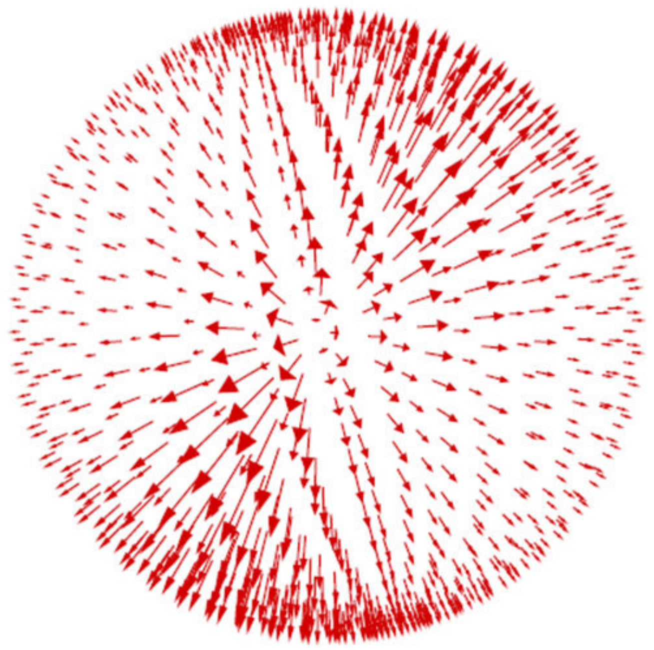
$$\sum_i C_i = 0$$



(BZ is a closed manifold)





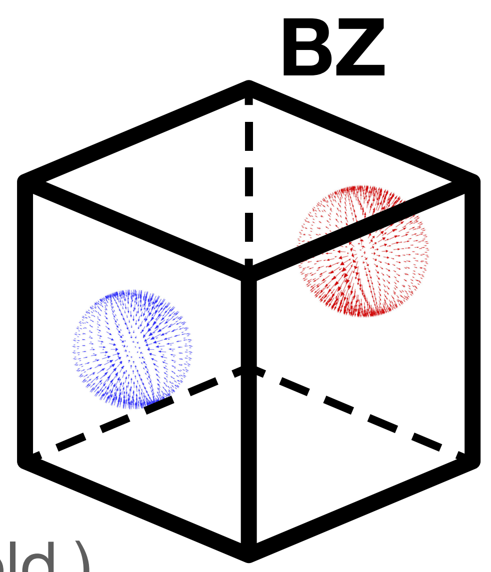


$$\mathscr{B}_{1,2}(\mathbf{k}) = \mp \frac{1}{2} \frac{\mathbf{k}}{|\mathbf{k}|^3}$$

Total Berry flux penetrating the whole BZ is **zero**.

Weyl nodes come in pairs!

$$\sum_i C_i = 0$$



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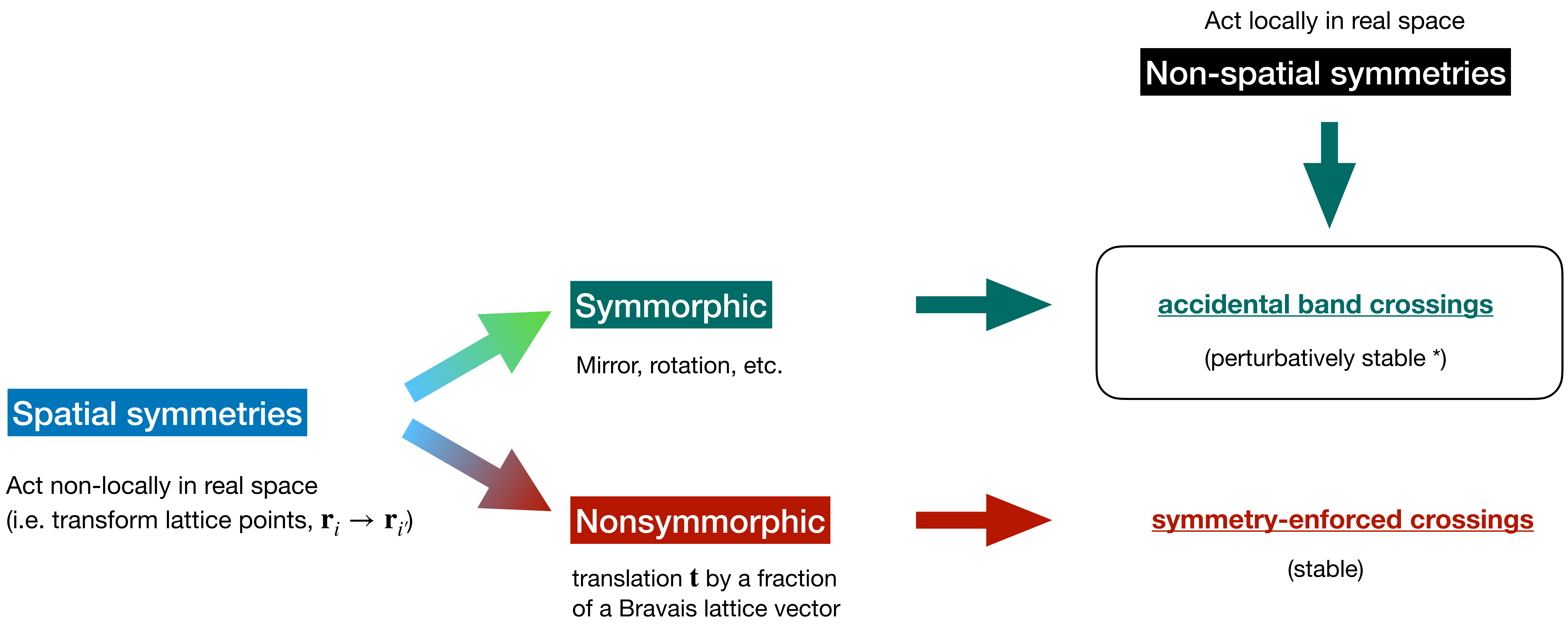
Part 2: Topological semi-metals protected by symmetry



* These can be removed by large symmetry-preserving deformations.

Part 2: Topological semi-metals protected by symmetry

Accidental band crossings

Use Clifford algebra $\{\mathbf{1}, \sigma_x, \sigma_y, \sigma_z\}$ to write a generic model for a band crossing in *d* spatial dimensions:

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$$H_{\mathbf{k}} = f_0(\mathbf{k})\,\mathbf{1} + f_x(\mathbf{k})\sigma_x + f_y(\mathbf{k})\sigma_y + f_z(\mathbf{k})\sigma_z$$

energy shift ($f_0 \equiv 0$)

$$\mathbf{k} = (k_1, \ldots, k_d)$$

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$$E_{\mathbf{k}} = \pm\sqrt{f_x^2(\mathbf{k}) + f_y^2(\mathbf{k}) + f_z^2(\mathbf{k})}$$

Recall:

$$\sigma_i^2 = \mathbf{1};\ \{\sigma_i, \sigma_j\} = 2\delta_{ij}\,\mathbf{1}$$

$$\Delta H^2 = (f_x^2 + f_y^2 + f_z^2)\,\mathbf{1}$$

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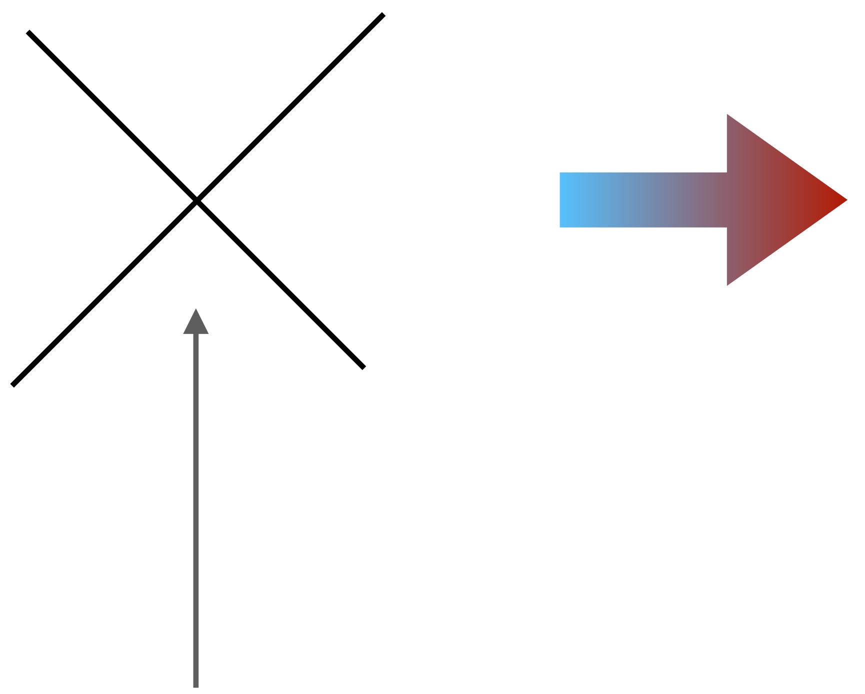
3D



$$f_i = \hbar\, v_i\, k_i$$

Assume crossings are pinned to a high-symmetry point like Γ

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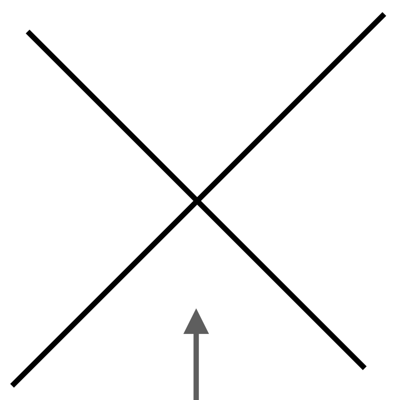

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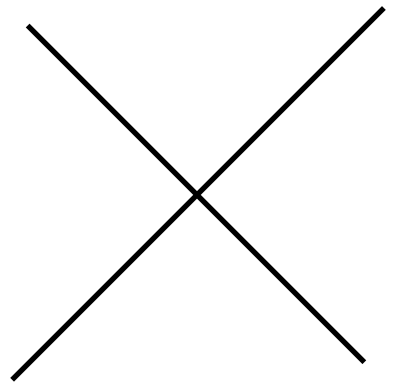
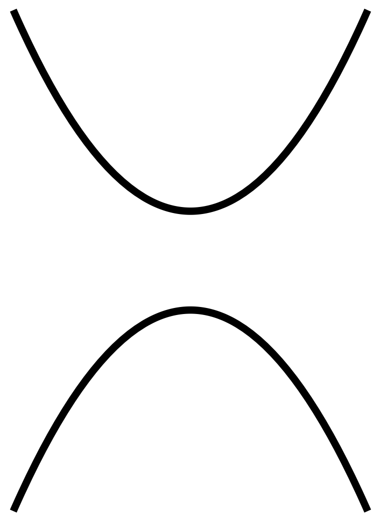
2D



$$f_z = 0 \quad (i = x, y, z)$$



$$f_z \equiv m \neq 0$$

Part 2: Topological semi-metals protected by symmetry

Accidental band crossings

Symmetry class A (unitary)

$\mathscr{T} = 0, \mathscr{C} = 0, \mathscr{S} = 0$

No spatial symmetries: $H_{\mathbf{k}} = \hbar v \left(\sigma_x k_x + \sigma_y k_y + \sigma_z k_z \right)$

3D

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σ_i perturbation just shifts the crossing point

stable

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3D σ_i perturbation just shifts the crossing point

stable

$H_{\mathbf{k}} = \hbar v \left(\sigma_x k_x + \sigma_y k_y \right)$

2D σ_z perturbation opens gap ➡ **unstable**

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⬇

To protect the 2D band crossing, we add a spatial symmetry!

Mirror plane: $H_{\mathbf{k}} = M_x^{-1}\, H_{-k_x,k_y}\, M_x$ **2D**

"Graphene"

Satisfied with $M_x = \sigma_y$

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Mirror plane:

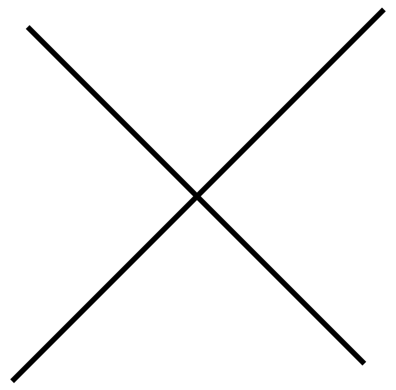
"Graphene”

$H_{\mathbf{k}} = M_x^{-1} H_{-k_x,k_y} M_x$

Satisfied with $M_x = \sigma_y$

2D σ_z is now symmetry forbidden! ➡ stable

$M_x^{-1} \sigma_z M_x = - \sigma_z$



Symmetry protected semi-metallic phase

Part 2: Topological semi-metals protected by symmetry

Accidental band crossings

Symmetry class AII (symplectic)

$$\mathscr{T} = 1$$

Example: surface of a 3D TI

2D

$$H_{\mathbf{k}} = \hbar v \left(\sigma_x k_x + \sigma_y k_y \right)$$

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*The TRS operation reverses momenta **and** spin*

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$$H_{\mathbf{k}} = \mathcal{T}^{-1} H_{-\mathbf{k}} \mathcal{T}$$

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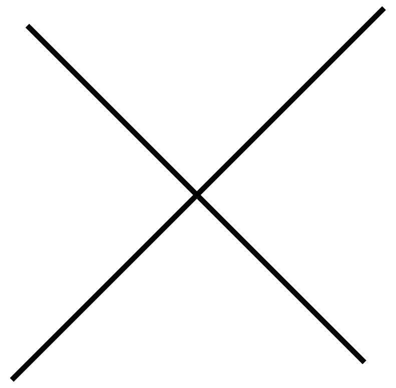
Band crossing is protected by TRS!



$\mathcal{T}^{-1} (m\sigma_z) \mathcal{T} = -m\sigma_z$

$H_{\mathbf{k}} = \mathcal{T}^{-1} H_{-\mathbf{k}} \mathcal{T}$

Overview

Symmetries provide a powerful toolbox in solid state physics, which allows, for example, for

- Understanding important features of the band structures of crystals
- Classifying topological insulators and topological semimetals
- Characterising spin arrangements in unconventional magnetic phases of matter

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Thank you for your attention!

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