ARPES of topological insulators and semi-metals

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GDR MEETICC
Matériaux, Etats ElecTroniques, Interactions et Couplages non-Conventionnels

Outline : Topology of the electronic structure probed by ARPES

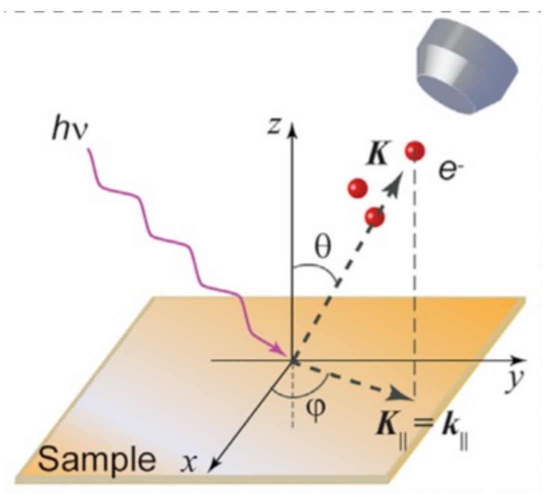
- Some generalities about topology, geometry and symmetry

  (Parallel transport, Berry connection and Berry curvature , magn. monopoles,

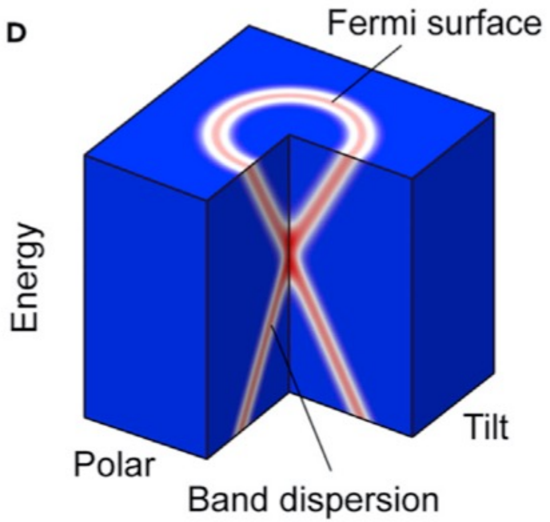
- The Chern topological and Kane-Mele topological insulators in 2D
- ARPES of Kane-Mele topological insulators in 3D
- Dirac semi-Metals and Weyl semi-metals (ARPES and Spin-ARPES)

Angle-resolved photoemission spectroscopy

- a photon-in electron-out technique
- one measures the kinetic energy and the momentum of the photoemitted electrons
- mapping the electronic band structure



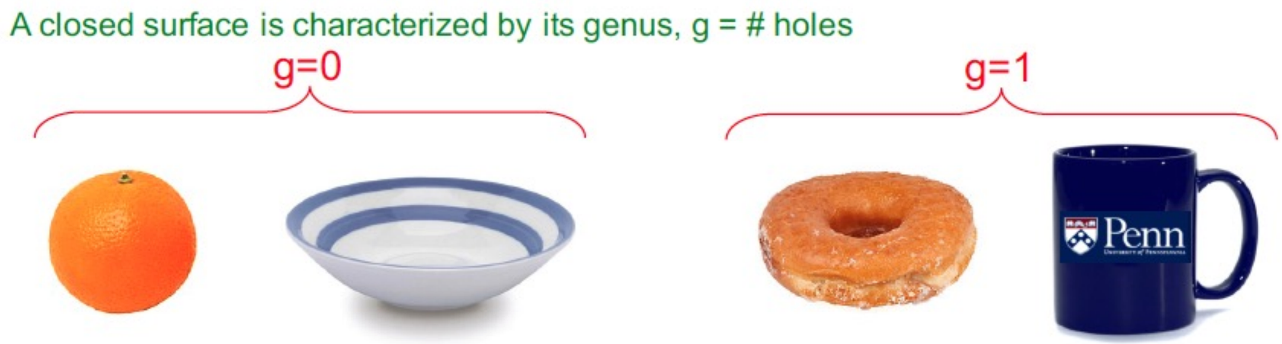
- determination of the Fermi surface (momentum distribution curves)
- and band dispersions (energy distribution curves)



Topology

Global properties preserved under continuous deformation

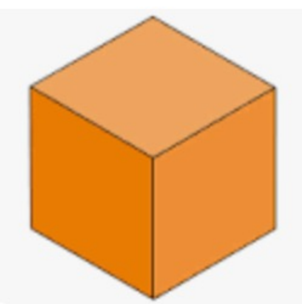
Topological number (number of holes)

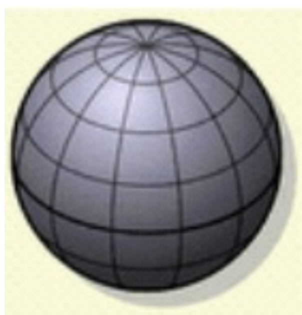


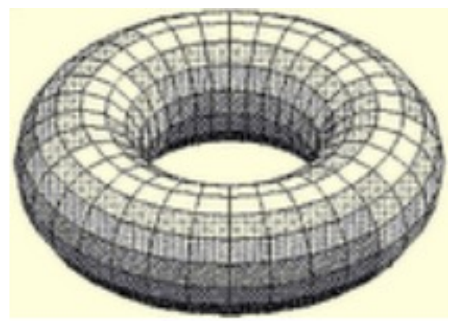
Trivial and non-trivial topology : the Euler characteristic for polyedra

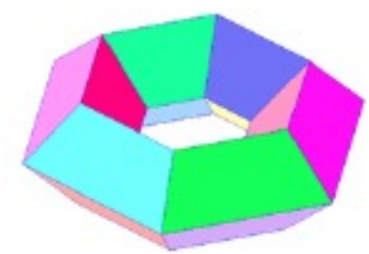
$$\chi = V - E + F$$

Vertices, Edges, Faces









$$\chi = 0$$

Topologically non trivial

$$\chi = 2$$

Topologically trivial

$$\chi = 0$$

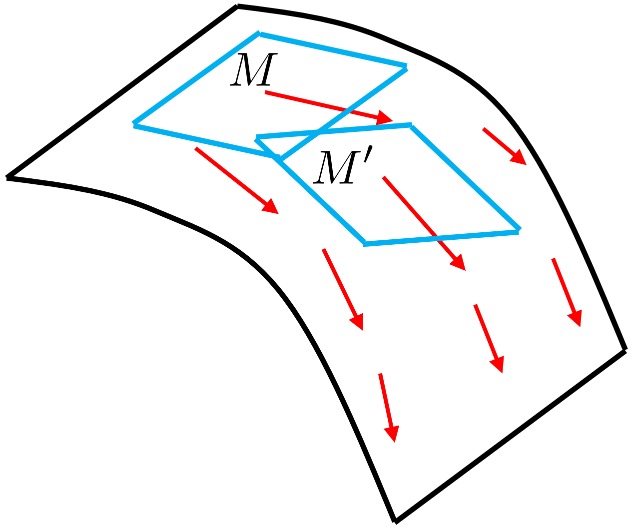
Euler characteristic

Topological number = global property

Relation with genus number :

$$\chi = 2(1 - g)$$

Geometry : connection and curvature



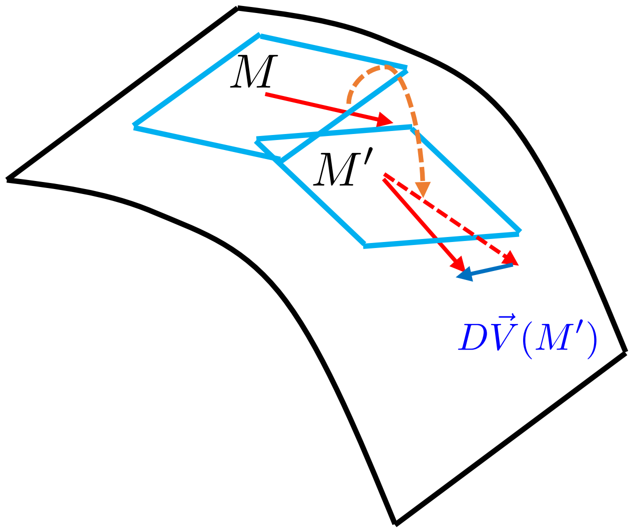
Vector field on a curved surface

Impossible to compare 2 vectors at 2 neighboring points (they belong to 2 different vector spaces)

An additionnal structure is needed : THE CONNECTION

A rule to transport a vector from one point to neighboring points (parallell transport)

Geometry : connection and curvature



Impossible to compare 2 vectors at 2 neighboring points (they belong to 2 different vector spaces)

An additionnal structure is needed : THE CONNECTION

A rule to transport a vector from one point to neighboring points (parallell transport)

$$\vec{V}(M) \to \vec{V}_{||}(M')$$

Possibility to derive the vector field

$$D\vec{V}(M') = \vec{V}(M') - \vec{V}_{||}(M')$$

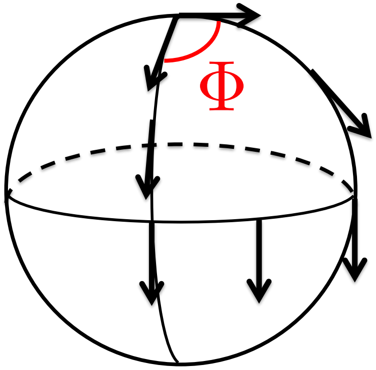
COVARIANT DERIVATIVE

Relation between geometry and topology

Example of parallel transport on a sphere

Geometric prop. : curvature

Transport on a flat surface :
no rotation



Parallel transport :

After a round trip, there is an angle proportionnal to the curvature

Non-integrable angle

(depends on trip)

Relation between global (topology) and local (geometry) properties

Gauss-Bonnet theorem :

$$\chi = \frac{1}{2\pi} \oint_S K dS$$

K : Gauss curvature
(sphere : $K = 1/R^2$: $\chi = 2$)

Euler characteristic global local curvature

Local (Gauge) symmetry

Gauge principle (electromagnetism) : one imposes a local symmetry by changing the local phase

$$\Psi \longrightarrow \Psi'(\vec{r}) = e^{i\frac{q}{\hbar}\Lambda(\vec{r})}\ \Psi(\vec{r})$$ $\Lambda(\vec{r})$ is an arbitrary function

it is necessary to introduce an interaction (gauge field $(\vec{A}, \varphi)$) to preserve the invariance

$$H = \frac{\left(\vec{p} - q\vec{A}(\vec{r},t)\right)^2}{2m} + q\varphi(\vec{r},t)$$

Change of phase compensated by the change of connection

$$\vec{A}' = \vec{A} + \vec{\nabla}\Lambda$$

Local (Gauge) symmetry and geometrical phase

Gauge principle (electromagnetism) : one imposes a local symmetry by changing the local phase

$$\Psi \longrightarrow \Psi' = e^{i\frac{q}{\hbar}\Lambda(\vec{r})}\ \Psi$$ $\Lambda(\vec{r})$ is an arbitrary function

it is necessary to introduce an interaction (gauge field ($\vec{A}, \varphi$)) to preserve the invariance

- $\vec{A}$ gives the evolution of the geometrical phase between two points (Aharonov-Bohm exp.) : $\vec{A}$ plays the role of connection

$$\Phi_{geo}(P \rightarrow Q) = \frac{q}{\hbar}\int_P^Q \vec{A}\cdot d\vec{\ell}$$

- $\Phi = \Phi_{Berry}$ on a closed curve is gauge invariant (Berry phase) $\left(\oint \vec{\nabla}\Lambda \cdot d\vec{\ell} = 0\right)$

$$\Phi_{Berry} = \frac{q}{\hbar}\oint \vec{A}\cdot d\vec{\ell} = \frac{q}{\hbar}\int \vec{B}\cdot d^2\vec{S}$$

Berry phase Berry connection Berry curvature

Consequence : Non trivial topology of electromagnetism (Monopole)

Monopole of charge q_m at $\vec{r}=0$

$$\vec{B}_m(\vec{r}) = \frac{\mu_0 q_m}{4\pi}\frac{\vec{r}}{r^3}.$$

Maxwell equation :

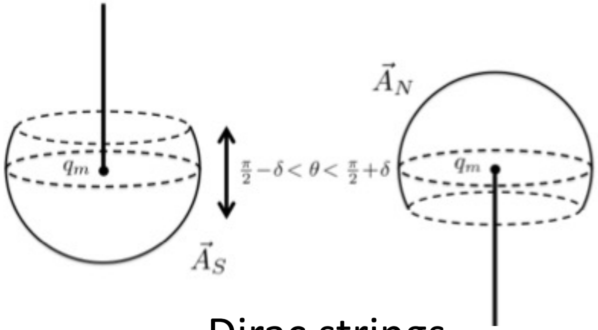
$$\vec{\nabla}\cdot\vec{B}_m = \mu_0\rho_m = \mu_0 q_m \delta(\vec{r})$$

$$\text{pour} \quad \vec{r}\neq 0,\ \vec{\nabla}\cdot\vec{B}_m = 0, \quad \vec{B}_m = \vec{\nabla}\wedge\vec{A}$$

But there is no unique $\vec{A}(\vec{r})$ function describing $\vec{B}_m$ everywhere!

$$\vec{A}_S(r,\theta,\phi) = -\frac{\mu_0}{4\pi}\frac{q_m(1+\cos\theta)}{r\sin\theta}\,\vec{u}_\phi$$

$\vec{A}_S$ not defined for $\theta=0$



Dirac strings

$$\vec{A}_N(r,\theta,\phi) = \frac{\mu_0}{4\pi}\frac{q_m(1-\cos\theta)}{r\sin\theta}\,\vec{u}_\phi$$

$\vec{A}_N$ not defined for $\theta=\pi$

(Dirac 1931, quantification of the electric charge)

The topology of the electromagnetism with monopole is non-trivial :
impossible to have only one regular $\vec{A}$ function, (topology of the sphere!)

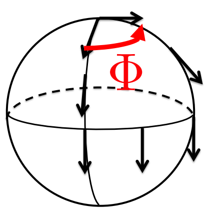
Geometrical interpretation of Gauge theory

Wu & Yang (1975)

Geometry

Connection (parallel transport)

Rotation of a vector transported
along a closed curve



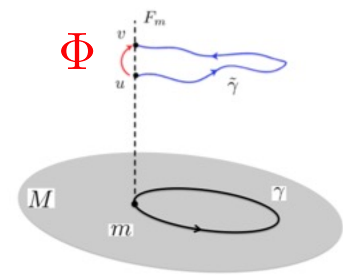
Curvature

Gauge invariance

vector potential $\vec{A}$

Phase shift
along a closed curve

$$\Phi = \frac{q}{\hbar}\oint \vec{A}\cdot d\vec{\ell}$$



Magnetic field $\vec{B} = \vec{\nabla} \wedge \vec{A}$

curl of A

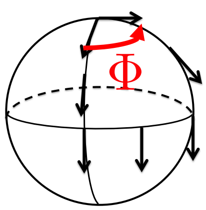
$$\oint_{\mathcal{C}} \vec{A}\cdot d\vec{\ell} = \int_{\mathcal{S}} \vec{B}\cdot d\vec{S}$$

Geometrical interpretation of Gauge theory

Geometry

Connection (parallel transport)

Rotation of a vector transported along a closed curve

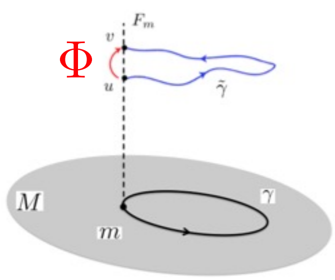


Curvature associated with Φ

Gauge invariance

Vector potential $\vec{A}$

Phase shift along a closed curve



$$\Phi = \frac{q}{\hbar} \oint \vec{A} \cdot d\vec{\ell}$$

Magnetic field

$$\vec{B} = \vec{\nabla} \wedge \vec{A}$$

What about the topology of the electronic structure in crystal?

Berry connection

$\vec{A}(\vec{k})$ in BZ

Berry phase

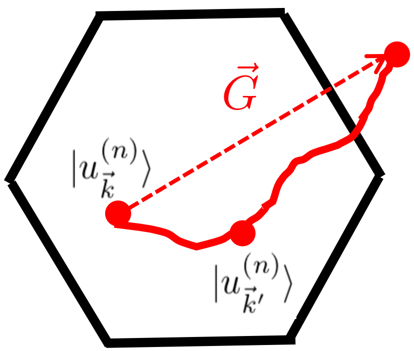
$$\Phi_{Berry} = \oint_{C} \vec{A}^{(n)}(\vec{k}) \cdot d\vec{k}$$

Berry curvature

$$\vec{\nabla}_{\vec{k}} \wedge \vec{A}(\vec{k})$$

Topology of the electronic structure

Bloch states $\mathcal{H}(\vec{k})\,|u_{\vec{k}}^{(n)}\rangle = \varepsilon_{\vec{k}}^{(n)}\,|u_{\vec{k}}^{(n)}\rangle$



Brillouin Zone

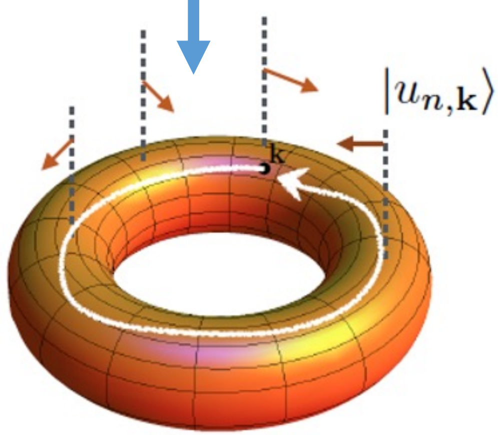
$$|u_{\vec{k}+\vec{G}}^{(n)}\rangle = |u_{\vec{k}}^{(n)}\rangle\; e^{i\alpha(\vec{k})}$$

Equivalent points

Closed curve since

$$\vec{k} \equiv \vec{k} + \vec{G}$$

Periodicity of the reciprocal space : 2 or 3 D-torus



The phase of $|u_{\vec{k}}^{(n)}\rangle$ must vary continuously from point to point in the Brillouin zone

Topologically non-trivial if

$$\alpha(k) \neq 2\pi \times p$$

Geometrical phase

$$d\theta_{geo} = \vec{A}^{(n)}(\vec{k}) \cdot d\vec{k}$$

Berry connection

$$\vec{A}^{(n)}(\vec{k}) = i\langle u_{\vec{k}}^{(n)}|\vec{\nabla}_{\vec{k}}\, u_{\vec{k}}^{(n)}\rangle$$

Berry curvature

$$\vec{\Omega}^{(n)}(\vec{k}) = \vec{\nabla}_{\vec{k}} \wedge \vec{A}^{(n)}(\vec{k})$$

Analogs to vector potential and magnetic field in reciprocal space

Topological number : Chern number

Generalisation of Gauss-Bonnet theorem :

$$C_1 = \frac{1}{2\pi} \oint_{\vec{k} \in ZB} \vec{\Omega}(\vec{k}) \cdot d^2\vec{k} \qquad C_1 \in Z$$

Chern number

(analogy with the Euler characteristic)

Berry curvature in k space : same behavior than magnetic field

Time reversal symmetry (TRS) $\vec{\Omega}^{(n)}(\vec{k}) = -\vec{\Omega}^{(n)}(-\vec{k})$ $C_1 = 0$

Inversion symmetry (IS) $\vec{\Omega}^{(n)}(\vec{k}) = \vec{\Omega}^{(n)}(-\vec{k})$

In presence of both TRS and IS : $\vec{\Omega}^{(n)}(\vec{k}) = 0 \quad \forall \vec{k}$

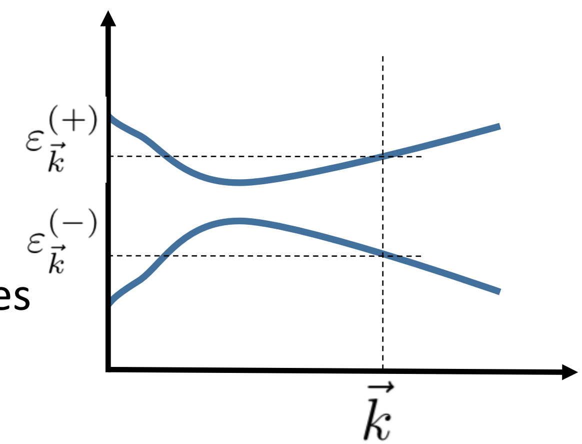
Chern topological insulators

Haldane model : for a two-band insulator (**spinless** electrons) (2 sites A &B per unit cell)

In each k point, we have a two-level system :

periodic on the BZ $$\mathcal{H}(\vec{k}) = \begin{pmatrix} h_z & h_x + ih_y \\ h_x - ih_y & -h_z \end{pmatrix} = \vec{h}(\vec{k}) \cdot \vec{\sigma}$$

Pauli matrices (A & B sites)



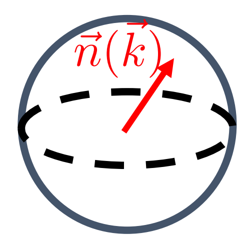
$$\mathcal{H}(\vec{k})|u^{(\pm)}_{\vec{k}}\rangle = \varepsilon^{(\pm)}_{\vec{k}}|u^{(\pm)}_{\vec{k}}\rangle \qquad \boxed{\varepsilon^{(\pm)}_{\vec{k}} = \pm h(\vec{k})}$$

parametrization by the spherical coordinates of $\vec{h}(\vec{k})$

$$\vec{h}(\vec{k}) = h(\vec{k}) \begin{pmatrix} \sin\theta_{\vec{k}} \cos\phi_{\vec{k}} \\ \sin\theta_{\vec{k}} \sin\phi_{\vec{k}} \\ \cos\theta_{\vec{k}} \end{pmatrix}$$

The Bloch sphere

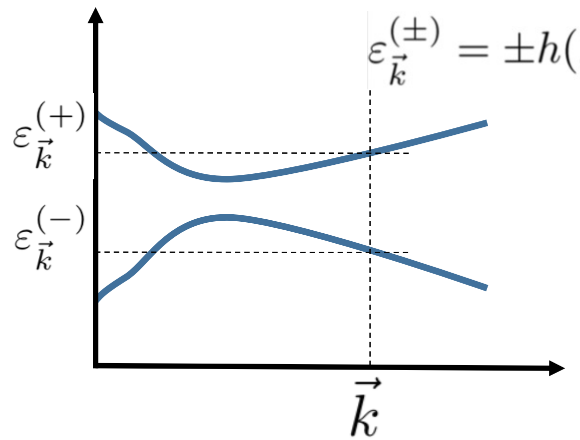
$$\vec{n}(\vec{k}) = \frac{\vec{h}(\vec{k})}{h(\vec{k})}$$



Chern topological insulators

Haldane model : for a two-band insulator (**spinless** electrons without time reversal symmetry)

In each k point, we have a two-level system :



periodic on the BZ

$$\mathcal{H}(\vec{k}) = \begin{pmatrix} h_z & h_x + i h_y \\ h_x - i h_y & -h_z \end{pmatrix} = \vec{h}(\vec{k}) \cdot \vec{\sigma}$$

parametrization by the spherical coordinates of $\vec{h}(\vec{k})$

$$\vec{h}(\vec{k}) = h(\vec{k}) \begin{pmatrix} \sin\theta_{\vec{k}} \cos\phi_{\vec{k}} \\ \sin\theta_{\vec{k}} \sin\phi_{\vec{k}} \\ \cos\theta_{\vec{k}} \end{pmatrix}$$

eigenvectors : $|u^{(-)}_{\vec{k}}\rangle = \begin{pmatrix} -\sin\frac{\theta}{2} \\ e^{i\phi}\cos\frac{\theta}{2} \end{pmatrix}$ $\qquad |u^{(+)}_{\vec{k}}\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}$

For $\theta = 0$, $|u^{(-)}_{\vec{k}}\rangle = \begin{pmatrix} 0 \\ e^{i\phi} \end{pmatrix}$ is ill-defined : ϕ undefined between 0 and 2π

multiplying by $e^{-i\phi}$ solves the problem in $\theta = 0$ but same problem appears at $\theta = \pi$!

Non trivial topology : not possible to use unique set of eigenvectors

The connection and curvature can be calculated :

$$A_\phi^{(S)} = i\langle u_{\vec{k}}^{(-)S} | \nabla_\phi u_{\vec{k}}^{(-)S} \rangle = -\frac{1}{2} \cdot \frac{1+\cos\theta}{h \sin\theta} \qquad \text{in } U_S$$

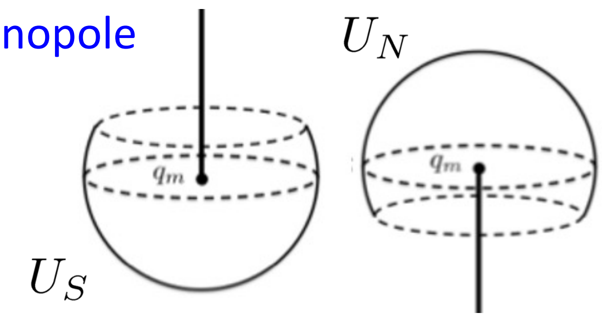
$$A_\phi^{(N)} = i\langle u_{\vec{k}}^{(-)N} | \nabla_\phi u_{\vec{k}}^{(-)N} \rangle = \frac{1}{2} \cdot \frac{1-\cos\theta}{h \sin\theta} \qquad \text{in } U_N$$

$$\vec{\Omega}^{(n)} = (\vec{\nabla} \wedge \vec{A}) = \frac{1}{2} \cdot \frac{\vec{h}}{h^3}$$

« magnetic field » of a Monopole in parameter space at $\vec{h} = 0$

We recognize the topology of the monopole

two eigenstates defined in U_N and U_S resp.



Chern-Gauss-Bonnet Th. :

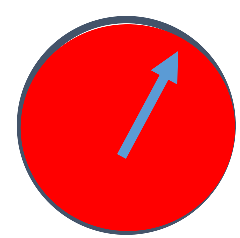
$$C_1 = \frac{1}{2\pi} \oint \vec{\Omega}(\vec{h}) \cdot d^2\vec{h}$$

Chern number = number of « magnetic monopoles »

topologically non trivial band

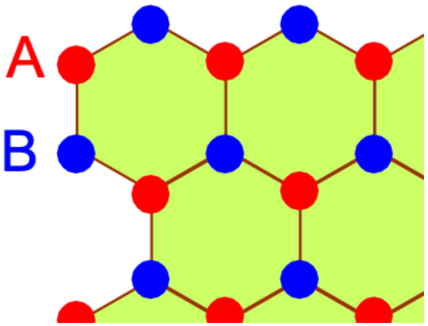
$C_1 \neq 0$

entire covering of the Bloch sphere



$\vec{n}(\vec{k})$

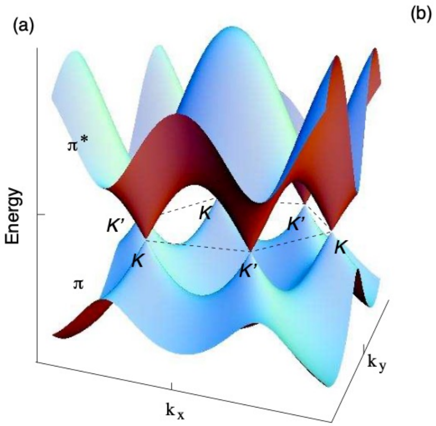
Case of graphene



Honeycomb lattice with two atoms per cell (2 sub-lattices A, B)

Inversion and time reversal symmetries $\vec{\Omega}^{(\pm)}(\vec{k}) = 0$

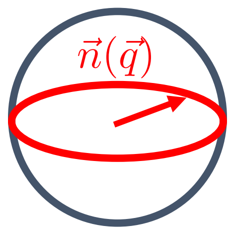
Semi-metal with 2 p_z bands with a linear dispersion to the K point



Close to the K points : $$\mathcal{H}^{\xi}(\vec{q}) = \hbar v_F(\xi q_x \sigma_x + q_y \sigma_y)$$

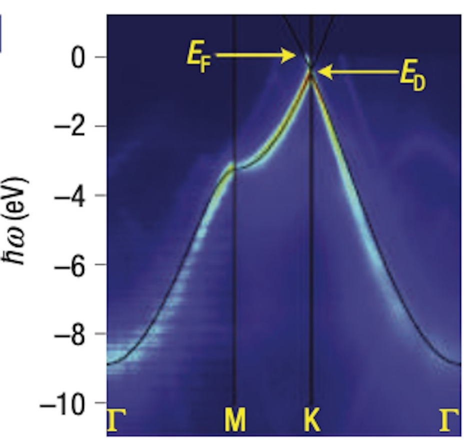
$\xi = \pm 1 \ (K, K')$

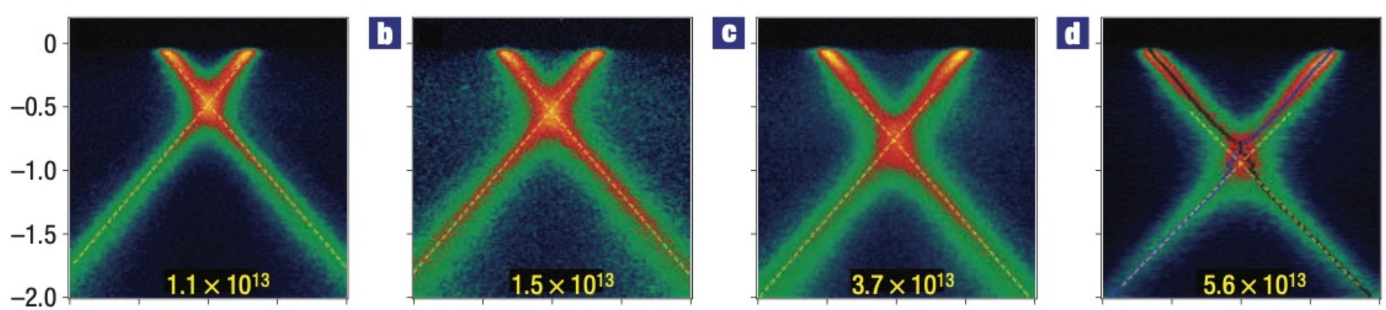
Massless (2+1) Dirac equation



Domain of parameters : circle (does not cover the entire Bloch sphere)

Topologically trivial bands





ARPES effect of doping

Bostwick et al, Nature Physics (2007)

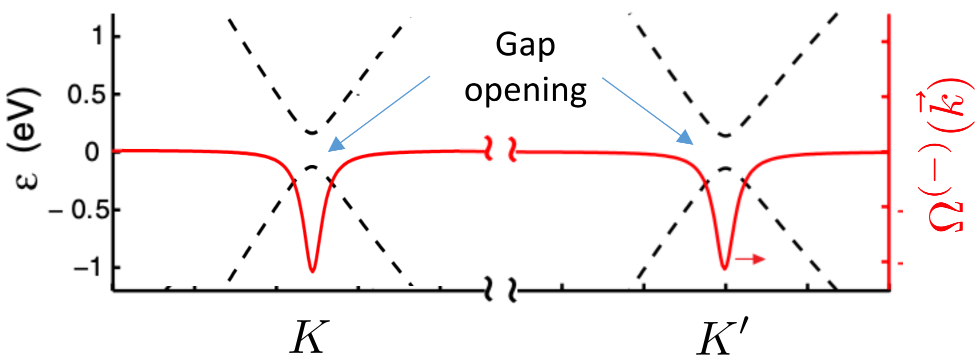
Chern insulator

To have a topologically non-trivial band : breakdown of the time reversal symmetry

To break TRS, Haldane introduced a complexe second neighbor hopping : $t_2 e^{\pm i\phi}$

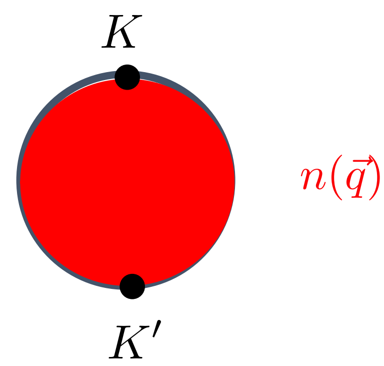
$$\mathcal{H}^{\xi}(\vec{q}) = \hbar v_F(\xi\, q_x\sigma_x + q_y\sigma_y) - \xi\, 3\sqrt{3}t_2 \sin\phi\ \sigma_z$$

Change of sign in K and K' points



Same curvature

in K and K'



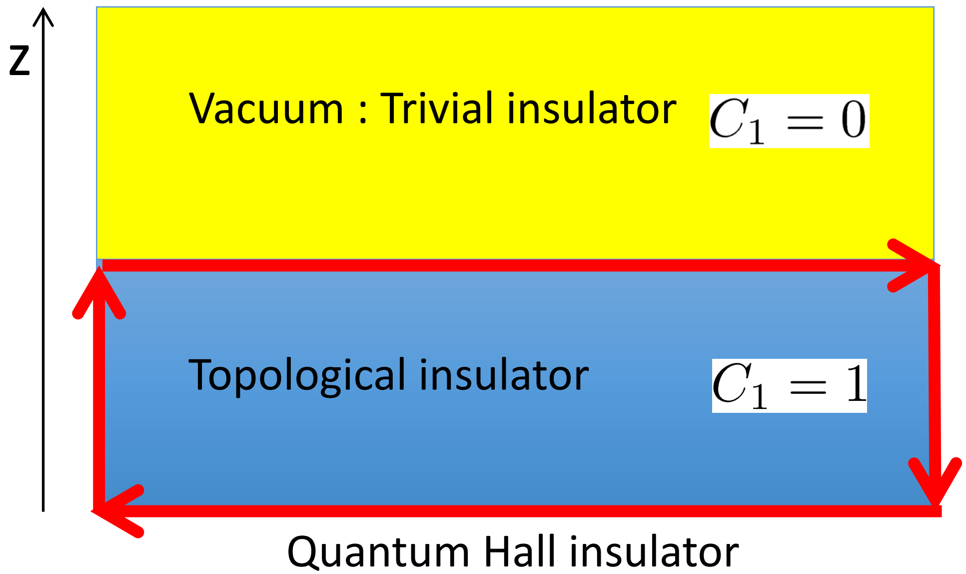
Same sign of the curvature on K and K'

$$C_1^{(-)} = \frac{1}{2\pi}\oint_{\vec{k}\in ZB} \vec{\Omega}^{(-)}(\vec{k})\cdot d^2\vec{k} \neq 0$$

$\vec{n}(\vec{q})$ covers the entire Bloch sphere (2 poles)

Topologically non-trivial band

Topolological edge states of a Chern insulator

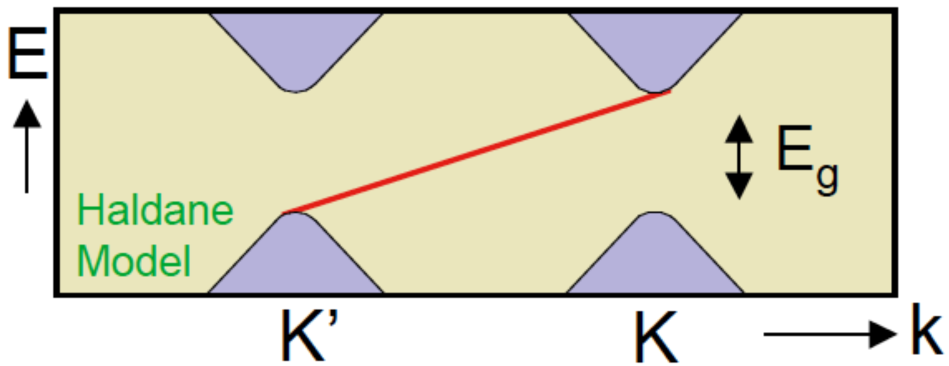


The gap has to be closed at the surface : metallic surface state

-Band edge states are robust against weak time-reversal invariant perturbations

-No scattering to the left! (edge states are chiral)

Chiral edge state : propagation to the right (to the left on the opposite edge)



TRS broken!

Quantum Hall insulator

Kane-Mele topological insulators in 2D : Z_2 invariant

New kind of topological insulator induced by time reversal symmetry (Chern number=0).

Kane & Mele model = 2 copies of the Haldane model (one for each spin direction, 4 bands)

« Spin-orbit » interaction with preserving S_z

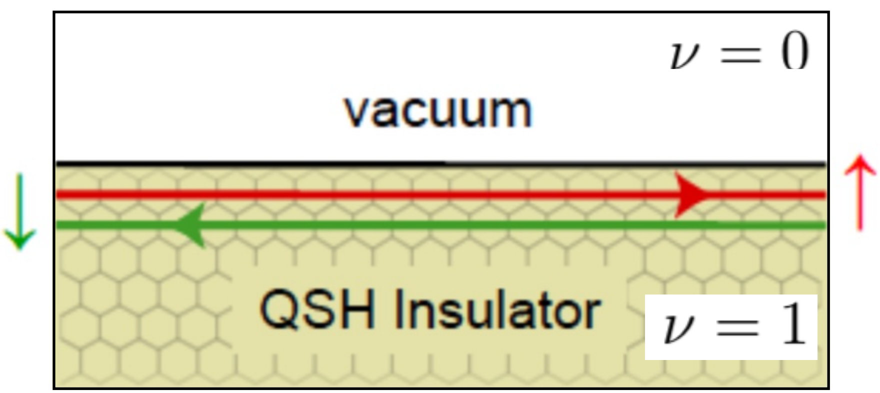
But for each spin band, time reversal is not a symmetry

two « Chern numbers » $C_\uparrow, C_\downarrow$ with opposite sign $C_\uparrow + C_\downarrow = 0$

$C_s = (C_\uparrow - C_\downarrow)/2$ $\mathbb{Z}_2$ Invariant index : $\nu = 0,\ 1$

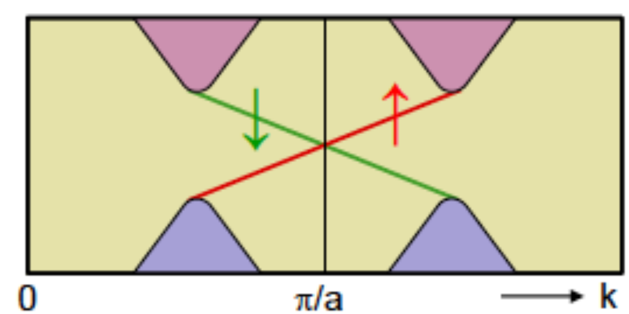
Trivial Non-trivial

Band edge are spin polarized



Quantum spin Hall insulator

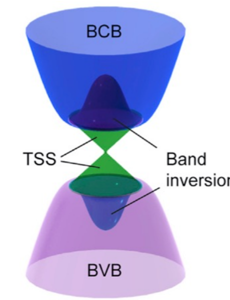
Edge band structure



Kane-Mele topological insulators in 3D

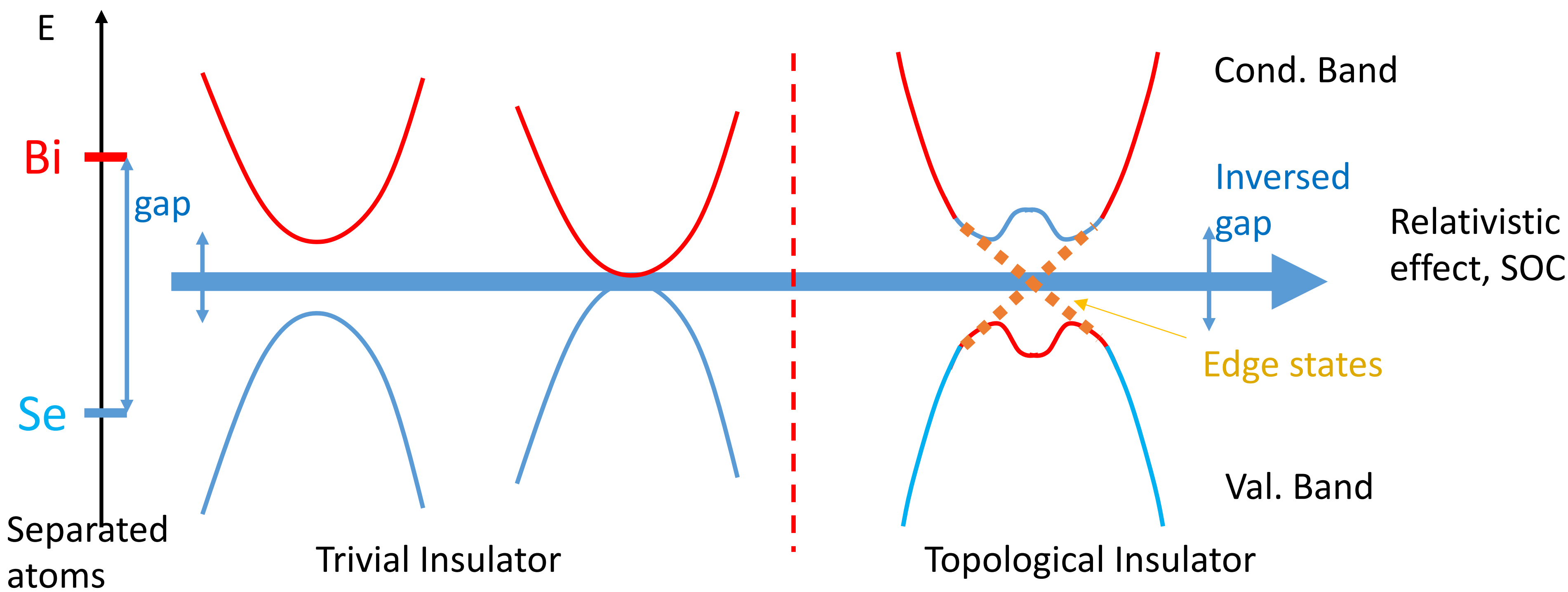
Similar to 2D topological insulators but with 4 invariant Z_2 numbers $(\nu_0; \nu_1, \nu_2, \nu_3)$

For strong TI $\nu_0 = 1$
- Odd number of gapless topological edge states (odd number of Fermi surface crossings (between 2 TRIMs)
- Spin-momentum locked (spin-polarized surface states)



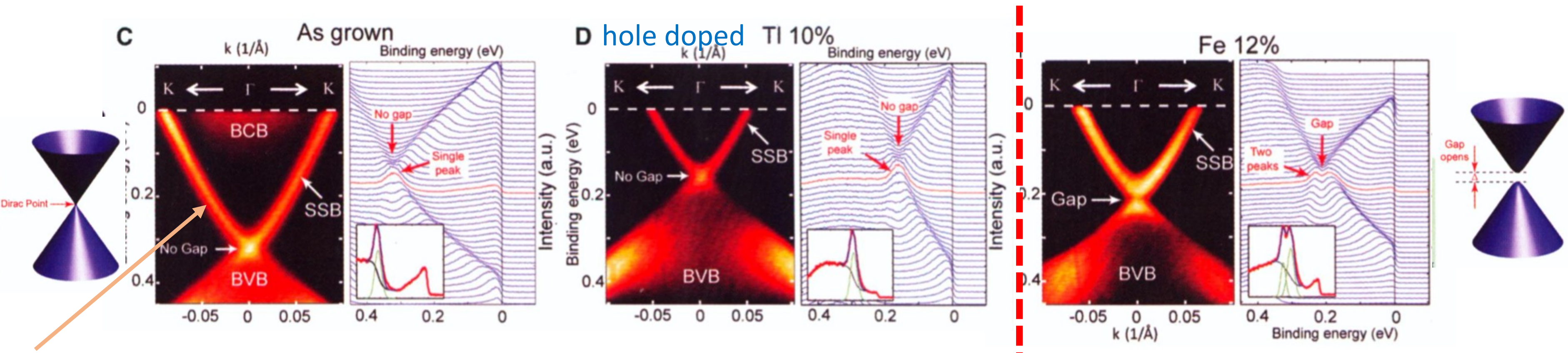
In Bi_2Se_3 ,Bi_2Te_3 : single Dirac cone surface states

bulk band inversion



Kane-Mele topological insulators in 3D

ARPES can probe the topological edge states! 2D surface states



Surface state
(topol. edge state)

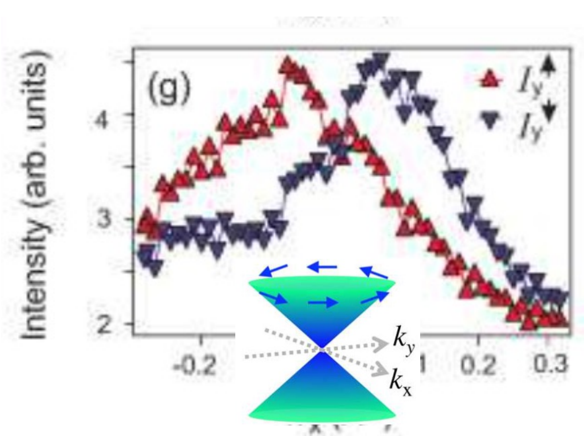
$\Delta \propto 0.3eV$ Room Temp. TI

Bi_2Te_3 Chen et al.
Science 329, 659 (2010)

Topological insulator

Doped with magnetic atoms
Breakdown of the TRS

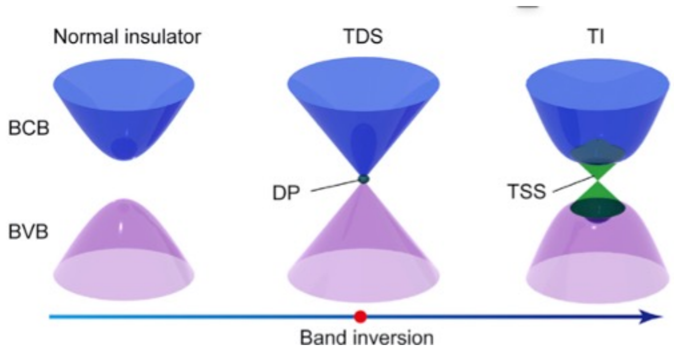
trivial insulator



Spin texture of edge state probed by spin-ARPES
Hsieh… Hasan et al., Nature 460, 1101 (2009)

Spin-momentum locking

Topological states in semi-metals : Dirac semi-metals



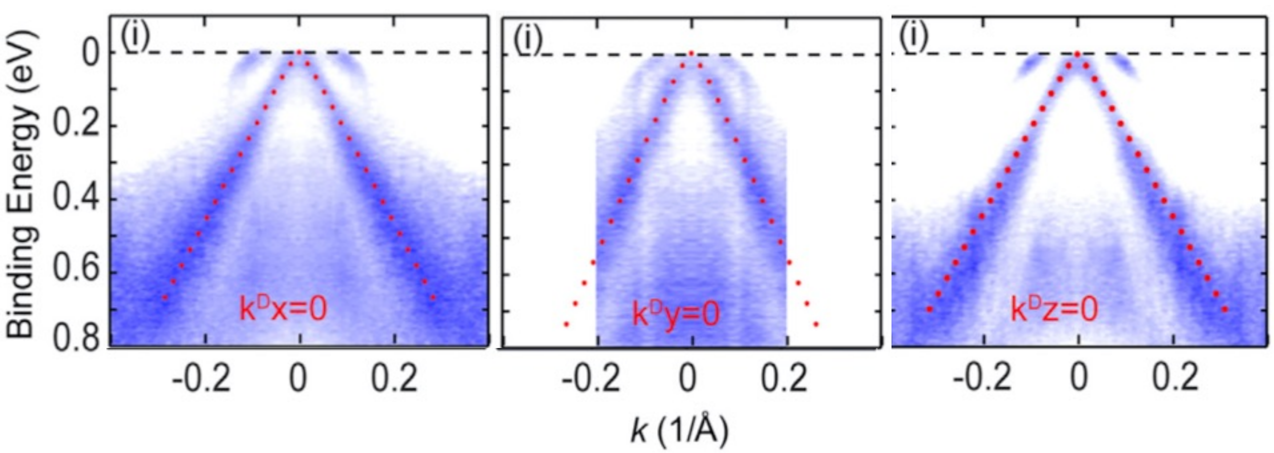
topological quantum phase transition

Dirac semi-metals can be found at the transition between normal and topological Insulators
(3D analogs of graphene)

crystal symmetries can help stabilize the 3D Dirac fermions (C3 axis in Na_3Bi)

First observation of a 3D Dirac semi-metal (Liu et al. Science 343, 864 (2014))

-linear dispersions across the Dirac point along all 3 momentum directions



Topological Weyl semi-metals

In particle physics, a Dirac fermion is described by a bispinor whereas a Weyl fermion is described by a spinor (well defined chirality) : Weyl fermion $\simeq$½ Dirac fermion

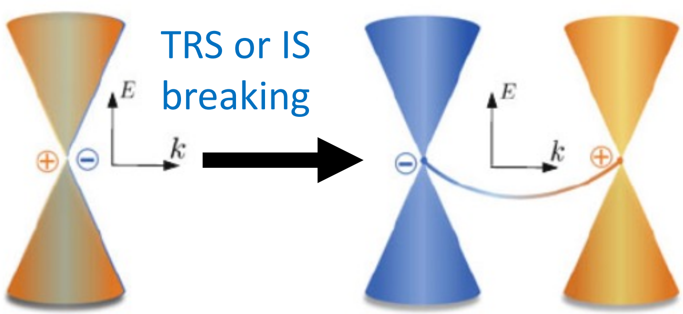
crossing of two spin-deg bands deg. 4

crossing of two non-deg bands deg. 2

similar behavior in condensed matter

TR and I symmetries

TRS or IS breaking



$\vec{\Omega}(\vec{k})=0$

$\vec{\Omega}(\vec{k})\neq 0$

One Dirac node

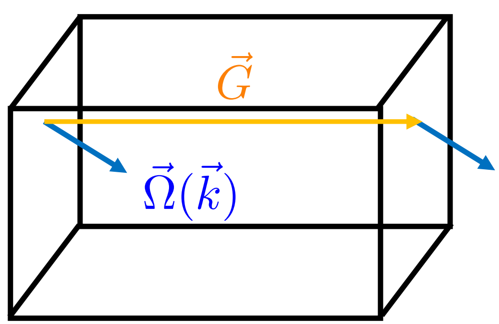
Two Weyl nodes

Weyl nodes of opposite chiral charges
= magnetic monopoles in k space
Source of Berry curvature $\vec{\Omega}(\vec{k})$

Weyl nodes appear by pairs

periodicity

$$\vec{\Omega}(\vec{k}) = \vec{\Omega}(\vec{k}+\vec{G})$$



Gauss Th. : flux of Berry curvature

$$\oint_{S_{BZ}} \vec{\Omega}(\vec{k})\cdot d^2\vec{k} = (n_+ + n_-) = 0$$

Positive & negative
Monopoles (chiral charges)

Topological Weyl semi-metals

In particle physics, a Dirac fermion is described by a bispineur whereas a Weyl fermion is described by a spineur (well defined chirality) : Weyl fermion $\simeq$ ½ Dirac fermion

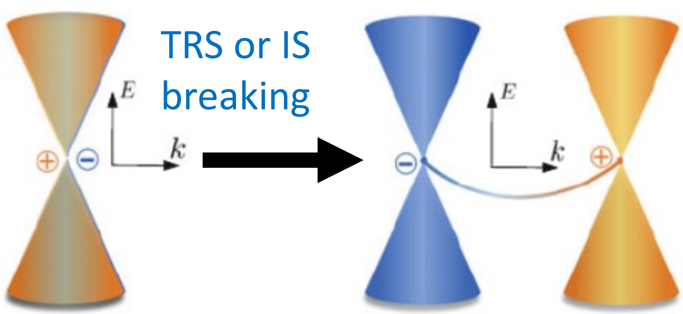
similar behavior in condensed matter

crossing of two spin-deg bands deg. 4

crossing of two non-deg bands deg. 2

TR and I symmetries

TRS or IS breaking



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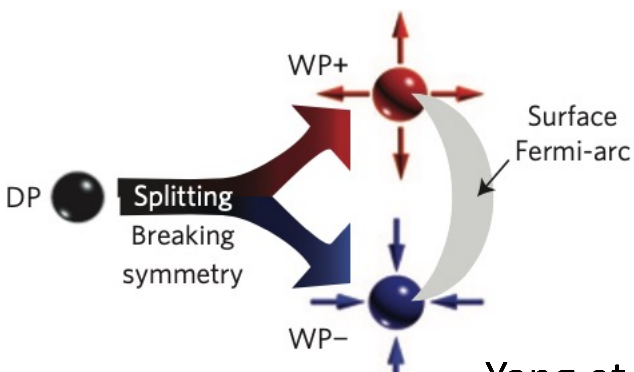
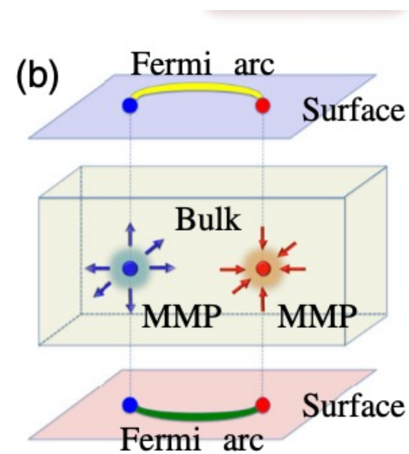


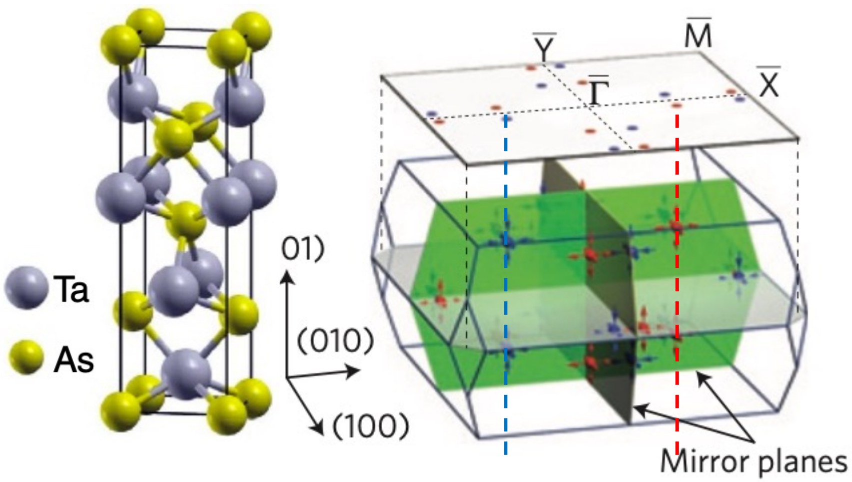
Topological edge state : open Fermi -arc

Yang et al. Nature Phys. (2015)



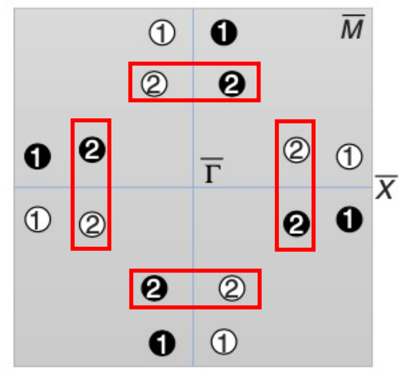
Discovery of a Weyl semimetal by three groups in non-centrosymmetric TaAs (NbAs)

Xu et al. science (7 Aug. 2015)
Yang et al. Nature Phys. (17 Aug. 2015)
Lv et al. Phys. Rev. X (31 July 2015)



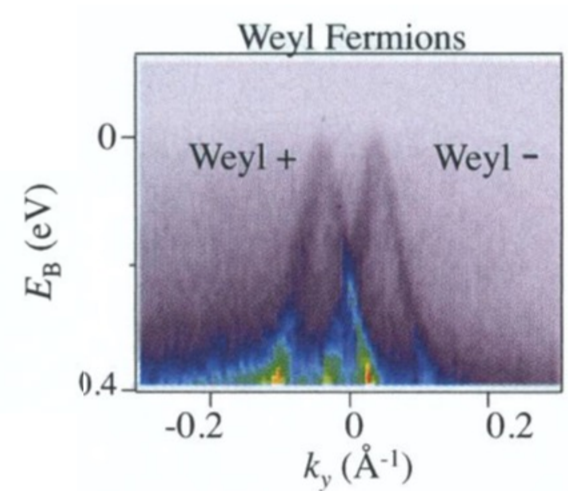
24 Weyl nodes
(12 pairs) in the BZ!

Surface Brillouin zone



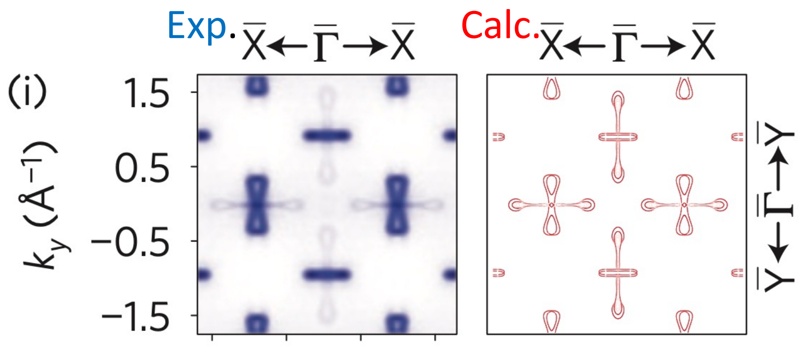
2 Weyl nodes of the same chiral charge are projected on the same surface point

ARPES measurements
of the Bulk Weyl cones
(k_z selected by the choice
of the photon energy)

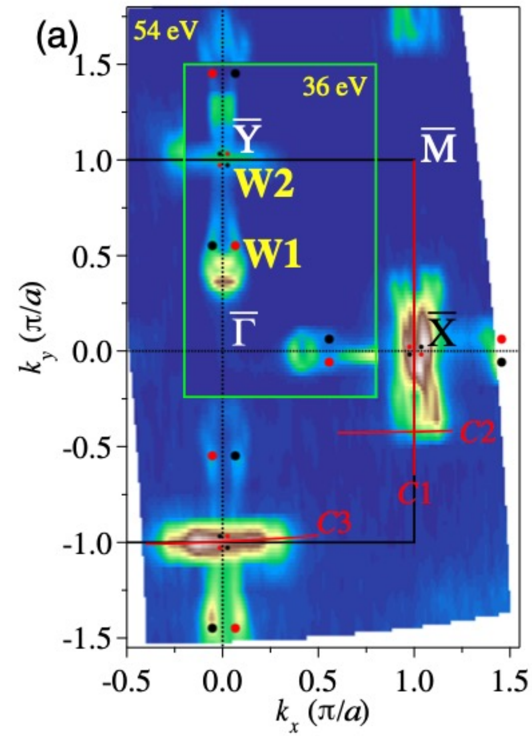


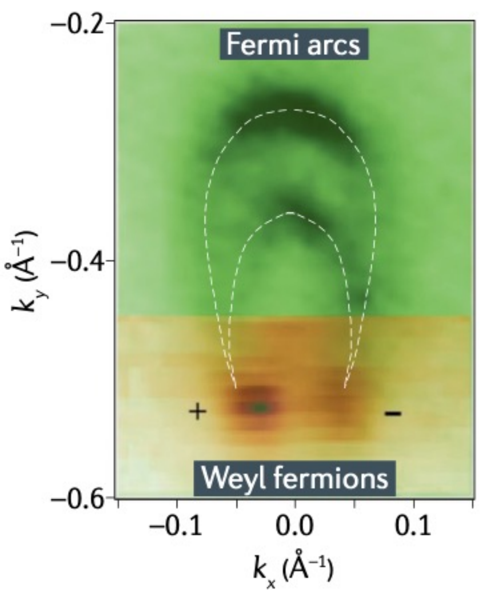
Yang et al.
Nature Phys. (2015)

Fermi surface of the edge states
(trivial and nontrivial states)



Lv et al. Phys. Rev. X (2015)





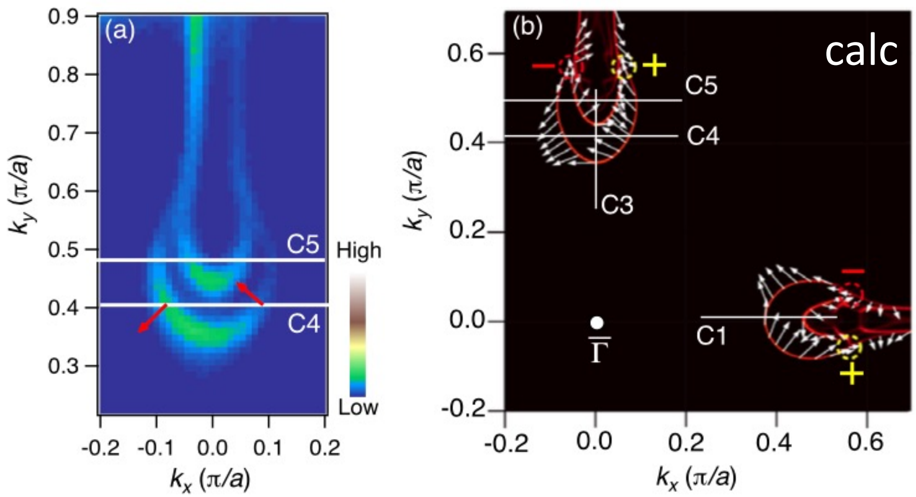
Surface
UV-ARPES
(90 eV)

Bulk
SX-ARPES
(650 eV)

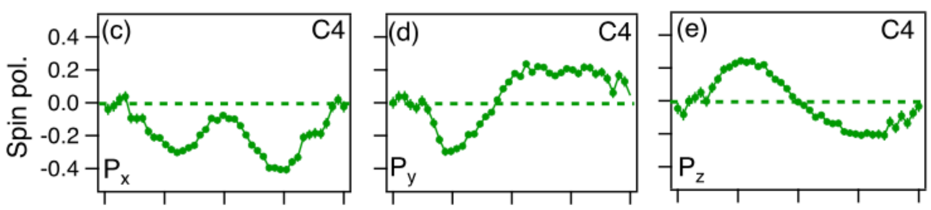
Surface-Bulk correspondence
of the non trivial topological
states in TaAs

Yang et al.
Nature Phys. (2015)

SPIN-ARPES → Spin texture in Weyl semi-metals



Spin texture in the TaAs Weyl semi-metal



Lv et al., PRL 115, 217601 (2015)

CONCLUSION

ARPES probes the non-trivial topology in insulators and in semi-metals

- Non-trivial topology due to inversion of bands (generally due to spin-orbit) and usually protected by symmetry
- Topological edge states with spin texture
- Quasiparticle analogs to particles in high energy physics
- Topological states in condensed matter with no analogs in particle physics : space-group symmetry instead of Lorentz (space-time) symmetry (topological cristalline insulators, type II Dirac and Weyl semi-metals, etc….)

THANK YOU FOR YOUR ATTENTION