# Topological insulators

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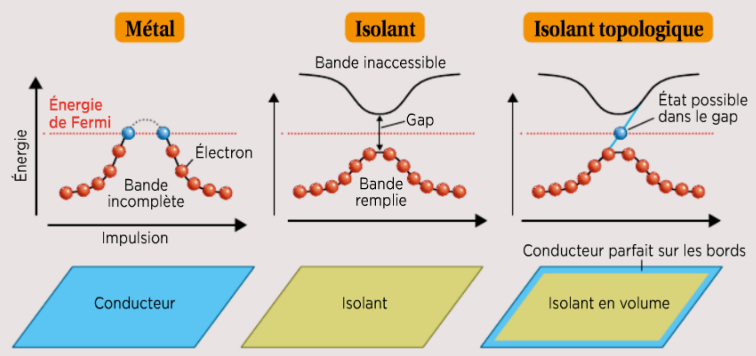
# 1) INTRODUCTION

# 1) INTRODUCTION

A material is either a **metal** or an **insulator**, however

**Some materials are insulators in their bulk and conductors on their edges !**



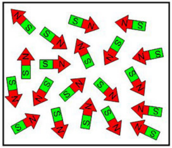
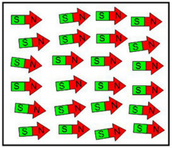
# 1) INTRODUCTION

## NEW CLASSIFICATION OF MATERIALS

1. **Conventional material**

   Phase transition = Symmetry breaking + Non-zero order parameter

   Example : paramagnetic → ferromagnetic transition with decreasing $T$ shows a reduction of its symmetry properties and the appearance of a finite magnetization $\langle M \rangle$.

2. **Topological material**

   → No symmetry breaking

   → Laudau-Ginzburg theory does not apply

   Pioneering examples : Kosterlitz-Thouless transition (1973)

   Quantum Hall effect (1980)

# 1) INTRODUCTION

## SOME FEATURES

- The **edge states** play a fundamental role, since they allow to the electrical current to circulate in topological insulators :

*Living on the edge*

- The current propagate **without dissipation** on the edge states.
- The Hall conductivity is equal to the quantum of conductance $e^2/h$ times an **integer value** $\mathcal{C}$, called Chern number :

$$\boxed{\sigma_H = \frac{e^2}{h}\mathcal{C}}$$

# 1) INTRODUCTION

## HOW COULD THEY BE USED ?

Electronics $\rightarrow$ Spintronics $\rightarrow$ **Topotronics**

## ADVANTAGES

- Do not require any external magnetic field :
  internal spin-orbit coupling plays the role of magnetic field
- Spin-filtering counter-propagating modes (helical edge modes)
- Room temperature device
- No dissipation

## NEXT GENERATION TRANSISTOR ?

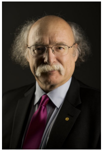
Click to see the video

# 1) INTRODUCTION

**NOBEL PRIZE IN PHYSICS IN 2016 : the tools of topology are used to study the exotic states in matter**

D.J. Thouless :

- Concept of topological order
- Notion of topological invariants



F.D.M. Haldane :

- Theory of the fractional quantum Hall effect

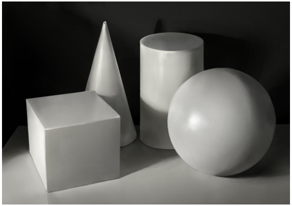
J.M. Kosterlitz :

- Study of phase transitions in topological materials (Kosterlitz-Thouless transition)

# 1) INTRODUCTION

**Definition**

The **topology** is the branch of mathematics which studies the spatial deformations of objects under continuous transformations, i.e. without cutting or re-collations applied to the structures. See the video



A cup can be transform to a donut (torus) with a continuous deformation : these two objects have the same topological index $\chi$, called the Euler characteristic. We have : $\boxed{\chi = 2(1-g)}$ where $g$ (genus) is the number of holes.

**Torus :** $g = 1 \Rightarrow \chi = 0$

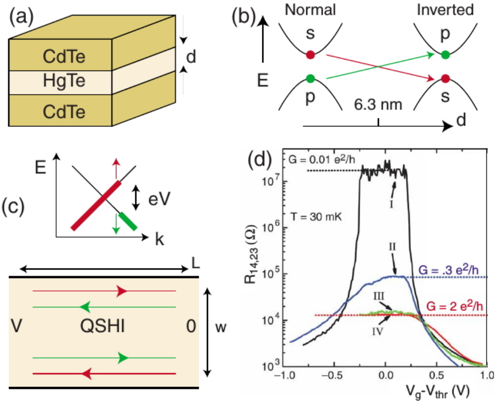
Cube, cylinder cone and sphere are topologically equivalent.

**Sphere :** $g = 0 \Rightarrow \chi = 2$

We have also $\chi = n_V - n_E + n_F$

# 1) INTRODUCTION

## TOPOLOGY OF THE ENERGY BANDS IN A SOLID




Band inversion
at $d_c = 6.3$ nm

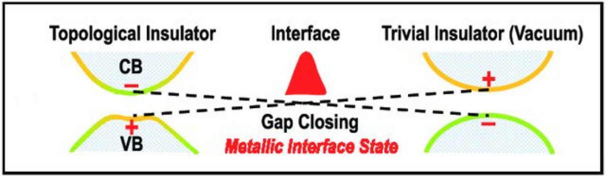
I : $d = 5.5$ nm
$\rightarrow$ **Trivial insulator**
II, III, IV : $d = 7.3$ nm
$\rightarrow$ **Topological insulator**

# 1) INTRODUCTION

## GAP CLOSURE

At the interface between two insulators :

- **If they are both trivial, or both topological**, they have the same Chern number $\mathcal{C}$ : it is possible to go from one to the other thanks to a continuous transformation without closing the gap.
- **If one is trivial and the other topological**, they have distinct Chern numbers : $\mathcal{C}_1 \neq \mathcal{C}_2$. The gap will be closed at the interface, leading to the appearance of conducting edge states. This is precisely what it is observed at the interface between a topological insulator and the vacuum ($=$ trivial insulator).



# 2) HISTORY

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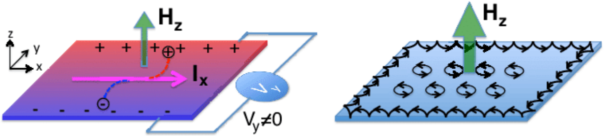
## QUANTUM HALL EFFECT

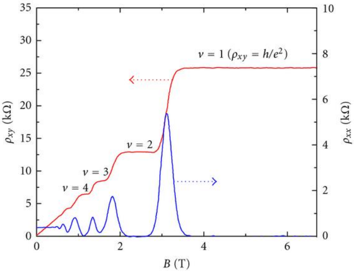


(a) Hall effect

(b) Quantum Hall effect

$$R = \frac{mv_0}{eH}$$

## GALLIUM ARSENIDE 2DEG




(1980) $\boxed{\rho_H = \frac{h}{e^2}\frac{1}{\mathcal{C}}}$

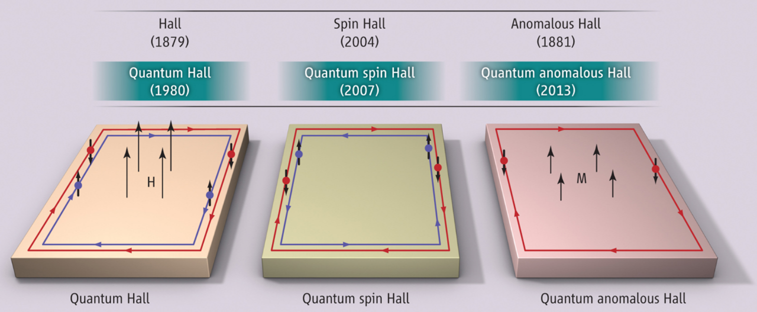
(1982) D.J. Thouless and co-workers showed that $\mathcal{C}$ is a topological invariant

(1985) Klaus von Klitzing got the Nobel prize in physics

# 2) HISTORY

## 2D TOPOLOGICAL INSULATORS

- Magnetic field → Hall effect
- Spin-orbit coupling → Spin Hall effect
- Magnetic material → Anomalous Hall effect

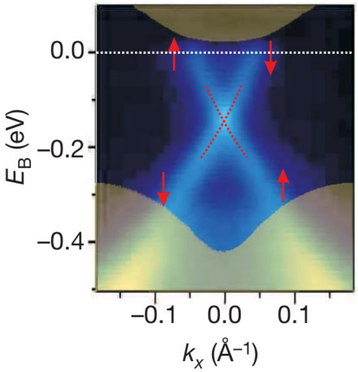


# 2) HISTORY

## 3D TOPOLOGICAL INSULATORS (2009)

Material with strong spin-orbit coupling : $Bi_2Se_3$

ARPES




Surface states

See the video on ARPES

# 3) CHARACTERIZATION

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## BERRY CONNEXION

$$\boxed{\vec{\mathcal{A}}_n(\vec{k}) = i\Psi_n^\dagger(\vec{k})\vec{\nabla}_{\vec{k}}\Psi_n(\vec{k})}$$

where $\Psi_n(\vec{k})$ are the eigenvectors of the Hamiltonian $H$ :

$$H\Psi_n(\vec{k}) = E_n(\vec{k})\Psi_n(\vec{k})$$

Michael Berry

## BERRY CURVATURE

$$\boxed{\vec{\mathcal{B}}_n(\vec{k}) = \vec{\nabla}_{\vec{k}} \times \vec{\mathcal{A}}_n(\vec{k}) = \overrightarrow{\mathrm{rot}}_{\vec{k}}\vec{\mathcal{A}}_n(\vec{k})}$$

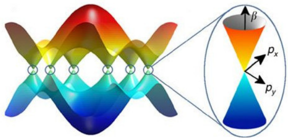
## ANALOGY

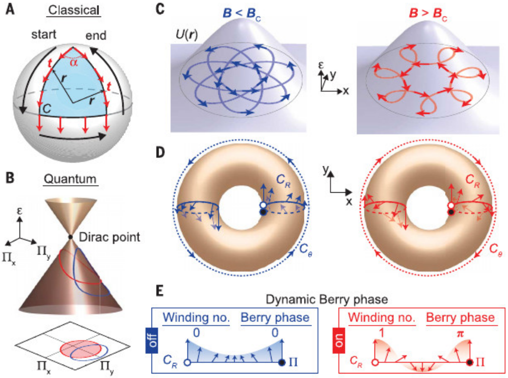
Berry connexion $\vec{\mathcal{A}}_n(\vec{k}) \longrightarrow$ Potential vector $\vec{A}(\vec{r})$
Berry curvature $\vec{\mathcal{B}}_n(\vec{k}) = \vec{\nabla}_{\vec{k}} \times \vec{\mathcal{A}}_n(\vec{k}) \longrightarrow$ Magnetic field $\vec{B}(\vec{r}) = \vec{\nabla}_{\vec{r}} \times \vec{A}(\vec{r})$

# 3) CHARACTERIZATION

**BERRY PHASE** $\boxed{\Phi_B = \int \vec{\mathcal{B}}(\vec{k}) \cdot d\vec{S}}$

The Berry phase can be seen as the phase gained by the wave function when the wave vector follows a close trajectory in the Brillouin zone.




See the video

# 3) CHARACTERIZATION

## ANOMALOUS VELOCITY

$$\boxed{\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}}E_n(\vec{k}) - \dot{\vec{k}} \times \vec{\mathcal{B}}_n(\vec{k})}$$

Similar in form with the Lorentz force : $\vec{F} = -e\vec{\mathcal{E}} - e\vec{v} \times \vec{B}$

$\Rightarrow$ Exercise 1 : use the anomalous velocity to show that $\sigma_H = (e^2/h)\mathcal{C}$

## CHERN NUMBER

$$\boxed{\mathcal{C} = \frac{1}{2\pi}\sum_n \int \vec{\mathcal{B}}_n(\vec{k}) \cdot d\vec{S} = \frac{\Phi_B}{2\pi}}$$

## TOPOLOGICAL INVARIANT $\mathbb{Z}_2$

$$\boxed{\mathbb{Z}_2 = \frac{1}{2\pi}\left[\oint_{\delta 1\mathrm{BZ}} \vec{\mathcal{A}}(\vec{k}) \cdot d\vec{k} - \int_{1\mathrm{BZ}} \vec{\mathcal{B}}(\vec{k}) \cdot d\vec{S}\right] \mathrm{mod}(2)}$$

# EXERCISE 1 : SHOW THAT $\sigma_H = (e^2/h)\mathcal{C}$

Electrical current : $\vec{I} = -en\langle\vec{v}\rangle$
Average velocity in the framework of Boltzmann equation theory :

$$\langle\vec{v}\rangle = \frac{\int_{1\mathrm{BZ}} \frac{d^3k}{(2\pi)^3}\vec{v}(\vec{k})f(\vec{k})}{\int_{1\mathrm{BZ}} \frac{d^3k}{(2\pi)^3}f(\vec{k})}$$

where

- $n = \int_{1\mathrm{BZ}} \frac{d^3k}{(2\pi)^3}f(\vec{k})$ is the electron density
- $f(\vec{k})$ is the out-of-equilibrium distribution function
- $\vec{v}(\vec{k}) = -\sum_n \dot{\vec{k}} \times \vec{\mathcal{B}}_n(\vec{k})$ is the anomalous velocity, with $\hbar\dot{\vec{k}} = \vec{F}$

Thus,

$$\vec{I} = e\sum_n \int_{1\mathrm{BZ}} \frac{d^3k}{(2\pi)^3}\dot{\vec{k}} \times \vec{\mathcal{B}}_n(\vec{k})f(\vec{k}) = \frac{e}{\hbar}\sum_n \int_{1\mathrm{BZ}} \frac{d^3k}{(2\pi)^3}\vec{F} \times \vec{\mathcal{B}}_n(\vec{k})f(\vec{k})$$

# EXERCISE 1 : SHOW THAT $\sigma_H = (e^2/h)\mathcal{C}$

For $\vec{B} = \vec{0}$, one has $\vec{F} = -e\vec{\mathcal{E}}$, where $\vec{\mathcal{E}}$ is the electrical field, thus

$$\vec{I} = -\frac{e^2}{\hbar}\sum_n \int_{1BZ} \frac{d^3k}{(2\pi)^3}\vec{\mathcal{E}} \times \vec{\mathcal{B}}_n(\vec{k}) f(\vec{k})$$

We expand the curl product :

$$\begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix} = -\frac{e^2}{\hbar}\sum_n \int_{1BZ} \frac{d^3k}{(2\pi)^3} \begin{pmatrix} \mathcal{E}_y \mathcal{B}_{n,z}(\vec{k}) - \mathcal{E}_z \mathcal{B}_{n,y}(\vec{k}) \\ \mathcal{E}_z \mathcal{B}_{n,x}(\vec{k}) - \mathcal{E}_x \mathcal{B}_{n,z}(\vec{k}) \\ \mathcal{E}_x \mathcal{B}_{n,y}(\vec{k}) - \mathcal{E}_y \mathcal{B}_{n,x}(\vec{k}) \end{pmatrix} f(\vec{k})$$

Since one has $\vec{I} = \sigma\vec{\mathcal{E}}$ and $\sigma_H = |\sigma_{xy}|$, one deduces that

$$\sigma_H = \frac{e^2}{2\pi\hbar}\sum_n \underbrace{\frac{1}{2\pi}\int_{1BZ} dk_x dk_y \mathcal{B}_{n,z}(\vec{k})}_{=\frac{1}{2\pi}\int_{1BZ} d\vec{S}\cdot\vec{\mathcal{B}}_n(\vec{k}) = \mathcal{C}_n} \underbrace{\frac{1}{2\pi}\int_{1BZ} dk_z f(\vec{k})}_{=1}$$

Result : $\boxed{\sigma_H = \frac{e^2}{h}\sum_n \mathcal{C}_n = \frac{e^2}{h}\mathcal{C}}$

# 4) DIRAC-WEYL HAMILTONIAN

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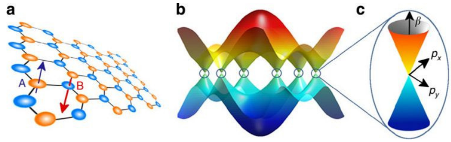
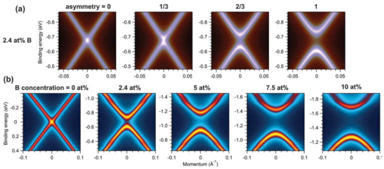
## DOPED GRAPHENE




## HAMILTONIAN

$$\boxed{H = \hbar v_F \vec{k} \cdot \vec{\sigma} = \vec{q} \cdot \vec{\sigma} + m\sigma_z}$$

with $q_x \equiv \hbar v_F k_x$, $q_y \equiv \hbar v_F k_y$, $m \equiv \hbar v_F k_z$
and $\sigma_x$, $\sigma_y$, $\sigma_z$, the Pauli matrices

# 4) DIRAC-WEYL HAMILTONIAN

## HAMILTONIAN

Pauli matrices :

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

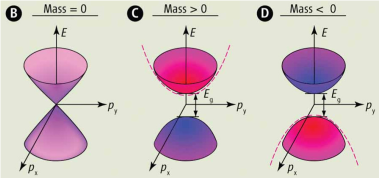
Matrix form :

$$H = \begin{pmatrix} m & q_x - iq_y \\ q_x + iq_y & -m \end{pmatrix}$$

## BAND STRUCTURE

$$\boxed{E_m^\pm(\vec{q}) = \pm\sqrt{q^2 + m^2}}$$

- $m = 0 \rightarrow$ massless Dirac cone
- $m \neq 0 \rightarrow$ massive Dirac cone




$\Rightarrow$ Exercise 2 : Berry phase calculation

# EXERCISE 2 : Berry phase calculation

## WORK TO DO

Starting from the Dirac-Weyl Hamiltonian :

$$H = \begin{pmatrix} m & q_x - iq_y \\ q_x + iq_y & -m \end{pmatrix}$$

It is asked you to calculate :

1. The eigenvalues $E_m^{\pm}(\vec{q})$ of $H$
2. The eigenvector $\Psi_m(\vec{q})$ associated to $E_m^{+}$
3. The Berry connexion $\vec{\mathcal{A}}_m(\vec{q}) = i\Psi_m^{\dagger}(\vec{q})\vec{\nabla}_{\vec{q}}\Psi_m(\vec{q})$
4. The Berry curvature $\vec{\mathcal{B}}_m(\vec{q}) = \vec{\nabla}_{\vec{q}} \times \vec{\mathcal{A}}_m(\vec{q})$
5. The Berry phase $\Phi_B = \int \vec{\mathcal{B}}_m(\vec{q}) \cdot d\vec{S}$

# EXERCISE 2 : Berry phase calculation

## RESULTS

1. Eigenvalues : $E_m^{\pm}(\vec{q}) = \pm\sqrt{q^2+m^2}$
2. Eigenvector $\Psi_m(\vec{q})$ associated to $E_m^+$ :

$$\Psi_m(\vec{q}) = \frac{1}{\sqrt{q^2+(m-\sqrt{q^2+m^2})^2}} \begin{pmatrix} q_x - iq_y \\ \sqrt{q^2+m^2}-m \end{pmatrix}$$

3. Berry connexion :

$$\vec{\mathcal{A}}_m(\vec{q}) = \frac{-q_y\vec{e}_x + q_x\vec{e}_y}{2\sqrt{q^2+m^2}(\sqrt{q^2+m^2}-m)}$$

4. Berry curvature : $\vec{\mathcal{B}}_m(\vec{q}) = \frac{m\vec{e}_z}{2(q^2+m^2)^{3/2}}$
5. Berry phase : $\Phi_B = \pm\pi\mathrm{sgn}(m)$

# 5) OTHER TOPOLOGICAL OBJECTS

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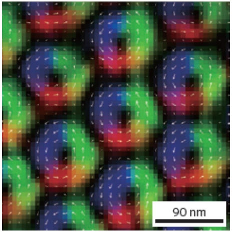
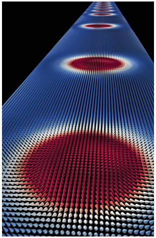
## SKYRMIONS = SPIN VORTICES



Lattice of skyrmions observed by Lorentz microscopy at the surface of $Fe_{1-x}Co_xSi$ (2011)

**Dzyaloshinsky-Moriya** interaction :

$$\boxed{\vec{D}_{ij} \cdot (\vec{S}_i \times \vec{S}_j)}$$

**Conditions :**

Symmetry lowering + Spin-orbit coupling

**Topological protected :**

Cannot be removed by continuous transformation

May be used for high density data storage

See the video

# 5) OTHER TOPOLOGICAL OBJECTS

## MAJORANA FERMIONS (1937)

Real solution of the Dirac equation such as the particle and anti-particle coincide : $\Psi = \Psi^*$.

As a consequence, creation and annihilation operators are equal :

$$\boxed{\gamma = \gamma^\dagger}$$

## EXAMPLE : KITAEV SUPERCONDUCTING CHAIN (2001)

$$H = -\mu \sum_{n=1}^{N} (c_n^\dagger c_n - 1/2) + \sum_{n=1}^{N-1} [t(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) - \Delta(c_n c_{n+1} + c_{n+1}^\dagger c_n^\dagger)]$$

We use $\gamma_n^A = (c_n + c_n^\dagger)/\sqrt{2}$ and $\gamma_n^B = i(c_n - c_n^\dagger)/\sqrt{2}$, then :

$$H = i\mu \sum_{n=1}^{N} \gamma_n^A \gamma_n^B + i \sum_{n=1}^{N-1} [(t + \Delta)\gamma_n^B \gamma_{n+1}^A - (t - \Delta)\gamma_n^A \gamma_{n+1}^B]$$

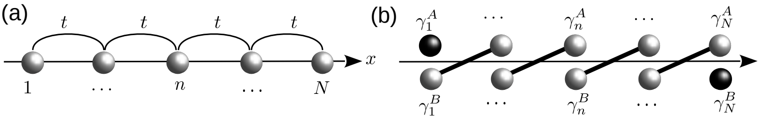
# 5) OTHER TOPOLOGICAL OBJECTS

## EXAMPLE : KITAEV SUPERCONDUCTING CHAIN

We set $\mu = 0$ and $\Delta = t$ :

$$\boxed{H = 2it \sum_{n=1}^{N-1} \gamma_n^B \gamma_{n+1}^A}$$

Two Majorana fermions appear at the extremities of the chain.




See the video

# 6) SUMMARY

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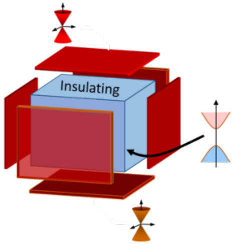
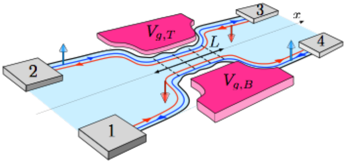
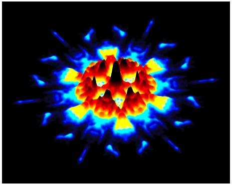
- Insulator in the bulk but **conductor on the surfaces/edges**
- Current propagate **without dissipation**
- Crucial role played by **the spin-orbit coupling**
- Opposite spins propagate in opposite direction
- Phase transitions are not related to symmetry breaking
- Instead, the system is characterized by **topological invariants**
- New field of research : **Topotronics**



Book : Introduction à la physique de la matière condensée, Dunod (2019)