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# A short introduction to Topological insulators

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### Outline

I) Semimetallic graphene: massless Dirac fermions

II) h-BN and Haldane model: massive Dirac fermions trivial vs Chern insulators

III) Kane-Mele model: massive Dirac fermions with spin-orbit coupling Z2 topological insulators

IV) Experimental realizations of topological insulators

C. Kane and Z. Hasan RMP 2010; X-L Qi and S-C Zhang RMP 2012

0- Brief reminder aboutDirac and Weyl equationsin high-energy physics



# Dirac equation (1928)



Wave-equation for relativistic et quantum particle (electron)

$$E^2 = p^2 c^2 + m^2 c^4$$

$$i\hbar\frac{\partial\Psi}{\partial t} = c\left(-i\hbar\frac{\alpha_i}{\partial x_i}\frac{\partial}{\partial x_i} + \beta mc\right)\Psi$$

$$E\Psi = c\left(\alpha_{i}p_{i} + \beta mc\right)\Psi$$
$$\{\alpha_{i}, \beta\} = 0 \qquad \{\alpha_{i}, \alpha_{j}\} = 2\delta_{ij}$$



# Clifford algebra



 $E\Psi = c\left(\frac{\alpha_i}{p_i}p_i + \beta mc\right)\Psi$ 

Coefficients must be Hermitian anti-commuting matrices squaring to identity

Pauli matrices (2x2): only 3 matrices which is not enough in 3D for a massive particle, but is enough for a massless particle

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

Dirac matrices (4x4): 15 matrices (more than needed)

Implies 4 components wave-functions: spin x particle/antiparticle



# Dirac and Weyl equations (1928)



 $E^2 = p^2 c^2 + m^2 c^4$ 

 $E = \pm cp$ 



At low velocity, one gets the non relativistic Schrödinger equation and the spin gets decoupled from the motion up to small corrective spin-orbit terms I- Graphene: Massless Dirac fermions

## Graphene: Dirac-like equation

Carbon is a light element: spin-orbit coupling is weak spin is basically decoupled from motion

### But:

Graphene has a particular lattice structure which leads to an additional internal degree of freedom: the sublattice isospin.

It turns out that this sublattice isospin is tied to electronic motion.

Low energy electrons are described by a « Dirac-like » equation.

### Graphene: honeycomb structure

 $d_{C-C} = 0.142 \,\mathrm{nm}$ 



internal degree of freedom: sub lattice isospin  $(a_k, b_k)$ 

# Tight-binding (TB) model

Schrödinger equation + projections on A and B orbitals

$$H \left| \Psi_{\vec{k}} \right\rangle \ = \ E_k \left| \Psi_{\vec{k}} \right\rangle$$

TB Hamiltonian in real space (only nearest neighbors hopping terms)

$$H_0 = -t \sum_{\vec{R}, \vec{\delta}_{\alpha}} c_B^{\dagger}(\vec{R}) c_A(\vec{R} + \vec{\delta}_{\alpha}) + H.c. \quad t = 2.7 \text{ eV}$$

with:

$$-t = \int d^3 r \, \phi^* (\vec{r} - \vec{R}_A - \vec{\delta}_3) (V(\vec{r}) - V_{\text{ato}}(\vec{r} - \vec{R}_B)) \phi(\vec{r} - \vec{R}_B)$$

# Diagonalization

$$H_{0} = -t \sum_{\vec{k},\vec{\delta}_{\alpha}} e^{i\vec{k}.\vec{\delta}_{\alpha}} c_{B}^{\dagger}(\vec{k}) c_{A}(\vec{k}) + H.c.$$
$$= -t \sum_{\vec{k}} c_{\alpha}^{\dagger}(\vec{k}) [h_{0}]_{\alpha\beta} c_{\beta}(\vec{k}) \qquad \alpha, \beta = A, B$$

$$h_0(\vec{k}) = -t \sum_{\vec{k},\vec{\delta}_{\alpha}} \left( \cos(\vec{k}.\vec{\delta}_{\alpha})\sigma_1 + \sin(\vec{k}.\vec{\delta}_{\alpha})\sigma_2 \right)$$

#### even function

#### odd function

Both functions periodic in reciprocal space

### Electronic structure

Two bands (2 sites/unit cell)



$$E(\vec{k}) = d_1(\vec{k})\sigma_1 + d_2(\vec{k})\sigma_2$$

$$\vec{E}(\vec{k}) = \pm || \vec{d}(\vec{k}) ||$$

Band touching points (two valleys)

$$d_1(\vec{k}) = d_2(\vec{k}) = 0 \rightarrow \vec{k} = \pm \vec{K}$$

1 electron/orbital (half-filling)

Electrostatic doping: it is possible to raise/lower the Fermi level in a reversible manner and without adding impurities.

### Linearization near Dirac points

$$\vec{k} = \boldsymbol{\xi}\vec{K} + \vec{q} \qquad \boldsymbol{\xi} = \pm 1 \quad \text{(Valley index)}$$
$$h_0(\boldsymbol{\xi}\vec{K} + \vec{q}) \simeq \hbar v_F \left(\boldsymbol{\xi}\boldsymbol{q}_x\boldsymbol{\sigma}_1 + \boldsymbol{q}_y\boldsymbol{\sigma}_2\right)$$

Linear dispersion (Dirac cone): electrons (or holes) behave as if they were massless

$$E(\boldsymbol{\xi}\vec{K}+\vec{q}\,)=\hbar v_F\sqrt{q_x^2+q_y^2}$$
 valley independent

Fermi velocity: 
$$v_F = 3at/2\hbar \simeq 10^6 {
m m.s}^{-1}$$

### Transport in ballistic graphene



Tworzydlo et al. , PRL 2006

No off-state !

 $k_F L$ 

### Electronic transport









# **Electronic optics**

From Cory Dean's group (Columbia), Science 2016









## Protection of Dirac points

The possible perturbations: only the third Pauli matrix can open a gap at the Dirac points

$$h_0(\vec{k}) = d_1(\vec{k})\sigma_1 + d_2(\vec{k})\sigma_2 + d_3(\vec{k})\sigma_3$$

Inversion symmetry enforces the relation:

$$h_0(\vec{k}) = \sigma_1 h_0(-\vec{k})\sigma_1 \quad \longrightarrow \quad d_3(\vec{k}) = -d_3(-\vec{k})$$

Time-reversal symmetry (for spinless electrons) enforces the relation:

$$h_0(\vec{k}) = h_0^*(-\vec{k}) \longrightarrow d_3(\vec{k}) = d_3(-\vec{k})$$

Hence if both T and P are satisfied:  $d_3(\vec{k}) = 0$ 

# II)- Graphene: Massive spinless Dirac fermions

How to transform a semimetal into an insulator ?

How to provide a mass to Dirac fermions ?

Add a perturbation that anticommutes with graphene's kinetic Hamiltonian and breaks either T or P

$$h_0(\vec{k}) = d_1(\vec{k})\sigma_1 + d_2(\vec{k})\sigma_2 + \frac{d_3(\vec{k})\sigma_3}{d_3(\vec{k})\sigma_3}$$

### Dirac mass 1: Semenov model (1984)

The simplest perturbation is a staggered potential on A/B sites (Semenov, PRL 1984): +M on A sites and -M on B-sites

$$d_3(\vec{k})\sigma_3 = M\sigma_3$$

This k-independent perturbation breaks inversion symmetry (A and B orbitals are no longer identical)

The resulting insulator is a trivial band insulator

Relevant for hexagonal boron-nitride (h-BN) which is 2D insulator with a large gap (around 5 eV)

# Dirac mass 2: Haldane model (1988)

A (far) less evident perturbation was proposed by D. Haldane. His initial motivation was to induce Quantum Hall effect in 2D lattice without Landau levels

Ingredients are :

- 2D crystal: graphene
- Break time-reversal symmetry (to generate Quantum Hall Effect)
- No net magnetic flux per unit cell (to avoid Landau Levels)



Haldane found that complex valued local fluxes with zero net average value meet all these criteria and do the job (PRL 1988).



# Haldane mass

Fractional topological phases and broken time re  $d_3(\vec{k}) = 2t_2 \sin 2\pi 2 \sin 2$ 

 $\boldsymbol{a}$ 

functions as gaps/masses are opposite atmates and -K



### Hall response

Hamiltonian

$$H = d_x(\vec{k})\sigma_x + d_y(\vec{k})\sigma_y + d_z(\vec{k})\sigma_z$$

Current operator:

$$j_i = \frac{\partial \mathcal{H}(\mathbf{k})}{\partial k_i} = \frac{\partial \varepsilon_0(\mathbf{k})}{\partial k_i} \mathbf{I}_{2\mathbf{x}2} + \sum_j^3 \frac{\partial \mathbf{d}(\mathbf{k})}{\partial k_i} .\boldsymbol{\sigma}$$

Hall conductivity (Kubo formalism)

$$\sigma_{xy} = \frac{e^2}{4\pi h} \int d^2 \mathbf{k} (f_+(\mathbf{k}) - f_-(\mathbf{k})) \left( \frac{\partial \hat{\mathbf{d}}(\mathbf{k})}{\partial k_x} \times \frac{\partial \hat{\mathbf{d}}(\mathbf{k})}{\partial k_y} \right) .\hat{\mathbf{d}}(\mathbf{k})$$
BZ

Insulator at T=0:

This winding number is often zero, and has to be an integer

# Topology: mapping BZ to BS



# Topological invariant



### Trivial insulator (TR invariant)





### Haldane insulator







### Interfaces between insulators



 $k_y$ 

# III)- Graphene: massive Dirac fermions with spin

How to provide a mass to Dirac fermions without breaking T or P ?

### Dirac mass 3: Kane-Mele model

In 2004, Kane and Mele realized that it is possible to open gaps without breaking any of the fundamental symmetries (P, T).

<u>Their initial motivation</u>: combining spin Hall effect + graphene





### Kane-Mele model

Spin-orbit coupling  

$$H = t \sum_{\langle i,j \rangle} c^{\dagger}_{i\alpha} c_{j\alpha} + it_2 \sum_{\langle \langle i,j \rangle \rangle} v_{ij} c^{\dagger}_{i\alpha} (s_3)_{\alpha\beta} c_{j\beta}$$
Spin-conserving model: two copies of Haldane model





#### Quantum Spin Hall insulator

### Robustness of the QSH insulator

#### One can add time-reversal invariant perturbations



FIG. 1 (color online). Energy bands for a one-dimensional "zigzag" strip in the (a) QSH phase  $\lambda_v = 0.1t$  and (b) the insulating phase  $\lambda_v = 0.4t$ . In both cases  $\lambda_{SO} = .06t$  and  $\lambda_R = .05t$ . The edge states on a given edge cross at  $ka = \pi$ . The inset shows the phase diagram as a function of  $\lambda_v$  and  $\lambda_R$  for  $0 < \lambda_{SO} \ll t$ .



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## Comparison Chern versus Z2 insulators

#### Chern insulator



#### Chiral edge state

- Time-reversal breaking
- Bulk topological invariant: Z
- Minimal bulk model: 2 bands

$$h_0(\vec{k}) = d_1(\vec{k})\sigma_1 + d_2(\vec{k})\sigma_2 + d_3(\vec{k})\sigma_3$$



helical edge state Time-reversal symmetric Bulk topological invariant: Z2 Minimal bulk model: 4 bands  $\mathcal{H}(\mathbf{k}) = \sum_{k=1}^{5} d_{a}(\mathbf{k})\Gamma^{a} + \sum_{k=1}^{5} d_{ab}(\mathbf{k})\Gamma^{a}$ 

$$(\mathbf{k}) = \sum_{a=1}^{5} d_a(\mathbf{k})\Gamma^a + \sum_{a < b=1}^{5} d_{ab}(\mathbf{k})\Gamma^{ab}$$

### Topology and Dirac mass

• Jackiw-Rebbi mechanism (1976):

$$i\hbar\partial_t\Psi(x,t) = (-i\hbar\partial_x\sigma_1 + m(x)\sigma_2)\Psi(x,t)$$



D-1 interfacial state E=0, localised at x=0 between two insulators

### 3D topological insulators

- Semiconductor: weak gap and strong SO coupling
- Dirac surface state (ARPES, STM, transport)





Each Bloch state k has only one spin direction

Surface state is spin-polarized

# IV)- Topological insulators in real materials

Spin orbit is too weak in graphene

HgTe and Bi-based compounds: strong spin-orbit and close to band inversion

# HgTe/CdTe



3D semiconductor

3D semimetal: no gap

This can be described by 8 (or 6) band model (within k.p theory)

### 4-band model

« Ab-initio » 6-band model + envelope functions leads to BHZ model



Symmetry allowed terms (both linear and quadratic in momentum)

$$H_{\rm eff}(k_x, k_y) = \begin{pmatrix} H(k) & 0\\ 0 & H^*(-k) \end{pmatrix}$$

$$d_1 + id_2 = A(k_x + ik_y) \equiv Ak_+$$
  

$$d_3 = M - B(k_x^2 + k_y^2)$$
  

$$\varepsilon(k) = C - D(k_x^2 + k_y^2)$$

# HgTe/CdTe quantum well

From B.A. Bernevig, T.L. Hughes, and S.C. Zhang, Science 314, 1757 (2006)



### Experiments

Koenig, Wiedmann, Brune, Buhmann, Molenkamp, Qi and Zhang, Science 2007



Edge conduction in III-IV cases (suppressed by magnetic field)

*Theory:* B.A. Bernevig, T.L. Hughes, and S.C. Zhang, Science **314**, 1757 (2006) *Experiments:* 

Konig, Wiedmann, Brune, Buhmann, Molenkamp, Qi and Zhang, Science 2007 Roth, Brune, Buhmann, Molenkamp, Maciejko, Qi and Zhang, Science 2009

### Experiments

Roth, Brune, Buhmann, Molenkamp, Maciejko, Qi and Zhang, Science 2009



**Fig. 1.** Two-terminal  $(R_{14,14})$  (top two traces) and four-terminal  $(R_{14,23})$  (bottom traces) resistance versus (normalized) gate voltage for the Hall bar devices D1 and D2 with dimensions (length × width) as indicated. The dotted blue lines indicate the resistance values expected from the Landauer-Büttiker approach.

#### Landauer-Buttiker analysis

### Bi2Se3 and Bi2Te3





from Y. Ando, JSPJ review 2013

### 2D Surface states versus graphene



from J. Bardarson<sup>k</sup>and J. Moore<sub>k</sub> Rep<sub>k</sub> Phone  $k_x$  Phone Phon

### Chern insulator: experiment



## Conclusions

Edge states provide new low dimensional conductors (1D) which differ from previously known 1D systems: nanowires, 1D organic conductors, carbon nanotubes.

The spin-momentum locking leads to:

- suppression of some scattering channels

- absence of backscattering by non magnetic impurities
- unusual proximity effect with superconductors: realization of exotic phases (Majorana quasiparticles)

Surface states of TIs also provide new low dimensional conductors (2D) which differ from previously known 2D systems: graphene, 2DEG trapped in heterojunctions.

## Topologie: enroulement de Bloch 1D

• Nombre d'enroulement S1 vers S1:



Zone de Brillouin = cercle

Fonctions d'ondes parametrées par un seul angle

$$H(k) = d_1(k)\sigma_1 + d_2(k)\sigma_2$$

# Topologie: enroulement de Bloch 1D

• Enroulement trivial des états de Bloch





Enroulement non trivial







# Weyl equation (1929)

### Massless particle:

$$i \left(\partial_t - c\vec{\sigma} \cdot \partial_{\vec{r}}\right) \psi_L = 0$$
$$i \left(\partial_t + c\vec{\sigma} \cdot \partial_{\vec{r}}\right) \psi_R = 0$$



### Masse de Dirac:

4 nombres complexes

$$i \left(\partial_t - c\vec{\sigma} \cdot \partial_{\vec{r}}\right) \psi_L = m\psi_R$$
$$i \left(\partial_t + c\vec{\sigma} \cdot \partial_{\vec{r}}\right) \psi_R = m\psi_L$$

Masse de Majorana (1937): 2 nombres complexes (4 réels)

$$\psi_R = i\sigma_y \psi_L^*$$



Neutrinos massifs: Dirac ou Majoranas ?



### BHZ model on the square lattice

2 blocks

Spin-up block describes a Chern insulator

Edge states on finite lattices

It is the realization of a Z2 topological insulator

### BHZ model: topological properties

$$\mathcal{H}(k) = \sin k_x \sigma_1 + \sin k_y \sigma_2 + (M - 2B(2 - \cos k_x - \cos k_y))\sigma_3$$

Réseau carré avec 2 orbitales (s et p) sur chaque site (électrons sans spin)

Dirac points	(0,0)	$(\pi,0)$	$(0,\pi)$	$(\pi,\pi)$	Ch
mass	M	M - 4B	M - 4B	M - 8B	
chirality	+	—	_	+	
M < 0	_	+	+	_	0
$M \in (0, 4B)$	+	+	+	—	+
$M \in (4B, 8B)$	+	_	_	_	_
M > 8B	+	—	_	+	0

**Modèle:** B.A. Bernevig, T.L. Hughes, and S.C. Zhang, Science **314**, 1757 (2006) Doru Sticlet et al., Phys. Rev. B **85**, 165456 (2012)



Configuration "ferromagnétique"  $d_3({m k})$ 

### 0<M<4B



### Configuration skyrmionique $d_3(k)$

### 4B<M<8B



Autre configuration skyrmionique  $d_3(m{k})$ 

### 4B<M<8B



Autre configuration skyrmionique  $d_3(m{k})$ 





Configuration ferromagnétique  $d_3(\mathbf{k})$ 

## InAs/GaSb electron/hole bilayer

Transition can be driven by gating

 $\label{eq:h_0 = -t \sum_{\vec{R},\vec{\delta}_\alpha} c^\dagger_B(\vec{R}) c_A(\vec{R}+\vec{\delta}_\alpha) + H.c.$ 

 $\label{eq:h_0 = -t \sum_{\vec_k}, vec_{\delta}_alpha} e^{i \vec_k} . \vec_{\delta}_alpha} c^{\delta_k} + H.c.$ 

\, \, h\_0 (\vec{k})= - t \sum\_{\vec{k}, \vec{\delta}\_\alpha} \left( \cos( \vec{k} .
\vec{\delta}\_\alpha) \sigma\_1 + \sin( \vec{k} . \vec{\delta}\_\alpha) \sigma\_2 \right)

 $h_0 (\operatorname{k}) = 0 \operatorname{rightarrow} \operatorname{k} = \operatorname{m} \operatorname{k}$ 

\, \, \, h\_0 (\vec{k})= - t \sum\_{\vec{k}, \vec{\delta}\_\alpha} \left( {\color{red}
\cos( \vec{k} . \vec{\delta}\_\alpha) }\sigma\_1 + {\color{blue} \sin( \vec{k} . \vec{\delta}\_\
\alpha) } \sigma\_2 \right)

= - t  $\sum_{k} c^{k}$  c  $\lambda c_{k}$  [h\_{0}]\_{ alpha beta c\_beta( $vec_{k}$ )

- t= \int d^3r \, \phi^\*(\vec{r}-\vec{R}\_A-\vec{\delta}\_3) (V(\vec{r})-V\_{\rm ato}(\vec{r}- \vec{R}\_B)) \phi(\vec{r}-\vec{R}\_B)

h\_0 (\vec{k})= \sigma\_1 h\_0 (-\vec{k}) \sigma\_1 h\_0 (\vec{k})= h\_0^\* (-\vec{k})

 $E_F = hbar v_F \{color\{blue\} q_F\}$ 

{\color{red} d\_3(\vec{k}) =- d\_3(-\vec{k}) }

 $v_F = 3 at/2 hbar \simeq 10^6 {\rm m.s^{-1}}$ 

 $E(\{\color{red} \ xi \ } \vec{K} + \{\color{blue} \ vec{q} \ \} \,) = \hbar v_F \{\color{blue} \ sqrt{q_x^2+q_y^2}\}$ 

 $\operatorname{Vec}\{k\} = \operatorname{Vec}\{K\} + {\operatorname{Vec}} \operatorname{Vec}\{q\} \}$ 

\, \, \, h\_0 ({\color{red} \xi }\vec{K} + {\color{blue} \vec{q} } \,) \simeq \hbar v\_F
\left( {\color{red} \xi } {\color{blue} q\_x }\sigma\_1 + {\color{blue} q\_y } \sigma\_2 \right)

 $\operatorname{k} = {\operatorname{color}{red} \times i} \operatorname{vec}{K} + {\operatorname{color}{blue} \times c{q} }$ 

h\_0 (\vec{k})= h\_0^\* (-\vec{k})

{\color{blue}  $T^2 = -1$  }