17/09/19 Ecole de pointe du LIA

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Circuits et matériaux quantiques

Lectures on 2D materials

I Graphene

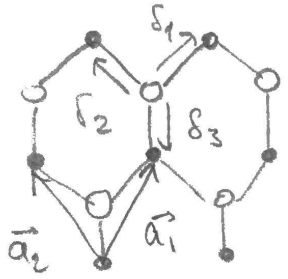
Outline

A| Band structure B| Wavefunctions

C| Symmetries and Wilson loop D| Edge states

A| Band structure

graphene = 2D plan of carbon atoms forming a honeycomb structure



○ A atoms
● B atoms

$$\vec{a}_1 = \frac{1}{2}\begin{pmatrix}\sqrt{3}\\ 3\end{pmatrix}$$

$$\vec{a}_2 = \frac{1}{2}\begin{pmatrix}-\sqrt{3}\\ 3\end{pmatrix}$$

$$\vec{\delta}_3 = (0,-1)$$

$$\vec{\delta}_{1/2} = \left(\pm\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$$

$\vec{a}_1$ and $\vec{a}_2$ generate the whole lattice - with $\vec{\delta}_3$ connecting A and B atoms

simplest tight-binding model (textbook)

$$H = -t \sum_{\langle i,j\rangle} c_i^\dagger c_j$$

nearest neighbor hopping

in Bloch space $c_{j A/B} = \frac{1}{\sqrt{N}} \sum_k e^{i \vec{k} \cdot \vec{R}_j} c_{k, A/B}$

$\vec{R}_j$ is the origin of a unit cell (same for A and B)

⚠ other choices are possible : gauge choice

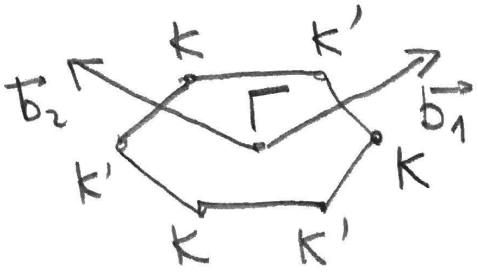
$\vec{R}_j = n \vec{a}_1 + m \vec{a}_2$

in A|B space $H_k = \begin{pmatrix} 0 & f^*(k) \\ f(k) & 0 \end{pmatrix}$ (AA, AB, BA, BB)

with $f(k) = -t \left\{ 1 + e^{i \vec{k} \cdot \vec{a}_1} + e^{i \vec{k} \cdot \vec{a}_2} \right\}$

→ with this gauge choice $f(k + b_{1/2}) = f(k)$

BZ:



$\vec{b}_1 = \frac{4\pi}{3}\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$

$\vec{b}_2 = \frac{4\pi}{3}\left(-\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$

reciproqual vectors $\vec{b}_j \cdot \vec{a}_\ell = 2\pi \delta_{j,\ell}$

Gapless point $f(\vec{k} = \vec{K}) = 0$ with $\vec{K} = \frac{\vec{b}_1 - \vec{b}_2}{3}$

$\left(\frac{4\pi}{3\sqrt{3}}, 0\right)$

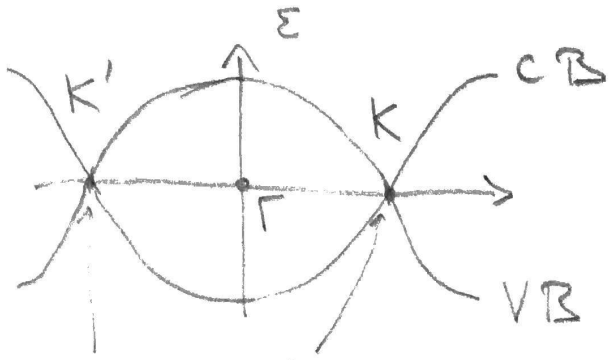
also $K' = K e^{i\pi/3}$, etc $f(K') = 0$

K, $K e^{2i\pi/3}$ and $K e^{4i\pi/3}$ are equivalent

(equal up to a reciproqual vector $\vec{b}_j$)

example: $K e^{2i\pi/3} = K + \vec{b}_2$

diagonalizat° of H_k: $\varepsilon_\pm(\vec{k}) = \pm |f(\vec{k})|$



$\varepsilon_F = 0$

(1 é per unit cell per spin direction)

semi-metal (gapless) : valence band is full up to the gap closing points K and K'

C : $1s^2\ 2s^2\ 2p^2 \rightarrow$ $1p_z$ orbital (π-band) described by n.n. tight-binding model

real model: gap closing points still at K, K' (protected by symmetries)

but no particle-hole symmetry

- linearizat° close to K : $k = K + q \quad q \ll K$

$$f(K+q) = -t\left\{1 + e^{i\vec{K}\cdot\vec{a}_1} + e^{i\vec{K}\cdot\vec{a}_2}\right\} \simeq -t\left\{1 + e^{i\vec{K}\vec{a}_1}(1+i\vec{q}\vec{a}_1) + e^{i\vec{K}\vec{a}_2}(1+i\vec{q}\vec{a}_2)\right\}$$

$$f(K+q) = \frac{3}{2} t a (q_x + i q_y)$$

$$H_{k=K+q} \simeq \frac{3}{2} t a \begin{pmatrix} 0 & q_x - i q_y \\ q_x + i q_y & 0 \end{pmatrix} = \hbar v_F (q_x \sigma_x + q_y \sigma_y) = \hbar v_F\, \vec{q}\cdot\vec{\sigma}$$

$\hbar v_F = \frac{3}{2} t a$ ← lattice spacing $\simeq 1.42$ Å

$v_F \simeq 10^6\ m.s^{-1}$

second Dirac point

$$H_{K'+q} \simeq \hbar v_F \left(-q_x \sigma_x + q_y \sigma_y\right)$$

$\longrightarrow$ 2 Dirac cones close to K and K'

B | Wavefunctions

for $f(k) \neq 0$ $\quad k \neq K$ and K'

$$f(k) = |f(k)| e^{i\theta(k)}$$

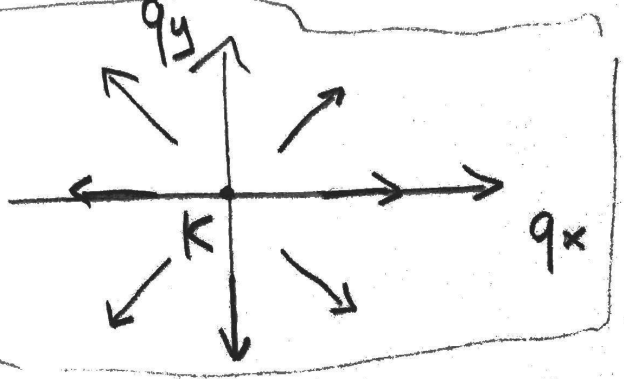
$$H = |f(k)| \underbrace{\begin{pmatrix} 0 & e^{-i\theta} \\ e^{i\theta} & 0 \end{pmatrix}}_{\cos\theta\, \sigma_x + \sin\theta\, \sigma_y}$$

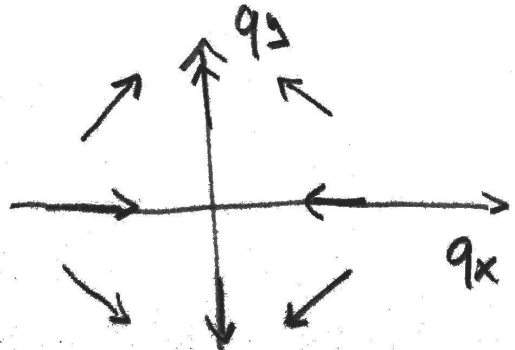
eigenstates are $\quad \psi_\pm = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm e^{i\theta} \end{pmatrix}$ $\quad +$ CB, $-$ VB

emulates a spinor (SU(2)) with direction θ_k on a 2D plan

We represent the direction of ψ_+ as funct° of k

vortex form close to K pt





anti-vortex next to K'

→ in both cases, topological winding k (or antiwinding k') of the phase θ_k with q moving around the K (K') point.

C| Symmetries and Wilson loop

among the symmetries of the model, there is:

1) time reversal symmetry T : $H^*(-k) = H(k)$
$(f^*(-k) = f(k))$

2) inversion symmetry $I = \sigma_x$ $\sigma_x H_{-k} \sigma_x = H_k$

T and I are robust symmetries of the lattice model of graphene - even when including next nearest couplings

Note 1: since $K' = -K$ both T and I send one valley to the other

Note 2: the model $H_k = \begin{pmatrix} 0 & f^*(k) \\ f(k) & 0 \end{pmatrix}$ has a chiral symmetry $\{\sigma_z, H_k\} = 0 \rightarrow \varepsilon_+(k) = -\varepsilon_-(k)$. This symmetry is broken for real graphene.

Including next nearest couplings gives $\left[-t' \sum_{\langle\langle i,j \rangle\rangle} c_i^+ c_j\right]$

$$H_k = \begin{pmatrix} \varepsilon_2(k) & f^*(k) \\ f(k) & \varepsilon_2(k) \end{pmatrix}$$

with $\varepsilon_2(K) = 0$
$\varepsilon_2(K') = 0$

$\rightarrow \{\sigma_z, H_k\} \neq 0$

$\varepsilon_2(-k) = \varepsilon_2(k)$

but <u>I and T still apply!</u>

The product $P = IT$ is local in momentum space $\sigma_x H_k \sigma_x = H_k^*$ - also conserves the valley index.

Wilson loop

discretizat° of a path in the BZ

$$W_{k_0,k_f} = \langle \psi^-_{k_f} | \psi^-_{k_{N-1}} \rangle \langle \psi^-_{k_{N-1}} | \psi^-_{k_{N-2}} \rangle \dots \langle \psi^-_{k_1} | \psi^-_{k_0} \rangle$$

and take the continuum limit $\delta k = k_{j+1} - k_j \to 0$, $N \to \infty$

$$W_{k_0,k_f} = e^{i \int_{k_0}^{k_f} d\vec{k} \cdot \vec{A}(\vec{k})}$$

$\vec{A}$ is the Berry connection

↳ Berry phase

$$\vec{A}(\vec{k}) = \frac{1}{i} \begin{pmatrix} \langle \psi^-_k | \partial_{k_x} | \psi^-_k \rangle \\ \langle \psi^-_k | \partial_{k_y} | \psi^-_k \rangle \end{pmatrix}$$

- instead of only ψ^-, this definition can be extended to a set of band → W becomes then a matrix

(see PRB 89, 155114 (2014)
PRB 96, 245115 (2017))

1 for a closed loop k_0, k_f, W is gauge invariant - in the sense that $\psi^-_{k_j} \to e^{i\varphi_j} \psi^-_{k_j}$ leaves it invariant

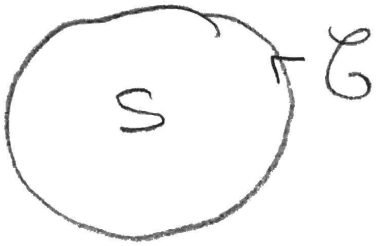
2 the Berry connect° $\vec{A}(\vec{k})$ plays a role similar to a potential vector with the associated B-field

$$\Omega = (\vec{\nabla} \times \vec{A})_z = \partial_{k_x} A_{y,} - \partial_{k_y} A_{x} \quad | \Omega \text{ real}$$

$$\boxed{\Omega = \frac{1}{i}\left(\langle \partial_x \psi^- | \partial_y \psi^- \rangle - \langle \partial_y \psi^- | \partial_x \psi^- \rangle \right)}$$

$\vec{A}$ is not gauge invariant but Ω is

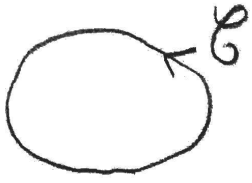
3 Stoke's theorem



Berry phase

$$\oint_C d\vec{k}.\vec{A}(\vec{k}) = \int_S dS\, \Omega_k$$

$P = IT$ symmetry $\quad \psi^{-*} = \sigma_x \psi^-$



$$W_C^* = \langle \psi^-_{k_0} | \underbrace{\sigma_x \sigma_x}_{=\mathbb{1}} | \overbrace{\psi^*_{k_{N-1}}}^{\psi_{k_{N-1}}} \rangle \cdots \langle \psi^-_{k_1} | \sigma_x \sigma_x | \psi^-_{k_0} \rangle$$

$$= W_C \qquad W_C \text{ is real} = \pm 1$$

$$\int_C d\vec{k}.\vec{A}(\vec{k}) = n\pi$$

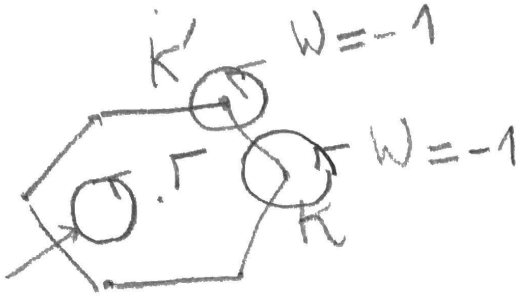
Berry phase has to be a multiple of π

In general $T : \Omega_k = -\Omega_{-k}$

$I : \Omega_k = \Omega_{-k}$

With $P = IT$ $\Omega_k = 0$ (except at K and K')

so $\int dS\, \Omega_k$ is quantified to $n\pi$



reminder

$$\psi_- = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -e^{i\theta} \end{pmatrix}$$

$$\frac{1}{i}\langle \psi_- | \partial_{k_x} | \psi_- \rangle = \frac{1}{2}\partial_{k_x}\theta_k$$

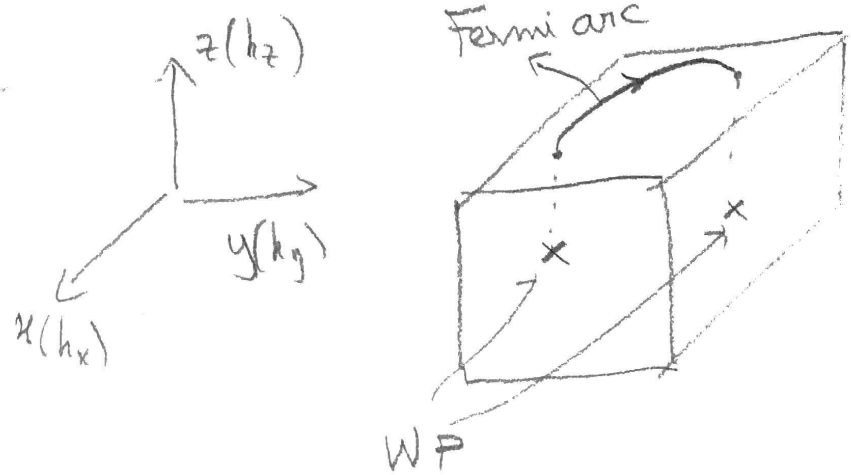
hence $\int \vec{A}\, d\vec{k} = \frac{1}{2}(\theta_{kf} - \theta_{ko})$

the Berry phase measure the winding of the pseudospin direction

$\Rightarrow$ <u>Topological protection</u> changing parameters of the model - without breaking $P = IT$ - cannot change $W = -1$ - $\int \vec{A}.d\vec{k} = \pi$ - around K and K' : protects the two Dirac points.

D| Edge states (of graphene)

Weyl semi-metals exhibit Fermi arcs on their surface



on the surface k_x and k_y are still good quantum numbers ⟶ line of zero-energy points connecting the projected WP on the $z=ct$ plane.

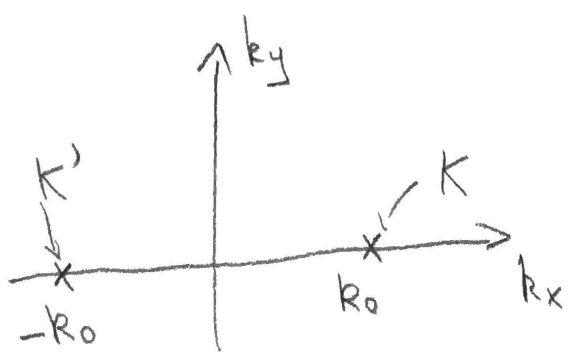
Same origin for the edge states of graphene.

Toy model in 2D

$$H_{k_x,k_y} = \frac{k_x^2 - k_0^2}{2k_0}\sigma_x + k_y\sigma_y$$

⟶ 2 DP with opposite chiralities

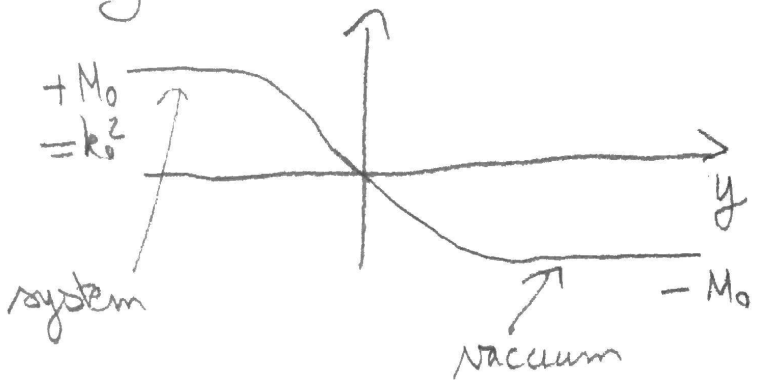
$$H(\pm k_0\vec{u_x} + \vec{q}) \simeq \pm q_x\sigma_x + q_y\sigma_y$$



I and T symmetries apply

• surface along x is modelled as

$k_0^2 \to M(y)$



we look for zero modes $H\psi = 0$ with $\psi_x e^{ik_x x}$

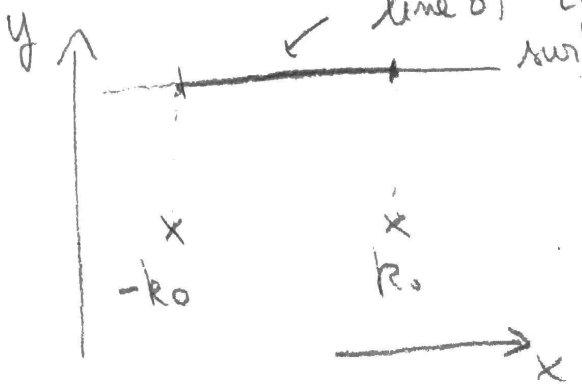
$$\left[\frac{k_x^2 - M(y)}{2k_0}\, \sigma_x \underbrace{-i\partial_y}_{p_y}\, \sigma_y \right] \psi_{k_x}(y) = 0$$

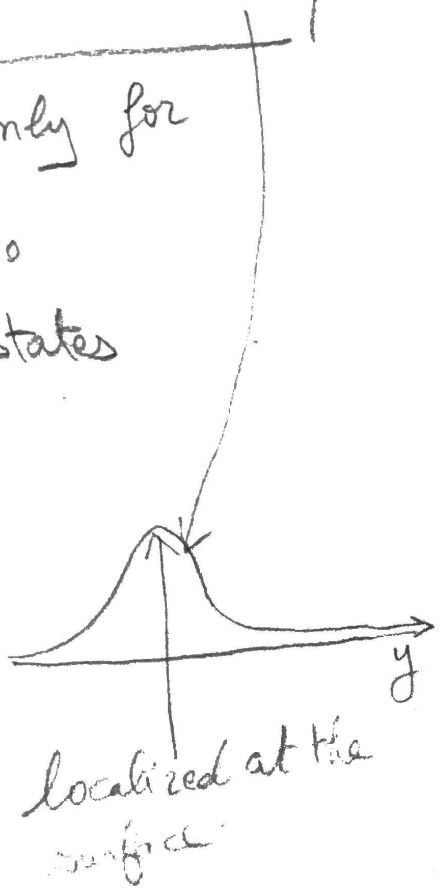
$$\to \left[\frac{k_x^2 - M(y)}{2k_0} + \sigma_z \partial_y \right] \psi_{k_x}(y) = 0$$

$$\boxed{\psi(y) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \exp\left[\int^y dy' \left(M(y') - k_x^2 \right) \right]}$$

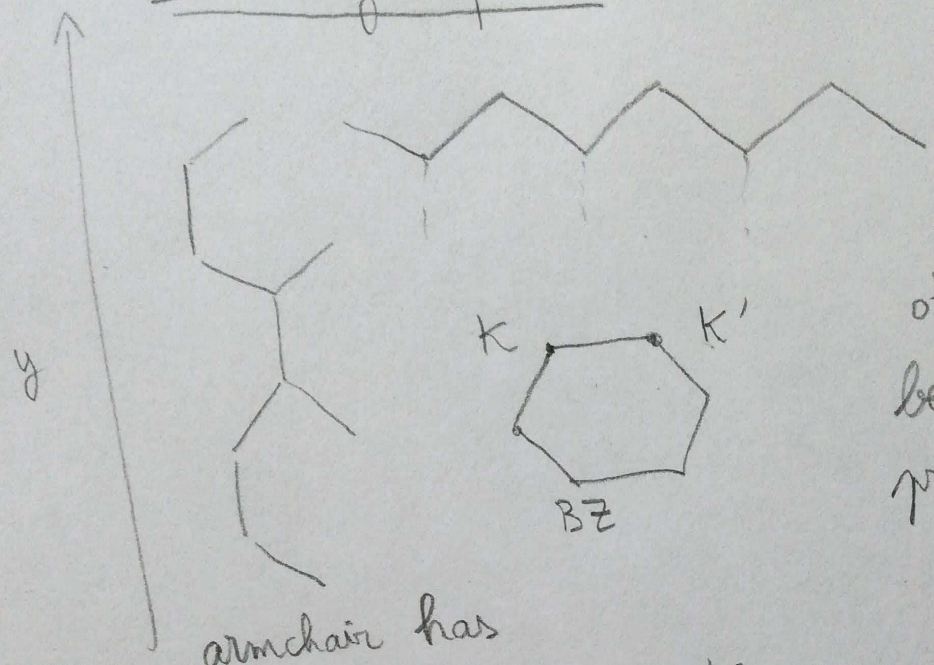
solut° is normalizable (exists) only for

$k_x^2 < M_0$ or $-k_0 < k_x < k_0$





In graphene



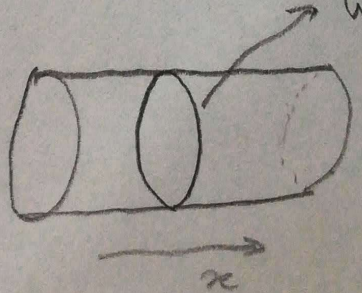
zig-zag edge exhibits a line of zero-energy states between K and K' projected

armchair has no edge states since K and K' project to the same point along y

x

$\Longrightarrow$ Any edge inbetween zig-zag and armchair has a line of zero-energy states (edge) connecting the projections of K and K'.

Wilson loop



W jumps from +1 to -1 each time a K(K') point is crossed : gives the $\mathbb{Z}_2$ invariant protecting the zero-energy edge states.

(similar to edge state of SSH)