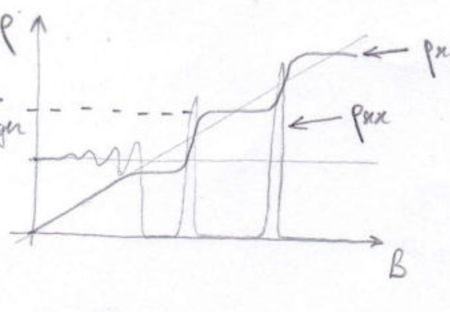
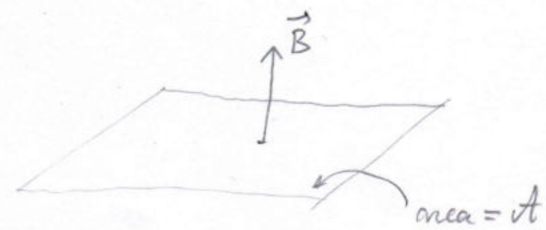
III. Time-reversal breaking topological insulators: QHE and the Haldane model

1) Definition of a T.I. from the example of the QHE

- 2D electron gas (metallic plane) in a strong $\perp$ $\vec{B}$ field and at low temperature





von Klitzing 1980

For certain filling factors (either tuned by B or by a backgate), there is a plateau in the Hall effect at a quantized value $\left(\frac{h}{e^2} \times \frac{1}{\text{integer}}\right)$ and a vanishing longitudinal resistance ($\rho_{xx} = 0$). The last feature indicates dissipationless transport.

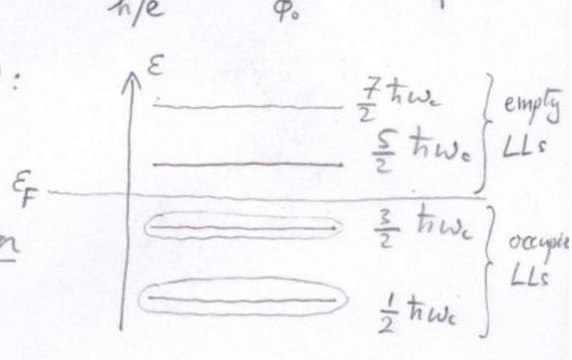
- Explanation:
  - Landau levels in the bulk of the system (quantized cyclotron orbits)

$$\mathcal{E}_n = \left(n + \frac{1}{2}\right) \underbrace{\hbar \frac{eB}{m}}_{\equiv \hbar\omega_c}, \; n \in \mathbb{N} \qquad \deg(\mathcal{E}_n) = \frac{B \times \mathcal{A}}{h/e} = \frac{\phi_{tot}}{\phi_0} = N_\phi$$

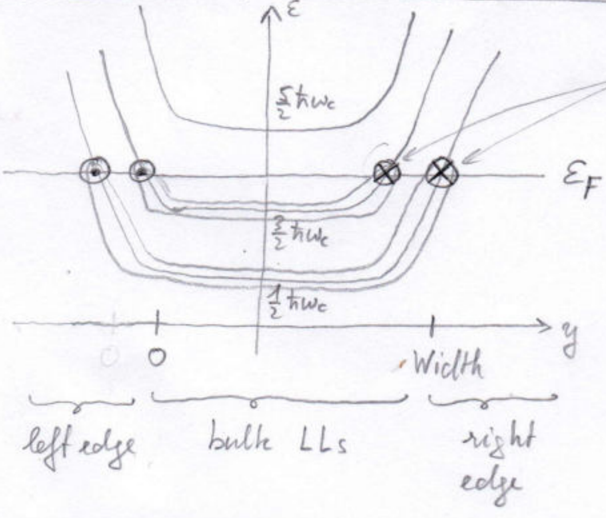
  - filling of the Landau levels (Pauli principle):

$$\nu \equiv \frac{N_{el}}{N_\phi} = \frac{n_{el}}{eB/h} = n_{el} \times 2\pi \ell_B^2$$

if ν is an integer $\Leftrightarrow$ bulk band insulator



  - chiral edge modes, immune to backscattering (i.e. robust to disorder)



two chiral 1D edge modes (quantized skipping orbits)

Halperin 1982

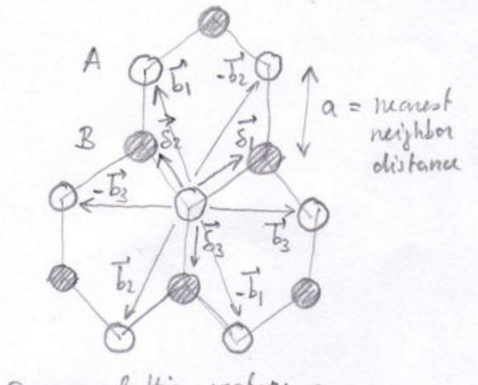
Bulk-edge correspondance:

number of filled LLs in the bulk = number of chiral edge modes (per edge)

2) The Haldane model : QHE without LLs

Haldane (1988) understood, after TKNN 1982, that the QHE can be seen as a band effect and does not require Landau levels. It requires a band insulator with a non-zero Chern number, which is only possible if TRS is broken (but breaking of translational symmetry is not required).

The Haldane model is a modified honeycomb tight-binding model, close to that of graphene.



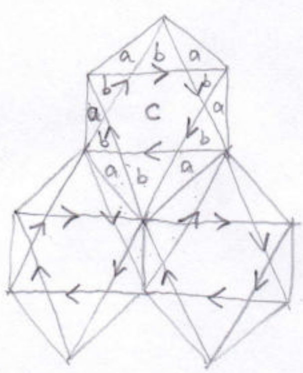
Bravais lattice vectors are $\vec{a}_1 \equiv -\vec{b}_2$ and $\vec{a}_2 \equiv \vec{b}_1$

Spinless electron hopping on a honeycomb lattice:

- triangular Bravais lattice (lattice spacing $= a\sqrt{3}$)
- unit cell with two inequivalent sites A and B
- 3 nearest neighbors: $\vec{\delta}_1, \vec{\delta}_2, \vec{\delta}_3$
- 6 next-nearest neighbors: $\vec{b}_1, \vec{b}_2, \vec{b}_3, -\vec{b}_1, -\vec{b}_2, -\vec{b}_3$
- hopping amplitudes: $\begin{cases} t_1 \in \mathbb{R} \\ \underset{\uparrow\atop >0}{t_2} \underbrace{e^{\pm i\varphi}} \in \mathbb{C} \end{cases}$

  >0 phase factors that break time-reversal symmetry

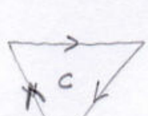
- staggered on-site potential energy: $\begin{cases} +M & \text{on } A \\ -M & \text{on } B \end{cases}$



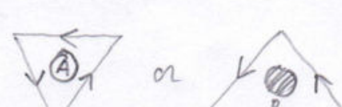
total flux around a hexagonal unit cell $= 0$ (because $t_1 \in \mathbb{R}$)

$j \to k$ means $t_2 e^{i\varphi}$ if hopping from j to k and $t_2 e^{-i\varphi}$ if hopping from k to j

phase when hopping with t_2:



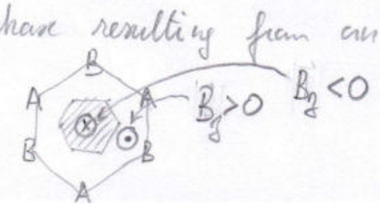
$\varphi_{\triangledown} = -3\varphi$ (triangle enclosing the center of the hexagon)



$\varphi_{\triangledown} = \varphi_{\triangle} = 3\varphi$

(triangles enclosing a site)

AB phase resulting from an inhomogeneous magnetic flux:

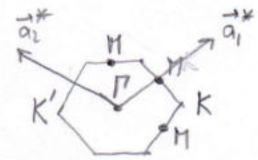


This breaks TRS.

The Bloch Hamiltonian is 2×2 in (A,B) subspace and reads:

$$H(\vec{k}) = \begin{pmatrix} AA & AB \\ BA & BB \end{pmatrix}$$

where $\vec{k}$ is in the BZ



BA: hopping from A to B

$$t_1 \sum_{j=1}^{3} e^{i\vec{k}\cdot\vec{\delta}_j} \equiv f(\vec{k})$$

AB: $f(\vec{k})^*$

$$AA: \quad \underset{\substack{\uparrow \\ \text{on-site energy} \\ \text{(no hopping)}}}{M} + \underbrace{t_2 \left\{ e^{i\vec{k}\cdot\vec{b}_1} e^{i\varphi} + e^{-i\vec{k}\cdot\vec{b}_3} e^{-i\varphi} + e^{i\vec{k}\cdot\vec{b}_2} e^{i\varphi} + e^{-i\vec{k}\cdot\vec{b}_1} e^{-i\varphi} + e^{i\vec{k}\cdot\vec{b}_3} e^{i\varphi} + e^{-i\vec{k}\cdot\vec{b}_2} e^{-i\varphi} \right\}}_{\text{hopping from A to A via } t_2} = M + t_2 \sum_{j=1}^{3} 2\cos(\vec{k}\cdot\vec{b}_j + \varphi)$$

$$BB: \; -M + t_2 \sum_{j=1}^{3} 2\cos(\vec{k}\cdot\vec{b}_j - \varphi) = -M + 2t_2 \left\{ \cos\varphi \sum_j \cos(\vec{k}\cdot\vec{b}_j) - \sin\varphi \sum_j \sin(\vec{k}\cdot\vec{b}_j) \right\}$$

In the end: $H(\vec{k}) = 2t_2\cos\varphi \sum_{j=1}^{3} \cos(\vec{k}\cdot\vec{b}_j)\cdot\sigma_0$ } This breaks particle-hole symmetry (as in graphene with NNN) but does not change the geometrical/topological properties

This is like graphene producing two Dirac cones at K and K' (gapless Dirac fermions)

$$\left\{ \begin{aligned} &+ t_1 \sum_{j=1}^{3} \cos(\vec{k}\cdot\vec{\delta}_j)\cdot\sigma_x \\ &+ t_1 \sum_{j=1}^{3} \sin(\vec{k}\cdot\vec{\delta}_j)\cdot\sigma_y \end{aligned} \right.$$

$$+ \left\{ M - 2t_2 \sin\varphi \sum_{j=1}^{3} \sin(\vec{k}\cdot\vec{b}_j) \right\}\cdot\sigma_z$$

$$= h_0(\vec{k})\sigma_0 + \vec{h}(\vec{k})\cdot\vec{\sigma} = h_0(\vec{k})\sigma_0 + |\vec{h}(\vec{k})|\, \vec{n}(\vec{k})\cdot\vec{\sigma}$$

This term gaps the Dirac cones. The Dirac fermions at K/K' become massive.

M breaks inversion symmetry (as in boron nitride, Semenoff 1984) : $H(\vec{k}) \xrightarrow{\;I\;} \sigma_x H(-\vec{k})\sigma_x \neq H(\vec{k})$

as $\sigma_x M\sigma_z \sigma_x = -M\sigma_z \neq M\sigma_z$

$t_2\sin\varphi$ breaks time-reversal : $H(\vec{k}) \xrightarrow{\;T\;} H(-\vec{k})^* \neq H(\vec{k})$

as $\left[-2t_2\sin\varphi \sum_j \sin(-\vec{k}\cdot\vec{b}_j)\sigma_z\right]^*$

$= 2t_2\sin\varphi \sum_j \sin(\vec{k}\cdot\vec{b}_j)\sigma_z \neq -2t_2\sin\varphi \sum_j \sin(\,)\sigma_z$

All the other terms (in $\sigma_0, \sigma_x, \sigma_y$) respect both I and T.

3) Low-energy effective description: massive Dirac fermions in 2D

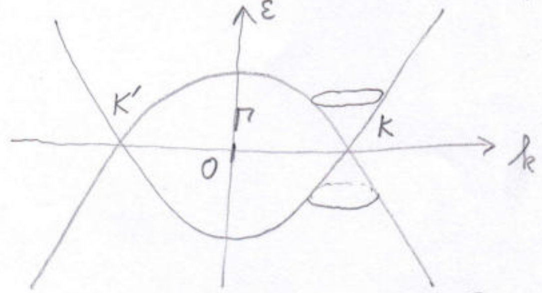
- The energy spectrum is $\mathcal{E}_\pm(\vec{k}) = h_0(\vec{k}) \pm |\vec{h}(\vec{k})|$ → breaks "$\mathcal{E} \to -\mathcal{E}$" symmetry but otherwise unimportant

[notice that $\vec{n}(\vec{k})$ does not appear here. It encodes the geometrical / topological properties.]

The two bands touch at $\pm\vec{K}$ when $M = 0$ and $t_2 = 0$ (graphene):

$$h_x(\pm\vec{K}) = h_y(\pm\vec{K}) = 0 \quad \text{i.e.} \quad f(\pm\vec{K}) = 0$$

$$f(\pm\vec{K}+\vec{q}) \simeq \hbar v\,(\pm q_x + i q_y) \qquad \text{where } \hbar v \equiv \frac{3}{2} t_1 a$$



$$\mathcal{E}_\pm(\pm\vec{K}+\vec{q}) = \pm\,\hbar v\,|\vec{q}|$$

(ultra-relativistic-like)

valley index, band index

two Dirac cones

Pauli matrices (pseudo-spin 1/2 due to sublattices A/B)

$$H(\pm\vec{K}+\vec{q}) \simeq \hbar v\,(\pm q_x \sigma_x + q_y \sigma_y)$$

Dirac Hamiltonian
in 2D → 2x2 matrices
(in 3D → 4x4 matrices)
massless: no σ_z term (Weyl)
two copies: two valleys.

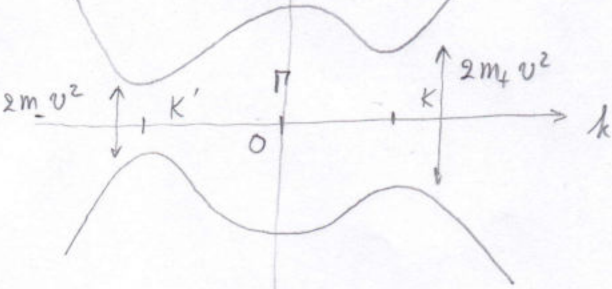
> remark: Dirac Hamiltonian 1928
> $H_D = c\,\vec{\alpha}\cdot\vec{p} + mc^2\beta$
> matrices $\alpha_1, \dots, \alpha_d$ and $\alpha_0 \equiv \beta$ satisfy the Clifford algebra: $\{\alpha_\mu, \alpha_\nu\} = 2\delta_{\mu\nu}$, $\mu = 0, 1, \dots, d$
> here $\alpha_x = \sigma_x$, $\alpha_y = \sigma_y$ and $\beta = \sigma_z$

If M and $t_2 \neq 0$: $h_z(\pm\vec{K}) = M - 2t_2 \sin\varphi \sum_{j=1}^{3} \sin(\pm\vec{K}\cdot\vec{b}_j) = M \pm 3\sqrt{3}\, t_2 \sin\varphi$

let $m_\pm v^2 \equiv M \pm 3\sqrt{3}\, t_2 \sin\varphi$

$$H(\pm\vec{K}+\vec{q}) \simeq \hbar v\,(\pm q_x\sigma_x + q_y\sigma_y) + m_\pm v^2 \sigma_z$$

massive Dirac Hamiltonian with 2 ≠ masses for the 2 copies



$$\mathcal{E}_\pm(\pm\vec{K}+\vec{q}) \simeq \pm\sqrt{\hbar^2 v^2 \vec{q}^{\,2} + m_\pm^2 v^4}$$

(relativistic-like)

M produces the same mass for the 2 Dirac fermions.

$t_2 \sin\varphi$ —— opposite masses ——

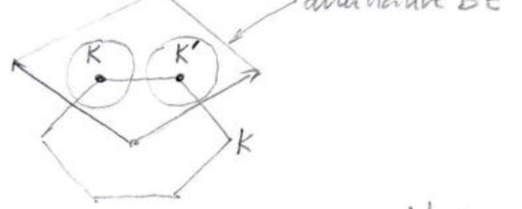
Is there something interesting contained in $\vec{n}(\vec{k}) \equiv \dfrac{\vec{h}(\vec{k})}{|\vec{h}(\vec{k})|}$?

In order to study the geometrical / topological properties of the Bloch bundle (that for the valence band, as we assume that $\varepsilon_F = 0$ such that ε_- is filled and ε_+ empty), we need to study $H(\vec{k})$ in the whole BZ. However, we know that the Berry curvature is large when the gap is small and small when the gap is large. We will assume that the gap $2 m_\pm v^2 \to 0$ and restrict to the vicinity of the two Dirac points:

$$H_\xi(\vec{q}) = \xi q_x \sigma_x + q_y \sigma_y + m_\xi \sigma_z$$

with $\hbar$ and $v \equiv 1$ and $\xi = \pm 1$ the valley index

$m_\xi = M + \xi 3\sqrt{3}\, t_2 \sin\varphi$



$$H_\xi(\vec{q}) = \varepsilon_+ \begin{pmatrix} \cos\theta & \sin\theta\, e^{-i\phi} \\ \sin\theta\, e^{i\phi} & -\cos\theta \end{pmatrix}$$

with $\varepsilon_\pm = \pm\sqrt{\vec{q}^2 + m_\xi^2}$

$\cos\theta = \dfrac{m_\xi}{\varepsilon_+} \qquad \sin\theta = \dfrac{|\vec{q}|}{\varepsilon_+}$

$e^{i\phi} = \dfrac{\xi q_x + i q_y}{|\vec{q}|}$ contains a vortex at $\xi = +$ and an antivortex at $\xi = -$

$$|u_+\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i\phi} \end{pmatrix} \qquad |u_-\rangle = \begin{pmatrix} -\sin\frac{\theta}{2} e^{-i\phi} \\ \cos\frac{\theta}{2} \end{pmatrix}$$

problem at the south pole of the Bloch sphere i.e. $\theta = \pi$

$$\vec{A}_\pm = \langle u_\pm | i \vec{\nabla}_q u_\pm \rangle = \mp \sin^2\frac{\theta}{2} \vec{\nabla}_q \phi = \mp \frac{1 - \cos\theta}{2} \vec{\nabla}_q \phi$$

$$\vec{\Omega}_\pm = \vec{\nabla}_q \times \vec{A}_\pm = \pm \frac{1}{2} \vec{\nabla}\cos\theta \times \vec{\nabla}\phi$$

but $\phi = \mathrm{Arctg}\left(\xi \dfrac{q_y}{q_x}\right) \rightarrow \vec{\nabla}\phi = \dfrac{\xi}{\vec{q}^2} \begin{vmatrix} -q_y \\ q_x \\ 0 \end{vmatrix}$

$\cos\theta = \dfrac{m_\xi}{\sqrt{\vec{q}^2 + m_\xi^2}} \rightarrow \vec{\nabla}\cos\theta = -\dfrac{m_\xi}{\varepsilon_+^3} \begin{vmatrix} q_x \\ q_y \\ 0 \end{vmatrix}$

$$\vec{\Omega}_\pm = \mp \frac{1}{2} \xi \frac{m_\xi}{\varepsilon_+^3} \vec{u}_z$$

Indeed the Berry curvature is concentrated where $\varepsilon_+(\vec{q})$ is small.

The Chern number for the valence band is:

$$C_- = \sum_\xi \int \frac{d^2 q}{2\pi} \Omega_- = \sum_\xi \frac{1}{2\pi} \times \frac{1}{2} \xi m_\xi \int d^2 q \frac{1}{\sqrt{\vec{q}^2 + m_\xi^2}^{\,3}}$$

$$\int d^2 q \rightarrow 2\pi \int_0^\infty dq\, q$$

but $\displaystyle\int_0^\infty dq \frac{q}{\sqrt{q^2 + m_\xi^2}^{\,3}} = \left[-\frac{1}{\sqrt{q^2 + m_\xi^2}} \right]_0^\infty = \frac{1}{|m_\xi|}$

$$\Rightarrow \boxed{C_\mp = \pm \sum_\xi \frac{1}{2} \xi\, \mathrm{sgn}(m_\xi)}$$

Remark: parity anomaly of Jackiw 1984 for a single massive Dirac fermion in 2D

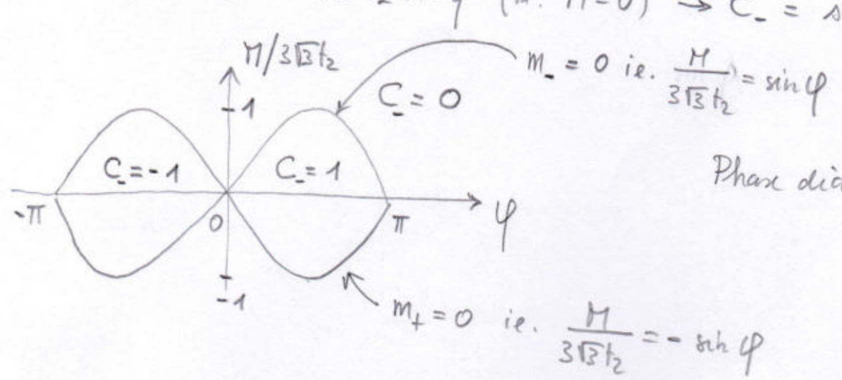
$$\sigma_{xy} = \frac{e^2}{h} \frac{1}{2} W_D\, \mathrm{sgn}(m_D)$$

We recover a well-known formula that a Dirac point contributes $\frac{1}{2} W_D \, \mathrm{sgn}(m_D)$ to the Chern number (ie. $\pm \frac{1}{2}$) depending on its chirality (winding number $W_D = \pm 1$, here $W_D = \xi$) and on the sign of its mass m_D. This is also related to fermion doubling as Chern $\in \mathbb{Z}$ $\Rightarrow$ even number of Dirac points.

Here $\boxed{C_- = -\frac{1}{2}\left[\mathrm{sgn}(m_+) - \mathrm{sgn}(m_-)\right]}$

Therefore if $m_+ = m_- = M$ (ie. $t_2 \sin\varphi = 0$) $\rightarrow$ $C_- = 0$ trivial band insulator

if $m_+ = -m_- = 3\sqrt{3}\, t_2 \sin\varphi$ (ie. $M = 0$) $\rightarrow$ $C_- = \mathrm{sgn}(m_+) = \pm 1$ Chern insulator



Phase diagram

Remark: on the boundaries where $m_\pm = 0$, there is a single massless Dirac cone and the C_- is ill-defined. At the phase transition the gap closes and C_- changes by 1. The mechanism is that there is a change in the mass sign of a single Dirac cone.

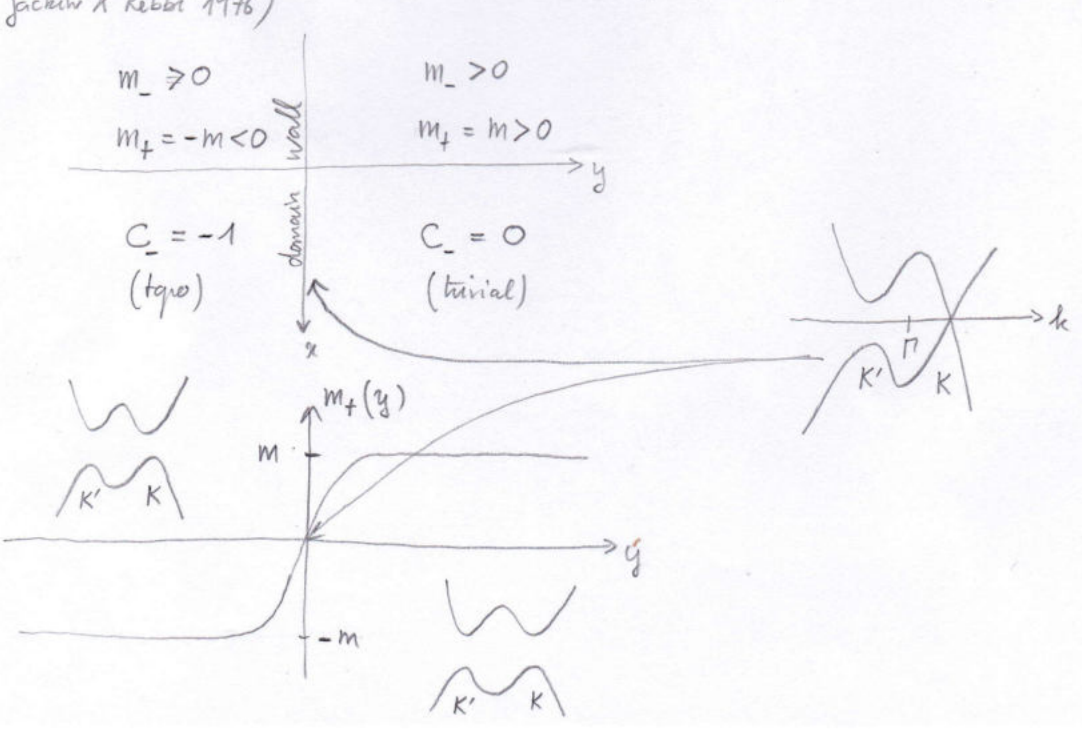
And according to TKNN: $\sigma_{xy} = \frac{e^2}{h} \sum_{\substack{\text{filled} \\ \text{bands}}} C = \frac{e^2}{h} C_-$

ie. QHE

What about edge modes?

4) Jackiw - Rebbi argument and the bulk-edge correspondance

A domain wall in the mass of a Dirac fermion produces a zero mode (a mid-gap state). (Jackiw & Rebbi 1976)



On the domain wall, the gap at K closes as $m_+(y=0) = 0$

$$H_+(\vec{q}) = q_x\sigma_x + q_y\sigma_y + m_+(y)\,\sigma_z = \hat{p}_x\sigma_x + \hat{p}_y\sigma_y + m_+(\hat{y})\,\sigma_z$$

Because $[\hat{H}_+, \hat{p}_x] = 0 \Rightarrow \psi(x,y) = e^{iq_x x}\phi(y)$

$H_+|\psi\rangle = \varepsilon|\psi\rangle$ and we search an eigenstate with $\varepsilon \approx 0$ ie. mid-gap state

$$\Rightarrow -i\sigma_x\, iq_x\,\phi(y) - i\sigma_y\,\phi'(y) + m_+(y)\,\sigma_z\,\phi(y) = \varepsilon\,\phi(y)$$

ansatz: $\phi(y) = f(y)\begin{pmatrix}1\\ \pm1\end{pmatrix}$ because $\sigma_x\begin{pmatrix}1\\ \pm1\end{pmatrix} = \pm\begin{pmatrix}1\\ \pm1\end{pmatrix}$ and $\hat{\vec{v}} = \dot{\hat{\vec{r}}} = \frac{1}{i}[\hat{\vec{r}}, \hat{H}] = \begin{vmatrix}\sigma_x\\ \sigma_y\end{vmatrix}$

also $\sigma_y\begin{pmatrix}1\\ \pm1\end{pmatrix} = \mp i\begin{pmatrix}1\\ \mp1\end{pmatrix}$ and $\sigma_z\begin{pmatrix}1\\ \pm1\end{pmatrix} = \begin{pmatrix}1\\ \mp1\end{pmatrix}$

$$\Rightarrow \pm q_x f(y)\begin{pmatrix}1\\ \pm1\end{pmatrix} - i\times\mp i\, f'(y)\begin{pmatrix}1\\ \mp1\end{pmatrix} + m_+(y)f(y)\begin{pmatrix}1\\ \mp1\end{pmatrix} = \varepsilon f(y)\begin{pmatrix}1\\ \pm1\end{pmatrix}$$

but $\begin{pmatrix}1\\ \pm1\end{pmatrix}$ and $\begin{pmatrix}1\\ \mp1\end{pmatrix}$ are $\perp$ $\Rightarrow \begin{cases}\pm q_x f(y) = \varepsilon f(y)\\ \mp f'(y) + m_+(y) f(y) = 0\end{cases}$

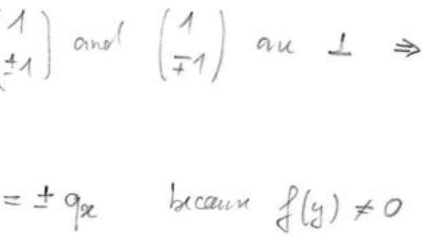
$\Rightarrow \varepsilon = \pm q_x$ because $f(y) \neq 0$

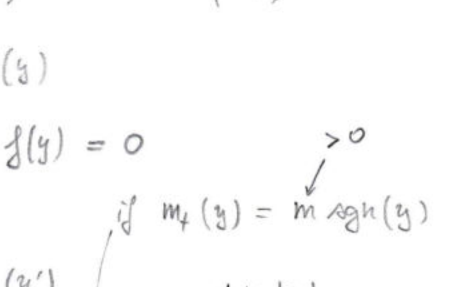
$\frac{df}{f} = \pm m_+(y)\,dy$ ie. $f(y) = f(0)\,e^{\pm\int_0^y dy'\, m_+(y')} = f(0)\,e^{\pm m|y|}$ if $m_+(y) = \underset{>0}{m}\,\mathrm{sgn}(y)$

normalisable iff $f(y) = f(0)\,e^{-m|y|}$, exp. localized near the interface on a distance $\frac{\hbar v}{mv^2} = \frac{\hbar}{mv}$

and $\varepsilon = -q_x$: chiral mode! $\quad \frac{d\varepsilon}{dq_x} = -1 < 0$

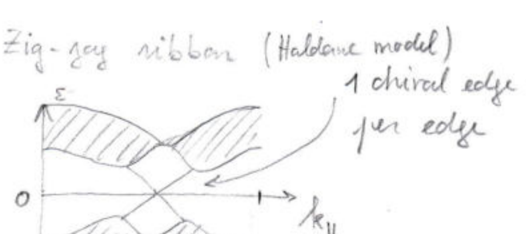
$$\psi(x,y) \sim e^{iq_x x}\, e^{-m|y|}\begin{pmatrix}1\\ 1\end{pmatrix}$$



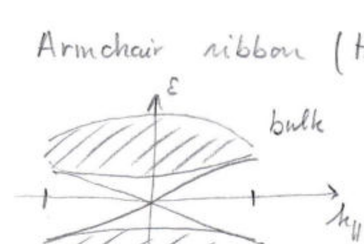


The chirality of the mode is due to the Dirac cone being chiral (related to its winding W_D and to the sign of its mass) : $\sigma_{xy}^D = \frac{e^2}{h}\frac{1}{2}W_D\,\mathrm{sgn}(m_D)$. Parity anomaly (Jackiw 1984).

Zig-zag ribbon (Haldane model)



Armchair ribbon (Haldane model)



Conclusion:

- Quantum Hall effect was thought to be due to the applied magnetic field to be due to the filling of Landau levels

- TKNN understood that there was a topological invariant explaining the robustness

- Haldane understood that it is a band insulator with a non-zero Chern number (and this requires TRS to be broken, for example with an inhomogeneous magnetic field). Chern $\in \mathbb{Z}$.
- Niu, Thouless and Wu 1985 further showed how the Chern number could be defined even in the absence of bands (ie presence of disorder) and for interacting electrons.

Next time we will see how to have a topological insulator that respects TRS.