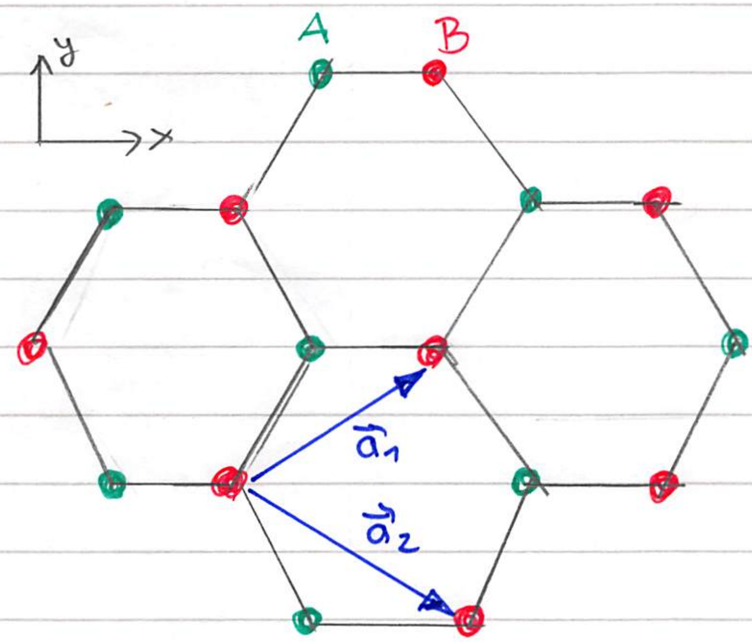
5. Graphene and Haldane model

An important and interesting class of Chern insulators is based on lattice models on a hexagonal lattice

5.1. Graphene and Dirac fermions

(A) lattice structure and tight-binding hamiltonian



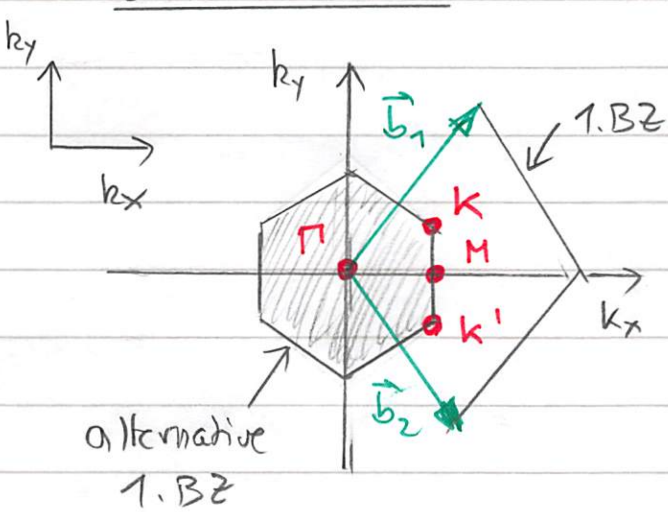
unit cell has two lattice points (A, B)

lattice vectors

$$\vec{a}_1 = \frac{a}{2}\left(3, \sqrt{3}\right) \qquad (214)$$

$$\vec{a}_2 = \frac{a}{2}\left(3, -\sqrt{3}\right)$$

Brillouin zone:



reciprocal lattice vectors:

$$\vec{b}_1 = \frac{2\pi}{3a}\left(1, \sqrt{3}\right) \qquad (215)$$

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

see e.g. Rev. Mod. Phys. 81, 109 (2009)

alternative Brillouin zone : hexagon with edges

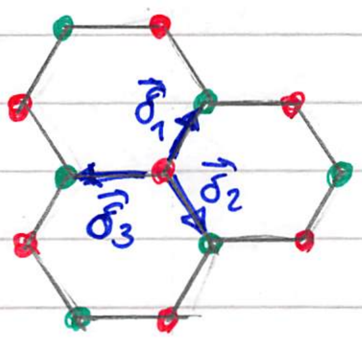
$$\vec{K} \hat{=} \frac{2\pi}{3a}\left(1, \frac{1}{\sqrt{3}}\right) \qquad \vec{K}' = \frac{2\pi}{3a}\left(1, -\frac{1}{\sqrt{3}}\right) \tag{216}$$

$\vec{K}$ and $\vec{K}'$ are TR partners since

$$\vec{K} \xrightarrow{T} -\vec{K} = \vec{K}' - (\vec{b}_1 + \vec{b}_2)$$

The simplest tight-binding hamiltonian on the hexagonal lattice reads

$$H = \sum_{\vec{k}} \begin{pmatrix} \tilde{C}_A^+(\vec{k}) \\ \tilde{C}_B^+(\vec{k}) \end{pmatrix}^T \begin{pmatrix} 0 & \sum_{j=1}^{3} t_j e^{i\vec{k}_j \vec{\sigma}_j} \\ \sum_{j=1}^{3} t_j e^{-i\vec{k}_j \vec{\sigma}_j} & 0 \end{pmatrix} \begin{pmatrix} \tilde{C}_A(\vec{k}) \\ \tilde{C}_B(\vec{k}) \end{pmatrix} \tag{217}$$



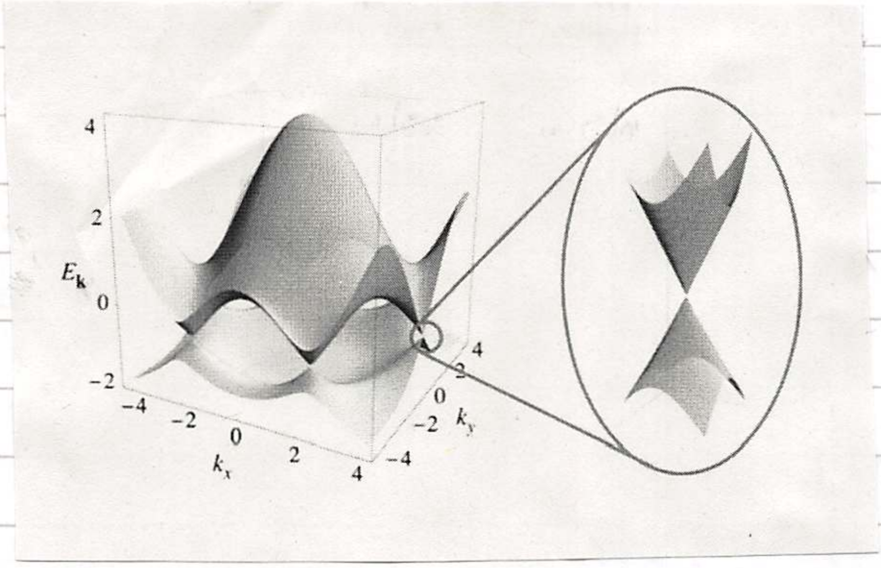
with a gauge trafo

$$\tilde{C}_B(\vec{k}) \rightarrow \tilde{C}_B(\vec{k}) e^{i\vec{k}\cdot\vec{\sigma}_3}$$

One obtains

$$\boxed{H = \sum_{\vec{k}} \begin{pmatrix} \tilde{C}_A(\vec{k}) \\ \tilde{C}_B(\vec{k}) \end{pmatrix}^+ \begin{pmatrix} 0 & -t_a e^{i\vec{k}\vec{a}_1} - t_b e^{i\vec{k}\vec{a}_2} - t_c \\ c.c. & 0 \end{pmatrix} \begin{pmatrix} \tilde{C}_A(\vec{k}) \\ \tilde{C}_B(\vec{k}) \end{pmatrix}} \tag{218}$$

Since the unit cell has two sites the tight-binding model has two bands



Dirac-like dispersion around $\vec{K}$ and $\vec{K}'$

Dirac fermions

Graphene is a semi-metal since the band gap closes, however only at two discrete points in the BZ. In the vicinity of these points

$$\boxed{\begin{aligned} \underline{\underline{h}}(\vec{K}+\delta\vec{k}) &= \delta k_x \underline{\underline{\sigma}}_x + \delta k_y \underline{\underline{\sigma}}_y \\ \underline{\underline{h}}(\vec{K}'+\delta\vec{k}) &= -\delta k_x \underline{\underline{\sigma}}_x + \delta k_y \underline{\underline{\sigma}}_y \end{aligned}} \tag{219}$$

(B) Symmetries of Graphene

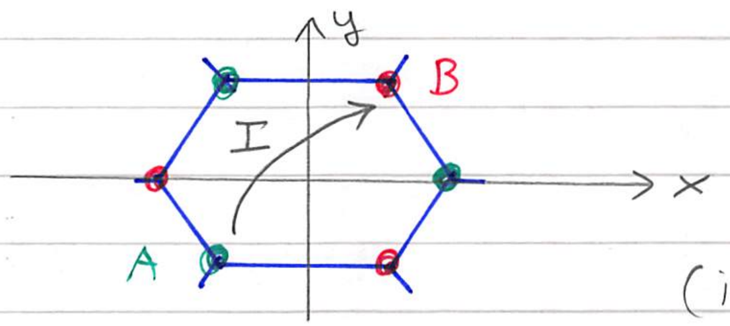
(i) in the vicinity of the Dirac points, i.e. for $E \approx 0$ holds (note $\vec{K}' \equiv -\vec{K}$)

$$\underline{\underline{h}}^*(\vec{K}+\delta\vec{k}) = \delta k_x \underline{\underline{\sigma}}_x - \delta k_y \underline{\underline{\sigma}}_y = \underline{\underline{h}}(-\vec{K}-\delta\vec{k}) \tag{220}$$

i.e $\quad THT^{-1} = H \quad$ TR invariant for $E \approx 0$

(ii) the hamiltonian is invariant under inversion

$$I: (x,y) \longleftrightarrow (-x,-y)$$



($i \equiv$ 2D index)

$$(221) \quad I \hat{c}_{iA} I^{-1} = \hat{c}_{-iB} \qquad I \hat{c}_{iB} I^{-1} = \hat{c}_{-iA}$$

$$(222) \quad \boxed{I \hat{c}_{i\mu} I^{-1} = \sigma^x_{\mu\mu'} \hat{c}_{-i\mu'}}$$

action of inversion I on real space operators

· in Fourier-space (momentum-space)

$$I \tilde{c}_\mu(\vec{k}) I^{-1} = \frac{1}{\sqrt{L}} \sum_j e^{i\vec{k}\vec{R}_j} I \hat{c}_{j\mu} I^{-1}$$

$$= \frac{1}{\sqrt{L}} \sum_j e^{i\vec{k}\vec{R}_j} \hat{c}_{-j\mu'} \sigma^x_{\mu\mu'}$$

$\vec{R}_{-j} = -\vec{R}_j \Rightarrow$

$$(223) \quad \boxed{I \tilde{c}_\mu(\vec{k}) I^{-1} = \sigma^x_{\mu\mu'} \tilde{c}_{\mu'}(-\vec{k})}$$

Note: Eq. (221) describes "active" inversion i.e. $\vec{R}_j$ is unaffected by particle operators $\hat{c}_j \to \hat{c}_{-j}$. Equivalently one could have used "passive" inversion where $\vec{R}_j \to -\vec{R}_j$ but $\hat{c}_j$ remains. In both cases we would get (223)

The Graphene hamiltonian is invariant under inversion

$$(224) \qquad I H I^{-1} = H \qquad \text{IR invariance}$$

In general the condition for IR invariance reads

$$I H I^{-1} = \sum_{\bar{k}} I \tilde{c}^{\dagger}_{\alpha}(\bar{k})\, h_{\alpha\beta}(\bar{k})\, \tilde{c}_{\beta}(\bar{k})\, I^{-1}$$

$$= \sum_{\bar{k}} \sigma^{x}_{\alpha\gamma}\, \tilde{c}^{\dagger}_{\gamma}(-\bar{k})\, I\, h_{\alpha\beta}(\bar{k})\, I^{-1} \sigma^{x}_{\beta\lambda}\, \tilde{c}_{\lambda}(-\bar{k})$$

$$= \sum_{\vec{k}} c^{\dagger}_{\gamma}(\bar{k}) \underbrace{\left[\sigma^{x}_{\alpha\gamma}\, I\, h_{\alpha\beta}(-\bar{k}) I^{-1} \sigma^{x}_{\beta\lambda}\right]}_{\stackrel{!}{=}\, h_{\gamma\lambda}(\bar{k})} \tilde{c}_{\lambda}(\bar{k})$$

$$(225) \qquad \boxed{\sigma^{x}_{\gamma\alpha}\, h_{\alpha\beta}(-\vec{k})\, \sigma^{x}_{\beta\lambda} \stackrel{!}{=} h_{\gamma\lambda}(\bar{k})} \qquad \text{IR invariance}$$

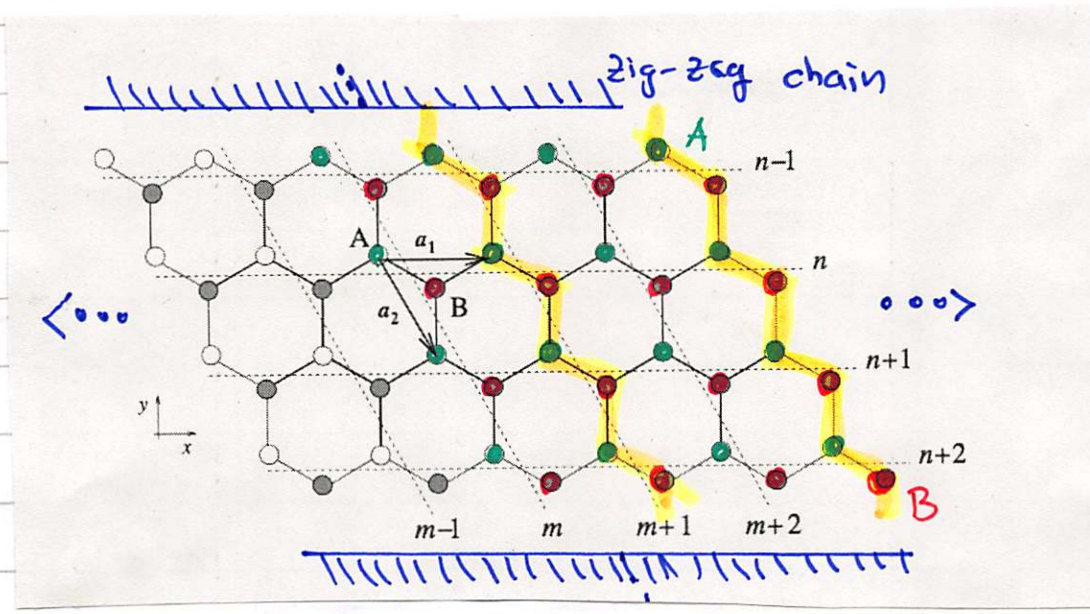
One can show:

> The existence of Dirac points is guaranteed by the combined TR <u>and</u> IR invariance

In order to open up a gap one needs to break either TR or IR symmetry.

(c) edge modes in Graphene

Although Graphene is not an insulator it does have edge modes: consider open boundary conditions in zig-zag direction and periodic BC in orthogonal



can be considered as coupled zig-zag chains

F-trafo in x and assume $t_a = t_b = t_c = t$

$$H = -t \sum_{n k_x} \left(C^+_{2n+1}(k_x)\, C_{2n}(k_x) + h.a. \right)$$

(226)

$$-t \sum_{n k_x} \left[C^+_{2n}(k_x)\, C_{2n-1}(k_x) \left(e^{i k_x \frac{a_1}{2}} + e^{-i k_x \frac{a_1}{2}} \right) + h.a. \right]$$

where $a_1 = \frac{a}{2}\sqrt{3}$; gauge trafo $C_{2n-1} \to C_{2n-1}\, e^{i k_x a_1/2}$

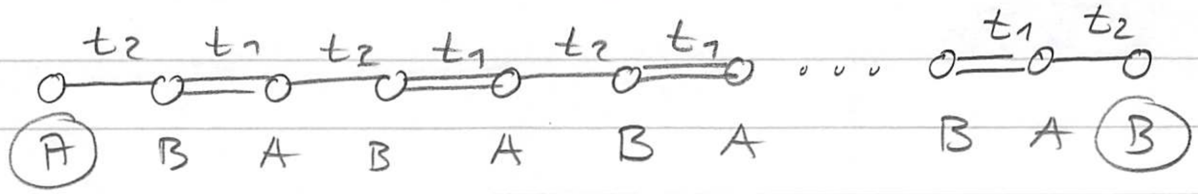
(227)
$$\boxed{H = -t \sum_{n k_x} \left[C^+_{2n+1}(k_x)\, C_{2n}(k_x) + C^+_{2n}(k_x)\, C_{2n-1}(k_x) \left(1 + e^{-i k_x a_1} \right) + h.a. \right]}$$

this is the SSH model for every k_x

$$2n-1 \longleftrightarrow 2n \qquad t\left(1+e^{-ik_x a_1}\right) = t_2$$

$$2n \longleftrightarrow 2n+1 \qquad t \qquad = t_1$$

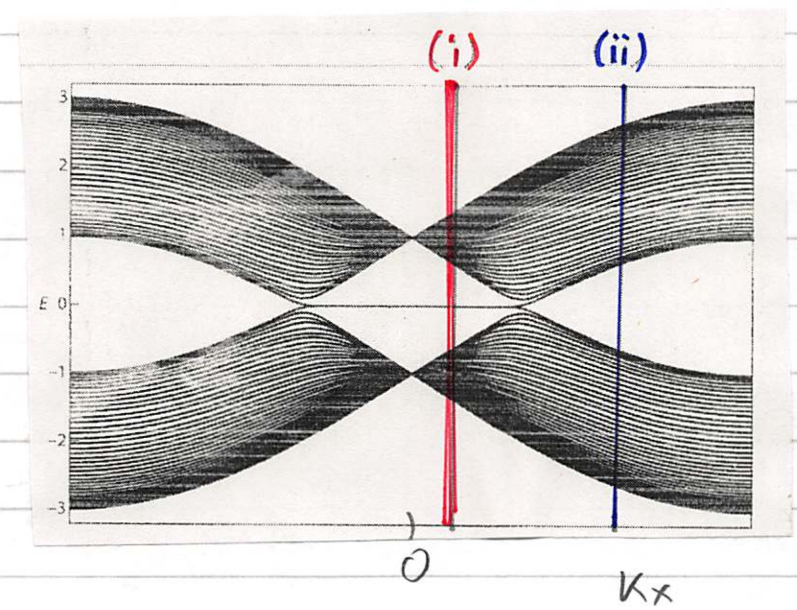
chains from "A" to "B"



$$|t_2| = |1+e^{-ik_x a_1}|\, t_1 = \sqrt{2}\cos\left(\frac{k_x a_1}{2}\right) t_1$$

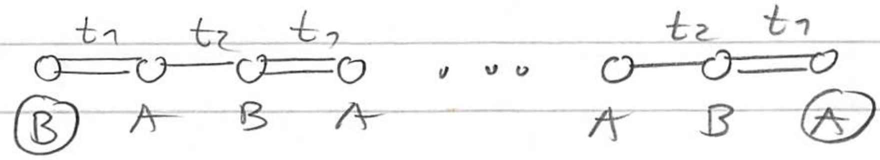
$\Rightarrow$ $\exists$ edge states with energy $E=0$ for all k_x for which

(228) $$\cos\frac{k_x a_1}{2} \leq \frac{1}{\sqrt{2}} \qquad \text{region (i)}$$



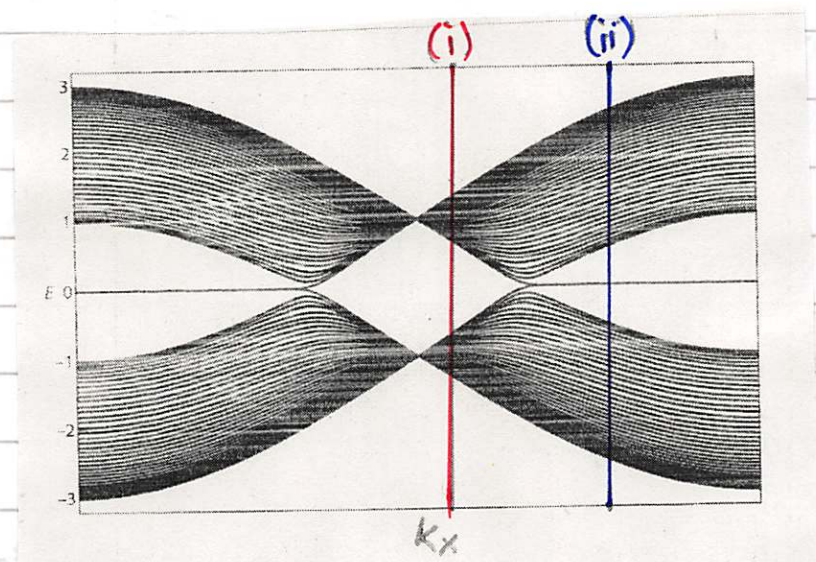
edge non-dispersive
$$\frac{\partial E}{\partial k_x} = 0$$

inverting the system leads to chains from "B" to "A"

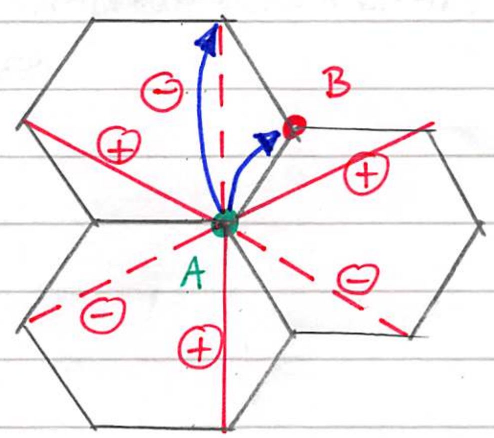


$\Rightarrow$ $\exists$ edge states with $E=0$ for all k_x for which

(229) $$\cos\frac{k_x a_1}{2} \geq \frac{1}{\sqrt{2}}$$



5.2 Haldane model



Haldane constructed a variant of Graphene which breaks both TR and IR

Phys. Rev. Lett. 61 2015 (1988)

nearest and next-nearest neighbor hopping

$$H = t_1 \sum_{\langle ij \rangle} c_i^+ c_j + t_2 \sum_{\langle\langle ij \rangle\rangle} e^{-i\nu_{ij}\phi} c_i^+ c_j + m \sum_j \varepsilon_j c_j^+ c_j \tag{230}$$

$\langle ij \rangle$ nearest neighbor hopping NN
$\langle\langle ij \rangle\rangle$ next-nearest -"- NNN

$$\varepsilon_j = \begin{cases} +1 & \text{A sites} \\ -1 & \text{B sites} \end{cases} \qquad \nu_{ij} = \mathrm{sgn}(\vec{d}_1 \times \vec{d}_2)_z$$

(see figure "$\oplus$" or "$\ominus$")

F-trafo of (230) yields

$$H = \sum_{\vec{k}} \begin{pmatrix} C_A^+(\vec{k}) \\ C_B^+(\vec{k}) \end{pmatrix}^T \underline{\underline{h}}(\vec{k}) \begin{pmatrix} C_A(\vec{k}) \\ C_B(\vec{k}) \end{pmatrix} \tag{231}$$

where

$$\boxed{\underline{\underline{h}}(\vec{k}) = \varepsilon(\vec{k}) + \sum_{j=1}^{3} d_j(\vec{k})\, \underline{\underline{\sigma}}_j} \tag{232}$$

$$\begin{aligned}
\varepsilon(\vec{k}) &= 2t_2 \cos\phi \left[\cos(\vec{k}\cdot\vec{a}_1) + \cos(\vec{k}\cdot\vec{a}_2) + \cos(\vec{k}\cdot(\vec{a}_1-\vec{a}_2))\right] \\
d_1(\vec{k}) &= t_1\left[\cos(\vec{k}\cdot\vec{a}_1) + \cos(\vec{k}\cdot\vec{a}_2) + 1\right] \\
\vec{d}_2(\vec{k}) &= t_1\left[\sin(\vec{k}\cdot\vec{a}_1) + \sin(\vec{k}\cdot\vec{a}_2)\right] \\
\vec{d}_3(\vec{k}) &= m + 2t_2\sin\phi\left[\sin(\vec{k}\vec{a}_1) - \sin(\vec{k}\vec{a}_2) - \sin(\vec{k}\cdot(\vec{a}_1-\vec{a}_2))\right]
\end{aligned} \tag{233}$$

(A) symmetry properties of the Haldane model

rem: Pauli-matrices in $\underline{\underline{h}}(\bar{k})$ correspond to pseudo spin

- TR invariance

$$\varepsilon(\bar{k}) = \varepsilon(-\bar{k}) \quad \checkmark$$

$$d_1(\bar{k}) = d_1(-\bar{k}) \quad \checkmark \qquad d_2(\bar{k}) = -d_2(-\bar{k}) \quad \checkmark$$

but $\quad d_3(\bar{k}) = d_3(-\bar{k})$ only at $\phi = 0, \pi$

$\Rightarrow$ Haldane model is TR invariant only for $\phi = 0, \pi$

- Inversion

$$\varepsilon(\bar{k}) = \varepsilon(-\bar{k}) \quad \checkmark$$

$$d_1(\bar{k}) = d_1(-\bar{k}) \quad \checkmark \qquad d_2(\bar{k}) = -d_2(-\bar{k}) \quad \checkmark$$

but $\quad d_3(\bar{k}) = -d_3(-\bar{k})$ only for $m = 0$

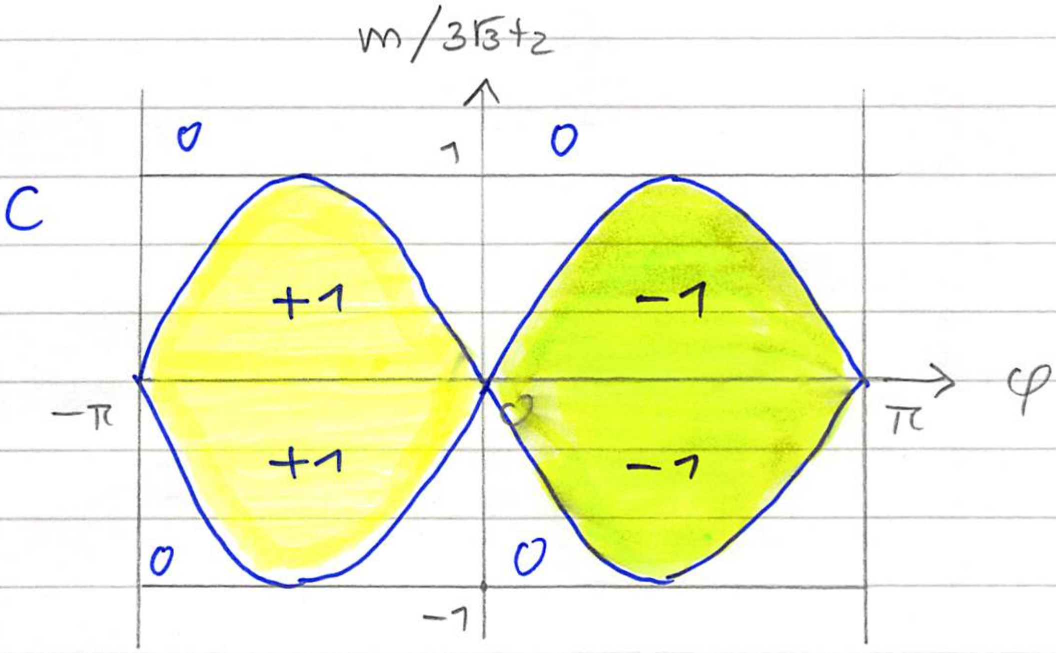
$\Rightarrow$ Haldane model is I-invariant only for vanishing mass term, i.e. $m = 0$

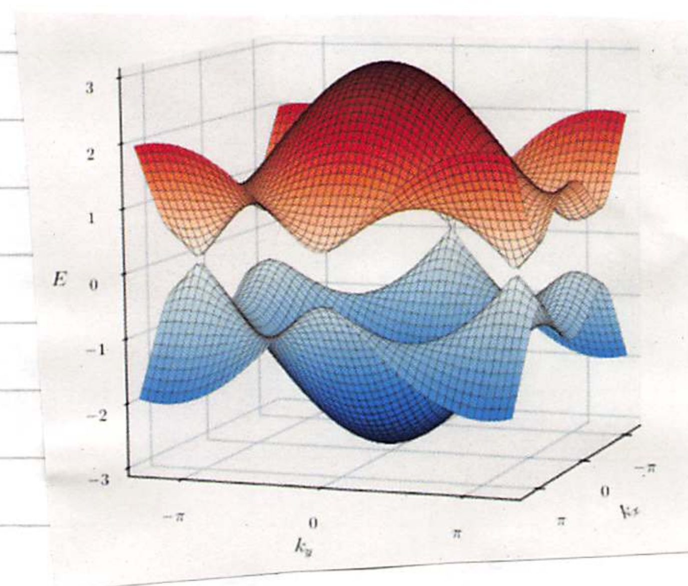
So we see that the d_3 component contains both an I-breaking and a TR breaking term.

$$d_3 = m + 2t_2 \sin\phi \left[\sin(\vec{b}\vec{a}_1) - \sin(\vec{b}\vec{a}_2) - \sin(\vec{b}\cdot(\vec{a}_1 - \vec{a}_2)) \right]$$

I breaking   TR breaking

As a consequence:
- gap opening
- non-trivial Chern number





gap openings!