- chiral symmetry

$$\sigma_x \underline{h}(\vec{k})\sigma_x = \sin k_x \sigma_x - \sin k_y \sigma_y - [u+\cos k_x + \cos k_y]\sigma_z$$

$$\sigma_y \underline{h}(\vec{k})\sigma_y = -\sin k_x \sigma_x + \sin k_y \sigma_y - [u+\cos k_x + \cos k_y]\sigma_z$$

$$\sigma_z \underline{h}(\vec{k})\sigma_z = -\sin k_x \sigma_x - \sin k_y \sigma_y + [u+\cos k_x + \cos k_y]\sigma_z$$

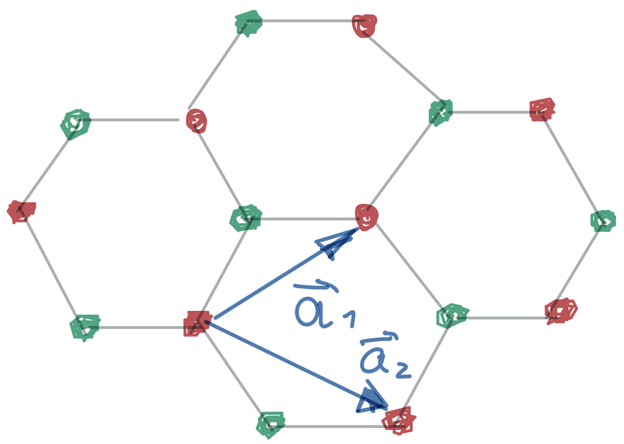
$S=0$ $\boxed{A}$ topological in 2D

5. Graphene and Haldane model

An important and interesting class of Chern insulators is based on honeycomb lattices

5.1 Graphene and Dirac fermions

(A) Lattice structure and Hamiltonian

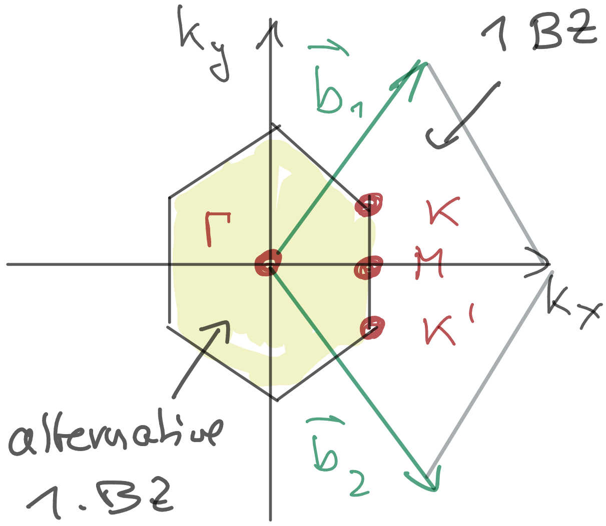


unit cell has two lattice points (A, B)

lattice vectors

$$\vec{a}_1 = \frac{a}{2}(3, \sqrt{3}) \qquad (260)$$
$$\vec{a}_2 = \frac{a}{2}(3, -\sqrt{3})$$

Brillouin zone



reciprocal lattice vectors

$$\vec{b}_1 = \frac{2\pi}{3a}\left(1, \sqrt{3}\right)$$
$$\vec{b}_2 = \frac{2\pi}{3a}\left(1, -\sqrt{3}\right) \qquad (261)$$

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

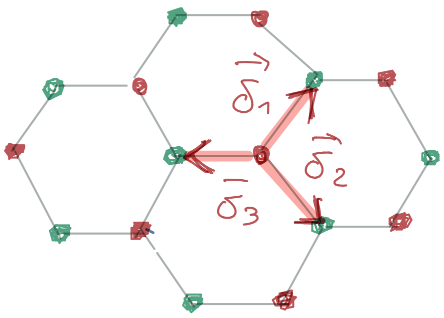
alternative BZ: Hexagon with edges

$$\vec{K} = \frac{2\pi}{3a}\left(1, \frac{1}{\sqrt{3}}\right) \qquad \vec{K}' = \frac{2\pi}{3a}\left(1, -\frac{1}{\sqrt{3}}\right) \qquad (262)$$

$\vec{K}$ and $\vec{K}'$ are Time-reversal partners since

$$T\,|u(\vec{k})\rangle \longrightarrow |u(-\vec{k})\rangle$$
$$-\vec{K} = \vec{K}' - (\vec{b}_1 + \vec{b}_2) \;\hat{=}\; \vec{K}'$$

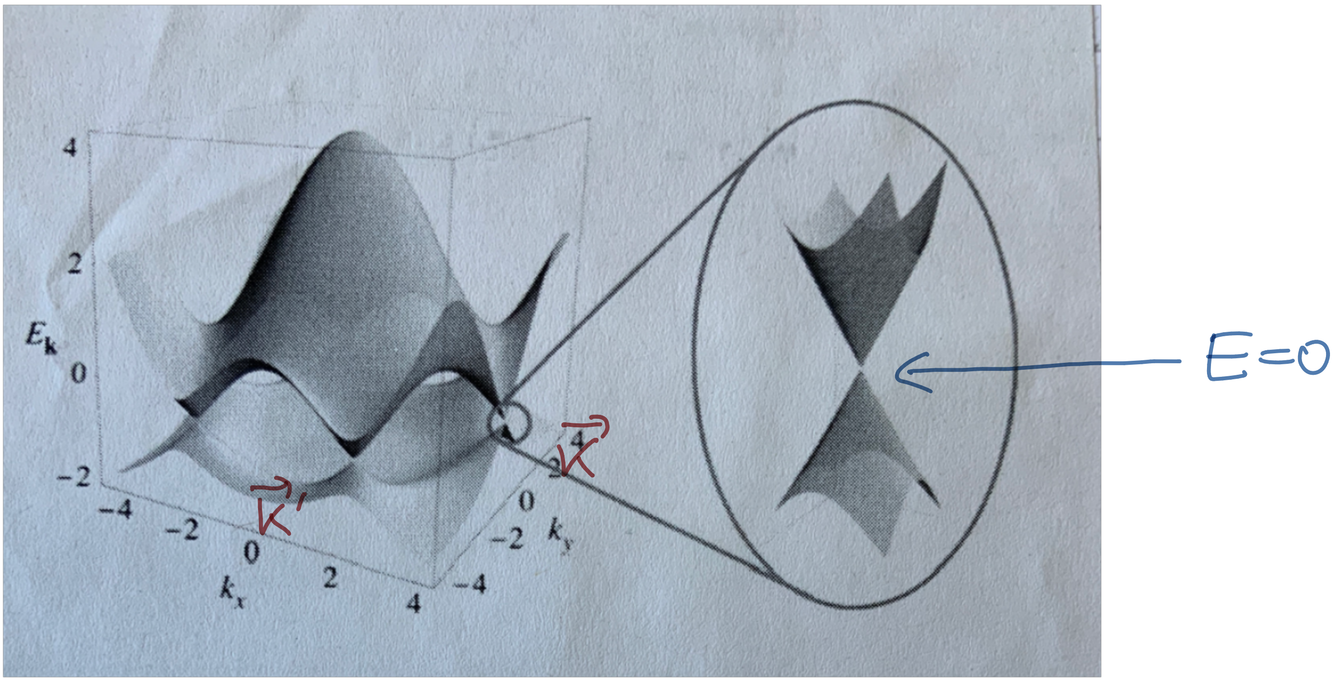
simple hopping on honeycomb lattice



$$H = \sum_{\vec{k}} \begin{pmatrix} \tilde{C}_A^+(\vec{k}) \\ \tilde{C}_B^+(\vec{k}) \end{pmatrix}^T \begin{pmatrix} 0 & \sum_{j=1}^{3} t_j e^{i\vec{k}\vec{\delta}_j} \\ \sum_{j=1}^{3} t_j e^{-i\vec{k}\vec{\delta}_j} & 0 \end{pmatrix} \begin{pmatrix} \tilde{C}_A(\vec{k}) \\ \tilde{C}_B(\vec{k}) \end{pmatrix} \qquad (263)$$

with a gauge trafo $\tilde{c}_B(\vec{k}) \to \tilde{c}_B(\vec{k})\, e^{i\vec{k}\cdot\vec{\delta}_3}$

$$\boxed{H = \sum_{\vec{k}} \begin{pmatrix} \tilde{c}_A^\dagger(\vec{k}) \\ \tilde{c}_B^\dagger(\vec{k}) \end{pmatrix}^T \begin{pmatrix} 0 & -t_a e^{i\vec{k}\vec{a}_1} - t_b e^{i\vec{k}\vec{a}_2} - t_c \\ c.c. & 0 \end{pmatrix} \begin{pmatrix} \tilde{c}_A(\vec{k}) \\ \tilde{c}_B(\vec{k}) \end{pmatrix}} \tag{264}$$



unit cell of 2 sites ⇒ 2 bands

Dirac-like spectrum around $\vec{K}, \vec{K}'$

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

$$\boxed{\begin{aligned} \underline{\underline{h}}(\vec{K}+\delta\vec{k}) &= \delta k_x \underline{\underline{\sigma_x}} + \delta k_y \underline{\underline{\sigma_y}} \\ \underline{\underline{h}}(\vec{K}'+\delta\vec{k}) &= -\delta k_x \underline{\underline{\sigma_x}} + \delta k_y \underline{\underline{\sigma_y}} \end{aligned}} \tag{265}$$

(B) Symmetries of Graphene

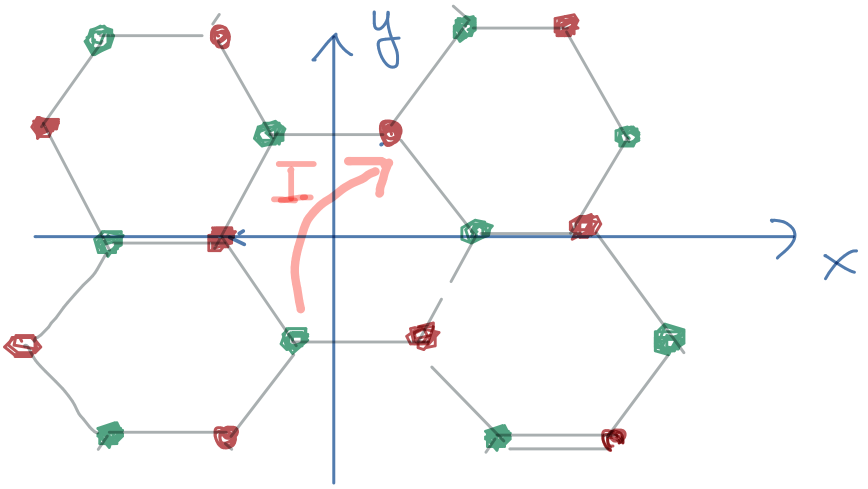
- In the vicinity of the Dirac points, i.e. for $E \simeq 0$

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

note that $-\vec{k} \mathrel{\hat{=}} \vec{k}'$

$\Rightarrow$ $$\boxed{THT^{-1} = H}$$ TR invariant (for $E \simeq 0$)

- The Hamiltonian is inversion symmetric



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

$i = (l,m)$ 2D index

- action of inversion ?

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

(268) $$\boxed{I\, \hat{c}_{i\mu} I^{-1} = \tau^x_{\mu\mu'}\, \hat{c}_{-i\mu'}}$$

τ^x Pauli matrix in "A", "B" pseudospins

$\to$ in Fourier space

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

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

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

(269) $$\boxed{I\,\tilde{c}_\mu(\vec{k})I^{-1} = \tau^x_{\mu\mu'}\,\tilde{c}_{\mu'}(-\bar{k})}$$

Note: • Eq. (267) describes "active" inversion, i.e. $\vec{R}_j \to \vec{R}_j$ remains the same but $\hat{c}_j \to \hat{c}_{-j}$

• In a "passive" inversion one would have $\vec{R}_j \to -\vec{R}_j$ but $\vec{c}_j \to \vec{c}_j$

In both cases eq. (269) follows

• Proof that Graphene Hamiltonian is inversion (IR) symmetric

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

$$= \sum_{\vec{k}} \tau^x_{\alpha\gamma}\,\tilde{c}^+_\gamma(-\bar{k})\, I h_{\alpha\beta}(\vec{k}) I^{-1}\, \tau^x_{\beta\lambda}\,\hat{c}_\lambda(-\bar{k})$$

only number!

$k \to -k$ $$= \sum_{\vec{k}} \tilde{c}^+_\gamma(\bar{k}) \underbrace{\left[\tau^x_{\alpha\gamma}\, I h_{\alpha\beta}(-\bar{k}) I^{-1}\, \tau^x_{\beta\lambda}\right]}_{\stackrel{?}{=}\, h_{\gamma\lambda}(\bar{k})} \tilde{c}_\lambda(\bar{k})$$

✓

$$\tau^x_{\alpha\beta} = \tau^x_{\beta\alpha}$$

(270) $$\tau^x_{\gamma\alpha}\, h_{\alpha\beta}(-\vec{k})\, \tau^x_{\beta\lambda} = h_{\gamma\lambda}(\vec{k})$$

IR invariance

One can show

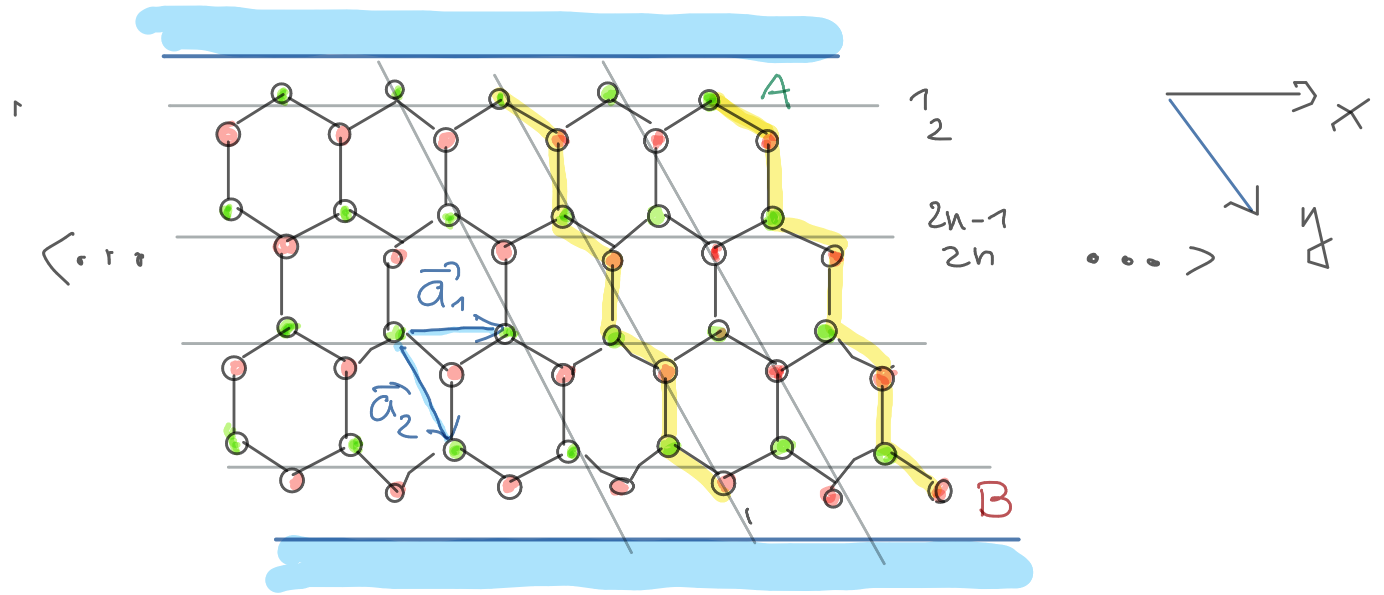
$$\boxed{\text{The existance of Dirac points is guaranteed by the combined TR \underline{and} IR invariance}}$$

$\Rightarrow$ in order to open a true gap one has to break either TR or IR invariance

(c) Edge modes of Graphene

Although Graphene is not an insulator nor does it have a Chern number (TR invariance) it has edge modes.

Consider <u>open boundary</u> conditions in <u>zig-zag</u> and <u>periodic boundary</u> conditions in orthogonal direction



can be considered as coupled zig-zag chains

F-trafo in x direction (periodic or infinite)

assume for simplicity

(271) $$t_a = t_b = t_c = t$$

with gauge trafo $C_{2n-1} \to C_{2n-1} e^{ik_x a_1/2}$

(272) $$\boxed{\bar{H} = -t \sum_{n,k_x} \Big[C^\dagger_{2n+1}(k_x)\, C_{2n}(k_x) + C^\dagger_{2n}(k_x)\, C_{2n-1}(k_x)\left(1+e^{-ik_x a_1}\right) + h.c. \Big]}$$

This is an SSH model for every k_x

$2n-1 \leftrightarrow 2n \qquad t(1+e^{-ik_x a_1}) = t_1$

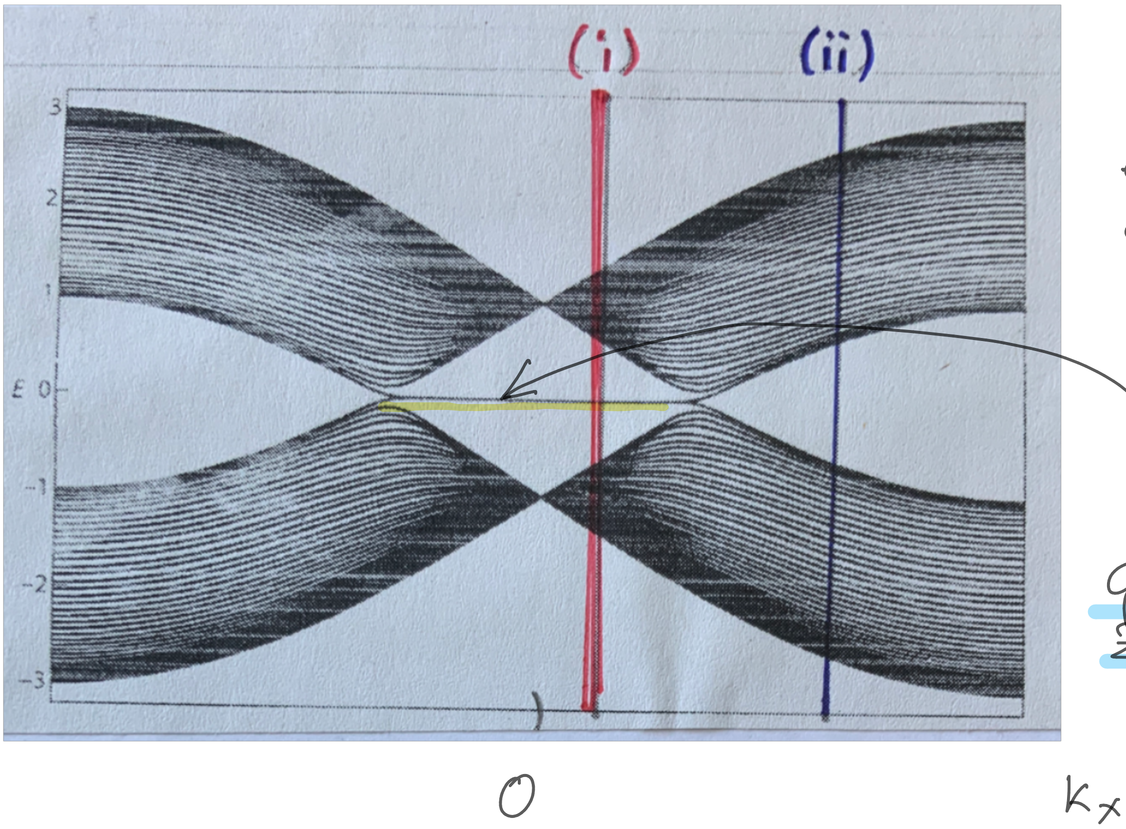
$2n \leftrightarrow 2n+1 \qquad t = t_2$

zig-zag chains run from "A" to "B"

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

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

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



edge states are dispersion-less

$$\frac{\partial E}{\partial k_x} = 0$$

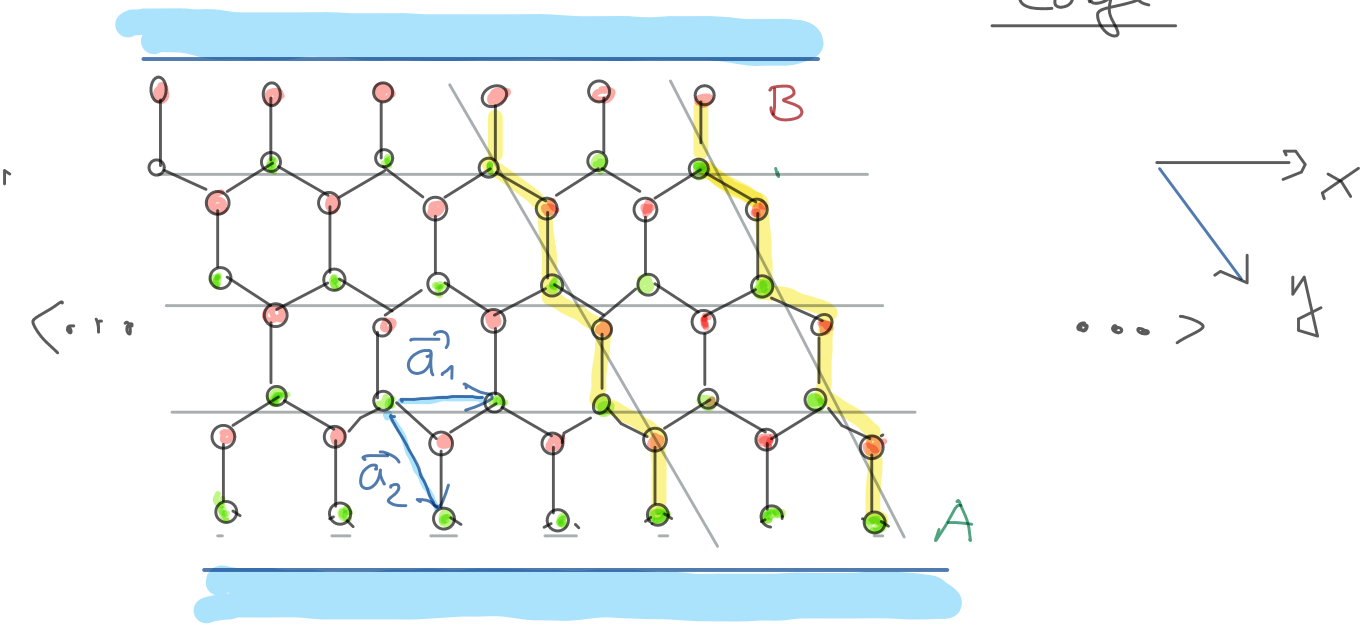
<u>graphene with zig-zag edge</u>

for k_x with

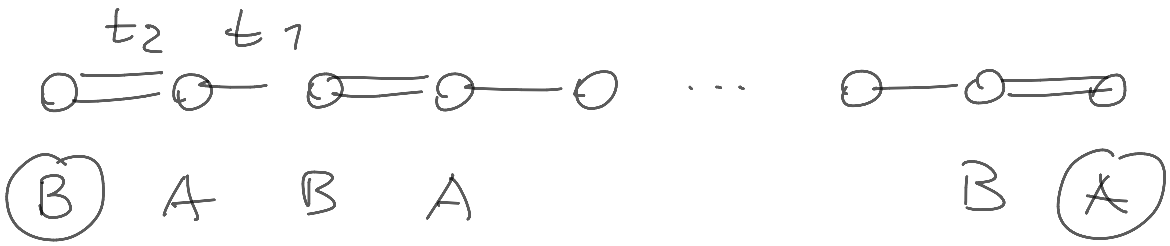
$$\cos\frac{k_x a_1}{2} \geq \frac{1}{\sqrt{2}} \qquad \text{region (ii)}$$

there are no edge states

- If we invert the system and consider a <u>bearded edge</u>

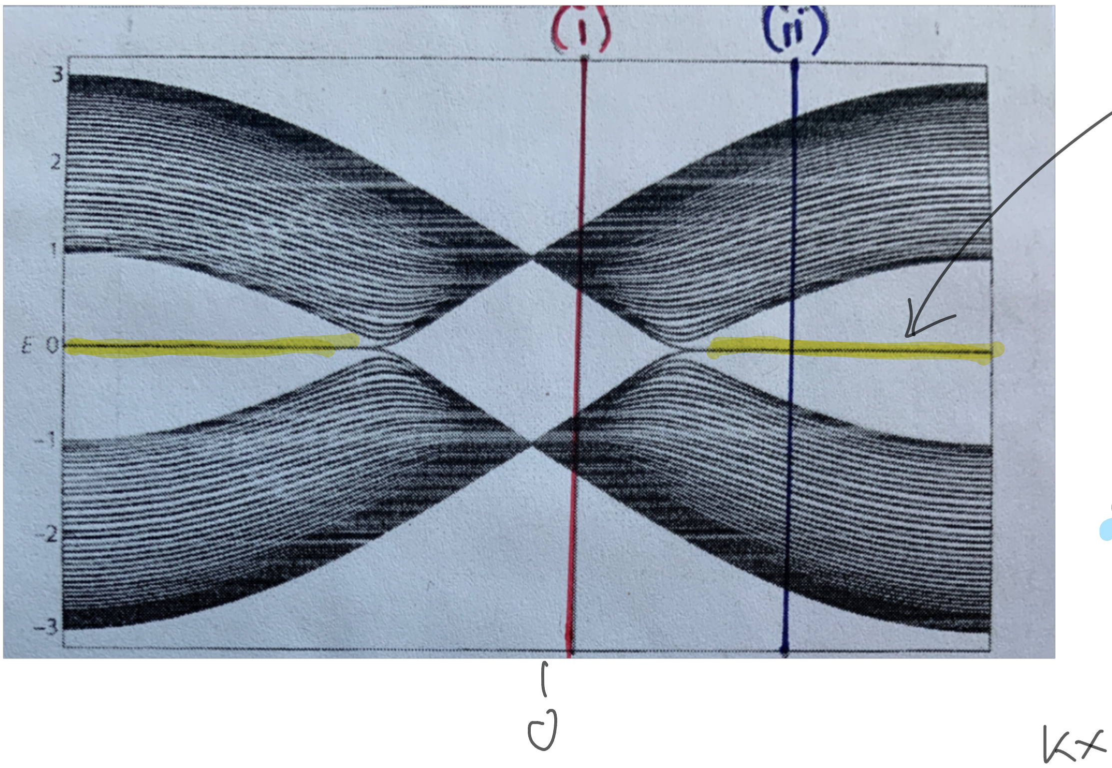


then we find SSH zig-zag chains from "B" to "A"



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

$$\cos\frac{k_x a_1}{2} \geq \frac{1}{\sqrt{2}} \quad \text{region (ii)} \tag{274}$$



dispersion-less edge modes

$$\frac{\partial E}{\partial k_x} = 0$$

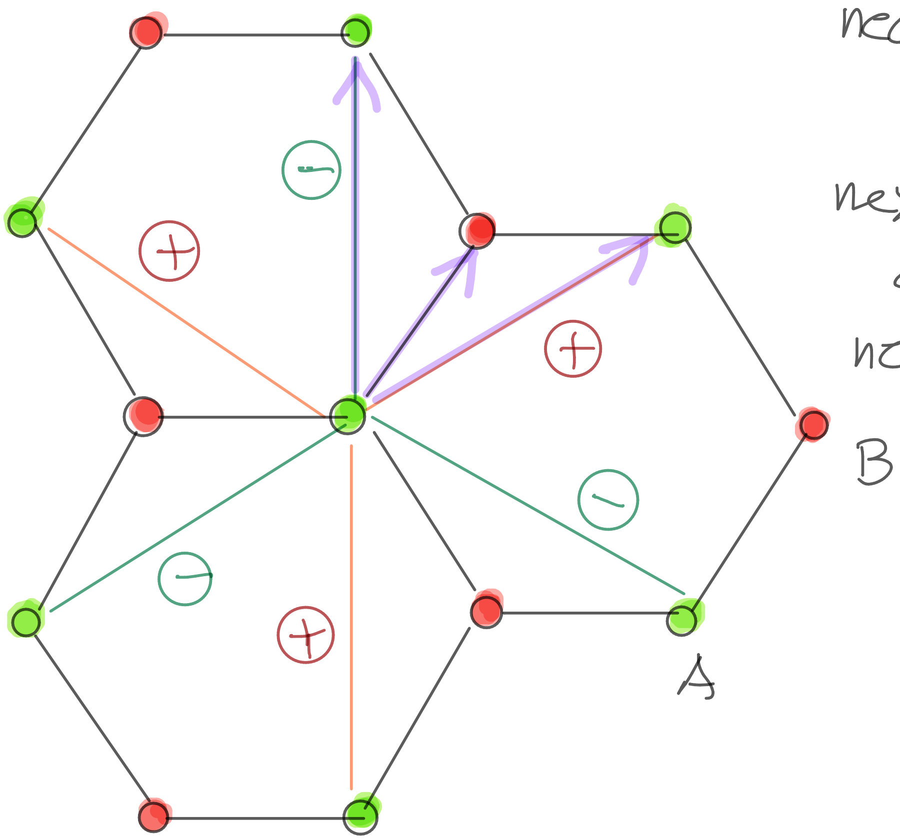
Graphene with bearded edge

5.3 Haldane model

Haldane constructed a variant of the Graphene model which breaks both TR and IR symmetry.

Phys. Rev. Lett 61, 2015 (1988)

TR breaking is achieved by NNN hopping with complex phases



nearest and

$\langle ij \rangle$

next-nearest

$\langle\langle ij \rangle\rangle$

neighbor hopping

(275)

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

Haldane Hamiltonian

$\langle ij \rangle$ NN hopping

$\langle\langle ij \rangle\rangle$ NNN hopping

$$\varepsilon_j = \begin{cases} +1 & \text{A sites} \\ -1 & \text{B sites} \end{cases}$$

$\nu_{ij} = \pm 1$ see figure above

momentum space

$$H = \sum_{\vec{k}} \begin{pmatrix} \tilde{c}_A^+(\vec{k}) \\ \tilde{c}_B^+(\vec{k}) \end{pmatrix}^T \underline{\underline{h}}(\vec{k}) \begin{pmatrix} \tilde{c}_A(\vec{k}) \\ \tilde{c}_B(\vec{k}) \end{pmatrix} \quad (276)$$

where

$$\boxed{\underline{\underline{h}}(\vec{k}) = \varepsilon(\vec{k}) + \sum_{j=1}^{3} d_j(\vec{k}) \underline{\underline{\tau}}_j} \quad (277)$$

$\underline{\underline{\tau}}_j$ Pauli matrices in pseudo spin A, B

$$\boxed{\begin{aligned} \varepsilon(\vec{k}) &= 2t_2 \cos\phi \left[\cos(\vec{k}\vec{a}_1) + \cos(\vec{k}\vec{a}_2) + \cos(\vec{k}\cdot(\vec{a}_1 - \vec{a}_2))\right] \\ d_1(\vec{k}) &= t_1\left[\cos(\vec{k}\cdot\vec{a}_1) + \cos(\vec{k}\cdot\vec{a}_2) + 1\right] \\ d_2(\vec{k}) &= t_1\left[\sin(\vec{k}\vec{a}_1) + \sin(\vec{k}\cdot\vec{a}_2)\right] \qquad (278) \\ d_3(\vec{k}) &= m \\ &\quad + 2t_2 \sin\phi\left[\sin(\vec{k}\vec{a}_1) - \sin(\vec{k}\vec{a}_2) - \sin(\vec{k}\cdot(\vec{a}_1 - \vec{a}_2))\right] \end{aligned}}$$

(A) Symmetries of the Haldane model

remark: the Haldane model is for spin-less fermions and the Pauli matrices $\underline{\underline{\tau}}_\mu$ are in pseudo-spin space "A" $\hat{=} \uparrow$ and "B" $\hat{=} \downarrow$

- TR invariance?

only $\underline{\underline{\tau}}_y^* = -\underline{\underline{\tau}}_y$

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

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

but $d_3(\vec{k}) = d_3(-\vec{k})$ only for $\underline{\underline{\phi = 0, \pi}}$

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

- Inversion?

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

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

but $d_3(\vec{k}) = -d_3(-\vec{k})$ only for $\underline{\underline{m = 0}}$

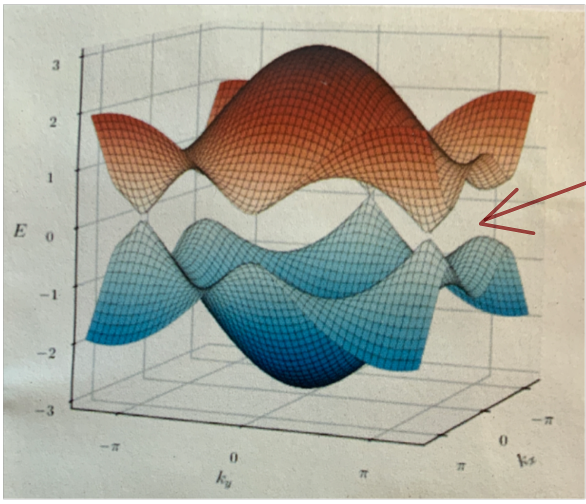
$\Rightarrow$ Haldane model is IR invariant only for $m = 0$

d_3-component contains TR and IR breaking terms

$$d_3 = \underbrace{m}_{\text{IR breaking}} + 2t_2 \sin\varphi \Big[\underbrace{\sin(\vec{b}\,\vec{a}_1) - \sin(\vec{b}\,\vec{a}_2) - \sin(\vec{b}(\vec{a}_1 - \vec{a}_2))}_{\text{TR breaking}} \Big]$$

A consequence of this is that

- a gap opens
- non-zero Chern number



gap opening at Dirac points