

1. Topology of Bloch Hamiltonians: an introduction

In the following we will consider lattice Hamiltonians $h(\vec{k})$ with discrete translational invariance. Here the lattice quasi-momentum is conserved and we will investigate the homotopy of mappings

$$(33) \quad \boxed{\vec{k} \longrightarrow h(\vec{k})}$$

no external
parameter

$$(34) \quad \boxed{k, \lambda \longrightarrow h(k, \lambda)}$$

with external
parameter

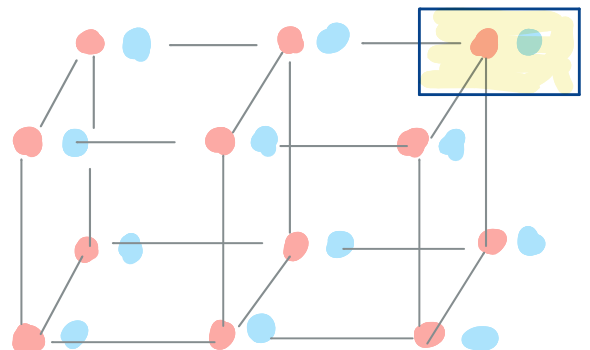
1.1 Bloch bands

crystals have discrete translational invariance

unit cell

• lattice vector

$$(35) \quad \vec{R} = \sum_{i=1}^3 n_i \vec{a}_i$$

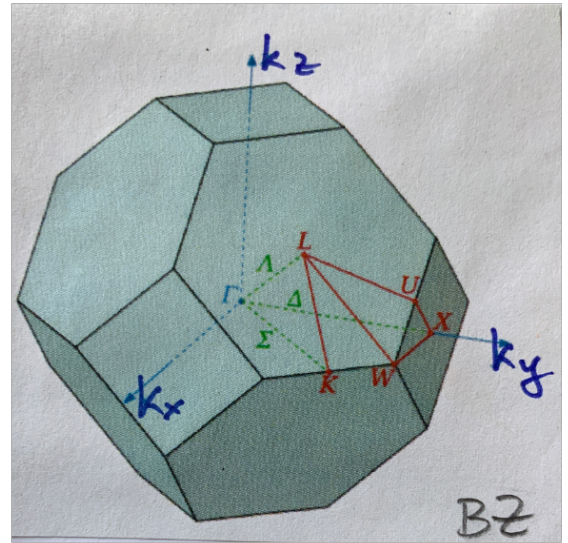


$\vec{a}_i$ basis vectors $n_i \in \mathbb{Z}$

• Dual lattice: Bravais lattice

$$(36) \quad \vec{G} = \sum_{i=1}^3 m_i \vec{b}_i$$

$$\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}$$



• Brillouin zone (BZ)

$$|\vec{b}| < |\vec{b} + \vec{G}| \quad \forall \vec{G}$$

Bloch theorem

$T_{\vec{R}}$: lattice translations

$$T_{\vec{R}}^{-1} H T_{\vec{R}} = H \Rightarrow \text{common eigenfunctions } |\psi_{n\vec{b}}\rangle$$

$$(37) \quad \langle \vec{r} | \psi_{n\vec{b}} \rangle = e^{i\vec{b}\vec{r}} \langle \vec{r} | \psi_{n\vec{b}} \rangle \quad n\text{-Bloch index}$$

with $\vec{b} \in 1\text{BZ}$ and Bloch states $|\psi_{n\vec{b}}\rangle$ are $\vec{R}$ periodic

$$(38) \quad \langle \vec{r} + \vec{R} | \psi_{n\vec{b}} \rangle = \langle \vec{r} | \psi_{n\vec{b}} \rangle$$

• single particle Hamiltonian factorizes in $\vec{b}$ -space

$$(39) \quad H = \sum_{\vec{b} \in 1\text{BZ}} \underline{h}(\vec{b})$$

$\underline{h}(\vec{b})$ still matrix since unit cell has multiple sites or equivalently there are multiple Bloch bands

$\underline{h}(\vec{k})$ is called Bloch Hamiltonian

$$(40) \quad \underline{h}(\vec{k} + \vec{b}_j) = \underline{h}(\vec{k}) \quad \forall \vec{k} \in 1BZ$$

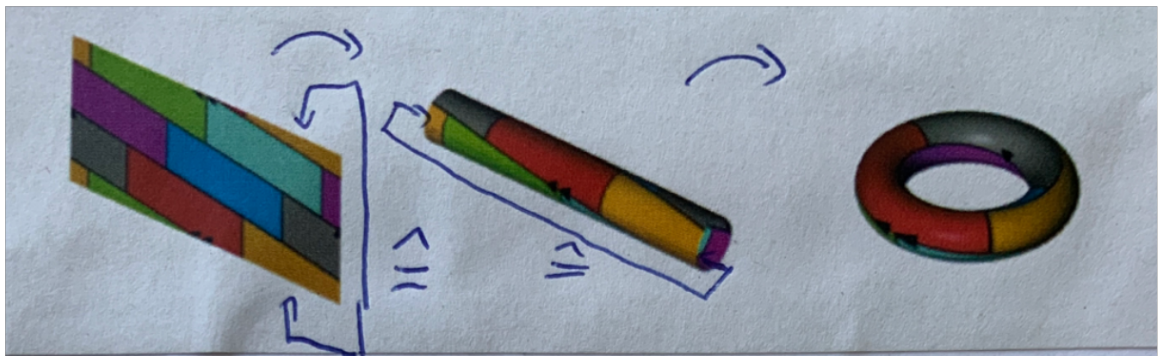
stationary Schrödinger equation

$$(41) \quad \underline{h}(\vec{k}) |u_{n\vec{k}}\rangle = \epsilon_n(\vec{k}) |u_{n\vec{k}}\rangle$$

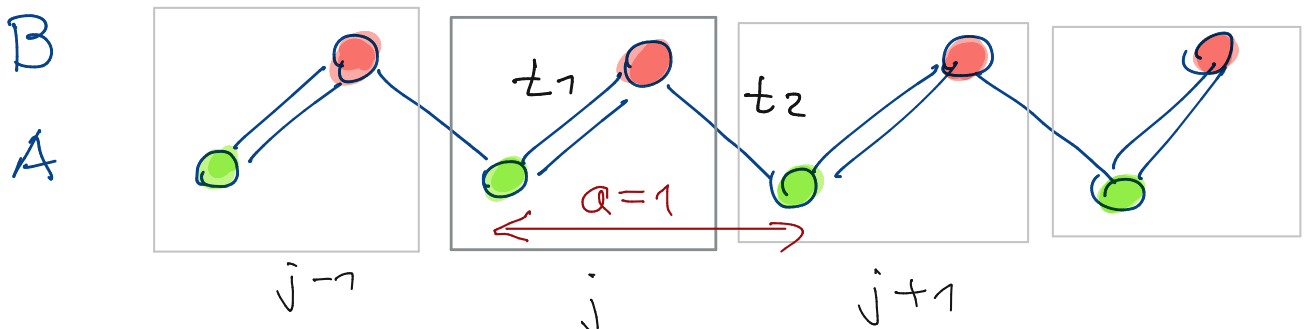
Bloch states defined only modulo gauge trafo

$$(42) \quad |u_{n\vec{k}}\rangle \longrightarrow e^{i\alpha(\vec{k})} |u_{n\vec{k}}\rangle$$

Brillouin zone is a Torus T_{BZ}^2 or T_{BZ}^3



1.2 One-dimensional Bloch Hamiltonians with "topology": Rice-Heale Model



Rice-
Mele
model

$$(43) \quad H = -t_1 \sum_j (C_{Bj}^\dagger C_{Aj} + \text{h.c.}) \\ - t_2 \sum_j (C_{Aj+1}^\dagger C_{Bj} + \text{h.c.}) \\ + \Delta \sum_j (C_{Aj}^\dagger C_{Aj} - C_{Bj}^\dagger C_{Bj})$$

Bloch Hamiltonian? L : # of unit cells PBC
 $\rightarrow$ discrete Fourier transform

lattice momenta

$$\frac{2\pi k}{La} \quad k \in \left[-\frac{L}{2}, \frac{L}{2}\right) \quad a=1$$

$1BZ$

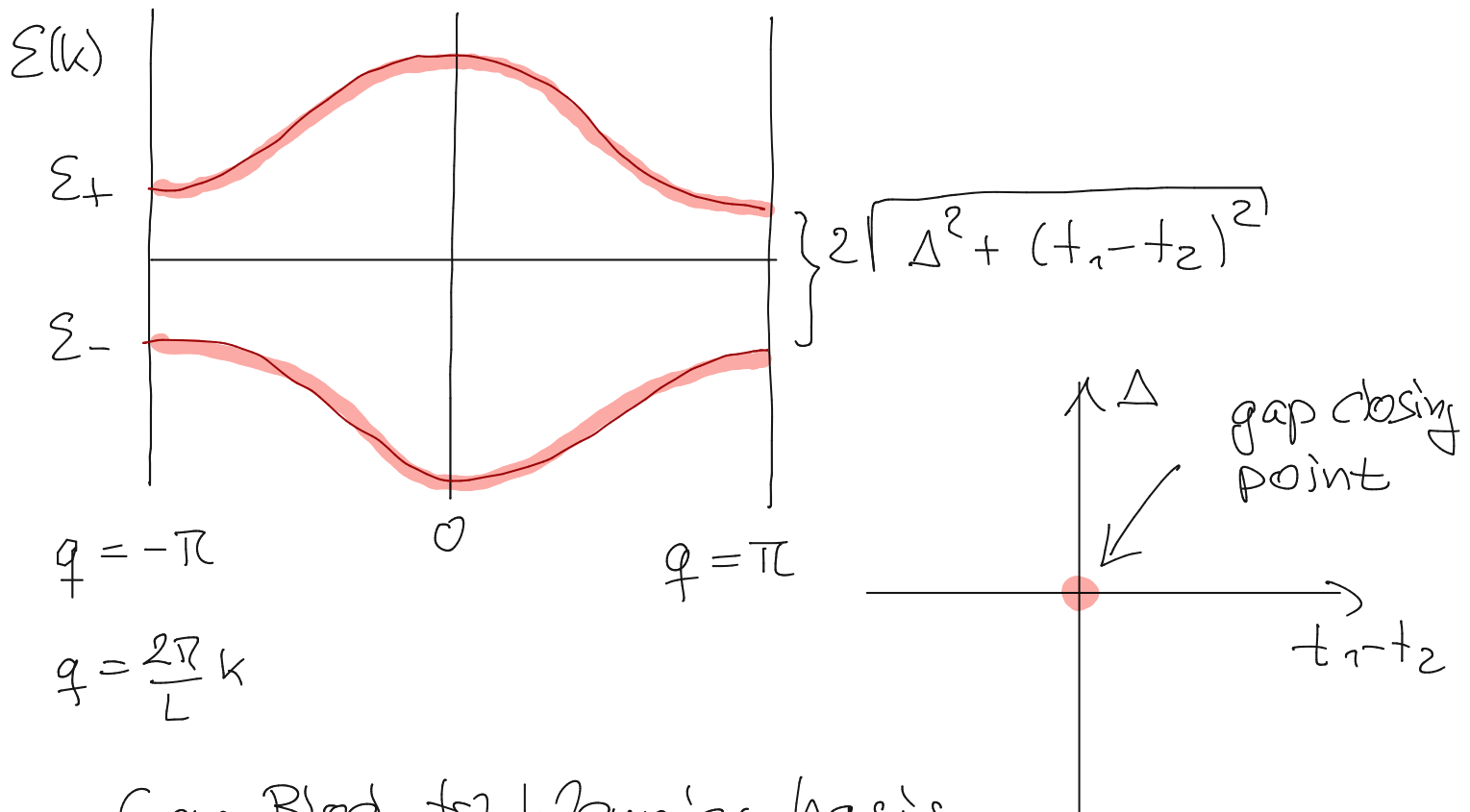
$$(44) \quad \tilde{C}_{Ak} = \frac{1}{L} \sum_{j=1}^L e^{\frac{2\pi i}{L} k j} C_{Aj}$$

$$(45) \Rightarrow H = \sum_{k \in BZ} \begin{pmatrix} \tilde{C}_{Ak}^\dagger \\ \tilde{C}_{Bk}^\dagger \end{pmatrix}^T \underbrace{\begin{pmatrix} \Delta & -t_1 - t_2 e^{-ik} \\ -t_1 - t_2 e^{ik} & -\Delta \end{pmatrix}}_{\text{Bloch Hamiltonian}} \begin{pmatrix} \tilde{C}_{Ak} \\ \tilde{C}_{Bk} \end{pmatrix}$$

2 energy bands

$$(46) \quad \mathcal{E}_\pm(k) = \pm \mathcal{E}(k) = \pm \left[\Delta^2 + (t_1^2 + t_2^2 + 2t_1 t_2 \cos k) \right]^{1/2}$$

$|u_{nk}\rangle$ eigenstates $n=1,2$



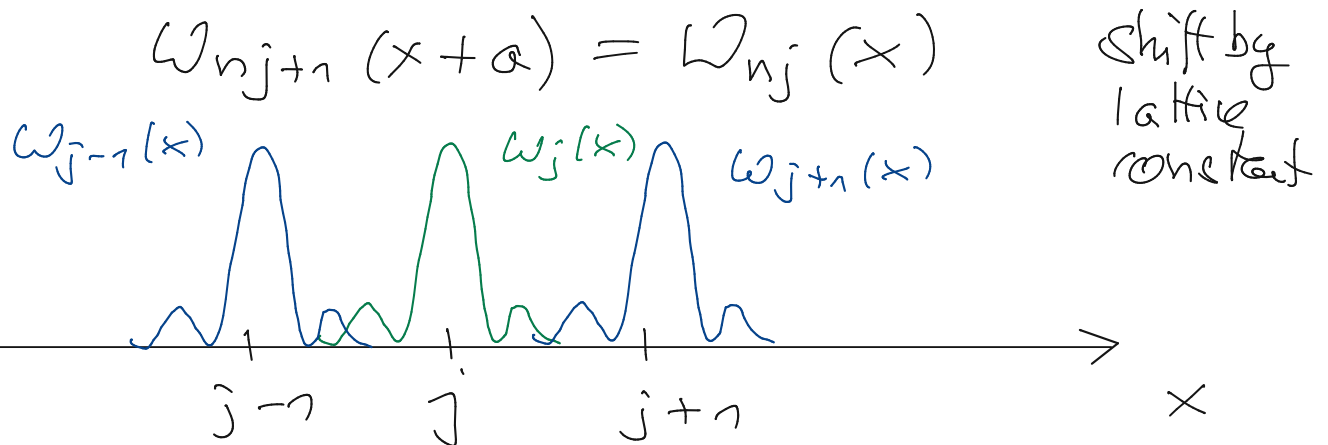
from Bloch to Wannier basis

going back from k -space to position space

$$(47) \quad |W_{nj}\rangle = \frac{1}{\sqrt{L}} \sum_{\mathbf{k}} e^{-\frac{2\pi i \mathbf{j} \mathbf{k}}{L}} e^{i\alpha(\mathbf{k})} |u_{\mathbf{k}}\rangle$$

$\alpha(\mathbf{k})$ is some appropriately chosen gauge (freedom!!)

$$(48) \quad \langle W_{nj} | W_{n'j'} \rangle = \delta_{jj'} \delta_{nn'}$$



an important quantity is the center of mass of Wannier function with respect to unit cell

$$(49) \quad \langle \omega_{nj} | \hat{x} + ja | \omega_{nj} \rangle$$

$j=0$ is sufficient ; also: include gauge in Bloch states

$$\begin{aligned} \hat{x} |\omega_n\rangle &= \frac{1}{2\pi} \int dk \underbrace{\sum_j e^{ikj}}_{\hat{x}} |u_{nk}\rangle \\ &= \frac{i}{2\pi} \int dk e^{ikj} \partial_k |u_{nk}\rangle \end{aligned}$$

$j e^{ikj} = -i \partial_k e^{ikj}$

i.e.

$$(50) \quad \langle \omega_n | \hat{x} | \omega_n \rangle = \frac{i}{2\pi} \int_{BZ} dk \langle u_{nk} | \partial_k u_{nk} \rangle$$

$\Rightarrow$ The center of mass of the Wannier function is the Berry phase of the Bloch function moving through the Brillouin zone called Zak phase

$$(51) \quad \varphi_n^{\text{ZAK}} = i \int_{BZ} dk \langle u_{nk} | \partial_k u_{nk} \rangle$$

- What happens if we adiabatically change the parameter

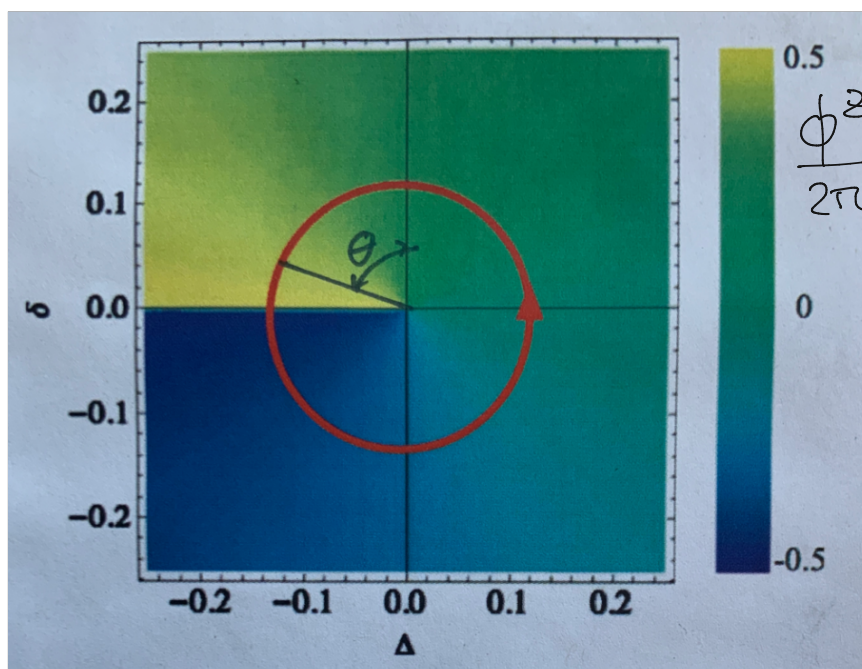
$$\vec{\lambda} = \begin{pmatrix} t_1 - t_2 \\ \Delta \end{pmatrix} \quad \vec{\lambda} \in \mathbb{R}^2$$

in a closed loop in parameter space?

The center of the Wannier functions will move:

$$\Delta x = \oint d\vec{\lambda} \frac{\partial \langle \hat{x} \rangle}{\partial \vec{\lambda}} = \frac{1}{2\pi} \oint d\vec{\lambda} \frac{\partial \phi_n^{2\Delta k}}{\partial \vec{\lambda}}$$

Let's pick a parameter path: $\theta: [0, 2\pi]$



$$\Delta x = \frac{i}{2\pi} \int_{BZ} dk \int_0^{2\pi} d\theta \frac{\partial}{\partial \theta} \langle u_{nk} | \partial_k u_{nk} \rangle$$

i.e.

$$(52) \quad \Delta x = \frac{1}{2\pi} \int dk \int d\theta \quad i \left[\langle \partial_\theta u_{nk} | \partial_k u_{nk} \rangle - \langle \partial_k u_{nk} | \partial_\theta u_{nk} \rangle \right]$$

Berry curvature $\nearrow$ in (k, θ) space

We recognize that the shift of center of mass in a closed loop is an integral over a Berry curvature, which must be an integer

integer-valued topological invariant

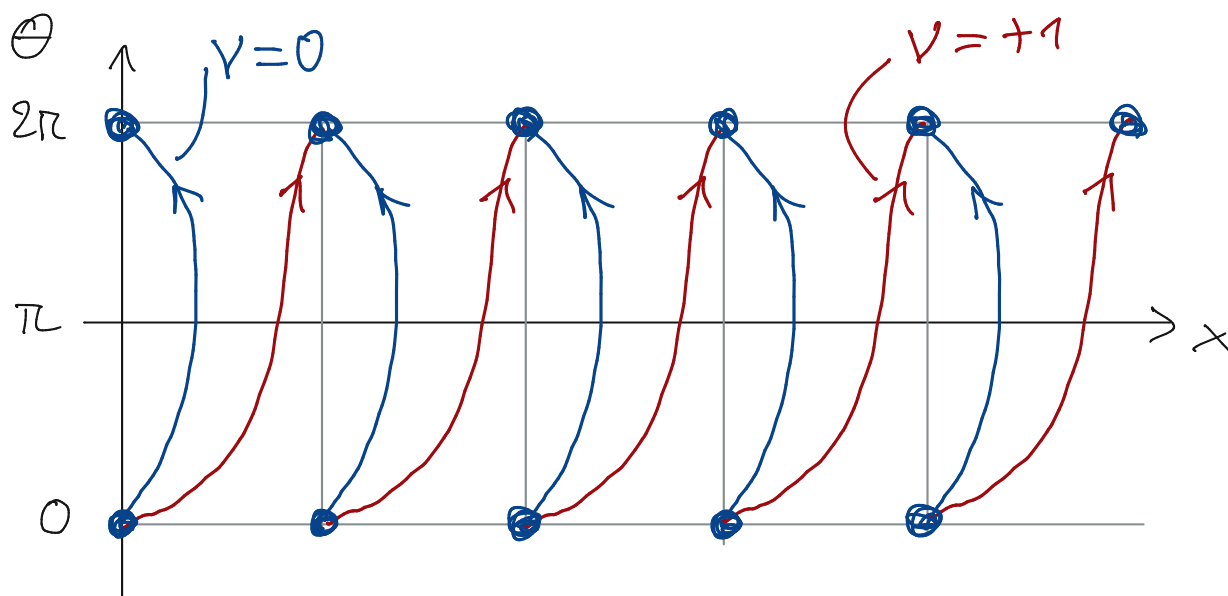
$$(53) \quad \Delta x = \gamma = \frac{1}{2\pi} \oint d\theta \frac{\partial \phi^{2A_k}}{\partial \theta} \in \mathbb{Z}$$

- if path includes origin in Figure above

$$\gamma = \pm 1$$

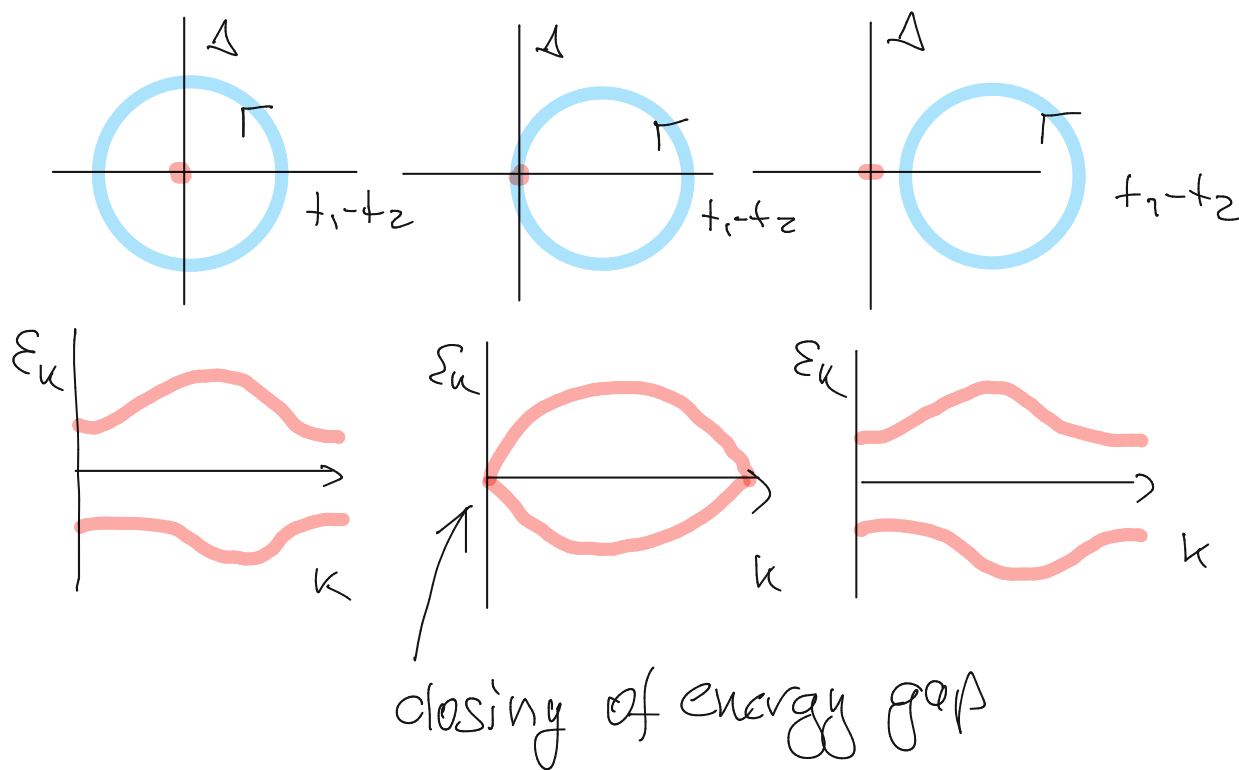
if path excludes origin in Figure above

$$\gamma = 0$$



$\Rightarrow$ physical consequence of nontrivial invariant:
quantized transport in bulk: Thouless pump

$\nu = +1 \longrightarrow \nu = 0$ topological phase transition



Now consider a many-body system with a completely filled lower band; i.e. each block state $|u_-(k)\rangle$ is occupied by one fermion. This is an insulator. Still, from the motion of Wannier centers we expect a quantized transport by ν particles per period. Let's calculate the current in period T

(54)

$\Delta n = \int_0^T dt j(t)$

Since we expect $j \sim 1/T$ we need first-order non-adiabatic corrections of time evolved Bloch states

$$t=0 \quad | \psi_n(t=0) \rangle = e^{ikx} | u_{nk}(t=0) \rangle$$

$t > 0$

$$(55) \quad | \psi_n(t) \rangle = e^{ikx} \left[| u_{nk}(t) \rangle - i t \sum_{n' \neq n} \frac{| u_{n'k} \rangle \langle u_{n'k} | \partial_t u_{nk} \rangle}{E_n(k) - E_{n'}(k)} \right]$$

velocity operator

$$(56) \quad \hat{v} = \frac{d}{dt} \hat{x} = \frac{i}{\hbar} [H, \hat{x}]$$

momentum representation $\hat{x} \rightarrow i \frac{\partial}{\partial q} \quad (m=1)$

$$(57) \quad \hat{v}(q) = \frac{1}{\hbar} \frac{\partial H(q, t)}{\partial q}$$

$$\Rightarrow v_n(q) = \langle \psi_n(t) | \hat{v} | \psi_n(t) \rangle = \frac{1}{\hbar} \frac{\partial E_n(k)}{\partial k}$$

$$(58) \quad - i \sum_{n' \neq n} \left(\frac{\langle u_{nk} | \partial_k H | u_{n'k} \rangle \langle u_{n'k} | \partial_t u_{nk} \rangle}{E_n(k) - E_{n'}(k)} - c.c. \right)$$

$$(59) \quad \text{Using} \quad \langle u_{nk} | \frac{\partial H}{\partial k} | u_{n'k} \rangle = (E_n - E_{n'}) \langle \frac{\partial u_{nk}}{\partial k} | u_{n'k} \rangle$$

yields

$$v_n(q) = \frac{1}{\hbar} \frac{\partial E_n(q)}{\partial q} + i \underbrace{\left[\langle \partial_t u_{nk} | \partial_k u_{nk} \rangle - \langle \partial_k u_{nk} | \partial_t u_{nk} \rangle \right]}_{\Omega_{tk}^{(n)} \text{ Berry curvature}}$$

$$(60) \quad v_n(q) = \frac{1}{\hbar} \frac{\partial E_n(q)}{\partial q} + \Omega_{tk}^{(n)}$$

If all states in the Brillouin zone of the n 'th Bloch band are occupied, the total particle current $j_\perp$ ($\alpha=1$)

$$(61) \quad j_\perp = \underbrace{\frac{1}{\hbar} \int_{BZ} \frac{dk}{2\pi} \frac{\partial E_n(k)}{\partial k}}_{=0} + \int \frac{dk}{2\pi} \Omega_{tk}^{(n)}$$

The integration over a whole cycle gives indeed a quantized transport

$$(62) \quad \Delta n = \frac{1}{2\pi} \int_{BZ} dk \int_0^T dt \Omega_{tk}^{(n)}$$

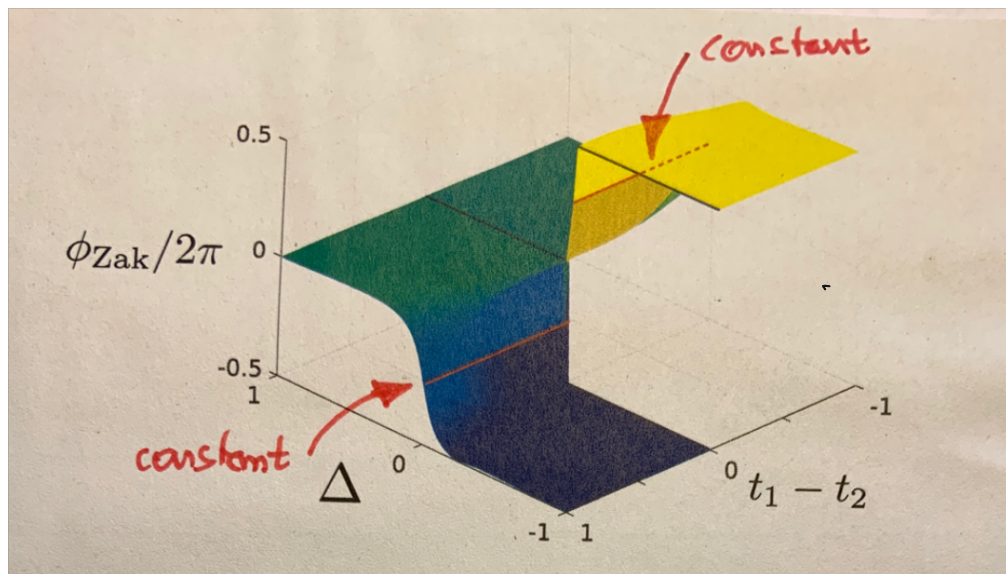
$$(63) \quad \Delta n = \nu = \frac{\Delta \phi_{ZAK}}{2\pi}$$

The winding of the Zak phase of the single-particle Bloch states implies an integer-quantized adiabatic particle transport in the insulating many-body state of a completely filled Bloch band.

Thouless pump (D.J. Thouless PRB 27, 6083 (1983))

1.3 The Su-Schrieffer Heeger (SSH) model

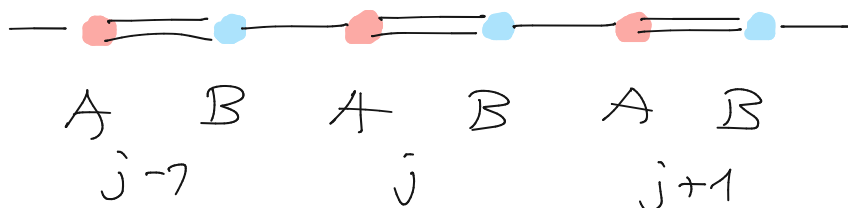
Let's have a look again at the Zak phase of the Rice-Mele model



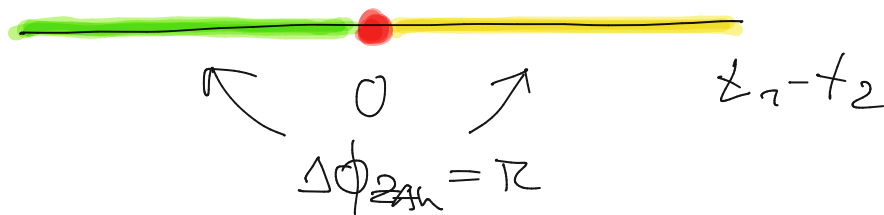
The Zak phase is constant for $\Delta=0$ and jumps by π between the two regions $t_1 - t_2 < 0$ and $t_1 - t_2 > 0$.

Rice-Mele model with $\Delta=0$: Su-Schrieffer Heeger (SSH) model

$$(64) \quad H = -t_1 \sum_j (c_{Bj}^\dagger c_{Aj} + \text{h.a.}) - t_2 \sum_j (c_{Aj+1}^\dagger c_{Bj} + \text{h.a.})$$



bulk properties are unchanged if $t_1 \leftrightarrow t_2$.
However we see the Zak phase differs by π .



Note that Zak phase depends on the choice of origin of the unit cell.

We will see that the SSH Hamiltonian has two topologically distinct ground states characterized by a

$$\underline{\mathbb{Z}_2} \text{ topological invariant } \begin{cases} \phi_{\text{Zak}} = 0 \\ \phi_{\text{Zak}} = \pi \end{cases}$$

Block Hamiltonian of SSH

$$(65) \quad \underline{H}(k) = \begin{pmatrix} 0 & -t_1 - t_2 e^{-ik} \\ -t_1 - t_2 e^{ik} & 0 \end{pmatrix} = d_x(k) \hat{\sigma}_x + d_y(k) \hat{\sigma}_y$$

$$(66) \quad d_x(k) = -t_1 - t_2 \cos k \quad d_y(k) = -t_2 \sin k$$

Since the Pauli matrix $\hat{\sigma}_z$ is missing, $\underline{h}(k)$ can be described by a unit vector $\vec{n}(k)$ which lies in the x-y plane

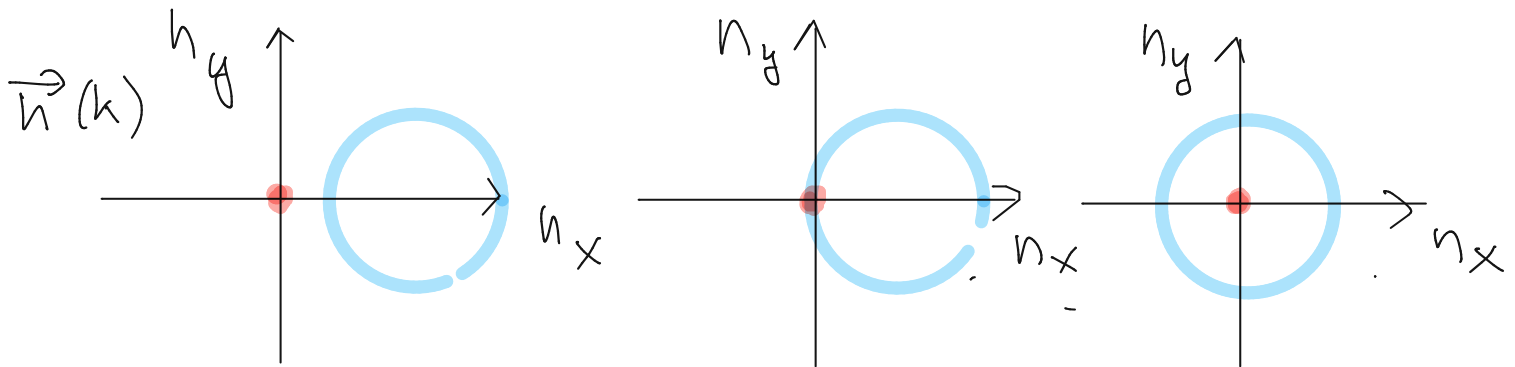
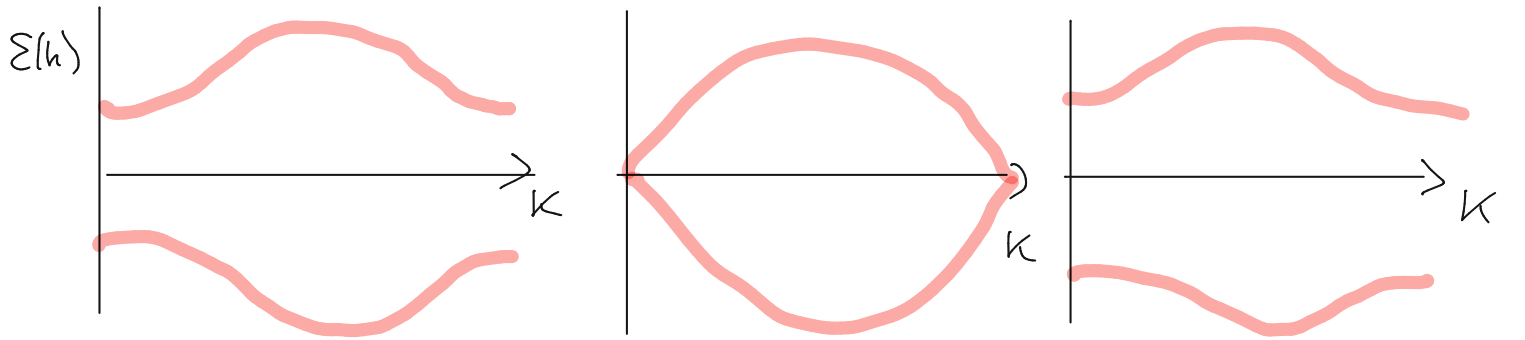
$$(67) \quad \underline{h}(k) = \varepsilon(k) \vec{n}(k) \cdot \vec{\sigma}$$

There is an interesting relation between the Zak phase and the winding of the vector $\vec{n}(k)$

$$t_1 > t_2$$

$$t_1 = t_2$$

$$t_1 < t_2$$



topolog. phase -
transition

In the Rice-Mele model there is also a z -component

$$(68) \quad d_z(k) = \Delta$$

i.e. here $\vec{n}(k)$ is not confined to the x,y plane.

The confinement of $\vec{n}(k)$ to the x,y plane is associated with a generalized (anti-unitary) symmetry. We will discuss these generalized symmetries in detail later but here a short remark:

Unitary Symmetry

if $U H U^\dagger = H$ $U = e^{i\hat{X}}$ $U^\dagger = U^{-1}$

(69) $\Leftrightarrow [\hat{X}, H] = 0$ $\hat{X}$ constant of motion

generalized (anti-unitary) symmetry

have Chiral symmetry

(70) $\Gamma H \Gamma^\dagger = -H$ $\Gamma^\dagger = \Gamma^{-1}$

(71) for SSH $\Gamma = \sigma_z = \Gamma^\dagger$ $\Gamma^2 = 1$

$$\begin{aligned} \sigma_z h(h) \sigma_z &= \underline{d_x} \sigma_z \underline{\sigma_x} \sigma_z + \underline{d_y} \sigma_z \underline{\sigma_y} \sigma_z \\ &\quad + \underline{d_z} \sigma_z \underline{\sigma_z} \sigma_z \\ &= -d_x \sigma_x - d_y \sigma_y + d_z \sigma_z \end{aligned}$$

SO
(72) $\sigma_z h_{SSH} \sigma_z = -h_{SSH} \Leftrightarrow d_z \equiv 0$

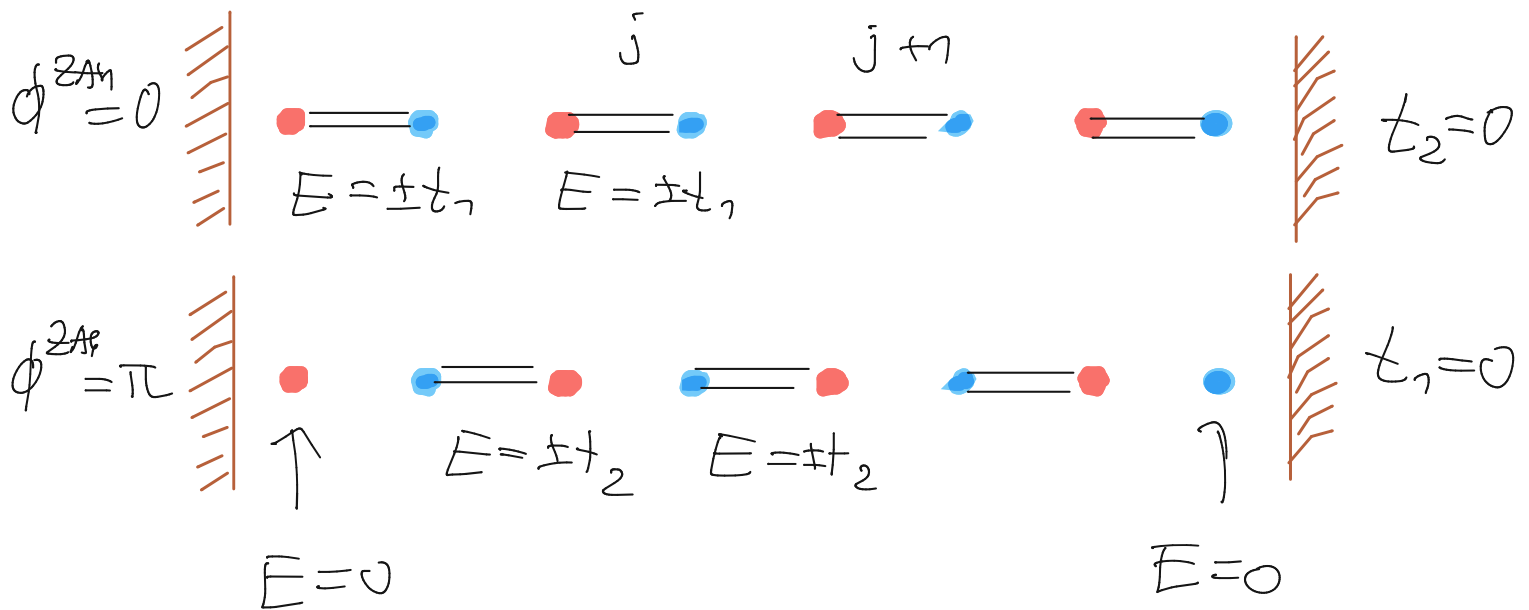
$\Rightarrow$ topological property of SSH is symmetry induced

symmetry protected topology

$\leftarrow$ 27.04,

physical consequence (here of symmetry protected) topology: edge states

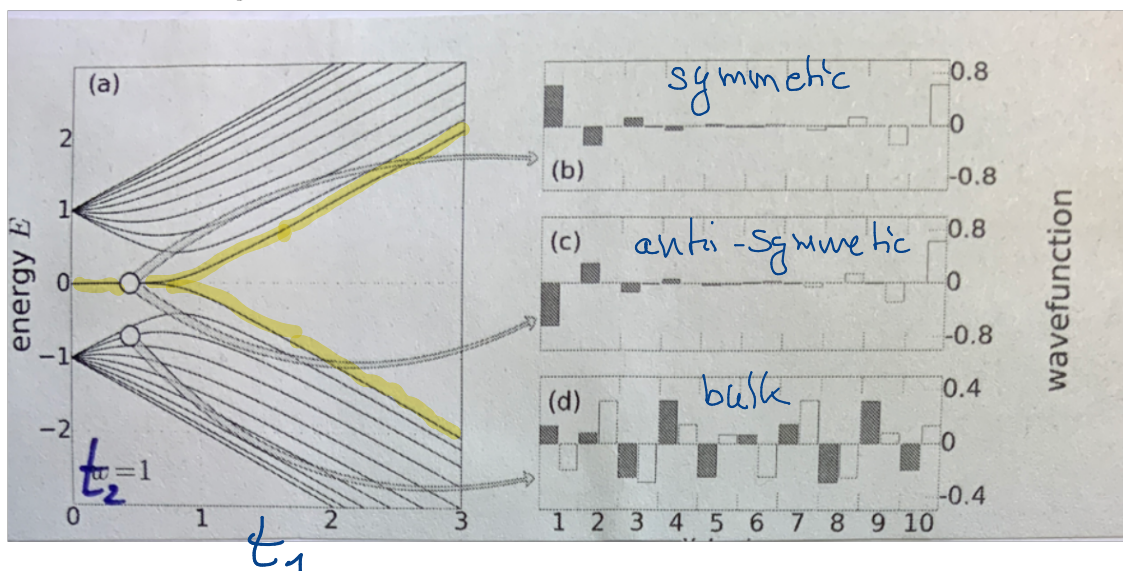
- consider finite lattice (open boundary conditions)
first in fully dimerized limit



In the case $\phi^{\text{ZAH}} = \pi$ there are two additional states with energy $E = 0$, localized at the edges

edge states

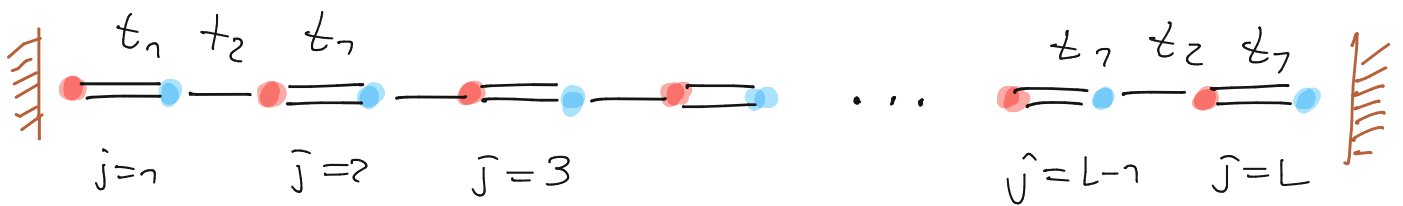
- away from dimerized limit:



two mid-gap states also away from dimerized limit

- localization length increases with $t_1, t_2 \rightarrow 0$
- as soon as edge state wavefunctions start to overlap in a finite lattice they hybridize and their energy splits

► finite lattice with L unit cells: (no translational invariance)



in first quantization

$$(83) \quad H_L = -t_1 \sum_{\hat{j}=1}^L (|j, B\rangle \langle j, A| + \text{h.c.}) - t_2 \sum_{\hat{j}=1}^L (|j+1, A\rangle \langle j, B| + \text{h.c.})$$

Ansatz for single-particle eigenstate

$$(84) \quad |\phi_0\rangle = \sum_{\hat{j}=1}^L \alpha_{\hat{j}} |j, A\rangle + \beta_{\hat{j}} |j, B\rangle$$

zero energy state?

$$H_L |\phi_0\rangle = 0$$

$$(85) \quad \begin{aligned} t_1 \alpha_{\hat{j}} + t_2 \alpha_{\hat{j}+1} &= 0 & \hat{j} &= 1, \dots, L-1 \\ t_2 \beta_{\hat{j}} + t_1 \beta_{\hat{j}+1} &= 0 \end{aligned}$$

boundary:

$$t_1 \alpha_L = 0$$

$$t_1 \beta_1 = 0$$

$$\Rightarrow \begin{aligned} (\text{86}) \quad \alpha_{\hat{j}} &= \left(-\frac{t_1}{t_2} \right)^{\hat{j}-1} \alpha_1 & \hat{j} &= 2, \dots, L \\ \beta_{\hat{j}} &= \left(-\frac{t_1}{t_2} \right)^{L-(\hat{j}+1)} \beta_L & \hat{j} &= 1, \dots, L-1 \end{aligned}$$

but since $\beta_1 = \alpha_L = 0 \neq$ zero energy solution
In any finite system there is an exponentially small hybridization of edge states which leads to small energy splitting.

Σ_{86} is however approximate solution

$$(\text{87}) \quad |L\rangle = \sum_{\hat{j}=1}^L \alpha_{\hat{j}} |j, A\rangle$$

only A sites

$$|R\rangle = \sum_{\hat{j}=1}^L \beta_{\hat{j}} |j, B\rangle$$

only B sites

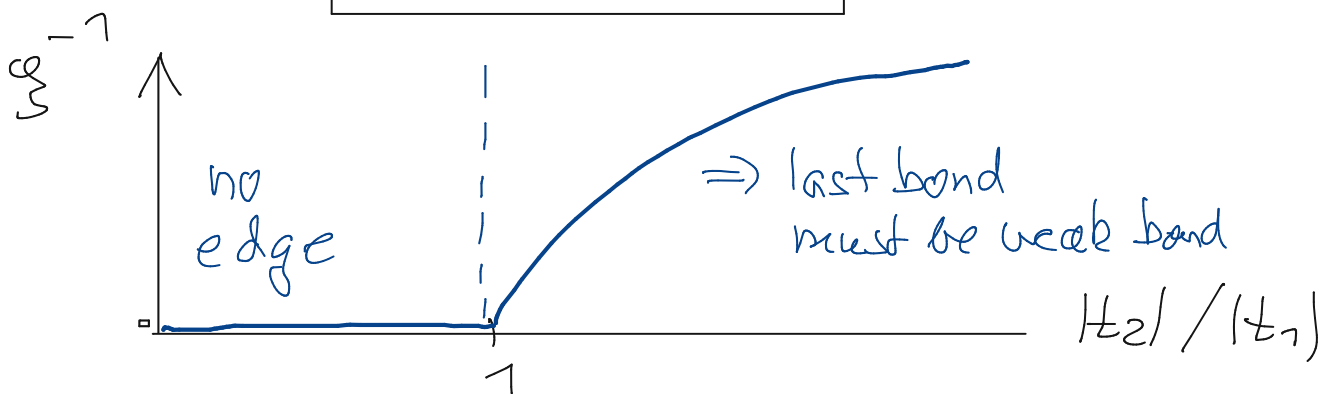
with

$$|\alpha_L| = |\alpha_1| e^{-(L-1)/\xi} \quad |\beta_1| = |\beta_L| e^{-(L-1)/\xi}$$

(88)

$$\xi^{-1} = \log \left| \frac{t_2}{t_1} \right|$$

localization length



1.4 A two-dimensional Bloch Hamiltonian with topological properties: The Qi-Wu-Zhang (QWZ)

In Sect. 1.3 we have discussed a one-dimensional Bloch Hamiltonian with an additional periodic parameter

$$(99) \quad \vec{\lambda} = \begin{pmatrix} t_1 - t_2 \\ \Delta \end{pmatrix} \quad \text{e.g.} \quad \begin{aligned} t_1 &= -(1 + \cos(2t)) \\ t_2 &= -1 \\ \Delta &= -\sin(2t) \end{aligned}$$

$$(100) \quad \text{So} \quad \underline{h}_{\text{RM}}(k, t) = [1 + \cos(2t) + \cos k] \hat{\sigma}_x + \sin k \hat{\sigma}_y + \sin 2t \hat{\sigma}_z$$

Now let's go to a 2D system and replace the periodic functions $\cos(2t)$ and $\sin(2t)$ by $\cos(k_x)$ and $\sin(k_y)$. After an additional (unimportant) rotation in space we obtain the

QWZ Hamiltonian

$$(101) \quad \underline{h}_{\text{QWZ}}(k_x, k_y) = \sin k_x \hat{\sigma}_x + \sin k_y \hat{\sigma}_y + (u + \cos k_x + \cos k_y) \hat{\sigma}_z$$

$$(92) \quad i\hbar \frac{\partial}{\partial t} \vec{d}(\vec{k}) = \begin{pmatrix} \sin k_x \\ \sin k_y \\ u + \cos k_x + \cos k_y \end{pmatrix} \quad \vec{k} = (k_x, k_y)$$

and
$$h_{\text{QWZ}} = \vec{d} \cdot \vec{\sigma}$$

$$(93) \quad h_{\text{QWZ}}^2 = |\vec{d}|^2 \cdot \mathbb{I}$$

$\Rightarrow$ eigenvalues $\pm |\vec{d}|$ 2 bands

$$(94) \quad E_{\pm}(\vec{k}) = \pm \sqrt{\sin^2 k_x + \sin^2 k_y + (u + \cos k_x + \cos k_y)^2}$$

gap closes for $u = 0, \pm 2$

$$u = -2 \quad k_x = k_y = 0$$

Γ point

$$u = 0 \quad k_x = 0 \quad k_y = \pi$$

two X points

or $k_x = \pi \quad k_y = 0$

$$u = +2 \quad k_x = k_y = \pi$$

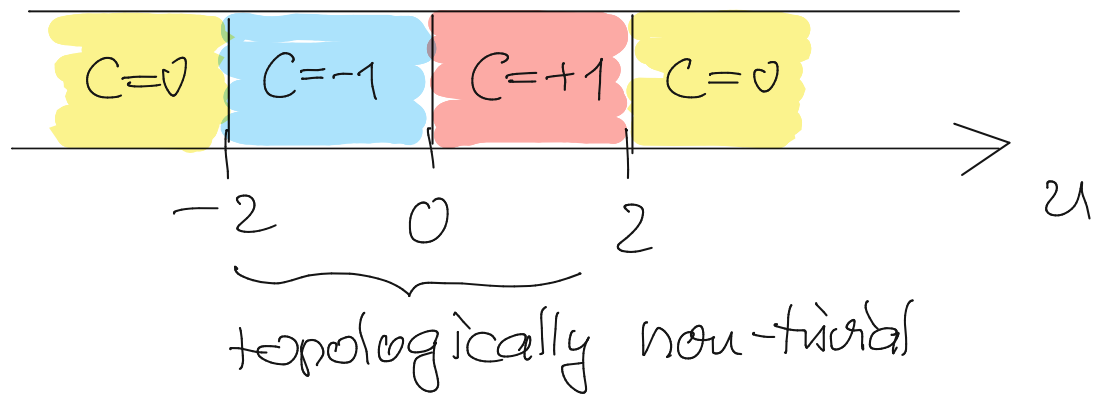
M point

From the Bloch eigenstates $|u_{\pm}(k_x, k_y)\rangle$ one can calculate the Chern numbers of the bands

$$(95) \quad C_{\pm} = \frac{1}{2\pi} \int_{\mathbb{B}^2} \int_{\mathbb{B}^2} i \left[\langle \partial_{k_x} u_{\pm} | \partial_{k_y} u_{\pm} \rangle - \text{c.c.} \right]$$

and finds

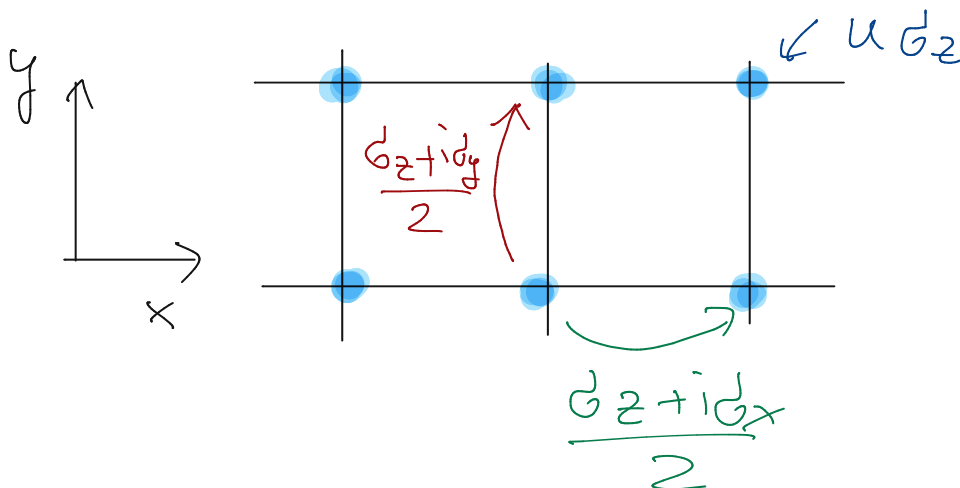
$$(96) \quad C_{\pm} = \mp C$$



real-space Hamiltonian

inverse Fourier transform $\Rightarrow$ real-space Hamiltonian for two "spin" components

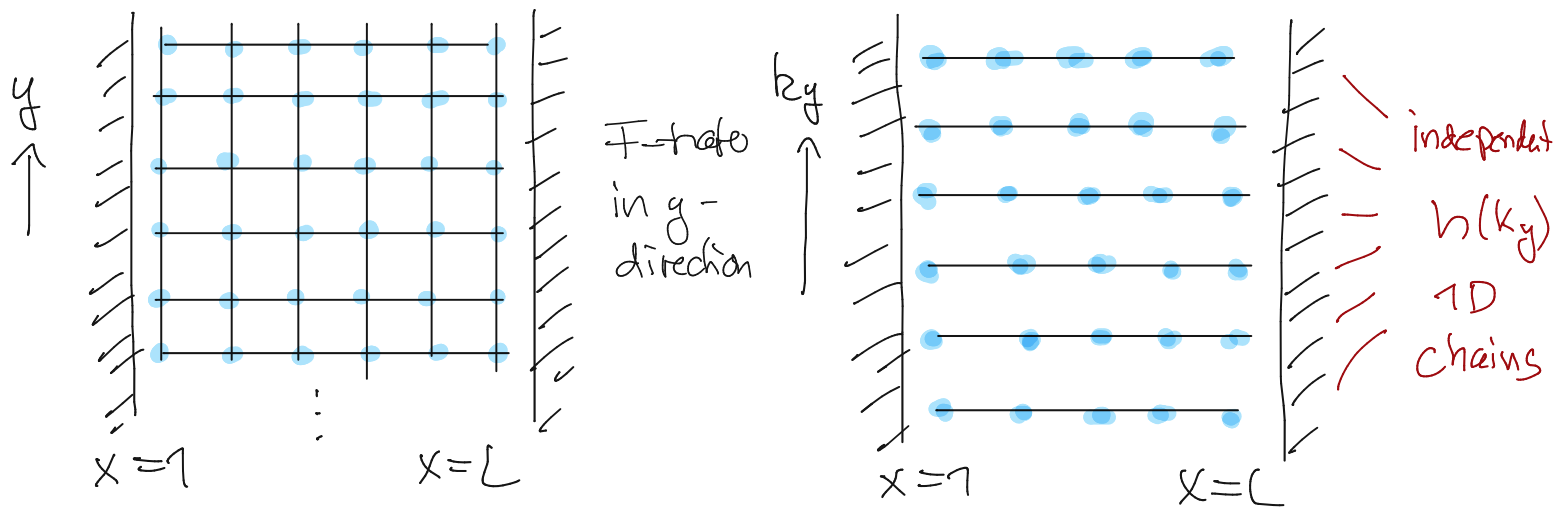
$$\begin{aligned}
 (97) \quad H = & \sum_{\bar{j}=1}^{L_x-1} \sum_{\ell=1}^{L_y} \left(|j+1, \ell\rangle \langle j, \ell| \frac{\sigma_z + i\sigma_x}{2} + \text{h.c.} \right) \\
 & + \sum_{\bar{j}=1}^{L_x} \sum_{\ell=1}^{L_y-1} \left(|j, \ell+1\rangle \langle j, \ell| \frac{\sigma_z + i\sigma_y}{2} + \text{h.c.} \right) \\
 & + u \sum_{\bar{j}=1}^{L_x} \sum_{\ell=1}^{L_y} |j, \ell\rangle \langle j, \ell| \sigma_z
 \end{aligned}$$



- hopping with "spin" rotation
- on-site energy $\pm u$

edge states

Now the edge is one-dimensional and this gives rise to additional interesting phenomena. Consider half-infinite stripe



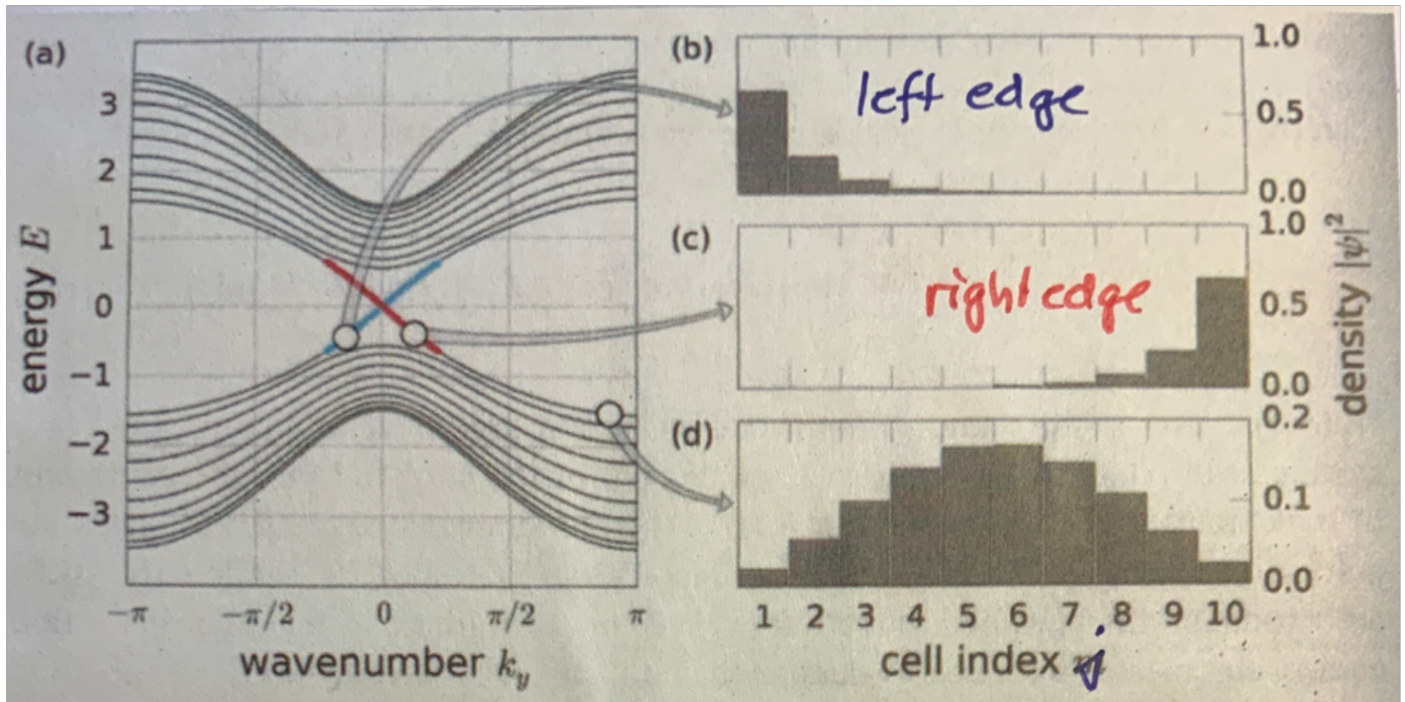
independent 1D chains

$$h(k_y) = \sum_{j=1}^{L_x-1} \left(|j+1\rangle \langle j| \frac{\sigma_z + i\sigma_x}{2} + \text{h.c.} \right)$$

(98)

$$+ \sum_{j=1}^{L_x} |j\rangle \langle j| \left(\cos k_y \hat{\sigma}_z + \sin k_y \hat{\sigma}_y + u \hat{\sigma}_z \right)$$

- for every chain with given k_y one finds edge states localized either at $x=1$ or $x=L$
- energies $\mathcal{E}_{L/R} = \mathcal{E}_{L/R}(k_y)$ are smooth functions of k_y 1D edge modes



- the edge modes have a dispersion with fixed sign!

$$(gg) \quad \frac{\partial \varepsilon_L(k_y)}{\partial k_y} > 0 \quad \frac{\partial \varepsilon_R(k_y)}{\partial k_y} < 0$$

they can carry a current, but only in one direction

chiral edge modes

At an interface between two topologically different bulk regions there have to be states that close the gap, since topological integers cannot change smoothly and only by closing the energy gap.

robustness of edge states / modes

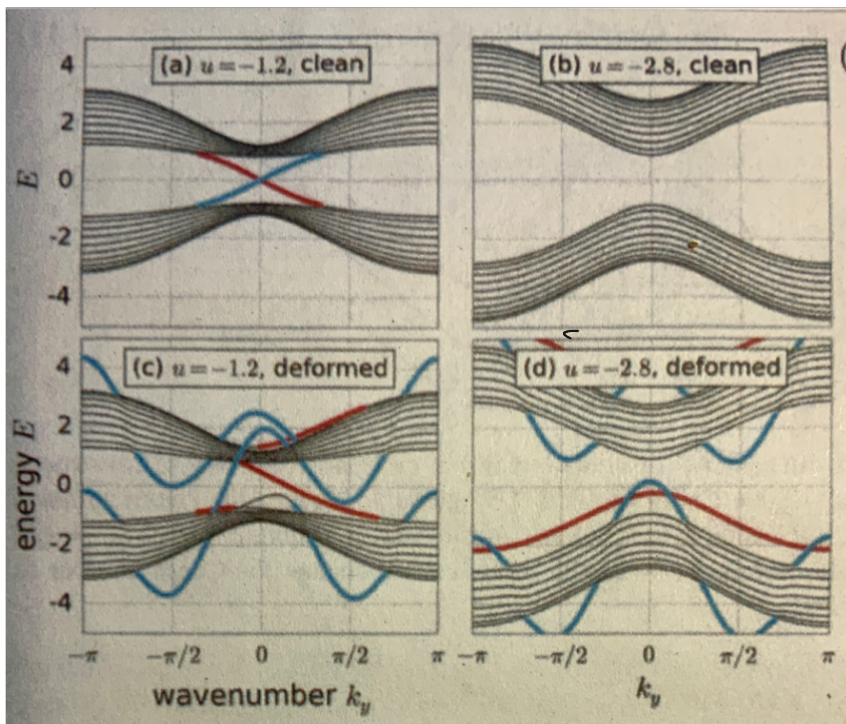
Perturbations that do not close the energy gap or break symmetries in the case of symmetry protected topology do not remove edge states / modes.

E.g. $h(k_y) \rightarrow h'(k_y)$

$$h'(k_y) = h(k_y) + |j=1\rangle\langle j=1| (\mu^{(1)} + h_2^{(1)} \cos(2k_y)) \\ + |j=L\rangle\langle j=L| (\mu^{(2)} + h_2^{(2)} \cos(2k_y))$$

$$C = -1$$

$$C = 0$$



presence of
edge modes
survives!

Furthermore, since edge modes are chiral a localized impurity cannot lead to a resistance because there is no backscattering.

$\Rightarrow$ robustness of edge currents to disorder